



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:54 AM GMT

PDB ID : 3K2B
Title : Crystal structure of photosynthetic A4 isoform glyceraldehyde-3-phosphate dehydrogenase complexed with NAD, from *Arabidopsis thaliana*
Authors : Fermani, S.; Falini, G.; Thumiger, A.; Sparla, F.; Marri, L.; Trost, P.
Deposited on : 2009-09-29
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

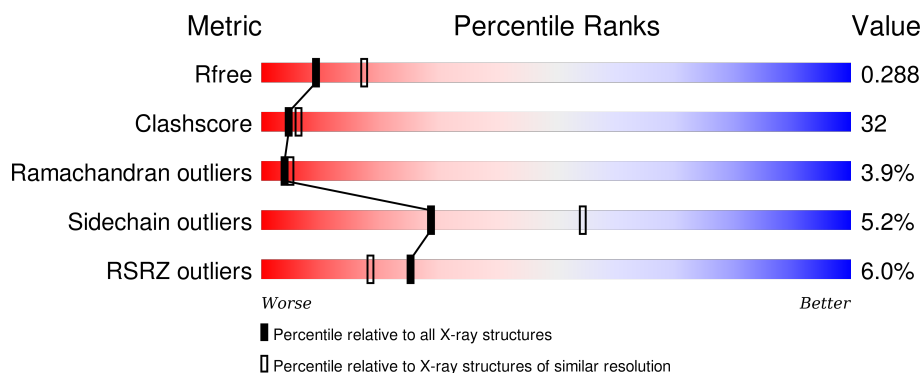
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	337	<div> <div>65%</div> <div>31%</div> <div>.</div> </div>
1	B	337	<div> <div>%</div> <div>61%</div> <div>36%</div> <div>.</div> </div>
1	C	337	<div> <div>%</div> <div>59%</div> <div>36%</div> <div>5%</div> </div>
1	D	337	<div> <div>%</div> <div>47%</div> <div>49%</div> <div>.</div> </div>
1	E	337	<div> <div>28%</div> <div>29%</div> <div>62%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	337	
1	G	337	
1	H	337	
1	O	337	
1	Q	337	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	H	334	-	-	-	X
3	SO4	O	337	-	-	-	X
3	SO4	O	340	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27072 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2557	1615	445	488	9			
1	B	337	Total	C	N	O	S	0	0	0
			2557	1615	445	488	9			
1	C	337	Total	C	N	O	S	0	0	0
			2557	1615	445	488	9			
1	D	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	E	336	Total	C	N	O	S	0	0	0
			2547	1609	443	486	9			
1	F	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	G	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	H	335	Total	C	N	O	S	0	0	0
			2542	1606	442	485	9			
1	O	337	Total	C	N	O	S	0	0	0
			2557	1615	445	488	9			
1	Q	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	Q	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	84	Total	O	0	0
			84	84		
4	C	94	Total	O	0	0
			94	94		
4	D	85	Total	O	0	0
			85	85		
4	E	79	Total	O	0	0
			79	79		
4	F	65	Total	O	0	0
			65	65		
4	G	81	Total	O	0	0
			81	81		
4	H	56	Total	O	0	0
			56	56		
4	O	129	Total	O	0	0
			129	129		

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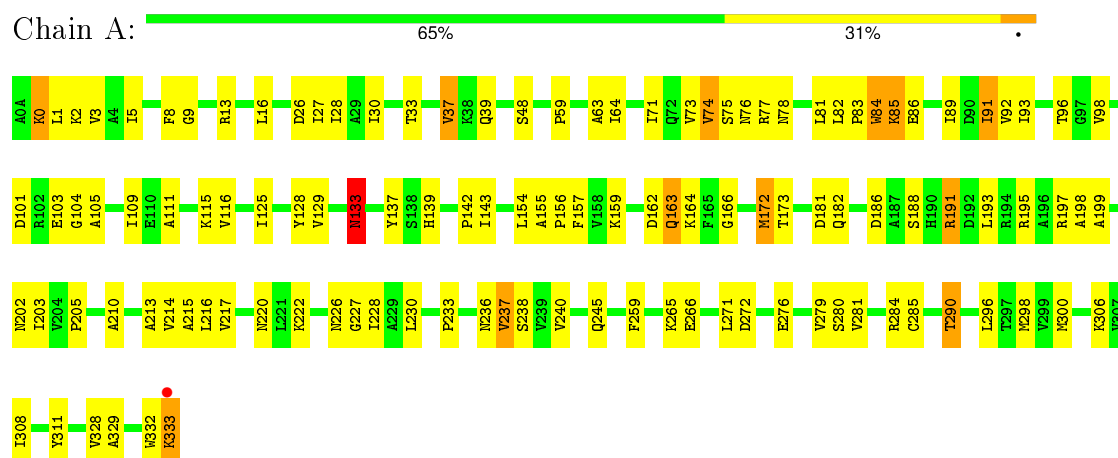
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	100	Total	O	0	0
			100	100		

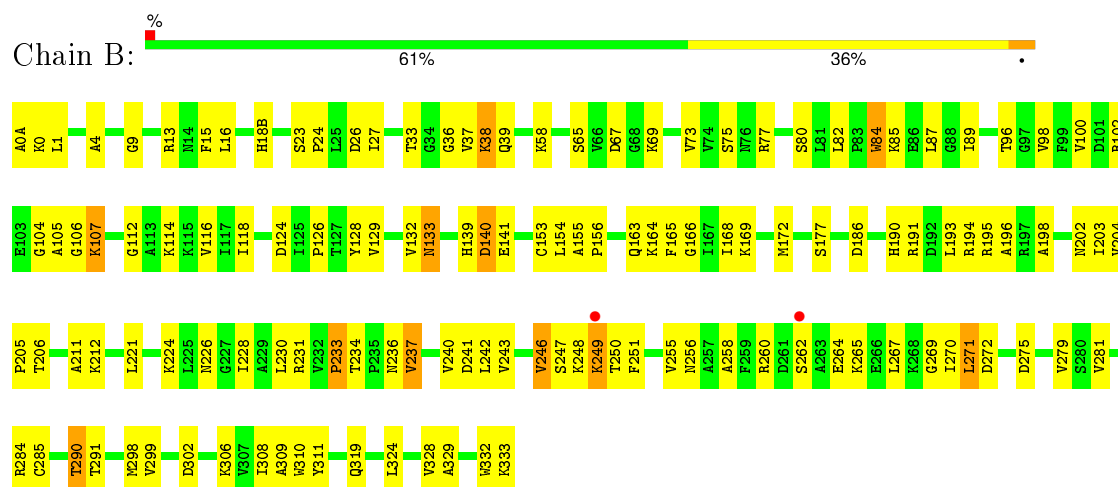
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

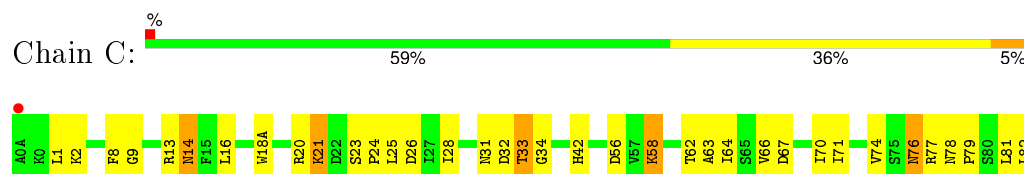
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic

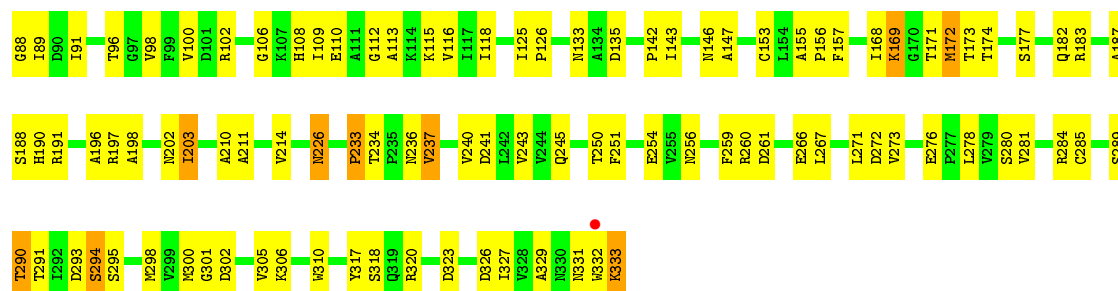


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic

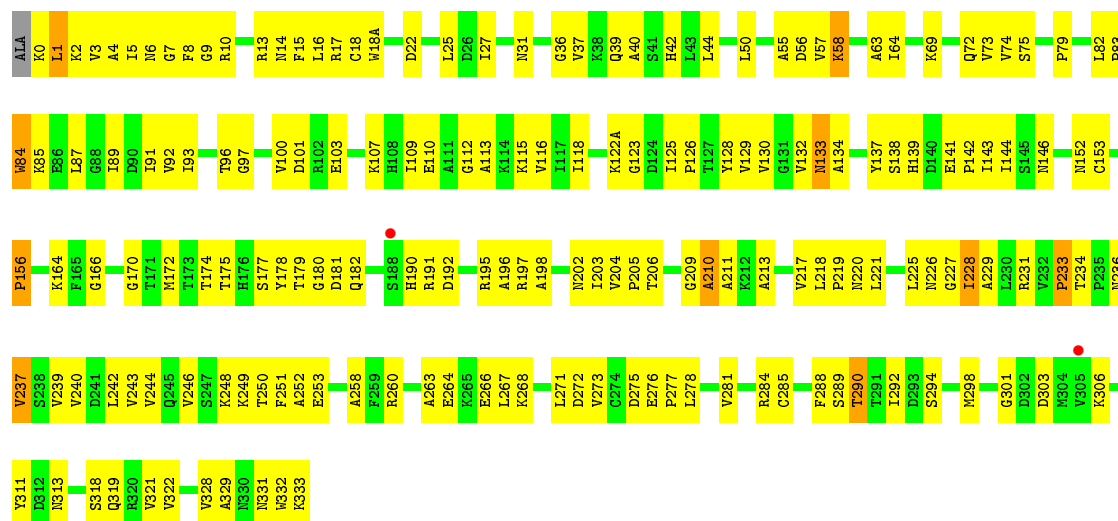


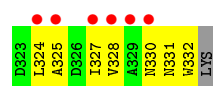
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic



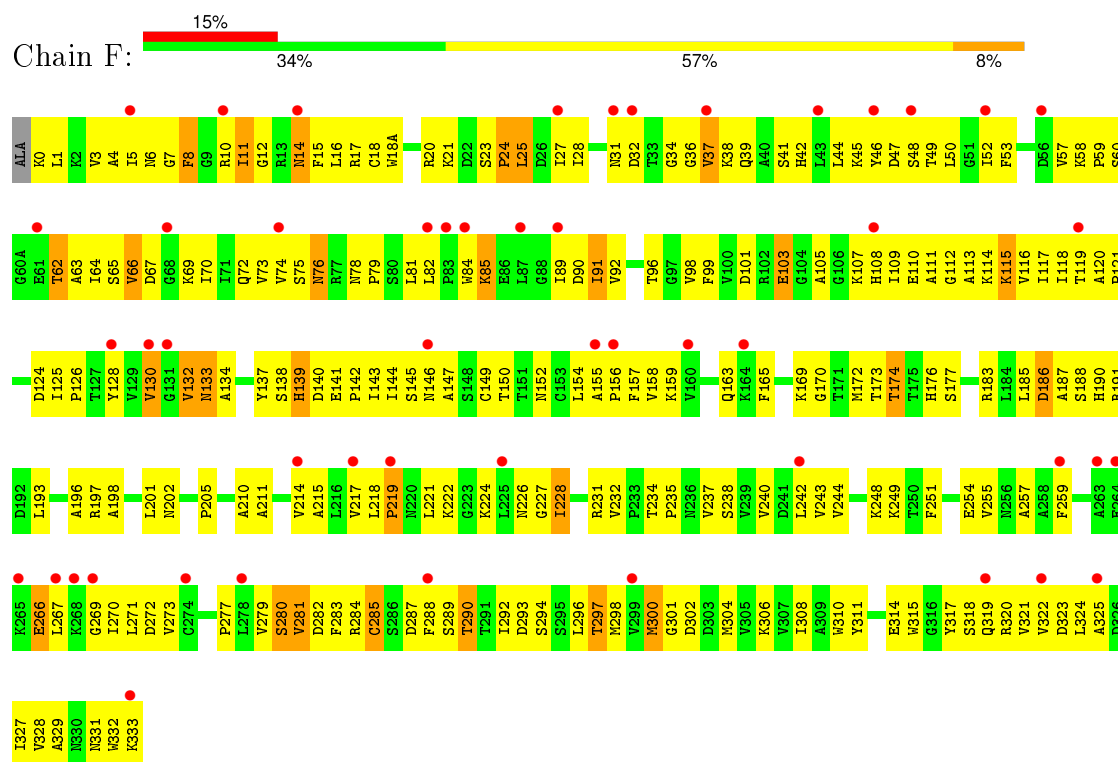


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic

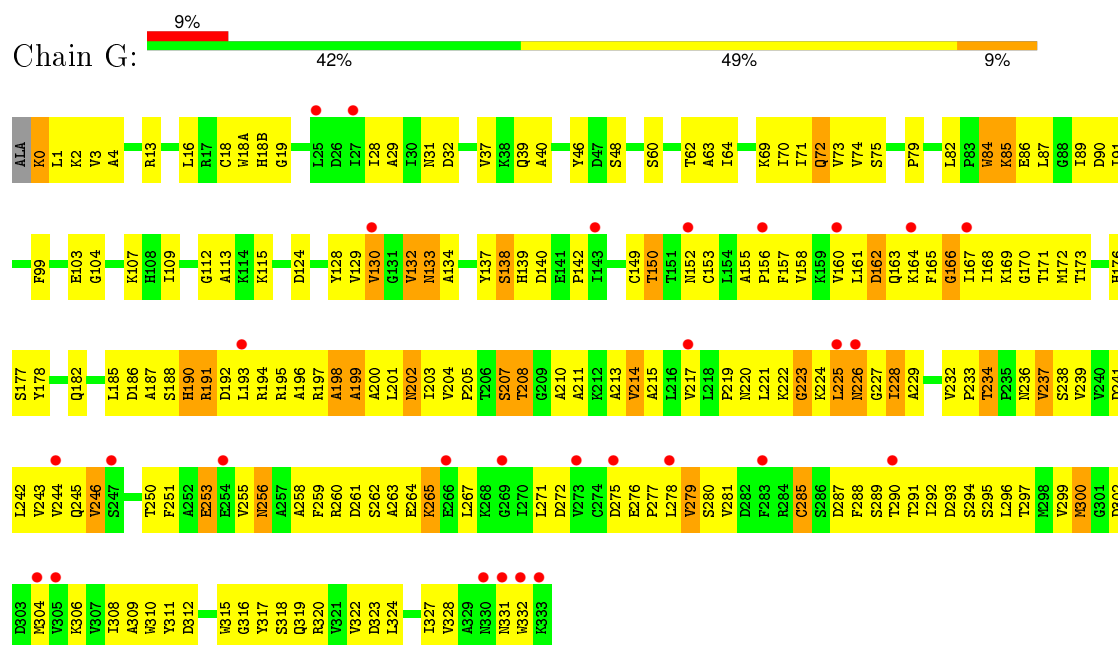




- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

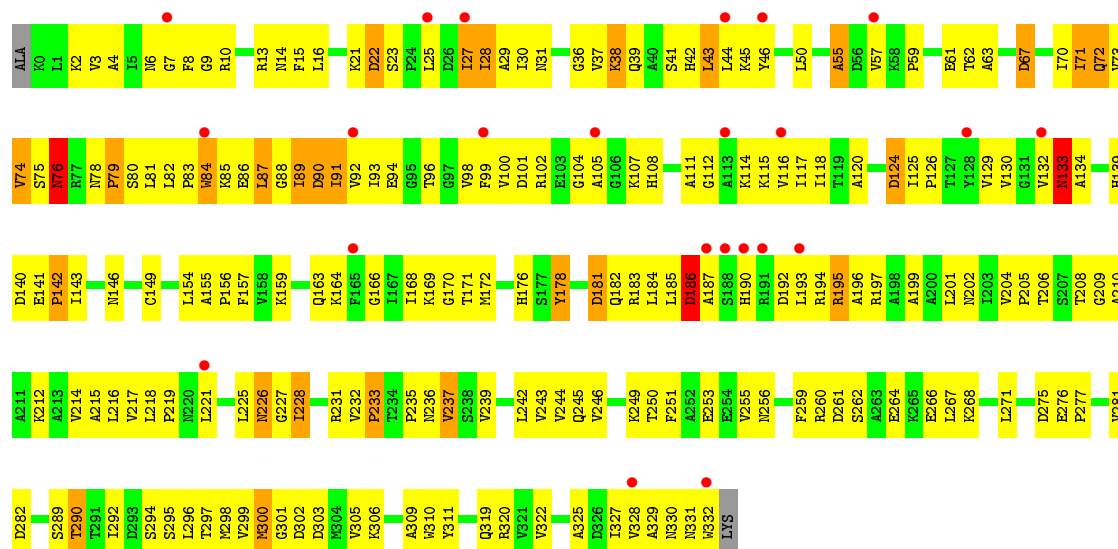


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplasic



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	150.74Å 188.62Å 314.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.22 – 2.60 94.22 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.8 (94.22-2.60) 95.9 (94.22-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.62Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.237 , 0.289 0.237 , 0.288	Depositor DCC
R_{free} test set	6671 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 69.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 131352 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27072	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	0/2601	0.66	1/3530 (0.0%)
1	B	0.38	0/2601	0.67	1/3530 (0.0%)
1	C	0.37	0/2601	0.66	1/3530 (0.0%)
1	D	0.34	0/2596	0.62	1/3523 (0.0%)
1	E	0.34	0/2591	0.60	0/3519
1	F	0.31	0/2596	0.59	0/3523
1	G	0.35	0/2596	0.62	0/3523
1	H	0.30	0/2586	0.57	0/3512
1	O	0.44	0/2601	0.72	1/3530 (0.0%)
1	Q	0.42	0/2596	0.70	1/3523 (0.0%)
All	All	0.37	0/25965	0.64	6/35243 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	203	ILE	N-CA-C	-5.86	95.18	111.00
1	D	203	ILE	N-CA-C	-5.66	95.71	111.00
1	O	203	ILE	N-CA-C	-5.62	95.82	111.00
1	A	203	ILE	N-CA-C	-5.56	95.99	111.00
1	C	203	ILE	N-CA-C	-5.42	96.35	111.00
1	B	203	ILE	N-CA-C	-5.42	96.37	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2557	0	2598	126	0
1	B	2557	0	2598	117	0
1	C	2557	0	2598	125	0
1	D	2552	0	2593	168	1
1	E	2547	0	2585	348	0
1	F	2552	0	2593	266	0
1	G	2552	0	2593	250	0
1	H	2542	0	2580	255	0
1	O	2557	0	2598	98	0
1	Q	2552	0	2593	122	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	0	0
2	D	44	0	26	3	0
2	E	44	0	26	5	0
2	F	44	0	26	2	0
2	G	44	0	26	1	0
2	H	44	0	26	2	0
2	O	44	0	26	1	0
2	Q	44	0	26	0	0
3	A	35	0	0	0	0
3	B	25	0	0	0	0
3	C	20	0	0	0	0
3	D	15	0	0	0	0
3	E	20	0	0	3	0
3	F	15	0	0	0	0
3	G	25	0	0	0	0
3	H	15	0	0	0	0
3	O	30	0	0	0	0
3	Q	25	0	0	0	0
4	A	109	0	0	1	0
4	B	84	0	0	1	0
4	C	94	0	0	4	0
4	D	85	0	0	6	0
4	E	79	0	0	9	0
4	F	65	0	0	1	0
4	G	81	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	56	0	0	0	0
4	O	129	0	0	2	0
4	Q	100	0	0	4	0
All	All	27072	0	26189	1682	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (1682) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:191:ARG:HB3	1:Q:191:ARG:HH11	1.22	1.04
1:G:63:ALA:HB1	1:G:70:ILE:HD11	1.34	1.04
1:E:17:ARG:HA	1:E:17:ARG:HE	1.18	1.03
1:F:90:ASP:HA	1:F:114:LYS:HD3	1.41	1.03
1:D:139:HIS:HB3	1:D:333:LYS:HE2	1.40	1.02
1:F:126:PRO:HG2	1:F:141:GLU:HG2	1.42	1.01
1:E:304:MET:HE3	1:G:245:GLN:HB2	1.45	0.98
1:G:221:LEU:HD21	1:G:225:LEU:HD11	1.46	0.98
1:O:17:ARG:NH1	1:O:53:PHE:HB2	1.79	0.98
1:H:72:GLN:H	1:H:72:GLN:NE2	1.62	0.97
1:E:226:ASN:HB3	1:G:300:MET:HE2	1.45	0.96
1:G:161:LEU:HB2	1:G:167:ILE:HD11	1.51	0.93
1:Q:38:LYS:HE3	1:Q:38:LYS:H	1.34	0.92
1:E:194:ARG:HH21	1:G:277:PRO:HA	1.34	0.91
1:G:256:ASN:HD21	1:G:297:THR:HG21	1.35	0.91
1:E:126:PRO:HB2	1:E:144:ILE:HG22	1.53	0.90
1:D:85:LYS:HG3	1:D:112:GLY:HA2	1.51	0.90
1:E:70:ILE:HD13	1:E:70:ILE:H	1.35	0.90
1:A:202:ASN:HD21	1:C:281:VAL:HG12	1.37	0.89
1:E:117:ILE:HG22	1:E:144:ILE:HD11	1.52	0.89
1:F:202:ASN:HD22	1:H:281:VAL:H	1.23	0.87
1:F:96:THR:OG1	1:F:98:VAL:HG22	1.76	0.86
1:F:85:LYS:HG2	1:F:112:GLY:HA2	1.57	0.86
1:E:154:LEU:HD21	1:E:172:MET:HG3	1.58	0.86
1:G:251:PHE:O	1:G:255:VAL:HG23	1.77	0.85
1:G:2:LYS:HD2	1:G:28:ILE:HG21	1.58	0.85
1:F:317:TYR:O	1:F:321:VAL:HG23	1.77	0.84
1:E:133:ASN:H	1:E:133:ASN:HD22	1.22	0.84
1:H:190:HIS:HB3	1:H:196:ALA:HB2	1.59	0.84
1:C:333:LYS:HE2	4:C:423:HOH:O	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:HIS:O	1:E:231:ARG:HA	1.78	0.82
1:E:139:HIS:CE1	1:E:332:TRP:HA	2.14	0.82
1:Q:191:ARG:HB3	1:Q:191:ARG:NH1	1.94	0.82
1:B:139:HIS:NE2	1:B:333:LYS:HD3	1.95	0.81
1:F:328:VAL:O	1:F:332:TRP:HB2	1.80	0.81
1:F:130:VAL:HB	1:F:320:ARG:HD3	1.61	0.81
1:F:31:ASN:HB2	1:F:74:VAL:HG13	1.61	0.81
1:H:96:THR:OG1	1:H:98:VAL:HG22	1.81	0.81
1:E:17:ARG:HA	1:E:17:ARG:NE	1.96	0.80
1:D:129:VAL:HG23	1:D:217:VAL:HG11	1.63	0.80
1:C:156:PRO:HB2	1:C:290:THR:HG21	1.63	0.80
1:E:232:VAL:HG21	1:G:203:ILE:HD11	1.61	0.80
1:D:264:GLU:HA	1:D:268:LYS:HE3	1.62	0.80
1:H:170:GLY:HA3	1:H:244:VAL:HG12	1.64	0.80
1:H:228:ILE:H	1:H:228:ILE:HD13	1.47	0.80
1:G:129:VAL:HG23	1:G:217:VAL:HG11	1.63	0.79
1:G:294:SER:O	1:G:297:THR:HG22	1.81	0.79
1:H:129:VAL:H	1:H:133:ASN:HD21	1.27	0.79
1:H:86:GLU:O	1:H:87:LEU:HB2	1.81	0.79
1:O:281:VAL:HB	1:Q:202:ASN:HD21	1.46	0.79
1:Q:0:LYS:HD2	1:Q:0:LYS:O	1.84	0.78
1:E:203:ILE:HD11	1:G:232:VAL:HG21	1.64	0.78
1:E:262:SER:HB3	1:E:267:LEU:HD12	1.65	0.78
1:G:211:ALA:CB	1:G:226:ASN:HA	2.14	0.78
1:H:195:ARG:HH21	1:H:206:THR:HG21	1.49	0.78
1:E:133:ASN:N	1:E:133:ASN:HD22	1.78	0.77
1:E:277:PRO:HA	1:G:194:ARG:HE	1.50	0.77
1:B:163:GLN:HE21	1:B:164:LYS:NZ	1.82	0.77
1:Q:159:LYS:HG2	1:Q:163:GLN:HE21	1.47	0.77
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.18	0.77
1:F:315:TRP:O	1:F:319:GLN:HG2	1.83	0.77
1:E:72:GLN:HG3	1:E:73:VAL:H	1.50	0.77
1:D:91:ILE:HA	1:D:115:LYS:O	1.85	0.77
1:E:171:THR:HB	1:G:300:MET:HG2	1.64	0.77
1:B:226:ASN:ND2	1:D:298:MET:SD	2.58	0.77
1:E:0(A):ALA:HB1	1:E:26:ASP:HB2	1.65	0.77
1:H:130:VAL:HA	1:H:134:ALA:HB2	1.67	0.77
1:F:79:PRO:HA	1:F:82:LEU:HD12	1.65	0.76
1:E:169:LYS:HE3	1:G:304:MET:HB2	1.66	0.76
1:Q:138:SER:HB3	1:Q:141:GLU:OE2	1.83	0.76
1:E:165:PHE:HD1	1:E:248:LYS:HD2	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:ILE:HG23	1:E:73:VAL:HG21	1.67	0.76
1:A:156:PRO:HB2	1:A:290:THR:HG21	1.66	0.75
1:A:85:LYS:N	1:A:85:LYS:HE3	2.02	0.75
1:E:167:ILE:HG23	1:E:244:VAL:HB	1.68	0.75
1:Q:78:ASN:HB3	1:Q:81:LEU:HD12	1.69	0.75
1:G:293:ASP:OD1	1:G:296:LEU:HG	1.87	0.75
1:F:243:VAL:HG11	1:H:171:THR:HG21	1.69	0.75
1:E:194:ARG:HG2	1:G:277:PRO:O	1.86	0.75
1:F:284:ARG:O	1:F:285:CYS:HB2	1.87	0.75
1:B:153:CYS:HA	1:B:290:THR:HG22	1.67	0.75
1:H:38:LYS:HD2	1:H:38:LYS:H	1.51	0.75
1:F:85:LYS:HG2	1:F:112:GLY:CA	2.17	0.75
1:E:58:LYS:HB2	1:E:59:PRO:HD2	1.69	0.74
1:E:204:VAL:HB	1:E:231:ARG:HB2	1.67	0.74
1:B:233:PRO:HB2	1:D:233:PRO:HB2	1.67	0.74
1:Q:210:ALA:O	1:Q:214:VAL:HG23	1.88	0.74
1:E:256:ASN:HD21	1:E:297:THR:HB	1.51	0.74
1:A:30:ILE:HG13	1:A:71:ILE:HD11	1.67	0.74
1:O:281:VAL:HB	1:Q:202:ASN:ND2	2.01	0.74
1:D:91:ILE:HG22	1:D:115:LYS:HB3	1.69	0.73
1:H:156:PRO:HB2	1:H:290:THR:HG21	1.69	0.73
1:C:76:ASN:HD22	1:C:77:ARG:N	1.85	0.73
1:H:81:LEU:H	1:H:81:LEU:HD12	1.53	0.73
1:B:271:LEU:HD13	1:B:272:ASP:N	2.03	0.73
1:F:78:ASN:HB3	1:F:81:LEU:HD13	1.69	0.73
1:E:279:VAL:CG1	1:G:204:VAL:HG22	2.18	0.73
1:G:129:VAL:H	1:G:133:ASN:HD21	1.35	0.73
1:H:168:ILE:HD12	1:H:245:GLN:HG2	1.69	0.73
1:E:156:PRO:HB2	1:E:290:THR:HG21	1.71	0.73
1:A:33:THR:HG22	1:A:77:ARG:HG2	1.69	0.73
1:F:60:SER:H	1:F:64:ILE:HA	1.54	0.73
1:F:82:LEU:HD13	1:F:84:TRP:CZ2	2.23	0.73
1:F:228:ILE:HD13	1:F:228:ILE:H	1.54	0.73
1:E:217:VAL:HG23	1:E:218:LEU:HG	1.71	0.73
1:H:183:ARG:HG2	1:H:196:ALA:HA	1.71	0.73
1:E:194:ARG:NH2	1:G:277:PRO:HA	2.03	0.73
1:H:70:ILE:HG22	1:H:71:ILE:H	1.53	0.73
1:F:267:LEU:HD22	1:F:270:ILE:HG21	1.68	0.72
1:E:7:GLY:HA2	2:E:335:NAD:H1B	1.70	0.72
1:F:222:LYS:HG2	1:F:224:LYS:HE2	1.71	0.72
1:D:153:CYS:HA	1:D:290:THR:HG22	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:VAL:HA	1:G:134:ALA:HB2	1.71	0.72
1:E:20:ARG:NH2	1:E:322:VAL:HB	2.03	0.72
1:F:16:LEU:HD22	1:F:44:LEU:HD11	1.71	0.72
1:F:249:LYS:HG2	1:F:302:ASP:HB3	1.71	0.72
1:H:155:ALA:HB3	1:H:156:PRO:HD3	1.70	0.72
1:G:193:LEU:HD22	1:G:193:LEU:H	1.54	0.72
1:D:0:LYS:HD2	4:D:363:HOH:O	1.90	0.71
1:B:105:ALA:HB1	1:B:116:VAL:HG11	1.71	0.71
1:E:194:ARG:HD3	1:E:205:PRO:HG2	1.73	0.71
1:D:74:VAL:HG22	1:D:75:SER:H	1.54	0.71
1:E:235:PRO:HB3	1:H:201:LEU:HD11	1.72	0.71
1:E:3:VAL:HG21	1:E:25:LEU:HD22	1.72	0.71
1:G:62:THR:HG22	1:Q:62:THR:HG22	1.73	0.71
1:E:195:ARG:HH22	1:E:231:ARG:NH2	1.89	0.70
1:E:186:ASP:HB2	1:H:10:ARG:NH1	2.06	0.70
1:F:21:LYS:N	1:F:21:LYS:HD2	2.05	0.70
1:G:241:ASP:OD1	1:G:308:ILE:HD11	1.91	0.70
1:B:139:HIS:CD2	1:B:333:LYS:HD3	2.25	0.70
1:G:186:ASP:OD1	1:G:197:ARG:HA	1.92	0.70
1:A:271:LEU:HD12	1:A:272:ASP:H	1.57	0.70
1:H:4:ALA:HB2	1:H:89:ILE:HD12	1.72	0.70
1:E:178:TYR:HA	1:E:182:GLN:OE1	1.92	0.70
1:D:83:PRO:HB3	1:H:72:GLN:OE1	1.92	0.70
1:A:27:ILE:HG22	1:A:71:ILE:HD12	1.74	0.70
1:A:48:SER:HA	1:B:281:VAL:HG11	1.73	0.70
1:F:318:SER:O	1:F:322:VAL:HG23	1.92	0.70
1:Q:82:LEU:HD13	1:Q:84:TRP:CZ2	2.27	0.70
1:E:119:THR:HG22	1:E:321:VAL:HG11	1.74	0.70
1:E:157:PHE:HE1	1:E:307:VAL:HG21	1.56	0.70
1:E:194:ARG:HE	1:G:277:PRO:C	1.95	0.70
1:H:181:ASP:HB3	1:H:195:ARG:HD3	1.74	0.70
1:B:281:VAL:HG12	1:D:202:ASN:HD21	1.57	0.70
1:Q:4:ALA:HB2	1:Q:89:ILE:HD12	1.74	0.70
1:H:37:VAL:HG21	1:H:62:THR:HA	1.74	0.70
1:F:11:ILE:O	1:F:11:ILE:HD13	1.92	0.70
1:H:72:GLN:HE21	1:H:72:GLN:H	1.37	0.69
1:E:192:ASP:HB3	1:E:195:ARG:HB2	1.73	0.69
1:F:228:ILE:HG21	1:H:296:LEU:HD22	1.74	0.69
1:F:222:LYS:HG2	1:F:224:LYS:CE	2.21	0.69
1:G:256:ASN:HD22	1:G:256:ASN:N	1.89	0.69
1:F:75:SER:O	1:F:76:ASN:HB2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:300:MET:HG2	1:H:226:ASN:ND2	2.07	0.69
1:E:194:ARG:HH12	1:G:296:LEU:HD21	1.57	0.69
1:F:298:MET:HE3	1:F:306:LYS:HD3	1.74	0.69
1:G:256:ASN:HB3	1:G:260:ARG:NH1	2.07	0.69
1:B:212:LYS:HE3	4:B:785:HOH:O	1.91	0.69
1:D:18:CYS:HB3	1:D:319:GLN:OE1	1.92	0.69
1:F:126:PRO:HB2	1:F:144:ILE:HG22	1.74	0.69
1:O:202:ASN:HD21	1:Q:281:VAL:HB	1.57	0.69
1:H:45:LYS:HB2	1:H:57:VAL:HB	1.74	0.69
1:A:3:VAL:HG22	1:A:91:ILE:HG23	1.72	0.69
1:E:63:ALA:HA	1:E:73:VAL:HG23	1.74	0.69
1:E:204:VAL:HG22	1:G:279:VAL:HG11	1.75	0.69
1:F:133:ASN:HD21	1:F:217:VAL:HG12	1.58	0.69
1:F:21:LYS:H	1:F:21:LYS:HD2	1.59	0.69
1:F:323:ASP:O	1:F:327:ILE:HG13	1.92	0.69
1:O:159:LYS:O	1:O:163:GLN:HG3	1.92	0.69
1:A:281:VAL:CG1	1:C:202:ASN:HD21	2.06	0.68
1:G:170:GLY:HA2	1:G:243:VAL:O	1.92	0.68
1:F:31:ASN:HB2	1:F:74:VAL:CG1	2.23	0.68
1:E:114:LYS:HB2	1:E:332:TRP:HH2	1.57	0.68
1:F:202:ASN:HD21	1:H:281:VAL:HB	1.58	0.68
1:E:154:LEU:O	1:E:158:VAL:HG23	1.94	0.68
1:G:256:ASN:ND2	1:G:297:THR:HG21	2.08	0.68
1:E:183:ARG:HD3	1:E:190:HIS:HB2	1.76	0.68
1:A:202:ASN:HD21	1:C:281:VAL:CG1	2.05	0.68
1:A:281:VAL:H	1:C:202:ASN:ND2	1.92	0.68
1:C:115:LYS:HE2	1:C:142:PRO:HA	1.76	0.68
1:E:55:ALA:O	1:E:57:VAL:HG23	1.94	0.68
1:Q:169:LYS:HE3	1:Q:245:GLN:NE2	2.09	0.68
1:E:134:ALA:HB3	4:E:490:HOH:O	1.93	0.67
1:A:281:VAL:HG12	1:C:202:ASN:HD21	1.59	0.67
1:D:172:MET:O	1:D:227:GLY:HA3	1.94	0.67
1:Q:85:LYS:HB2	1:Q:112:GLY:HA3	1.75	0.67
1:G:0:LYS:HB3	1:G:0:LYS:NZ	2.09	0.67
1:E:240:VAL:HG23	1:E:309:ALA:HB3	1.76	0.67
1:H:159:LYS:HE3	1:H:218:LEU:HD21	1.77	0.67
1:A:78:ASN:ND2	1:A:81:LEU:HG	2.08	0.67
1:E:31:ASN:HA	1:E:74:VAL:CG2	2.24	0.67
1:F:272:ASP:HB2	1:F:288:PHE:CD2	2.30	0.67
1:F:5:ILE:HD13	1:F:8:PHE:HD1	1.59	0.67
1:B:240:VAL:HG22	1:B:309:ALA:HB3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:ASP:OD1	1:E:296:LEU:HG	1.93	0.67
1:Q:206:THR:HG22	1:Q:229:ALA:HB3	1.77	0.67
1:F:210:ALA:O	1:F:214:VAL:HG23	1.94	0.67
1:F:133:ASN:ND2	1:F:217:VAL:HG12	2.10	0.67
1:E:194:ARG:HE	1:G:277:PRO:CA	2.07	0.67
1:E:5:ILE:CD1	1:E:27:ILE:HD12	2.25	0.67
1:G:262:SER:HB3	1:G:267:LEU:HG	1.75	0.67
1:F:222:LYS:H	1:F:224:LYS:HE3	1.57	0.67
1:F:152:ASN:O	1:F:289:SER:HB3	1.96	0.66
1:G:162:ASP:HA	1:G:167:ILE:HG13	1.75	0.66
1:B:38:LYS:H	1:B:38:LYS:HD2	1.60	0.66
1:E:25:LEU:HD11	1:E:325:ALA:HB3	1.76	0.66
1:Q:154:LEU:O	1:Q:158:VAL:HG23	1.95	0.66
1:F:202:ASN:ND2	1:H:281:VAL:HB	2.11	0.66
1:E:242:LEU:HB3	1:E:307:VAL:CG2	2.26	0.66
1:E:279:VAL:HG22	1:E:282:ASP:OD2	1.94	0.66
1:A:105:ALA:HB1	1:A:116:VAL:HG11	1.77	0.66
1:F:125:ILE:H	1:F:125:ILE:HD12	1.61	0.66
1:D:83:PRO:O	1:D:87:LEU:HD23	1.94	0.66
1:E:126:PRO:HD2	1:E:143:ILE:O	1.95	0.66
1:E:132:VAL:HG21	1:E:155:ALA:HB1	1.77	0.66
1:C:58:LYS:HE2	4:C:378:HOH:O	1.96	0.66
1:G:211:ALA:HB1	1:G:226:ASN:HA	1.76	0.66
1:D:109:ILE:HA	1:D:113:ALA:O	1.95	0.66
1:D:116:VAL:HB	1:D:143:ILE:HD12	1.78	0.66
1:F:169:LYS:HD2	1:H:301:GLY:HA3	1.77	0.66
1:F:280:SER:HB3	1:F:310:TRP:HZ3	1.61	0.66
1:A:154:LEU:HD22	1:A:172:MET:HE3	1.77	0.66
1:F:114:LYS:N	1:F:114:LYS:HD2	2.11	0.66
1:E:304:MET:CE	1:G:245:GLN:HB2	2.23	0.66
1:E:299:VAL:HG22	1:E:305:VAL:HG22	1.76	0.66
1:G:187:ALA:O	1:G:196:ALA:HB1	1.95	0.66
1:F:266:GLU:HG3	4:F:578:HOH:O	1.96	0.66
1:G:168:ILE:HG22	1:G:169:LYS:HG3	1.77	0.65
1:H:236:ASN:O	1:H:237:VAL:HB	1.96	0.65
1:H:129:VAL:HG23	1:H:217:VAL:HG11	1.78	0.65
1:B:38:LYS:N	1:B:38:LYS:HD2	2.10	0.65
1:F:176:HIS:O	1:F:231:ARG:HA	1.95	0.65
1:A:202:ASN:ND2	1:C:281:VAL:HG12	2.11	0.65
1:E:279:VAL:HG12	1:G:204:VAL:HG22	1.76	0.65
1:E:5:ILE:HD12	1:E:27:ILE:HD12	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:204:VAL:HB	1:H:231:ARG:HB2	1.79	0.65
1:E:297:THR:HG23	1:E:306:LYS:O	1.96	0.65
1:B:33:THR:HG21	1:B:77:ARG:HD3	1.79	0.65
1:E:13:ARG:HG3	1:E:13:ARG:HH11	1.62	0.65
1:F:226:ASN:HB3	1:H:300:MET:SD	2.37	0.65
1:B:193:LEU:HD13	1:C:42:HIS:CG	2.31	0.65
1:G:155:ALA:HB3	1:G:156:PRO:HD3	1.79	0.65
1:B:80:SER:OG	1:B:107:LYS:HG2	1.97	0.65
1:G:285:CYS:HA	1:G:315:TRP:CD1	2.31	0.65
1:E:210:ALA:O	1:E:214:VAL:HG23	1.97	0.65
1:E:170:GLY:N	1:E:224:LYS:O	2.30	0.65
1:F:226:ASN:ND2	1:H:298:MET:SD	2.70	0.65
1:E:151:THR:HG23	1:E:214:VAL:HG22	1.79	0.65
1:F:118:ILE:H	1:F:118:ILE:HD12	1.61	0.65
1:A:1:LEU:HD22	1:A:329:ALA:CB	2.27	0.65
1:G:293:ASP:HB3	1:G:296:LEU:HD12	1.78	0.64
1:H:182:GLN:HE22	1:H:231:ARG:HB3	1.61	0.64
1:A:64:ILE:HG13	1:A:71:ILE:HG23	1.78	0.64
1:F:188:SER:HB2	1:G:39:GLN:OE1	1.96	0.64
1:F:281:VAL:HB	1:H:202:ASN:HB3	1.79	0.64
1:B:168:ILE:HD11	1:B:247:SER:HB3	1.79	0.64
1:F:296:LEU:HD22	1:H:228:ILE:HG21	1.79	0.64
1:F:89:ILE:O	1:F:113:ALA:HA	1.97	0.64
1:G:221:LEU:HD21	1:G:225:LEU:CD1	2.25	0.64
1:G:130:VAL:CG2	1:G:320:ARG:HD3	2.28	0.64
1:H:239:VAL:HG23	1:H:309:ALA:O	1.97	0.64
1:F:280:SER:HB3	1:F:310:TRP:CZ3	2.33	0.64
1:A:228:ILE:C	1:A:228:ILE:HD12	2.18	0.64
1:F:187:ALA:O	1:F:196:ALA:HB1	1.97	0.64
1:D:284:ARG:O	1:D:285:CYS:HB2	1.95	0.64
1:B:82:LEU:HD13	1:B:84:TRP:CZ2	2.32	0.64
1:H:251:PHE:HE2	1:H:253:GLU:HB2	1.61	0.64
1:G:260:ARG:O	1:G:263:ALA:HB3	1.98	0.64
1:E:328:VAL:O	1:E:332:TRP:HB2	1.97	0.64
1:E:277:PRO:CA	1:G:194:ARG:HE	2.10	0.64
1:E:165:PHE:CD1	1:E:248:LYS:HD2	2.33	0.64
1:E:183:ARG:HA	1:E:183:ARG:HH11	1.62	0.64
1:G:64:ILE:O	1:G:70:ILE:HD12	1.98	0.64
1:G:18(A):TRP:C	1:G:19:GLY:H	1.99	0.64
1:H:129:VAL:CG2	1:H:217:VAL:HG11	2.26	0.64
1:H:78:ASN:HB3	1:H:81:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:124:ASP:HB2	4:G:634:HOH:O	1.97	0.64
1:E:79:PRO:HB2	1:E:107:LYS:HB2	1.79	0.64
1:F:324:LEU:O	1:F:328:VAL:HG23	1.97	0.63
1:E:176:HIS:N	1:E:230:LEU:O	2.28	0.63
1:F:285:CYS:HA	1:F:315:TRP:CD1	2.33	0.63
1:D:74:VAL:HG22	1:D:75:SER:N	2.12	0.63
1:B:132:VAL:HG21	1:B:155:ALA:HB1	1.80	0.63
1:E:250:THR:OG1	1:E:254:GLU:HB3	1.98	0.63
1:G:221:LEU:HD11	1:G:225:LEU:HD21	1.79	0.63
1:F:59:PRO:HA	1:F:64:ILE:HA	1.81	0.63
1:H:251:PHE:CE2	1:H:253:GLU:HB2	2.34	0.63
1:E:109:ILE:HD13	1:E:109:ILE:O	1.98	0.63
1:B:4:ALA:HB2	1:B:89:ILE:HG12	1.80	0.63
1:F:298:MET:HE2	1:H:228:ILE:HG23	1.79	0.63
1:O:78:ASN:ND2	1:O:81:LEU:HG	2.12	0.63
1:F:118:ILE:N	1:F:118:ILE:HD12	2.12	0.63
1:H:70:ILE:HG22	1:H:71:ILE:N	2.12	0.63
1:H:299:VAL:HG22	1:H:305:VAL:HG22	1.81	0.63
1:E:58:LYS:NZ	1:E:58:LYS:HB3	2.13	0.63
1:C:77:ARG:O	1:C:79:PRO:HD3	1.99	0.63
1:G:130:VAL:HA	1:G:134:ALA:CB	2.28	0.63
1:O:17:ARG:HH11	1:O:53:PHE:HB2	1.61	0.63
1:E:72:GLN:HG3	1:E:73:VAL:N	2.13	0.63
1:F:11:ILE:HD12	1:F:119:THR:HG21	1.80	0.63
1:O:202:ASN:HD21	1:Q:281:VAL:CG1	2.12	0.63
1:E:79:PRO:HB2	1:E:107:LYS:CB	2.28	0.63
1:D:272:ASP:HB2	1:D:288:PHE:CD2	2.33	0.63
1:G:150:THR:HG23	1:G:311:TYR:OH	1.99	0.63
1:D:125:ILE:HD12	1:D:126:PRO:HD2	1.80	0.63
1:F:64:ILE:O	1:F:70:ILE:HG23	1.99	0.63
1:O:204:VAL:HB	1:O:231:ARG:HB2	1.81	0.63
1:G:166:GLY:O	1:G:246:VAL:HA	1.98	0.63
1:E:74:VAL:O	1:E:75:SER:HB2	1.98	0.62
1:E:155:ALA:HB3	1:E:156:PRO:HD3	1.81	0.62
1:B:281:VAL:H	1:D:202:ASN:ND2	1.97	0.62
1:E:208:THR:HG23	1:E:208:THR:O	1.99	0.62
1:E:250:THR:HG1	1:E:254:GLU:HB3	1.64	0.62
1:O:155:ALA:HB3	1:O:156:PRO:HD3	1.80	0.62
1:G:171:THR:O	1:G:242:LEU:HB2	2.00	0.62
1:F:27:ILE:N	1:F:27:ILE:HD12	2.15	0.62
1:E:28:ILE:HA	1:E:71:ILE:HG12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:183:ARG:HE	1:H:187:ALA:HB3	1.62	0.62
1:C:26:ASP:O	1:C:28:ILE:HG23	1.99	0.62
1:O:33:THR:CG2	1:O:77:ARG:HG2	2.30	0.62
1:A:306:LYS:HD2	1:C:171:THR:OG1	2.00	0.62
1:B:15:PHE:HE2	1:B:27:ILE:HD11	1.64	0.62
1:O:134:ALA:HB3	4:O:401:HOH:O	1.97	0.62
1:G:259:PHE:CD2	1:G:292:ILE:HG21	2.34	0.62
1:E:119:THR:CG2	1:E:321:VAL:HG11	2.29	0.62
1:O:202:ASN:ND2	1:Q:281:VAL:HB	2.14	0.62
1:A:173:THR:HG23	1:A:228:ILE:HD11	1.82	0.62
1:Q:8:PHE:N	1:Q:32:ASP:OD2	2.31	0.62
1:E:270:ILE:HD11	4:E:491:HOH:O	1.99	0.62
1:D:318:SER:O	1:D:322:VAL:HG23	2.00	0.62
1:E:183:ARG:CZ	1:E:187:ALA:HB3	2.30	0.62
1:B:281:VAL:H	1:D:202:ASN:HD22	1.48	0.62
1:Q:272:ASP:O	1:Q:291:THR:HA	1.99	0.62
1:F:108:HIS:O	1:F:111:ALA:HB3	1.99	0.61
1:B:262:SER:HB3	1:B:267:LEU:HD12	1.82	0.61
1:G:239:VAL:HG23	1:G:309:ALA:O	1.99	0.61
1:E:263:ALA:O	1:E:268:LYS:HA	1.99	0.61
1:E:174:THR:HB	1:E:240:VAL:HG12	1.81	0.61
1:A:281:VAL:H	1:C:202:ASN:HD22	1.47	0.61
1:A:154:LEU:HD22	1:A:172:MET:CE	2.29	0.61
1:E:260:ARG:HD2	4:E:538:HOH:O	2.01	0.61
1:O:202:ASN:HD22	1:Q:281:VAL:H	1.46	0.61
1:D:138:SER:O	1:D:141:GLU:HG2	2.01	0.61
1:H:85:LYS:HB2	1:H:111:ALA:O	2.01	0.61
1:H:84:TRP:HA	1:H:89:ILE:HG13	1.81	0.61
1:E:84:TRP:CE3	1:E:89:ILE:HG13	2.35	0.61
1:E:117:ILE:O	1:E:117:ILE:HG13	2.00	0.61
1:C:62:THR:HG22	1:C:62:THR:O	2.00	0.61
1:F:138:SER:HA	1:F:331:ASN:OD1	2.01	0.61
1:G:221:LEU:HD11	1:G:225:LEU:CD2	2.30	0.61
1:G:18:CYS:SG	1:G:319:GLN:HG2	2.41	0.61
1:F:279:VAL:O	1:F:281:VAL:N	2.34	0.61
1:F:38:LYS:HG3	1:F:39:GLN:N	2.16	0.61
1:E:264:GLU:HG3	4:E:535:HOH:O	2.00	0.61
1:H:176:HIS:HB3	1:H:231:ARG:HD3	1.83	0.61
1:H:192:ASP:HB3	1:H:195:ARG:HB3	1.83	0.61
1:C:250:THR:OG1	1:C:251:PHE:N	2.34	0.61
1:D:240:VAL:HG13	1:D:311:TYR:CE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:LYS:HB2	1:F:218:LEU:HD11	1.82	0.61
1:G:225:LEU:O	1:G:226:ASN:HB2	2.01	0.61
1:G:294:SER:C	1:G:296:LEU:H	2.03	0.61
1:F:6:ASN:OD1	1:F:31:ASN:ND2	2.34	0.60
1:E:265:LYS:HB2	1:E:266:GLU:OE1	2.00	0.60
1:O:224:LYS:O	1:O:225:LEU:HD23	2.01	0.60
1:H:31:ASN:OD1	1:H:74:VAL:HG23	2.01	0.60
1:G:177:SER:HB3	1:G:234:THR:O	2.01	0.60
1:E:270:ILE:HG13	4:E:828:HOH:O	2.00	0.60
1:A:298:MET:SD	1:C:226:ASN:OD1	2.59	0.60
1:E:209:GLY:HA3	1:E:212:LYS:HE2	1.84	0.60
1:G:162:ASP:CA	1:G:167:ILE:HG13	2.31	0.60
1:E:186:ASP:O	1:H:13:ARG:NH2	2.35	0.60
1:H:38:LYS:CD	1:H:38:LYS:H	2.12	0.60
1:O:202:ASN:HD21	1:Q:281:VAL:CB	2.15	0.60
1:A:142:PRO:HB2	1:A:143:ILE:HD12	1.82	0.60
1:C:155:ALA:HB3	1:C:156:PRO:HD3	1.83	0.60
1:F:251:PHE:CZ	1:F:254:GLU:HB2	2.37	0.60
1:E:6:ASN:ND2	1:E:108:HIS:HE1	1.99	0.60
1:O:124:ASP:CG	1:O:124:ASP:O	2.40	0.60
1:O:281:VAL:CB	1:Q:202:ASN:HD21	2.14	0.60
1:E:94:GLU:OE1	1:E:99:PHE:HB2	2.00	0.60
1:F:126:PRO:CG	1:F:141:GLU:HG2	2.26	0.60
1:F:243:VAL:HG22	1:F:306:LYS:HG3	1.82	0.60
1:A:5:ILE:HD11	1:A:27:ILE:HD13	1.84	0.60
1:B:281:VAL:CG1	1:D:202:ASN:HD21	2.14	0.60
1:G:208:THR:C	1:G:210:ALA:H	2.05	0.60
1:Q:31:ASN:OD1	1:Q:74:VAL:HG23	2.01	0.60
1:E:320:ARG:HA	1:E:320:ARG:NE	2.17	0.60
1:G:129:VAL:CG2	1:G:217:VAL:HG11	2.30	0.60
1:H:133:ASN:N	1:H:133:ASN:HD22	1.99	0.60
1:H:264:GLU:HA	1:H:268:LYS:HG3	1.84	0.60
1:D:133:ASN:HD22	1:D:133:ASN:C	2.05	0.59
1:H:27:ILE:O	1:H:28:ILE:HB	2.02	0.59
1:Q:183:ARG:NH1	4:Q:463:HOH:O	2.27	0.59
1:H:256:ASN:O	1:H:260:ARG:HG3	2.02	0.59
1:F:14:ASN:ND2	1:F:314:GLU:HG2	2.17	0.59
1:F:277:PRO:HB2	1:H:194:ARG:HG3	1.84	0.59
1:H:91:ILE:HD13	1:H:91:ILE:C	2.23	0.59
1:F:186:ASP:HA	1:F:196:ALA:O	2.02	0.59
1:E:31:ASN:HA	1:E:74:VAL:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:PHE:CE1	1:E:307:VAL:HG21	2.37	0.59
1:A:245:GLN:HE22	1:C:245:GLN:NE2	1.99	0.59
1:F:267:LEU:HD22	1:F:270:ILE:CG2	2.33	0.59
1:G:168:ILE:HG22	1:G:169:LYS:HE3	1.84	0.59
1:E:194:ARG:HH11	1:E:205:PRO:HG2	1.67	0.59
1:E:190:HIS:HB3	1:E:196:ALA:HB2	1.85	0.59
1:E:18:CYS:O	1:E:20:ARG:HG2	2.02	0.59
1:C:56:ASP:O	1:C:66:VAL:HA	2.02	0.59
1:O:129:VAL:H	1:O:133:ASN:HD21	1.48	0.59
1:F:149:CYS:HB3	2:F:335:NAD:H5N	1.84	0.59
1:E:195:ARG:NH2	1:E:231:ARG:NH2	2.51	0.59
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.83	0.59
1:A:271:LEU:HD12	1:A:272:ASP:N	2.17	0.59
1:A:245:GLN:HE22	1:C:245:GLN:HE22	1.51	0.59
1:D:164:LYS:HD2	1:D:258:ALA:HB1	1.85	0.59
1:F:271:LEU:HD13	1:F:290:THR:HG23	1.84	0.59
1:A:281:VAL:CB	1:C:202:ASN:HD21	2.16	0.59
1:Q:2:LYS:HE2	4:Q:451:HOH:O	2.02	0.59
1:F:271:LEU:HD13	1:F:290:THR:CG2	2.32	0.59
1:F:6:ASN:O	1:F:96:THR:HG23	2.03	0.59
1:G:205:PRO:HA	1:G:229:ALA:O	2.03	0.59
1:E:202:ASN:HD22	1:G:281:VAL:CG1	2.16	0.59
1:E:44:LEU:O	1:E:53:PHE:HD1	1.86	0.59
1:E:117:ILE:HG22	1:E:144:ILE:CD1	2.31	0.59
1:F:243:VAL:CG1	1:H:171:THR:HG21	2.33	0.59
1:E:3:VAL:CG2	1:E:25:LEU:HD22	2.32	0.59
1:F:183:ARG:NE	1:F:187:ALA:HB3	2.18	0.59
1:E:109:ILE:HA	1:E:113:ALA:O	2.03	0.59
1:E:318:SER:O	1:E:322:VAL:HG23	2.03	0.58
1:F:145:SER:C	1:F:147:ALA:H	2.06	0.58
1:F:271:LEU:HD11	1:F:292:ILE:HD11	1.84	0.58
1:E:157:PHE:HB2	1:E:259:PHE:CE1	2.37	0.58
1:E:159:LYS:O	1:E:163:GLN:HG3	2.03	0.58
1:E:279:VAL:HG22	1:G:197:ARG:NH1	2.18	0.58
1:H:108:HIS:HB2	1:H:116:VAL:HG21	1.85	0.58
1:E:199:ALA:HB2	1:H:184:LEU:HD21	1.85	0.58
1:E:293:ASP:CG	1:E:296:LEU:HG	2.23	0.58
1:C:241:ASP:OD1	1:C:306:LYS:HE3	2.03	0.58
1:G:172:MET:O	1:G:227:GLY:HA3	2.03	0.58
1:G:243:VAL:HG22	1:G:306:LYS:HE2	1.85	0.58
1:E:228:ILE:H	1:E:228:ILE:HD13	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:276:GLU:HB2	1:Q:278:LEU:HG	1.86	0.58
1:B:269:GLY:C	1:B:270:ILE:HD12	2.24	0.58
1:O:1:LEU:CD1	1:O:329:ALA:HA	2.34	0.58
1:O:277:PRO:HA	1:Q:194:ARG:NH2	2.19	0.58
1:Q:129:VAL:H	1:Q:133:ASN:ND2	2.01	0.58
1:G:192:ASP:CG	1:G:195:ARG:HG3	2.24	0.58
1:G:228:ILE:H	1:G:228:ILE:HD13	1.69	0.58
1:F:115:LYS:HD2	1:F:332:TRP:HZ3	1.68	0.58
1:E:115:LYS:HD2	1:E:328:VAL:HG11	1.86	0.58
1:F:154:LEU:HG	1:F:158:VAL:HG21	1.84	0.58
1:C:210:ALA:O	1:C:214:VAL:HG23	2.03	0.58
1:H:27:ILE:HG22	1:H:28:ILE:H	1.68	0.58
1:F:140:ASP:O	1:F:142:PRO:HD3	2.03	0.58
1:F:202:ASN:HD21	1:H:281:VAL:CG1	2.17	0.58
1:H:195:ARG:HH21	1:H:206:THR:CG2	2.15	0.58
1:F:235:PRO:HB3	1:G:201:LEU:HD11	1.86	0.58
1:G:251:PHE:HA	1:G:299:VAL:HG21	1.86	0.58
1:E:267:LEU:HD13	1:E:271:LEU:HD23	1.86	0.58
1:E:183:ARG:NE	1:E:187:ALA:HB3	2.19	0.58
1:H:328:VAL:O	1:H:332:TRP:HB2	2.03	0.58
1:O:33:THR:HG22	1:O:77:ARG:HG2	1.86	0.58
1:Q:123:GLY:O	1:Q:125:ILE:N	2.32	0.58
1:E:298:MET:SD	1:G:226:ASN:ND2	2.74	0.57
1:G:294:SER:O	1:G:296:LEU:N	2.37	0.57
1:E:277:PRO:HG2	1:F:42:HIS:CE1	2.39	0.57
1:O:168:ILE:HG22	1:O:169:LYS:HG2	1.86	0.57
1:F:205:PRO:HG2	1:H:310:TRP:HZ2	1.68	0.57
1:G:157:PHE:O	1:G:161:LEU:HG	2.05	0.57
1:F:0:LYS:HD2	1:F:24:PRO:HA	1.85	0.57
1:E:193:LEU:HB3	1:H:42:HIS:CD2	2.39	0.57
1:E:71:ILE:HD13	1:E:72:GLN:N	2.19	0.57
1:A:271:LEU:HD13	1:A:290:THR:OG1	2.04	0.57
1:H:38:LYS:HD2	1:H:38:LYS:N	2.19	0.57
1:B:155:ALA:HB3	1:B:156:PRO:HD3	1.86	0.57
1:D:3:VAL:HG21	1:D:25:LEU:HD22	1.86	0.57
1:D:58:LYS:HB3	1:D:58:LYS:NZ	2.20	0.57
1:E:203:ILE:HA	1:E:231:ARG:O	2.04	0.57
1:H:134:ALA:HB1	1:H:327:ILE:CD1	2.35	0.57
1:E:160:VAL:O	1:E:164:LYS:HB2	2.05	0.57
1:G:264:GLU:HG2	1:G:264:GLU:O	2.04	0.57
1:G:271:LEU:HD11	1:G:292:ILE:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:CYS:O	1:G:156:PRO:HD2	2.05	0.57
1:E:74:VAL:HG23	1:E:75:SER:N	2.18	0.57
1:Q:129:VAL:H	1:Q:133:ASN:HD21	1.53	0.57
1:Q:236:ASN:O	1:Q:237:VAL:HB	2.05	0.57
1:D:82:LEU:HD13	1:D:84:TRP:CZ2	2.39	0.57
1:E:205:PRO:HA	1:E:229:ALA:O	2.05	0.57
1:H:83:PRO:HB2	1:H:86:GLU:CG	2.34	0.57
1:E:15:PHE:CE1	1:E:322:VAL:HG22	2.40	0.57
1:Q:190:HIS:HB3	1:Q:196:ALA:HB2	1.87	0.57
1:H:246:VAL:HG22	1:H:303:ASP:O	2.05	0.57
1:D:4:ALA:HB2	1:D:89:ILE:HG12	1.87	0.57
1:F:16:LEU:HD23	1:F:16:LEU:C	2.24	0.57
1:A:115:LYS:HD2	1:A:332:TRP:CZ3	2.39	0.57
1:A:181:ASP:OD2	1:A:195:ARG:NH1	2.38	0.57
1:C:172:MET:HG2	1:C:173:THR:N	2.20	0.57
1:E:24:PRO:HG2	1:E:330:ASN:HD21	1.70	0.57
1:F:37:VAL:N	1:F:73:VAL:HG11	2.20	0.56
1:B:38:LYS:CD	1:B:38:LYS:H	2.13	0.56
1:B:255:VAL:O	1:B:258:ALA:HB3	2.05	0.56
1:E:33:THR:O	1:E:33:THR:HG22	2.05	0.56
1:F:156:PRO:O	1:F:159:LYS:HB3	2.05	0.56
1:A:91:ILE:HD13	1:A:91:ILE:C	2.25	0.56
1:E:13:ARG:HG3	1:E:13:ARG:NH1	2.20	0.56
1:C:18(A):TRP:O	1:C:20:ARG:HB2	2.06	0.56
1:F:304:MET:HB2	1:H:169:LYS:NZ	2.19	0.56
1:E:272:ASP:HB2	1:E:288:PHE:CD2	2.40	0.56
1:B:256:ASN:HB3	1:B:260:ARG:HH12	1.68	0.56
1:B:128:TYR:HA	1:B:133:ASN:HD21	1.70	0.56
1:G:185:LEU:HA	1:G:198:ALA:HB2	1.87	0.56
1:F:279:VAL:HG12	1:H:204:VAL:HA	1.88	0.56
1:H:91:ILE:HA	1:H:115:LYS:O	2.06	0.56
1:A:281:VAL:HG12	1:C:202:ASN:ND2	2.20	0.56
1:H:21:LYS:O	1:H:22:ASP:C	2.44	0.56
1:E:64:ILE:O	1:E:70:ILE:HA	2.06	0.56
1:E:279:VAL:HG11	1:G:204:VAL:HG22	1.85	0.56
1:O:236:ASN:O	1:O:237:VAL:HB	2.04	0.56
1:G:28:ILE:HD11	1:G:89:ILE:CD1	2.35	0.56
1:H:132:VAL:O	1:H:133:ASN:HB3	2.05	0.56
1:Q:84:TRP:CE3	1:Q:89:ILE:HG13	2.40	0.56
1:Q:169:LYS:HE3	1:Q:245:GLN:HE22	1.69	0.56
1:C:243:VAL:HG22	1:C:306:LYS:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:251:PHE:CZ	1:Q:254:GLU:HB2	2.40	0.56
1:C:21:LYS:HE3	1:C:21:LYS:H	1.70	0.56
1:D:209:GLY:O	1:D:211:ALA:N	2.39	0.56
1:B:15:PHE:CE2	1:B:27:ILE:HD11	2.40	0.56
1:D:133:ASN:ND2	1:D:133:ASN:C	2.58	0.56
1:H:157:PHE:HB2	1:H:259:PHE:CE1	2.41	0.56
1:A:103:GLU:HB2	1:G:253:GLU:OE1	2.05	0.56
1:F:202:ASN:HD21	1:H:281:VAL:CB	2.17	0.56
1:E:279:VAL:CG2	1:E:281:VAL:HG12	2.36	0.56
1:B:193:LEU:HD13	1:C:42:HIS:CD2	2.41	0.56
1:E:171:THR:HG23	1:G:306:LYS:HE3	1.88	0.56
1:E:158:VAL:HG11	1:E:225:LEU:HD11	1.87	0.56
1:A:210:ALA:O	1:A:214:VAL:HG23	2.05	0.56
1:C:266:GLU:HG2	1:C:267:LEU:N	2.19	0.56
1:D:292:ILE:HD12	1:D:292:ILE:N	2.19	0.56
1:F:172:MET:O	1:F:227:GLY:HA3	2.06	0.55
1:E:241:ASP:OD1	1:E:306:LYS:HE2	2.06	0.55
1:F:37:VAL:H	1:F:73:VAL:HG11	1.71	0.55
1:E:25:LEU:HD11	1:E:325:ALA:CB	2.36	0.55
1:E:4:ALA:HB3	1:E:92:VAL:HG22	1.89	0.55
1:G:192:ASP:OD1	1:G:195:ARG:HG3	2.07	0.55
1:D:246:VAL:O	1:D:303:ASP:HB2	2.05	0.55
1:F:115:LYS:HD2	1:F:332:TRP:CZ3	2.41	0.55
1:B:177:SER:HB3	1:B:234:THR:O	2.07	0.55
1:G:222:LYS:O	1:G:224:LYS:N	2.39	0.55
1:E:183:ARG:HB3	1:E:187:ALA:HB3	1.88	0.55
1:H:9:GLY:HA2	1:H:13:ARG:HH12	1.72	0.55
1:D:75:SER:HB3	1:H:61:GLU:HB3	1.87	0.55
1:Q:187:ALA:O	1:Q:196:ALA:HB1	2.05	0.55
1:H:102:ARG:NE	1:H:124:ASP:OD1	2.40	0.55
1:F:170:GLY:HA3	1:F:244:VAL:HG12	1.88	0.55
1:F:157:PHE:HB2	1:F:259:PHE:CE1	2.41	0.55
1:D:79:PRO:HA	1:D:82:LEU:HD12	1.88	0.55
1:H:194:ARG:C	1:H:196:ALA:H	2.10	0.55
1:E:119:THR:HG22	1:E:321:VAL:CG1	2.36	0.55
1:E:202:ASN:HD22	1:G:281:VAL:HG12	1.72	0.55
1:D:37:VAL:HG22	1:D:73:VAL:HB	1.89	0.55
1:E:276:GLU:OE2	1:E:277:PRO:HD2	2.06	0.55
1:E:85:LYS:N	1:E:112:GLY:HA3	2.21	0.55
1:E:257:ALA:HB2	4:E:537:HOH:O	2.07	0.55
1:A:333:LYS:C	1:A:333:LYS:HE2	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:181:ASP:CB	1:H:195:ARG:HD3	2.36	0.55
1:H:132:VAL:HG12	1:H:132:VAL:O	2.06	0.55
1:E:256:ASN:HD21	1:E:297:THR:CB	2.19	0.55
1:G:193:LEU:CD2	1:G:193:LEU:H	2.20	0.55
1:H:2:LYS:HD2	1:H:88:GLY:CA	2.37	0.55
1:D:182:GLN:HE22	1:D:231:ARG:HB3	1.72	0.55
1:D:91:ILE:CG2	1:D:115:LYS:HB3	2.35	0.55
1:A:85:LYS:H	1:A:85:LYS:HE3	1.71	0.55
1:H:294:SER:C	1:H:296:LEU:H	2.09	0.55
1:B:172:MET:HE3	1:B:211:ALA:HB2	1.87	0.55
1:O:213:ALA:O	1:O:216:LEU:HB2	2.07	0.55
1:H:266:GLU:HG2	1:H:267:LEU:HG	1.89	0.55
1:O:192:ASP:CG	1:O:195:ARG:HG3	2.27	0.55
1:D:266:GLU:HG2	1:D:267:LEU:HG	1.89	0.55
1:D:84:TRP:HB2	1:D:112:GLY:HA3	1.89	0.55
1:E:179:THR:HG22	1:E:180:GLY:N	2.22	0.55
1:G:194:ARG:HH11	1:G:205:PRO:HB2	1.72	0.55
1:F:301:GLY:HA3	1:H:169:LYS:HD2	1.89	0.55
1:B:240:VAL:CG2	1:B:309:ALA:HB3	2.37	0.55
1:O:162:ASP:OD2	1:O:220:ASN:ND2	2.40	0.55
1:Q:317:TYR:O	1:Q:320:ARG:HB2	2.07	0.55
1:H:90:ASP:O	1:H:114:LYS:HB2	2.07	0.55
1:D:129:VAL:CG2	1:D:217:VAL:HG11	2.35	0.55
1:Q:78:ASN:OD1	1:Q:80:SER:HB2	2.07	0.55
1:B:193:LEU:HB3	1:C:42:HIS:CD2	2.42	0.55
1:C:243:VAL:HA	1:C:305:VAL:O	2.06	0.55
1:H:125:ILE:HD12	1:H:125:ILE:N	2.23	0.55
1:G:271:LEU:HD13	1:G:290:THR:HG23	1.89	0.54
1:E:210:ALA:HB2	3:E:337:SO4:O4	2.06	0.54
1:E:172:MET:HG2	1:E:173:THR:N	2.23	0.54
1:C:272:ASP:O	1:C:291:THR:HA	2.07	0.54
1:O:202:ASN:ND2	1:Q:281:VAL:H	2.04	0.54
1:Q:160:VAL:HG13	1:Q:164:LYS:HE3	1.89	0.54
1:C:85:LYS:N	1:C:112:GLY:HA3	2.22	0.54
1:Q:135:ASP:OD2	1:Q:135:ASP:N	2.36	0.54
1:A:129:VAL:H	1:A:133:ASN:ND2	2.05	0.54
1:D:84:TRP:CE3	1:D:84:TRP:HA	2.42	0.54
1:H:130:VAL:HG21	1:H:320:ARG:HD3	1.90	0.54
1:F:169:LYS:CD	1:H:301:GLY:HA3	2.37	0.54
1:O:84:TRP:CE3	1:O:84:TRP:HA	2.42	0.54
1:E:166:GLY:O	1:E:246:VAL:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:296:LEU:HD12	1:E:308:ILE:HG21	1.90	0.54
1:D:313:ASN:O	2:D:335:NAD:H4N	2.08	0.54
1:E:70:ILE:HD13	1:E:70:ILE:N	2.16	0.54
1:H:194:ARG:HD3	1:H:205:PRO:O	2.07	0.54
1:E:14:ASN:HB3	1:E:318:SER:OG	2.08	0.54
1:G:201:LEU:O	1:G:233:PRO:HG2	2.07	0.54
1:A:128:TYR:HA	1:A:133:ASN:HD21	1.72	0.54
1:A:226:ASN:ND2	1:C:300:MET:HB2	2.22	0.54
1:A:2:LYS:HG2	1:A:28:ILE:HD13	1.90	0.54
1:E:87:LEU:HD12	1:E:87:LEU:N	2.22	0.54
1:A:9:GLY:HA3	2:A:335:NAD:O5B	2.08	0.54
1:E:17:ARG:HH11	1:E:18(B):HIS:HB3	1.72	0.54
1:E:169:LYS:HE2	1:E:245:GLN:CD	2.27	0.54
1:A:91:ILE:HD11	1:A:93:ILE:HD13	1.89	0.54
1:Q:133:ASN:HD22	1:Q:133:ASN:H	1.55	0.54
1:G:256:ASN:ND2	1:G:256:ASN:N	2.54	0.54
1:F:310:TRP:HZ2	1:H:205:PRO:HG2	1.72	0.54
1:B:271:LEU:HD22	1:B:290:THR:OG1	2.07	0.54
1:C:76:ASN:ND2	1:C:78:ASN:H	2.06	0.54
1:F:255:VAL:C	1:F:257:ALA:H	2.10	0.54
1:G:176:HIS:HA	1:G:238:SER:OG	2.08	0.54
1:G:161:LEU:O	1:G:165:PHE:HB2	2.08	0.54
1:F:38:LYS:HG3	1:F:39:GLN:H	1.72	0.54
1:E:151:THR:HG23	1:E:214:VAL:CG2	2.37	0.54
1:F:28:ILE:HG22	1:F:89:ILE:HD11	1.90	0.54
1:E:270:ILE:HG22	1:E:270:ILE:O	2.07	0.54
1:E:209:GLY:O	1:E:212:LYS:HG2	2.07	0.54
1:E:138:SER:O	1:E:140:ASP:N	2.41	0.54
1:E:58:LYS:CG	1:E:65:SER:HB3	2.38	0.54
1:A:30:ILE:HG13	1:A:71:ILE:CD1	2.35	0.54
1:O:84:TRP:HE3	1:O:84:TRP:HA	1.73	0.54
1:D:152:ASN:O	1:D:289:SER:HB3	2.08	0.54
1:D:84:TRP:HA	1:D:84:TRP:HE3	1.72	0.53
1:E:240:VAL:CG2	1:E:309:ALA:HB3	2.38	0.53
1:B:242:LEU:O	1:B:306:LYS:HA	2.08	0.53
1:G:90:ASP:HB3	1:G:332:TRP:CH2	2.43	0.53
1:H:15:PHE:CE2	1:H:93:ILE:HG13	2.44	0.53
1:Q:90:ASP:HA	1:Q:114:LYS:HG2	1.90	0.53
1:C:82:LEU:HD13	1:C:84:TRP:CZ2	2.43	0.53
1:E:252:ALA:HB1	1:E:298:MET:HA	1.90	0.53
1:F:202:ASN:ND2	1:H:281:VAL:H	1.98	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:ILE:H	1:F:228:ILE:CD1	2.21	0.53
1:G:291:THR:CG2	1:G:310:TRP:HB2	2.39	0.53
1:O:192:ASP:OD2	1:O:195:ARG:HG3	2.08	0.53
1:Q:38:LYS:CE	1:Q:38:LYS:H	2.16	0.53
1:E:279:VAL:HB	1:G:203:ILE:O	2.08	0.53
1:E:199:ALA:HB3	1:H:184:LEU:HD11	1.90	0.53
1:A:281:VAL:HB	1:C:202:ASN:HD21	1.72	0.53
1:C:115:LYS:HG3	1:C:142:PRO:O	2.08	0.53
1:E:77:ARG:CZ	1:E:77:ARG:HB3	2.38	0.53
1:F:126:PRO:HD2	1:F:143:ILE:O	2.07	0.53
1:E:211:ALA:CB	1:E:226:ASN:HA	2.39	0.53
1:F:296:LEU:O	1:F:298:MET:HG3	2.08	0.53
1:H:105:ALA:HB3	1:H:143:ILE:HD13	1.91	0.53
1:O:277:PRO:HA	1:Q:194:ARG:CZ	2.38	0.53
1:C:1:LEU:HD23	1:C:91:ILE:HD11	1.89	0.53
1:A:300:MET:HE3	1:C:226:ASN:HB3	1.90	0.53
1:Q:155:ALA:HB3	1:Q:156:PRO:HD3	1.91	0.53
1:G:188:SER:O	1:G:190:HIS:HB2	2.07	0.53
1:C:70:ILE:HD12	1:C:70:ILE:N	2.24	0.53
1:D:263:ALA:O	1:D:268:LYS:HA	2.09	0.53
1:E:317:TYR:O	1:E:321:VAL:HG23	2.09	0.53
1:F:120:ALA:O	1:F:145:SER:HB2	2.08	0.53
1:E:130:VAL:HA	1:E:134:ALA:HB2	1.91	0.53
1:F:176:HIS:HA	1:F:238:SER:HB3	1.91	0.53
1:O:162:ASP:HB2	1:O:167:ILE:HD12	1.91	0.53
1:G:152:ASN:O	1:G:289:SER:HB3	2.09	0.53
1:A:191:ARG:HH11	1:A:191:ARG:HB2	1.73	0.53
1:G:13:ARG:HH11	1:G:13:ARG:HG3	1.73	0.53
1:E:153:CYS:O	1:E:156:PRO:HD2	2.08	0.53
1:C:289:SER:OG	1:C:320:ARG:HD2	2.09	0.53
1:F:279:VAL:HG12	1:H:205:PRO:CD	2.39	0.53
1:H:81:LEU:HD12	1:H:81:LEU:N	2.21	0.53
1:O:133:ASN:HD22	1:O:133:ASN:H	1.55	0.53
1:A:101:ASP:OD1	1:A:103:GLU:HG3	2.09	0.53
1:G:138:SER:HB2	1:G:140:ASP:OD2	2.09	0.53
1:E:242:LEU:HB3	1:E:307:VAL:HG23	1.91	0.53
1:G:31:ASN:OD1	1:G:74:VAL:HG23	2.09	0.53
1:G:79:PRO:HA	1:G:82:LEU:HD12	1.91	0.53
1:O:18(A):TRP:CD2	1:O:27:ILE:HD13	2.44	0.53
1:D:79:PRO:HB2	1:D:107:LYS:HB2	1.90	0.53
1:H:83:PRO:O	1:H:86:GLU:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:125:ILE:HD12	1:H:125:ILE:H	1.72	0.53
1:H:25:LEU:HD11	1:H:325:ALA:HB1	1.91	0.53
1:D:236:ASN:O	1:D:237:VAL:HB	2.09	0.53
1:F:301:GLY:HA3	1:H:169:LYS:CD	2.39	0.52
1:H:250:THR:OG1	1:H:251:PHE:N	2.42	0.52
1:H:94:GLU:OE2	1:H:99:PHE:HD2	1.92	0.52
1:F:198:ALA:HB1	1:F:201:LEU:HG	1.91	0.52
1:H:186:ASP:OD2	1:H:197:ARG:NE	2.42	0.52
1:D:251:PHE:CE2	1:D:253:GLU:HG2	2.44	0.52
1:H:242:LEU:HD12	1:H:243:VAL:H	1.74	0.52
1:B:163:GLN:HE21	1:B:164:LYS:HZ2	1.53	0.52
1:E:58:LYS:HG3	1:E:65:SER:HB3	1.90	0.52
1:B:205:PRO:HA	1:B:230:LEU:HD23	1.92	0.52
1:E:162:ASP:HA	1:E:167:ILE:HG13	1.91	0.52
1:E:204:VAL:HG22	1:G:279:VAL:CG1	2.40	0.52
1:H:83:PRO:HB2	1:H:86:GLU:HG3	1.89	0.52
1:C:1:LEU:HD21	1:C:332:TRP:CE3	2.45	0.52
1:F:18(A):TRP:HA	1:F:20:ARG:HG2	1.90	0.52
1:G:16:LEU:O	1:G:16:LEU:HD23	2.09	0.52
1:E:129:VAL:HG21	1:E:217:VAL:HG11	1.91	0.52
1:E:192:ASP:OD2	1:E:195:ARG:HD2	2.10	0.52
1:H:115:LYS:HE2	1:H:332:TRP:HZ3	1.74	0.52
1:C:21:LYS:CE	1:C:21:LYS:H	2.23	0.52
1:G:236:ASN:O	1:G:237:VAL:HB	2.09	0.52
1:F:296:LEU:HD13	1:F:308:ILE:HG13	1.91	0.52
1:E:185:LEU:HA	1:E:198:ALA:HB2	1.91	0.52
1:F:60:SER:N	1:F:64:ILE:HA	2.24	0.52
1:H:294:SER:O	1:H:296:LEU:N	2.41	0.52
1:E:79:PRO:HA	1:E:82:LEU:HG	1.90	0.52
1:B:87:LEU:HB2	1:B:89:ILE:HD13	1.91	0.52
1:O:133:ASN:N	1:O:133:ASN:HD22	2.08	0.52
1:Q:211:ALA:HB1	1:Q:226:ASN:HA	1.92	0.52
1:Q:219:PRO:O	1:Q:222:LYS:HB2	2.09	0.52
1:A:16:LEU:HD23	1:A:16:LEU:O	2.10	0.52
1:D:220:ASN:C	1:D:221:LEU:HD22	2.30	0.52
1:G:276:GLU:HB3	1:G:277:PRO:HD2	1.91	0.52
1:H:134:ALA:HB1	1:H:327:ILE:HD13	1.91	0.52
1:Q:156:PRO:HB2	1:Q:290:THR:HG21	1.92	0.52
1:B:102:ARG:NH1	1:B:102:ARG:HG2	2.24	0.52
1:G:160:VAL:CG1	1:G:258:ALA:HB1	2.40	0.52
1:E:279:VAL:HG22	1:G:197:ARG:HH12	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:129:VAL:N	1:H:133:ASN:HD21	2.04	0.52
1:E:183:ARG:HG2	1:E:196:ALA:HA	1.91	0.52
1:O:129:VAL:H	1:O:133:ASN:ND2	2.08	0.52
1:Q:128:TYR:HA	1:Q:133:ASN:HD21	1.75	0.52
1:O:226:ASN:HB2	1:Q:300:MET:CE	2.40	0.52
1:Q:181:ASP:OD2	1:Q:195:ARG:NH1	2.36	0.52
1:E:181:ASP:OD2	1:E:195:ARG:NH1	2.43	0.52
1:C:271:LEU:HD12	1:C:290:THR:HG23	1.92	0.52
1:F:243:VAL:HG11	1:H:171:THR:CG2	2.39	0.52
1:F:186:ASP:OD1	1:F:197:ARG:HA	2.09	0.52
1:G:168:ILE:CG2	1:G:169:LYS:HE3	2.40	0.52
1:D:4:ALA:HB3	1:D:92:VAL:HG22	1.92	0.52
1:G:243:VAL:CG2	1:G:306:LYS:HE2	2.40	0.52
1:E:115:LYS:HD2	1:E:328:VAL:CG1	2.40	0.52
1:G:197:ARG:O	1:G:199:ALA:N	2.43	0.52
1:F:306:LYS:HD2	1:H:171:THR:OG1	2.09	0.52
1:Q:84:TRP:HA	1:Q:84:TRP:HE3	1.75	0.52
1:C:64:ILE:CD1	1:C:66:VAL:HG23	2.40	0.52
1:D:218:LEU:HB3	1:D:221:LEU:HD23	1.92	0.52
1:B:310:TRP:HZ2	1:D:205:PRO:HG2	1.74	0.52
1:G:137:TYR:CE2	1:G:328:VAL:HA	2.44	0.52
1:G:161:LEU:HD13	1:G:244:VAL:HG21	1.91	0.51
1:G:243:VAL:HG13	1:G:306:LYS:HB2	1.92	0.51
1:H:330:ASN:C	1:H:332:TRP:H	2.13	0.51
1:B:9:GLY:HA3	2:B:335:NAD:O5B	2.10	0.51
1:F:128:TYR:HA	1:F:133:ASN:HD21	1.76	0.51
1:H:72:GLN:N	1:H:72:GLN:NE2	2.46	0.51
1:E:171:THR:CG2	1:G:306:LYS:HE3	2.41	0.51
1:G:296:LEU:HD13	1:G:308:ILE:HG21	1.93	0.51
1:D:130:VAL:HA	1:D:134:ALA:HB2	1.90	0.51
1:D:89:ILE:O	1:D:113:ALA:HA	2.10	0.51
1:C:76:ASN:HD22	1:C:76:ASN:C	2.13	0.51
1:F:4:ALA:HB3	1:F:89:ILE:HG21	1.92	0.51
1:Q:1:LEU:HG	1:Q:1:LEU:O	2.10	0.51
1:D:101:ASP:CB	1:D:122(A):LYS:HB2	2.40	0.51
1:H:14:ASN:OD1	1:H:50:LEU:HD11	2.11	0.51
1:D:175:THR:HB	1:D:239:VAL:CG1	2.41	0.51
1:Q:86:GLU:N	1:Q:86:GLU:OE2	2.44	0.51
1:H:81:LEU:CD1	1:H:81:LEU:H	2.21	0.51
1:H:264:GLU:O	1:H:268:LYS:HD2	2.11	0.51
1:E:202:ASN:CB	1:G:280:SER:OG	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:176:HIS:HB3	1:Q:231:ARG:HD3	1.92	0.51
1:D:79:PRO:HA	1:D:82:LEU:CD1	2.40	0.51
1:F:79:PRO:HB3	1:F:108:HIS:CE1	2.46	0.51
1:E:175:THR:HB	1:E:239:VAL:HG12	1.92	0.51
1:E:203:ILE:HD11	1:G:232:VAL:CG2	2.36	0.51
1:H:242:LEU:HD12	1:H:243:VAL:N	2.26	0.51
1:H:92:VAL:HG11	1:H:108:HIS:CE1	2.46	0.51
1:Q:84:TRP:HA	1:Q:84:TRP:CE3	2.46	0.51
1:E:253:GLU:HG3	3:E:334:SO4:O3	2.10	0.51
1:E:320:ARG:HA	1:E:320:ARG:HE	1.75	0.51
1:A:83:PRO:HA	1:A:85:LYS:HE2	1.93	0.51
1:D:271:LEU:HD11	1:D:292:ILE:HD11	1.93	0.51
1:G:137:TYR:OH	1:G:328:VAL:HG13	2.11	0.51
1:F:174:THR:HB	1:F:240:VAL:HG12	1.92	0.51
1:O:0:LYS:NZ	1:O:23:SER:O	2.44	0.51
1:B:37:VAL:HG22	1:B:73:VAL:HB	1.93	0.51
1:H:72:GLN:N	1:H:72:GLN:HE21	2.07	0.51
1:E:27:ILE:HD11	1:E:30:ILE:CG1	2.40	0.51
1:F:279:VAL:HG12	1:H:205:PRO:HD2	1.92	0.51
1:B:228:ILE:HG23	1:D:298:MET:HE1	1.93	0.51
1:H:289:SER:OG	1:H:320:ARG:NH1	2.43	0.51
1:A:172:MET:HG2	1:A:173:THR:N	2.25	0.51
1:A:280:SER:HB3	1:C:203:ILE:HB	1.93	0.51
1:B:221:LEU:HA	1:B:224:LYS:HD2	1.91	0.51
1:B:324:LEU:O	1:B:328:VAL:HG23	2.11	0.51
1:D:170:GLY:O	1:D:225:LEU:HA	2.11	0.51
1:G:99:PHE:HB3	1:G:104:GLY:O	2.11	0.51
1:Q:191:ARG:HG2	1:Q:192:ASP:N	2.26	0.51
1:F:218:LEU:N	1:F:219:PRO:HD3	2.26	0.51
1:E:43:LEU:HD11	1:H:187:ALA:O	2.11	0.51
1:G:130:VAL:HG21	1:G:320:ARG:HD3	1.92	0.51
1:A:193:LEU:HD13	1:D:42:HIS:CG	2.46	0.51
1:B:114:LYS:HD2	1:B:332:TRP:HZ2	1.76	0.51
1:E:226:ASN:CB	1:G:300:MET:HE2	2.30	0.51
1:C:76:ASN:OD1	1:C:81:LEU:HB2	2.11	0.51
1:E:199:ALA:CB	1:H:184:LEU:HD21	2.40	0.51
1:C:64:ILE:HD11	1:C:71:ILE:HD12	1.93	0.51
1:F:174:THR:HA	1:F:240:VAL:HA	1.93	0.51
1:C:301:GLY:O	1:C:302:ASP:HB2	2.10	0.51
1:D:16:LEU:HD23	1:D:16:LEU:O	2.11	0.51
1:A:74:VAL:HG23	1:A:75:SER:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:HD12	1:A:290:THR:O	2.11	0.51
1:A:78:ASN:HD22	1:A:81:LEU:HG	1.76	0.51
1:E:272:ASP:HB2	1:E:288:PHE:CG	2.46	0.51
1:F:157:PHE:HB2	1:F:259:PHE:HE1	1.76	0.51
1:E:32:ASP:OD2	1:E:40:ALA:HB2	2.11	0.51
1:O:17:ARG:HD2	1:O:53:PHE:CD1	2.46	0.50
1:E:89:ILE:HG21	1:E:92:VAL:HG22	1.93	0.50
1:E:212:LYS:O	1:E:215:ALA:HB3	2.10	0.50
1:Q:1:LEU:HD23	1:Q:91:ILE:HD11	1.93	0.50
1:G:85:LYS:HG3	1:G:86:GLU:N	2.26	0.50
1:B:0(A):ALA:HB3	1:B:23:SER:O	2.11	0.50
1:E:267:LEU:HD13	1:E:271:LEU:CD2	2.41	0.50
1:F:287:ASP:OD1	1:F:319:GLN:NE2	2.44	0.50
1:F:60:SER:OG	1:F:70:ILE:HD13	2.12	0.50
1:H:75:SER:O	1:H:76:ASN:HB2	2.11	0.50
1:B:84:TRP:HA	1:B:84:TRP:CE3	2.46	0.50
1:C:9:GLY:O	1:C:13:ARG:HG3	2.11	0.50
1:G:168:ILE:C	1:G:169:LYS:HG3	2.32	0.50
1:G:129:VAL:H	1:G:133:ASN:ND2	2.07	0.50
1:A:143:ILE:HD12	1:A:143:ILE:N	2.27	0.50
1:O:279:VAL:HG11	1:Q:204:VAL:HG22	1.93	0.50
1:Q:107:LYS:O	1:Q:110:GLU:HB2	2.10	0.50
1:G:18(A):TRP:C	1:G:19:GLY:N	2.64	0.50
1:F:169:LYS:HA	1:F:224:LYS:HB3	1.92	0.50
1:E:15:PHE:CD1	1:E:322:VAL:HG22	2.47	0.50
1:C:62:THR:O	1:C:63:ALA:HB2	2.11	0.50
1:F:232:VAL:HG11	1:H:232:VAL:HG11	1.93	0.50
1:D:103:GLU:OE1	1:D:103:GLU:N	2.41	0.50
1:O:9:GLY:O	1:O:13:ARG:HG3	2.12	0.50
1:H:129:VAL:H	1:H:133:ASN:ND2	2.03	0.50
1:E:79:PRO:HA	1:E:82:LEU:CD1	2.42	0.50
1:O:26:ASP:OD1	1:O:69:LYS:HE2	2.11	0.50
1:G:226:ASN:ND2	1:G:227:GLY:H	2.09	0.50
1:E:194:ARG:NH1	1:E:205:PRO:HG2	2.26	0.50
1:G:256:ASN:HB3	1:G:260:ARG:HH11	1.75	0.50
1:A:1:LEU:HD22	1:A:329:ALA:HB2	1.94	0.50
1:H:8:PHE:CE1	1:H:16:LEU:HD12	2.46	0.50
1:H:3:VAL:HG23	1:H:91:ILE:O	2.11	0.50
1:B:169:LYS:CD	1:D:301:GLY:HA3	2.42	0.50
1:C:187:ALA:O	1:C:196:ALA:HB1	2.11	0.50
1:O:1:LEU:HD11	1:O:329:ALA:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:181:ASP:OD2	1:O:195:ARG:NH1	2.43	0.50
1:D:97:GLY:HA2	2:D:335:NAD:O3D	2.12	0.50
1:G:278:LEU:HD21	1:H:46:TYR:CZ	2.46	0.50
1:F:155:ALA:HB3	1:F:156:PRO:HD3	1.92	0.50
1:G:182:GLN:HB3	1:G:199:ALA:HB2	1.93	0.50
1:A:156:PRO:HB2	1:A:290:THR:CG2	2.39	0.50
1:E:146:ASN:ND2	1:E:324:LEU:HD22	2.27	0.50
1:F:150:THR:O	1:F:150:THR:HG22	2.12	0.50
1:F:177:SER:HB3	1:F:234:THR:O	2.12	0.49
1:A:245:GLN:NE2	1:C:245:GLN:HE22	2.08	0.49
1:O:219:PRO:O	1:O:222:LYS:HG2	2.12	0.49
1:D:206:THR:HG23	1:D:229:ALA:HB3	1.93	0.49
1:G:109:ILE:CD1	1:G:142:PRO:HB2	2.41	0.49
1:B:39:GLN:NE2	1:C:190:HIS:H	2.09	0.49
1:H:55:ALA:HB1	1:H:67:ASP:OD1	2.11	0.49
1:B:194:ARG:CZ	1:D:277:PRO:HA	2.41	0.49
1:G:3:VAL:HG22	1:G:91:ILE:HB	1.93	0.49
1:F:159:LYS:O	1:F:163:GLN:HB2	2.13	0.49
1:E:277:PRO:HA	1:G:194:ARG:NE	2.23	0.49
1:H:228:ILE:H	1:H:228:ILE:CD1	2.22	0.49
1:O:281:VAL:H	1:Q:202:ASN:HD22	1.59	0.49
1:Q:151:THR:OG1	1:Q:210:ALA:HA	2.13	0.49
1:H:91:ILE:HD11	1:H:117:ILE:CG2	2.42	0.49
1:E:312:ASP:CG	1:E:315:TRP:HB3	2.32	0.49
1:H:82:LEU:HD13	1:H:84:TRP:CZ2	2.47	0.49
1:H:63:ALA:HA	1:H:73:VAL:HG23	1.93	0.49
1:F:4:ALA:O	1:F:92:VAL:HG13	2.13	0.49
1:A:245:GLN:NE2	1:C:245:GLN:NE2	2.60	0.49
1:D:204:VAL:HB	1:D:231:ARG:HB2	1.94	0.49
1:A:236:ASN:O	1:A:237:VAL:HB	2.12	0.49
1:F:133:ASN:N	1:F:133:ASN:HD22	2.10	0.49
1:E:30:ILE:O	1:E:74:VAL:HG22	2.12	0.49
1:E:129:VAL:HB	1:E:133:ASN:HD21	1.77	0.49
1:H:84:TRP:CE3	1:H:84:TRP:HA	2.47	0.49
1:E:109:ILE:HG12	1:E:113:ALA:O	2.12	0.49
1:O:33:THR:HG22	1:O:77:ARG:CG	2.42	0.49
1:C:251:PHE:CZ	1:C:254:GLU:HB2	2.47	0.49
1:G:210:ALA:O	1:G:214:VAL:HG23	2.12	0.49
1:E:77:ARG:HB3	1:E:77:ARG:NH1	2.28	0.49
1:F:240:VAL:O	1:F:240:VAL:HG23	2.12	0.49
1:H:319:GLN:OE1	1:H:319:GLN:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2:LYS:HD2	1:H:88:GLY:HA2	1.94	0.49
1:G:158:VAL:HG13	1:G:167:ILE:CD1	2.43	0.49
1:E:211:ALA:HB1	1:E:226:ASN:HA	1.95	0.49
1:E:260:ARG:HB3	4:E:534:HOH:O	2.11	0.49
1:Q:190:HIS:CB	1:Q:196:ALA:HB2	2.42	0.49
1:C:1:LEU:HD22	1:C:329:ALA:CB	2.42	0.49
1:C:256:ASN:OD1	1:C:294:SER:HB2	2.12	0.49
1:H:6:ASN:ND2	1:H:96:THR:HG21	2.27	0.49
1:H:157:PHE:HE1	1:H:242:LEU:HD23	1.76	0.49
1:O:221:LEU:HA	1:O:224:LYS:HD2	1.93	0.49
1:E:6:ASN:ND2	1:E:108:HIS:CE1	2.80	0.49
1:O:129:VAL:HG23	1:O:217:VAL:HG11	1.94	0.49
1:E:202:ASN:HB2	1:G:280:SER:OG	2.12	0.49
1:B:250:THR:OG1	1:B:251:PHE:N	2.43	0.49
1:G:13:ARG:NH1	1:G:13:ARG:HG3	2.27	0.49
1:B:85:LYS:HB2	1:B:112:GLY:HA3	1.94	0.49
1:Q:109:ILE:HA	1:Q:113:ALA:O	2.12	0.49
1:Q:239:VAL:HG23	1:Q:309:ALA:O	2.12	0.49
1:Q:191:ARG:H	1:Q:191:ARG:CZ	2.26	0.49
1:E:139:HIS:CG	1:E:139:HIS:O	2.66	0.49
1:H:28:ILE:C	1:H:71:ILE:HG13	2.32	0.49
1:D:172:MET:CE	1:D:211:ALA:HB2	2.43	0.49
1:E:79:PRO:O	1:E:82:LEU:HG	2.13	0.49
1:F:32:ASP:OD2	2:F:335:NAD:H1B	2.13	0.49
1:E:16:LEU:HD13	1:E:44:LEU:HD21	1.94	0.49
1:C:1:LEU:HD23	1:C:91:ILE:CD1	2.42	0.49
1:Q:137:TYR:CZ	1:Q:328:VAL:HG22	2.48	0.49
1:B:140:ASP:OD2	1:B:140:ASP:N	2.45	0.49
1:F:292:ILE:HG22	1:F:293:ASP:N	2.27	0.49
1:E:70:ILE:H	1:E:70:ILE:CD1	2.15	0.49
1:E:172:MET:HA	1:E:242:LEU:HA	1.95	0.49
1:H:182:GLN:HE22	1:H:231:ARG:CB	2.26	0.49
1:E:232:VAL:O	1:E:234:THR:N	2.38	0.49
1:F:228:ILE:HG21	1:H:296:LEU:CD2	2.43	0.49
1:D:123:GLY:O	1:D:125:ILE:HG22	2.12	0.49
1:E:16:LEU:HD23	1:E:16:LEU:O	2.12	0.49
1:B:0(A):ALA:N	1:B:26:ASP:HB2	2.28	0.49
1:D:107:LYS:HA	1:D:110:GLU:HB3	1.95	0.49
1:D:85:LYS:HG3	1:D:112:GLY:CA	2.33	0.49
1:E:171:THR:HB	1:G:300:MET:CG	2.39	0.49
1:H:142:PRO:HG2	1:H:143:ILE:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:TRP:HA	1:B:84:TRP:HE3	1.78	0.49
1:C:84:TRP:CE3	1:C:84:TRP:HA	2.48	0.49
1:F:193:LEU:HD12	1:H:277:PRO:HG3	1.95	0.49
1:C:260:ARG:HG2	1:C:273:VAL:HG21	1.95	0.49
1:G:168:ILE:HB	1:G:245:GLN:O	2.12	0.49
1:E:252:ALA:HB2	4:E:545:HOH:O	2.12	0.49
1:G:2:LYS:HE3	1:G:87:LEU:O	2.13	0.49
1:O:281:VAL:CG1	1:Q:202:ASN:HD21	2.25	0.49
1:C:109:ILE:CD1	1:C:142:PRO:HB2	2.42	0.49
1:A:173:THR:HG23	1:A:228:ILE:CD1	2.43	0.49
1:O:226:ASN:HB2	1:Q:300:MET:HE2	1.95	0.49
1:B:251:PHE:C	1:B:299:VAL:HG21	2.34	0.49
1:O:242:LEU:HD11	1:O:244:VAL:HG13	1.94	0.49
1:F:152:ASN:O	1:F:156:PRO:HG2	2.13	0.48
1:G:0:LYS:HB3	1:G:0:LYS:HZ2	1.75	0.48
1:C:317:TYR:O	1:C:320:ARG:HB2	2.13	0.48
1:C:108:HIS:HB2	1:C:116:VAL:HG21	1.95	0.48
1:D:190:HIS:HB3	1:D:196:ALA:HB2	1.95	0.48
1:A:188:SER:HA	1:D:39:GLN:OE1	2.13	0.48
1:F:202:ASN:ND2	1:H:281:VAL:CB	2.76	0.48
1:D:260:ARG:O	1:D:263:ALA:HB3	2.13	0.48
1:A:101:ASP:OD1	1:A:104:GLY:N	2.40	0.48
1:H:126:PRO:HG2	1:H:141:GLU:OE2	2.13	0.48
1:C:323:ASP:O	1:C:327:ILE:HG13	2.14	0.48
1:F:118:ILE:CD1	1:F:118:ILE:H	2.26	0.48
1:E:299:VAL:CG2	1:E:305:VAL:HG22	2.42	0.48
1:D:84:TRP:HA	1:D:89:ILE:HD13	1.94	0.48
1:H:242:LEU:O	1:H:306:LYS:HA	2.14	0.48
1:H:84:TRP:HE3	1:H:84:TRP:HA	1.78	0.48
1:F:327:ILE:O	1:F:327:ILE:HG22	2.14	0.48
1:B:270:ILE:N	1:B:270:ILE:HD12	2.27	0.48
1:D:292:ILE:H	1:D:292:ILE:HD12	1.78	0.48
1:A:191:ARG:NH1	4:A:770:HOH:O	2.45	0.48
1:E:32:ASP:C	1:E:34:GLY:H	2.17	0.48
1:D:44:LEU:HD23	1:D:57:VAL:CG1	2.44	0.48
1:A:157:PHE:HB2	1:A:259:PHE:CE1	2.48	0.48
1:C:168:ILE:HG22	1:C:169:LYS:HD3	1.95	0.48
1:B:36:GLY:HA3	1:B:38:LYS:HE3	1.94	0.48
1:D:272:ASP:OD2	1:D:273:VAL:N	2.46	0.48
1:D:93:ILE:HD12	1:D:93:ILE:N	2.28	0.48
1:C:329:ALA:O	1:C:332:TRP:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:PRO:HB2	1:G:107:LYS:HB2	1.95	0.48
1:F:17:ARG:HD3	1:F:50:LEU:HD12	1.95	0.48
1:H:249:LYS:HA	1:H:302:ASP:O	2.13	0.48
1:C:182:GLN:HB3	4:C:396:HOH:O	2.12	0.48
1:E:90:ASP:OD1	1:E:114:LYS:HD2	2.14	0.48
1:G:194:ARG:HD3	1:G:205:PRO:HD2	1.94	0.48
1:A:64:ILE:CG1	1:A:71:ILE:HG23	2.42	0.48
1:E:208:THR:C	1:E:210:ALA:H	2.15	0.48
1:A:133:ASN:ND2	1:A:133:ASN:C	2.67	0.48
1:F:132:VAL:HG13	1:F:218:LEU:HD21	1.95	0.48
1:H:7:GLY:CA	1:H:96:THR:HG22	2.44	0.48
1:E:169:LYS:HE2	1:E:245:GLN:OE1	2.13	0.48
1:E:251:PHE:CE1	1:E:254:GLU:HB2	2.49	0.48
1:O:1:LEU:HD12	1:O:329:ALA:CB	2.44	0.48
1:D:132:VAL:HG13	1:D:218:LEU:HD21	1.96	0.48
1:H:16:LEU:HD23	1:H:16:LEU:O	2.13	0.48
1:B:126:PRO:HG2	1:B:141:GLU:HG2	1.95	0.48
1:O:15:PHE:CE1	1:O:321:VAL:HG12	2.48	0.48
1:C:177:SER:HB2	1:C:237:VAL:O	2.14	0.48
1:G:318:SER:O	1:G:322:VAL:HG23	2.13	0.48
1:G:48:SER:HA	1:H:281:VAL:HG11	1.96	0.48
1:E:187:ALA:O	1:H:43:LEU:HD11	2.14	0.48
1:G:130:VAL:HG23	1:G:320:ARG:HD3	1.96	0.48
1:A:296:LEU:HB3	1:A:308:ILE:HD12	1.96	0.48
1:B:251:PHE:O	1:B:255:VAL:HG23	2.14	0.48
1:C:31:ASN:HB2	1:C:74:VAL:HG23	1.95	0.48
1:D:84:TRP:HB3	1:D:113:ALA:H	1.79	0.48
1:E:18:CYS:HB3	1:E:319:GLN:CD	2.34	0.48
1:H:79:PRO:HB2	1:H:107:LYS:HB3	1.95	0.48
1:A:64:ILE:HG13	1:A:71:ILE:CG2	2.43	0.48
1:G:191:ARG:HG3	1:G:192:ASP:N	2.29	0.48
1:F:144:ILE:HD12	1:F:324:LEU:HD21	1.95	0.48
1:E:71:ILE:HD13	1:E:72:GLN:O	2.14	0.48
1:G:250:THR:OG1	1:G:251:PHE:N	2.46	0.48
1:H:178:TYR:HA	1:H:182:GLN:OE1	2.13	0.48
1:E:279:VAL:HG23	1:E:281:VAL:HG12	1.95	0.48
1:B:228:ILE:HG23	1:D:298:MET:CE	2.44	0.48
1:H:28:ILE:HG23	1:H:29:ALA:N	2.29	0.48
1:E:14:ASN:OD1	1:E:315:TRP:HA	2.13	0.48
1:C:109:ILE:HA	1:C:113:ALA:O	2.14	0.48
1:H:132:VAL:HG21	1:H:155:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:38:LYS:HG2	1:H:39:GLN:N	2.29	0.47
1:F:59:PRO:HA	1:F:64:ILE:HG22	1.95	0.47
1:D:44:LEU:HA	4:D:341:HOH:O	2.13	0.47
1:C:280:SER:HA	1:C:310:TRP:CZ3	2.48	0.47
1:H:149:CYS:HB3	2:H:335:NAD:C5N	2.44	0.47
1:C:23:SER:C	1:C:25:LEU:H	2.16	0.47
1:D:14:ASN:OD1	1:D:50:LEU:HD11	2.14	0.47
1:D:87:LEU:HB2	1:D:89:ILE:CD1	2.44	0.47
1:G:299:VAL:HG11	4:G:872:HOH:O	2.13	0.47
1:F:280:SER:OG	1:H:202:ASN:HB2	2.14	0.47
1:G:194:ARG:NH1	1:G:205:PRO:HB2	2.29	0.47
1:G:194:ARG:O	1:G:204:VAL:HG11	2.15	0.47
1:E:83:PRO:O	1:E:87:LEU:HD13	2.14	0.47
1:C:236:ASN:O	1:C:237:VAL:HB	2.14	0.47
1:C:284:ARG:O	1:C:285:CYS:HB2	2.14	0.47
1:O:293:ASP:HB3	1:O:296:LEU:HD12	1.96	0.47
1:D:85:LYS:CG	1:D:112:GLY:HA2	2.33	0.47
1:E:226:ASN:HD22	1:G:300:MET:CE	2.26	0.47
1:F:321:VAL:O	1:F:325:ALA:HB2	2.14	0.47
1:E:58:LYS:HB2	1:E:59:PRO:CD	2.39	0.47
1:F:62:THR:O	1:F:63:ALA:HB2	2.14	0.47
1:E:236:ASN:CG	1:E:237:VAL:H	2.17	0.47
1:Q:115:LYS:HG3	1:Q:142:PRO:O	2.14	0.47
1:G:128:TYR:CZ	1:G:137:TYR:HA	2.49	0.47
1:O:9:GLY:HA3	2:O:335:NAD:O5B	2.14	0.47
1:G:312:ASP:HB3	1:G:316:GLY:H	1.79	0.47
1:F:90:ASP:HA	1:F:114:LYS:CD	2.28	0.47
1:E:300:MET:SD	1:G:170:GLY:O	2.72	0.47
1:C:331:ASN:O	1:C:333:LYS:HD3	2.15	0.47
1:E:115:LYS:HE3	1:E:137:TYR:OH	2.14	0.47
1:D:126:PRO:HB2	1:D:144:ILE:HG22	1.95	0.47
1:Q:126:PRO:HD2	1:Q:143:ILE:O	2.14	0.47
1:G:198:ALA:O	1:G:200:ALA:N	2.48	0.47
1:E:115:LYS:HE3	1:E:328:VAL:HG13	1.96	0.47
1:G:62:THR:CG2	1:Q:62:THR:HG22	2.44	0.47
1:G:239:VAL:HB	1:G:310:TRP:CE3	2.49	0.47
1:H:15:PHE:CE1	1:H:322:VAL:HG22	2.49	0.47
1:B:102:ARG:O	1:B:106:GLY:N	2.47	0.47
1:F:240:VAL:HG13	1:F:311:TYR:CE1	2.49	0.47
1:B:194:ARG:NH1	1:D:278:LEU:O	2.47	0.47
1:Q:44:LEU:O	1:Q:44:LEU:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:194:ARG:CG	1:G:277:PRO:O	2.60	0.47
1:E:5:ILE:HD12	1:E:27:ILE:CD1	2.43	0.47
1:E:190:HIS:N	1:H:39:GLN:OE1	2.47	0.47
1:G:208:THR:C	1:G:210:ALA:N	2.68	0.47
1:D:64:ILE:HG23	1:D:73:VAL:HG21	1.96	0.47
1:E:284:ARG:O	1:E:285:CYS:HB2	2.14	0.47
1:B:195:ARG:HH21	1:B:206:THR:HG21	1.79	0.47
1:A:63:ALA:HA	1:A:73:VAL:HG23	1.96	0.47
1:H:192:ASP:C	1:H:194:ARG:H	2.16	0.47
1:H:228:ILE:HD13	1:H:228:ILE:N	2.24	0.47
1:G:133:ASN:N	1:G:133:ASN:HD22	2.13	0.47
1:E:58:LYS:HB3	1:E:58:LYS:HZ2	1.79	0.47
1:D:0:LYS:O	1:D:1:LEU:HB2	2.15	0.47
1:F:4:ALA:HB3	1:F:92:VAL:HG22	1.96	0.47
1:B:154:LEU:HD21	1:B:172:MET:HE2	1.97	0.47
1:Q:272:ASP:HB2	1:Q:288:PHE:CD2	2.49	0.47
1:E:138:SER:C	1:E:140:ASP:H	2.17	0.47
1:B:102:ARG:HH11	1:B:102:ARG:HG2	1.79	0.47
1:D:177:SER:HB3	1:D:234:THR:O	2.14	0.47
1:Q:284:ARG:O	1:Q:285:CYS:HB2	2.15	0.47
1:B:165:PHE:HB3	1:B:246:VAL:HG11	1.96	0.47
1:Q:130:VAL:HA	1:Q:134:ALA:HB2	1.97	0.47
1:O:28:ILE:HD11	1:O:89:ILE:HD13	1.97	0.47
1:Q:28:ILE:HD12	1:Q:28:ILE:C	2.35	0.47
1:B:240:VAL:HG13	1:B:311:TYR:CE1	2.49	0.47
1:E:82:LEU:HD13	1:E:84:TRP:CZ2	2.49	0.47
1:B:186:ASP:HA	1:B:196:ALA:O	2.15	0.47
1:O:187:ALA:O	1:O:196:ALA:HB1	2.15	0.47
1:G:260:ARG:NH2	1:G:275:ASP:OD1	2.47	0.47
1:G:294:SER:C	1:G:296:LEU:N	2.68	0.47
1:F:298:MET:CE	1:H:228:ILE:HG23	2.45	0.47
1:F:255:VAL:C	1:F:257:ALA:N	2.68	0.47
1:D:134:ALA:HB3	4:D:396:HOH:O	2.15	0.47
1:H:8:PHE:HE1	1:H:16:LEU:HD12	1.80	0.47
1:Q:183:ARG:HG3	1:Q:196:ALA:HA	1.97	0.47
1:C:241:ASP:OD1	1:C:306:LYS:CE	2.63	0.47
1:O:169:LYS:HD2	1:Q:300:MET:HG3	1.97	0.47
1:C:84:TRP:HE3	1:C:84:TRP:HA	1.79	0.47
1:B:279:VAL:HG22	1:D:197:ARG:NH1	2.29	0.47
1:E:117:ILE:CG2	1:E:144:ILE:HD11	2.36	0.46
1:B:202:ASN:OD1	1:D:281:VAL:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:SER:O	1:F:231:ARG:HD2	2.15	0.46
1:A:226:ASN:HD21	1:C:300:MET:HB2	1.80	0.46
1:C:153:CYS:SG	1:C:240:VAL:HG13	2.55	0.46
1:F:107:LYS:HA	1:F:110:GLU:HG2	1.96	0.46
1:A:284:ARG:O	1:A:285:CYS:HB2	2.14	0.46
1:Q:18:CYS:HB3	1:Q:319:GLN:OE1	2.15	0.46
1:H:146:ASN:O	1:H:146:ASN:OD1	2.32	0.46
1:Q:271:LEU:C	1:Q:271:LEU:HD23	2.35	0.46
1:E:108:HIS:HB2	1:E:116:VAL:HG21	1.97	0.46
1:H:256:ASN:ND2	1:H:297:THR:OG1	2.31	0.46
1:G:85:LYS:N	1:G:112:GLY:HA3	2.31	0.46
1:H:149:CYS:HB3	2:H:335:NAD:H5N	1.96	0.46
1:B:284:ARG:O	1:B:285:CYS:HB2	2.13	0.46
1:F:85:LYS:HD2	1:F:85:LYS:HA	1.78	0.46
1:F:322:VAL:O	1:F:325:ALA:HB3	2.15	0.46
1:E:179:THR:HG22	1:E:180:GLY:H	1.80	0.46
1:E:179:THR:OG1	1:E:231:ARG:NH1	2.49	0.46
1:E:169:LYS:HE3	1:G:304:MET:CB	2.43	0.46
1:F:301:GLY:O	1:F:302:ASP:HB2	2.15	0.46
1:B:133:ASN:HD22	1:B:133:ASN:H	1.61	0.46
1:D:139:HIS:CB	1:D:333:LYS:HE2	2.27	0.46
1:F:65:SER:HA	1:F:70:ILE:HA	1.97	0.46
1:A:91:ILE:HD13	1:A:92:VAL:N	2.31	0.46
1:E:79:PRO:HB2	1:E:107:LYS:HB3	1.96	0.46
1:E:251:PHE:CZ	1:E:254:GLU:HB2	2.50	0.46
1:D:15:PHE:CE1	1:D:322:VAL:HG22	2.50	0.46
1:Q:194:ARG:HD2	1:Q:205:PRO:O	2.15	0.46
1:A:13:ARG:HH11	1:A:13:ARG:HG3	1.80	0.46
1:G:172:MET:HB2	1:G:242:LEU:CB	2.45	0.46
1:F:108:HIS:HB2	1:F:116:VAL:HG21	1.97	0.46
1:G:4:ALA:HB2	1:G:89:ILE:HD12	1.97	0.46
1:C:211:ALA:HB1	1:C:226:ASN:N	2.31	0.46
1:D:37:VAL:O	1:D:40:ALA:HB3	2.15	0.46
1:C:33:THR:HG21	1:C:77:ARG:CZ	2.45	0.46
1:E:178:TYR:CB	1:E:199:ALA:HB1	2.46	0.46
1:E:202:ASN:ND2	1:G:281:VAL:CG1	2.78	0.46
1:G:84:TRP:CE3	1:G:84:TRP:HA	2.50	0.46
1:A:159:LYS:NZ	1:A:163:GLN:HE22	2.13	0.46
1:O:253:GLU:H	1:O:253:GLU:CD	2.19	0.46
1:B:191:ARG:NH1	1:B:191:ARG:HB2	2.30	0.46
1:F:15:PHE:CE1	1:F:322:VAL:HG22	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:132:VAL:O	1:H:133:ASN:CB	2.63	0.46
1:F:18:CYS:SG	1:F:319:GLN:OE1	2.74	0.46
1:G:291:THR:O	1:G:291:THR:HG23	2.16	0.46
1:C:320:ARG:HA	1:C:320:ARG:NE	2.30	0.46
1:O:215:ALA:HB1	1:O:222:LYS:HD3	1.97	0.46
1:E:284:ARG:O	1:E:285:CYS:CB	2.63	0.46
1:O:285:CYS:N	1:O:312:ASP:OD2	2.45	0.46
1:F:45:LYS:HD3	1:F:57:VAL:HB	1.97	0.46
1:F:90:ASP:O	1:F:115:LYS:N	2.41	0.46
1:E:70:ILE:O	1:E:70:ILE:HG12	2.15	0.46
1:E:154:LEU:C	1:E:158:VAL:HG23	2.36	0.46
1:F:27:ILE:N	1:F:27:ILE:CD1	2.77	0.46
1:Q:271:LEU:HD23	1:Q:272:ASP:N	2.31	0.46
1:E:260:ARG:HD3	4:E:534:HOH:O	2.15	0.46
1:A:300:MET:HE3	1:C:226:ASN:CB	2.46	0.46
1:O:2:LYS:HD2	1:O:28:ILE:HD13	1.97	0.46
1:E:226:ASN:HD22	1:G:300:MET:HE1	1.81	0.46
1:E:183:ARG:CG	1:E:196:ALA:HA	2.46	0.46
1:D:322:VAL:HG12	1:D:322:VAL:O	2.16	0.46
1:H:210:ALA:O	1:H:214:VAL:HG23	2.16	0.46
1:G:162:ASP:C	1:G:164:LYS:H	2.19	0.45
1:E:133:ASN:H	1:E:133:ASN:ND2	2.01	0.45
1:E:133:ASN:N	1:E:133:ASN:ND2	2.51	0.45
1:B:163:GLN:NE2	1:B:164:LYS:NZ	2.58	0.45
1:A:84:TRP:HA	1:A:84:TRP:CE3	2.52	0.45
1:H:130:VAL:CG2	1:H:320:ARG:HD3	2.46	0.45
1:F:154:LEU:HD11	1:F:242:LEU:HD13	1.98	0.45
1:G:228:ILE:N	1:G:228:ILE:HD13	2.30	0.45
1:B:190:HIS:HB3	1:B:196:ALA:HB2	1.97	0.45
1:F:66:VAL:O	1:F:67:ASP:HB2	2.16	0.45
1:E:17:ARG:HE	1:E:17:ARG:CA	2.05	0.45
1:G:242:LEU:HD23	1:G:242:LEU:H	1.82	0.45
1:D:83:PRO:HB2	1:D:87:LEU:HD23	1.98	0.45
1:E:63:ALA:HB2	1:E:72:GLN:OE1	2.15	0.45
1:F:81:LEU:HD12	1:F:81:LEU:N	2.30	0.45
1:E:235:PRO:HG2	1:E:236:ASN:H	1.81	0.45
1:H:4:ALA:HB3	1:H:92:VAL:HG22	1.98	0.45
1:F:145:SER:O	1:F:147:ALA:N	2.49	0.45
1:F:139:HIS:CD2	1:F:333:LYS:HG2	2.51	0.45
1:F:109:ILE:CD1	1:F:142:PRO:HB3	2.45	0.45
1:D:101:ASP:HB3	1:D:122(A):LYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:ASN:HB3	1:C:318:SER:OG	2.16	0.45
1:D:242:LEU:HG	1:D:244:VAL:HG13	1.98	0.45
1:H:208:THR:HG23	1:H:208:THR:O	2.16	0.45
1:D:228:ILE:HD13	1:D:228:ILE:H	1.80	0.45
1:H:105:ALA:HB1	1:H:116:VAL:HG11	1.98	0.45
1:D:210:ALA:O	1:D:213:ALA:HB3	2.17	0.45
1:G:291:THR:HG22	1:G:310:TRP:O	2.15	0.45
1:A:296:LEU:O	1:A:298:MET:HG3	2.16	0.45
1:F:235:PRO:HB3	1:G:201:LEU:HD21	1.97	0.45
1:E:246:VAL:O	1:E:303:ASP:HB2	2.16	0.45
1:C:82:LEU:HA	1:C:83:PRO:HD3	1.79	0.45
1:A:213:ALA:O	1:A:216:LEU:HB2	2.17	0.45
1:H:88:GLY:O	1:H:89:ILE:C	2.55	0.45
1:B:38:LYS:N	1:B:38:LYS:CD	2.77	0.45
1:Q:183:ARG:CG	1:Q:196:ALA:HA	2.46	0.45
1:O:279:VAL:CG1	1:Q:204:VAL:HG22	2.46	0.45
1:Q:204:VAL:HB	1:Q:231:ARG:HB2	1.98	0.45
1:A:215:ALA:HB2	1:A:222:LYS:HA	1.98	0.45
1:E:290:THR:HA	1:E:310:TRP:O	2.17	0.45
1:G:267:LEU:HD12	1:G:271:LEU:HD22	1.99	0.45
1:G:193:LEU:HD22	1:G:193:LEU:N	2.26	0.45
1:F:27:ILE:CD1	1:F:27:ILE:H	2.30	0.45
1:D:3:VAL:CG1	1:D:93:ILE:HD13	2.45	0.45
1:F:23:SER:C	1:F:25:LEU:H	2.20	0.45
1:F:47:ASP:OD1	1:F:48:SER:N	2.49	0.45
1:D:10:ARG:HG2	4:D:377:HOH:O	2.16	0.45
1:B:319:GLN:HA	1:B:319:GLN:OE1	2.16	0.45
1:D:181:ASP:OD1	1:D:195:ARG:NE	2.50	0.45
1:A:227:GLY:N	1:C:298:MET:HE1	2.31	0.45
1:F:31:ASN:ND2	1:F:82:LEU:HD11	2.31	0.45
1:F:84:TRP:CE3	1:F:84:TRP:HA	2.52	0.45
1:E:186:ASP:HB2	1:H:10:ARG:HH12	1.82	0.45
1:F:119:THR:O	1:F:120:ALA:HB2	2.16	0.45
1:A:279:VAL:HG23	1:A:281:VAL:HG12	1.99	0.45
1:Q:178:TYR:CE1	1:Q:235:PRO:HA	2.52	0.45
1:H:185:LEU:O	1:H:186:ASP:C	2.55	0.45
1:C:126:PRO:HD2	1:C:143:ILE:O	2.17	0.45
1:O:176:HIS:HA	1:O:238:SER:HB3	1.99	0.45
1:F:101:ASP:OD1	1:F:103:GLU:HB3	2.16	0.45
1:D:18(A):TRP:CE3	1:D:27:ILE:HD12	2.51	0.45
1:D:27:ILE:O	1:D:69:LYS:HE3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:137:TYR:CE2	1:F:328:VAL:HA	2.52	0.45
1:F:271:LEU:HA	1:F:290:THR:HG23	1.99	0.45
1:E:102:ARG:O	1:E:106:GLY:N	2.50	0.45
1:C:2:LYS:HD3	1:C:28:ILE:HD13	1.98	0.45
1:A:129:VAL:H	1:A:133:ASN:HD21	1.65	0.45
1:C:293:ASP:O	1:C:295:SER:N	2.49	0.45
1:E:194:ARG:NH1	1:G:296:LEU:HD21	2.30	0.45
1:E:7:GLY:HA2	2:E:335:NAD:C1B	2.42	0.45
1:H:329:ALA:O	1:H:332:TRP:HB3	2.16	0.45
1:E:66:VAL:O	1:E:67:ASP:HB2	2.16	0.45
1:O:218:LEU:HB3	1:O:221:LEU:HD23	1.99	0.45
1:D:44:LEU:HD23	1:D:57:VAL:HG11	1.99	0.45
1:F:52:ILE:HG22	1:F:53:PHE:N	2.31	0.45
1:A:159:LYS:O	1:A:163:GLN:HB2	2.17	0.45
1:Q:69:LYS:HD3	4:Q:618:HOH:O	2.15	0.45
1:E:31:ASN:HA	1:E:74:VAL:HG23	1.98	0.45
1:E:9:GLY:N	2:E:335:NAD:H4B	2.31	0.45
1:F:74:VAL:HG22	1:F:75:SER:N	2.32	0.45
1:E:132:VAL:HG13	1:E:218:LEU:HD21	1.99	0.45
1:G:28:ILE:HD11	1:G:89:ILE:HD13	1.98	0.45
1:H:192:ASP:OD1	1:H:194:ARG:HB2	2.16	0.45
1:F:296:LEU:O	1:F:297:THR:C	2.56	0.45
1:H:218:LEU:HB3	1:H:221:LEU:HD23	1.99	0.45
1:B:271:LEU:HD13	1:B:272:ASP:H	1.76	0.45
1:H:3:VAL:HG13	1:H:27:ILE:HA	1.99	0.45
1:F:185:LEU:O	1:F:186:ASP:C	2.55	0.45
1:O:263:ALA:O	1:O:268:LYS:HA	2.17	0.45
1:F:132:VAL:HG11	1:F:218:LEU:HG	1.98	0.45
1:D:116:VAL:HB	1:D:143:ILE:CD1	2.47	0.45
1:H:132:VAL:HG13	1:H:218:LEU:HD21	1.98	0.45
1:D:74:VAL:CG2	1:D:75:SER:H	2.28	0.45
1:H:92:VAL:HB	1:H:116:VAL:HG22	1.99	0.45
1:G:287:ASP:OD1	1:G:319:GLN:HG3	2.16	0.45
1:Q:1:LEU:HD22	1:Q:329:ALA:CB	2.47	0.45
1:G:79:PRO:HB2	1:G:107:LYS:CB	2.47	0.45
1:B:241:ASP:HA	1:B:308:ILE:HD13	1.99	0.45
1:E:278:LEU:HD21	1:F:46:TYR:CE2	2.52	0.45
1:G:32:ASP:OD1	2:G:335:NAD:H1B	2.17	0.45
1:Q:212:LYS:HB3	4:Q:459:HOH:O	2.15	0.45
1:G:46:TYR:HB3	1:H:282:ASP:OD1	2.17	0.45
1:E:173:THR:HG23	1:E:228:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:176:HIS:HB3	1:H:231:ARG:CD	2.46	0.44
1:G:204:VAL:HA	1:G:205:PRO:HD3	1.83	0.44
1:H:133:ASN:N	1:H:133:ASN:ND2	2.65	0.44
1:F:190:HIS:HB3	1:F:196:ALA:HB2	1.99	0.44
1:Q:133:ASN:HD22	1:Q:133:ASN:N	2.13	0.44
1:Q:320:ARG:NE	1:Q:320:ARG:HA	2.32	0.44
1:H:276:GLU:HB3	1:H:277:PRO:HD2	1.98	0.44
1:O:157:PHE:HE1	1:O:242:LEU:HD23	1.83	0.44
1:H:139:HIS:C	1:H:141:GLU:H	2.20	0.44
1:A:215:ALA:CB	1:A:222:LYS:HA	2.47	0.44
1:B:248:LYS:O	1:B:249:LYS:C	2.55	0.44
1:O:54:ASP:HB3	4:O:425:HOH:O	2.16	0.44
1:F:132:VAL:HG12	1:F:133:ASN:N	2.31	0.44
1:F:215:ALA:O	1:F:219:PRO:HG3	2.18	0.44
1:G:172:MET:HA	1:G:242:LEU:HA	2.00	0.44
1:E:28:ILE:HG12	1:E:28:ILE:O	2.17	0.44
1:A:83:PRO:HA	1:A:85:LYS:CE	2.47	0.44
1:E:178:TYR:CA	1:E:182:GLN:OE1	2.63	0.44
1:H:292:ILE:HD13	1:H:309:ALA:HB2	1.99	0.44
1:F:251:PHE:CE1	1:F:254:GLU:HB2	2.52	0.44
1:D:191:ARG:NE	4:D:338:HOH:O	2.47	0.44
1:G:75:SER:HB2	1:Q:61:GLU:HG2	1.99	0.44
1:D:146:ASN:HD22	1:D:321:VAL:HG22	1.81	0.44
1:O:70:ILE:HD12	1:O:70:ILE:N	2.31	0.44
1:B:204:VAL:HB	1:B:231:ARG:HB2	2.00	0.44
1:Q:191:ARG:NH1	1:Q:191:ARG:CB	2.75	0.44
1:F:84:TRP:HE3	1:F:84:TRP:HA	1.82	0.44
1:H:157:PHE:CE1	1:H:242:LEU:HD23	2.53	0.44
1:A:33:THR:CG2	1:A:77:ARG:HG2	2.44	0.44
1:G:185:LEU:HA	1:G:198:ALA:CB	2.47	0.44
1:Q:1:LEU:O	1:Q:90:ASP:HB2	2.17	0.44
1:G:278:LEU:HD22	1:H:46:TYR:CD2	2.52	0.44
1:E:327:ILE:HG23	3:E:338:SO4:O3	2.18	0.44
1:D:13:ARG:HD2	4:D:341:HOH:O	2.17	0.44
1:D:197:ARG:N	1:D:197:ARG:HD2	2.32	0.44
1:B:298:MET:SD	1:D:226:ASN:ND2	2.90	0.44
1:F:98:VAL:HG23	1:F:99:PHE:CD1	2.52	0.44
1:E:203:ILE:CD1	1:G:232:VAL:HG21	2.42	0.44
1:H:170:GLY:H	1:H:225:LEU:HD23	1.83	0.44
1:H:226:ASN:OD1	1:H:227:GLY:N	2.51	0.44
1:E:251:PHE:O	1:E:253:GLU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:157:PHE:CE1	1:O:242:LEU:HD23	2.53	0.44
1:D:228:ILE:CD1	1:D:228:ILE:H	2.30	0.44
1:E:173:THR:HG23	1:E:228:ILE:CD1	2.47	0.44
1:E:170:GLY:O	1:E:225:LEU:HA	2.18	0.44
1:E:197:ARG:NH1	1:G:279:VAL:HG22	2.33	0.44
1:A:85:LYS:HZ2	1:A:86:GLU:HB3	1.81	0.44
1:B:272:ASP:O	1:B:291:THR:HA	2.17	0.44
1:E:50:LEU:HB2	1:E:53:PHE:CZ	2.52	0.44
1:D:221:LEU:N	1:D:221:LEU:HD22	2.33	0.44
1:D:17:ARG:HD3	1:D:50:LEU:HD13	2.00	0.44
1:D:329:ALA:O	1:D:332:TRP:HB2	2.18	0.44
1:D:298:MET:HE3	1:D:306:LYS:HD2	2.00	0.44
1:Q:3:VAL:HG12	1:Q:4:ALA:N	2.33	0.44
1:A:137:TYR:CZ	1:A:328:VAL:HG22	2.52	0.44
1:E:60(A):GLY:O	1:E:61:GLU:HG2	2.17	0.44
1:C:276:GLU:HB2	1:C:278:LEU:HG	1.99	0.44
1:A:205:PRO:HA	1:A:230:LEU:HD23	1.98	0.44
1:D:133:ASN:OD1	1:D:217:VAL:HA	2.18	0.44
1:A:84:TRP:HA	1:A:84:TRP:HE3	1.82	0.44
1:F:154:LEU:HD23	1:F:214:VAL:HG21	2.00	0.44
1:E:106:GLY:O	1:E:110:GLU:HG3	2.18	0.44
1:B:133:ASN:HD22	1:B:133:ASN:N	2.15	0.44
1:G:84:TRP:HA	1:G:84:TRP:HE3	1.81	0.44
1:Q:255:VAL:O	1:Q:258:ALA:HB3	2.18	0.44
1:C:146:ASN:O	1:C:147:ALA:HB3	2.17	0.44
1:C:16:LEU:HD23	1:C:16:LEU:C	2.38	0.44
1:E:194:ARG:HE	1:G:277:PRO:HA	1.82	0.44
1:G:251:PHE:CA	1:G:299:VAL:HG21	2.46	0.44
1:H:182:GLN:HB3	1:H:199:ALA:HB2	1.99	0.44
1:G:37:VAL:HG21	1:G:62:THR:HA	2.00	0.44
1:A:0:LYS:HG2	1:A:26:ASP:HB2	2.00	0.44
1:G:211:ALA:HB1	1:G:226:ASN:CA	2.44	0.44
1:E:158:VAL:O	1:E:158:VAL:HG12	2.18	0.44
1:H:30:ILE:HG13	1:H:71:ILE:HD11	2.00	0.44
1:H:2:LYS:HD2	1:H:88:GLY:HA3	1.99	0.44
1:E:8:PHE:CZ	1:E:13:ARG:HG2	2.53	0.44
1:C:56:ASP:N	1:C:67:ASP:OD1	2.35	0.44
1:Q:125:ILE:HG23	1:Q:143:ILE:O	2.17	0.44
1:G:222:LYS:HG2	1:G:223:GLY:N	2.32	0.44
1:F:259:PHE:HB3	1:F:273:VAL:HG21	1.98	0.44
1:Q:1:LEU:HD22	1:Q:329:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:THR:HB	1:D:239:VAL:HG13	2.00	0.44
1:E:201:LEU:HD11	1:H:235:PRO:HB3	1.99	0.44
1:Q:174:THR:O	1:Q:174:THR:HG23	2.18	0.44
1:G:162:ASP:O	1:G:164:LYS:N	2.49	0.43
1:F:38:LYS:CE	1:G:193:LEU:HD21	2.48	0.43
1:Q:206:THR:HG23	1:Q:207:SER:O	2.17	0.43
1:E:106:GLY:O	1:E:109:ILE:HG22	2.18	0.43
1:O:158:VAL:HG13	1:O:167:ILE:CD1	2.48	0.43
1:D:253:GLU:CD	1:D:253:GLU:H	2.21	0.43
1:D:276:GLU:HB2	1:D:278:LEU:HG	2.00	0.43
1:D:248:LYS:O	1:D:249:LYS:C	2.56	0.43
1:E:153:CYS:SG	1:E:240:VAL:HG21	2.58	0.43
1:F:279:VAL:O	1:F:279:VAL:HG23	2.17	0.43
1:H:70:ILE:CG2	1:H:71:ILE:H	2.27	0.43
1:G:153:CYS:C	1:G:156:PRO:HD2	2.39	0.43
1:O:236:ASN:O	1:O:237:VAL:CB	2.66	0.43
1:E:77:ARG:CB	1:E:77:ARG:NH1	2.81	0.43
1:O:2:LYS:CD	1:O:28:ILE:HD13	2.48	0.43
1:F:279:VAL:CG1	1:H:204:VAL:HA	2.47	0.43
1:F:10:ARG:HH11	1:G:186:ASP:HB2	1.84	0.43
1:F:301:GLY:HA3	1:H:169:LYS:CE	2.48	0.43
1:A:76:ASN:ND2	1:A:81:LEU:HB2	2.34	0.43
1:A:227:GLY:H	1:C:298:MET:HE1	1.83	0.43
1:F:125:ILE:CG2	1:F:143:ILE:HG22	2.48	0.43
1:G:167:ILE:O	1:G:167:ILE:HG22	2.18	0.43
1:E:228:ILE:HD13	1:E:228:ILE:N	2.32	0.43
1:F:277:PRO:HG3	1:H:193:LEU:HD12	2.00	0.43
1:E:277:PRO:HA	1:G:194:ARG:HH21	1.82	0.43
1:E:266:GLU:HG2	1:E:267:LEU:N	2.33	0.43
1:B:256:ASN:HB3	1:B:260:ARG:NH1	2.32	0.43
1:G:1:LEU:HD21	1:G:332:TRP:CE3	2.54	0.43
1:D:103:GLU:CD	1:D:103:GLU:H	2.19	0.43
1:H:79:PRO:HB2	1:H:107:LYS:CB	2.47	0.43
1:G:327:ILE:HG23	1:G:331:ASN:HD22	1.83	0.43
1:A:233:PRO:HB2	1:C:233:PRO:HB2	2.00	0.43
1:A:109:ILE:N	1:A:109:ILE:HD12	2.33	0.43
1:G:64:ILE:HG23	1:G:73:VAL:HG21	2.01	0.43
1:E:177:SER:OG	1:E:237:VAL:O	2.36	0.43
1:D:209:GLY:O	1:D:210:ALA:C	2.57	0.43
1:G:82:LEU:HD13	1:G:84:TRP:CZ2	2.53	0.43
1:B:9:GLY:O	1:B:13:ARG:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:THR:O	1:D:174:THR:HG23	2.19	0.43
1:E:312:ASP:O	1:E:314:GLU:N	2.51	0.43
1:H:61:GLU:HG3	1:H:61:GLU:O	2.19	0.43
1:E:55:ALA:HB1	1:E:67:ASP:OD1	2.19	0.43
1:A:101:ASP:HA	1:A:125:ILE:HD11	2.00	0.43
1:A:39:GLN:NE2	1:D:190:HIS:O	2.44	0.43
1:G:69:LYS:HE3	1:G:71:ILE:HD11	2.00	0.43
1:E:139:HIS:CG	1:E:331:ASN:O	2.72	0.43
1:F:304:MET:HB2	1:H:169:LYS:HZ2	1.82	0.43
1:H:37:VAL:HG22	1:H:73:VAL:HB	2.01	0.43
1:E:79:PRO:HA	1:E:82:LEU:HD11	1.99	0.43
1:O:33:THR:HG21	1:O:77:ARG:HG2	1.99	0.43
1:F:235:PRO:CB	1:G:201:LEU:HD11	2.48	0.43
1:B:251:PHE:N	1:B:251:PHE:CD1	2.87	0.43
1:A:133:ASN:C	1:A:133:ASN:HD22	2.22	0.43
1:D:250:THR:OG1	1:D:251:PHE:N	2.52	0.43
1:F:1:LEU:HD22	1:F:329:ALA:HB2	2.01	0.43
1:F:105:ALA:HB3	1:F:143:ILE:HD13	2.01	0.43
1:G:158:VAL:HG11	1:G:221:LEU:CD2	2.49	0.43
1:G:219:PRO:O	1:G:221:LEU:N	2.52	0.43
1:O:17:ARG:NH2	1:O:50:LEU:HB3	2.34	0.43
1:D:84:TRP:CB	1:D:112:GLY:HA3	2.48	0.43
1:E:9:GLY:CA	2:E:335:NAD:H4B	2.48	0.43
1:B:33:THR:HA	1:B:75:SER:OG	2.19	0.43
1:H:23:SER:O	1:H:25:LEU:N	2.43	0.43
1:D:100:VAL:HA	1:D:118:ILE:HD13	2.00	0.43
1:G:18(A):TRP:O	1:G:19:GLY:N	2.52	0.43
1:G:28:ILE:HD11	1:G:89:ILE:HD11	1.99	0.43
1:D:72:GLN:HE22	1:H:83:PRO:HG3	1.84	0.43
1:H:36:GLY:HA3	1:H:38:LYS:CD	2.49	0.43
1:H:3:VAL:O	1:H:28:ILE:HG22	2.19	0.43
1:O:202:ASN:HD21	1:Q:281:VAL:HG12	1.82	0.43
1:G:0:LYS:HG3	4:G:597:HOH:O	2.17	0.43
1:C:183:ARG:NH1	1:C:188:SER:O	2.52	0.43
1:B:236:ASN:O	1:B:237:VAL:HB	2.18	0.43
1:Q:162:ASP:HB2	1:Q:167:ILE:HD12	2.01	0.43
1:H:261:ASP:OD1	1:H:262:SER:N	2.52	0.43
1:A:238:SER:HB2	1:A:311:TYR:CE1	2.53	0.43
1:G:164:LYS:O	1:G:164:LYS:HG2	2.19	0.42
1:G:261:ASP:O	1:G:262:SER:C	2.57	0.42
1:H:195:ARG:NH2	1:H:206:THR:HG21	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TRP:CE3	1:A:89:ILE:HG13	2.54	0.42
1:A:84:TRP:HB2	1:A:111:ALA:O	2.19	0.42
1:F:173:THR:OG1	1:F:228:ILE:HD11	2.19	0.42
1:H:70:ILE:CG2	1:H:71:ILE:N	2.81	0.42
1:B:240:VAL:HG23	1:B:240:VAL:O	2.19	0.42
1:O:253:GLU:N	1:O:253:GLU:CD	2.72	0.42
1:D:179:THR:O	1:D:181:ASP:N	2.52	0.42
1:B:96:THR:OG1	1:B:98:VAL:HG22	2.19	0.42
1:A:37:VAL:CG1	1:A:59:PRO:HB3	2.49	0.42
1:B:18(B):HIS:HE1	1:B:67:ASP:OD2	2.01	0.42
1:C:174:THR:O	1:C:174:THR:HG23	2.19	0.42
1:Q:31:ASN:HA	1:Q:74:VAL:O	2.19	0.42
1:A:191:ARG:NH1	1:A:191:ARG:HB2	2.34	0.42
1:O:249:LYS:HB3	1:O:302:ASP:HB3	2.00	0.42
1:E:78:ASN:HB3	1:E:81:LEU:HG	1.99	0.42
1:Q:242:LEU:O	1:Q:306:LYS:HA	2.19	0.42
1:H:209:GLY:HA3	1:H:212:LYS:HE2	2.01	0.42
1:F:126:PRO:HB3	1:F:128:TYR:OH	2.18	0.42
1:E:242:LEU:HD21	1:E:244:VAL:HG13	2.00	0.42
1:H:154:LEU:O	1:H:155:ALA:C	2.58	0.42
1:B:163:GLN:HE21	1:B:164:LYS:CE	2.32	0.42
1:D:156:PRO:HB2	1:D:290:THR:HG21	2.01	0.42
1:F:37:VAL:HG12	1:F:38:LYS:N	2.34	0.42
1:F:154:LEU:O	1:F:158:VAL:HG23	2.19	0.42
1:F:234:THR:HG22	1:H:233:PRO:HG2	2.00	0.42
1:E:150:THR:HB	1:E:210:ALA:CB	2.49	0.42
1:E:29:ALA:HB1	1:E:84:TRP:HZ3	1.85	0.42
1:E:84:TRP:C	1:E:112:GLY:HA3	2.40	0.42
1:C:28:ILE:HD11	1:C:89:ILE:HD13	2.01	0.42
1:C:24:PRO:HD2	1:C:326:ASP:OD1	2.19	0.42
1:E:159:LYS:HB2	1:E:218:LEU:HD11	2.01	0.42
1:H:171:THR:HG23	1:H:243:VAL:HB	2.01	0.42
1:F:58:LYS:O	1:F:65:SER:N	2.52	0.42
1:C:241:ASP:OD2	1:C:306:LYS:HE2	2.19	0.42
1:E:269:GLY:HA2	1:E:288:PHE:CE1	2.54	0.42
1:D:178:TYR:HB2	1:D:182:GLN:OE1	2.18	0.42
1:G:236:ASN:O	1:G:237:VAL:CB	2.67	0.42
1:A:162:ASP:OD2	1:A:220:ASN:ND2	2.39	0.42
1:F:132:VAL:C	1:F:134:ALA:H	2.23	0.42
1:E:252:ALA:HA	1:E:299:VAL:HG23	2.02	0.42
1:D:264:GLU:CA	1:D:268:LYS:HE3	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:GLN:NE2	1:H:83:PRO:HG3	2.34	0.42
1:E:185:LEU:O	1:E:186:ASP:C	2.57	0.42
1:A:142:PRO:C	1:A:143:ILE:HD12	2.40	0.42
1:E:79:PRO:HA	1:E:82:LEU:CG	2.49	0.42
1:O:132:VAL:HG21	1:O:155:ALA:HB1	2.01	0.42
1:F:27:ILE:HD12	1:F:27:ILE:H	1.82	0.42
1:D:15:PHE:CD1	1:D:322:VAL:HG22	2.54	0.42
1:D:7:GLY:HA3	1:D:96:THR:HG22	2.01	0.42
1:Q:241:ASP:HA	1:Q:308:ILE:HD13	2.01	0.42
1:Q:16:LEU:HD23	1:Q:16:LEU:O	2.19	0.42
1:G:157:PHE:HZ	1:G:242:LEU:HD22	1.85	0.42
1:E:194:ARG:NH1	1:E:205:PRO:CG	2.83	0.42
1:G:256:ASN:HD21	1:G:297:THR:CG2	2.18	0.42
1:E:188:SER:HA	1:H:39:GLN:OE1	2.19	0.42
1:F:41:SER:OG	1:F:59:PRO:HD3	2.20	0.42
1:F:222:LYS:HG2	1:F:224:LYS:HE3	1.98	0.42
1:D:153:CYS:SG	1:D:290:THR:HB	2.59	0.42
1:A:1:LEU:HD21	1:A:332:TRP:CE3	2.54	0.42
1:D:240:VAL:HG13	1:D:311:TYR:HE1	1.82	0.42
1:E:202:ASN:OD1	1:E:202:ASN:N	2.52	0.42
1:B:260:ARG:NH2	1:B:275:ASP:OD1	2.52	0.42
1:O:205:PRO:HG2	1:Q:310:TRP:HZ2	1.85	0.42
1:A:197:ARG:O	1:A:198:ALA:C	2.57	0.42
1:E:239:VAL:HG22	1:E:240:VAL:H	1.83	0.42
1:B:243:VAL:HG11	1:D:243:VAL:HG11	2.00	0.42
1:H:275:ASP:OD1	1:H:294:SER:OG	2.34	0.42
1:H:251:PHE:O	1:H:255:VAL:HG23	2.19	0.42
1:B:129:VAL:H	1:B:133:ASN:ND2	2.18	0.42
1:D:192:ASP:HB3	1:D:195:ARG:HB2	2.01	0.42
1:O:194:ARG:HD2	1:O:205:PRO:O	2.18	0.42
1:O:271:LEU:HD23	1:O:271:LEU:C	2.40	0.42
1:F:156:PRO:HB2	1:F:290:THR:HG21	2.01	0.42
1:D:128:TYR:HA	1:D:133:ASN:HD21	1.85	0.42
1:E:183:ARG:CZ	1:E:187:ALA:CB	2.96	0.42
1:Q:79:PRO:HA	1:Q:82:LEU:HG	2.00	0.42
1:G:291:THR:CG2	1:G:291:THR:O	2.67	0.42
1:C:177:SER:OG	1:C:234:THR:O	2.34	0.42
1:B:191:ARG:HH11	1:B:191:ARG:HB2	1.84	0.42
1:O:60:SER:HB2	1:O:65:SER:HB2	2.02	0.42
1:A:182:GLN:HB3	1:A:199:ALA:HB2	2.00	0.42
1:B:65:SER:HA	1:B:69:LYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:PRO:HB2	1:D:107:LYS:CB	2.50	0.42
1:E:31:ASN:ND2	2:E:335:NAD:H2A	2.34	0.42
1:E:162:ASP:HB2	1:E:167:ILE:HD12	2.01	0.42
1:E:137:TYR:CZ	1:E:139:HIS:HA	2.55	0.42
1:H:84:TRP:HD1	1:H:111:ALA:HB3	1.85	0.42
1:A:139:HIS:CE1	1:A:333:LYS:HG2	2.55	0.42
1:B:23:SER:HA	1:B:24:PRO:HD3	1.78	0.42
1:C:237:VAL:CG2	1:C:284:ARG:HD3	2.50	0.42
1:E:129:VAL:HB	1:E:133:ASN:ND2	2.34	0.42
1:E:291:THR:HB	1:E:310:TRP:HB2	2.02	0.42
1:H:6:ASN:HD22	1:H:96:THR:HG21	1.85	0.42
1:D:2:LYS:HZ2	1:H:87:LEU:HD13	1.85	0.42
1:D:63:ALA:HB2	1:D:72:GLN:HA	2.02	0.42
1:C:106:GLY:O	1:C:110:GLU:HG3	2.19	0.42
1:G:255:VAL:HG12	1:G:259:PHE:CE2	2.56	0.41
1:H:36:GLY:C	1:H:38:LYS:HD2	2.40	0.41
1:F:36:GLY:O	1:F:37:VAL:C	2.58	0.41
1:A:228:ILE:CD1	1:A:228:ILE:C	2.87	0.41
1:O:170:GLY:HA3	1:O:244:VAL:HG12	2.02	0.41
1:G:213:ALA:O	1:G:215:ALA:N	2.53	0.41
1:O:256:ASN:O	1:O:260:ARG:HG3	2.20	0.41
1:F:118:ILE:HD11	1:F:143:ILE:HG23	2.02	0.41
1:F:218:LEU:O	1:F:221:LEU:HD23	2.20	0.41
1:F:85:LYS:HE3	1:F:85:LYS:O	2.20	0.41
1:E:154:LEU:CD1	1:E:240:VAL:HG11	2.50	0.41
1:C:156:PRO:HB2	1:C:290:THR:CG2	2.43	0.41
1:C:271:LEU:HG	1:C:272:ASP:N	2.35	0.41
1:E:185:LEU:O	1:E:187:ALA:N	2.53	0.41
1:F:37:VAL:HG22	1:F:63:ALA:H	1.85	0.41
1:A:116:VAL:HB	1:A:143:ILE:HG13	2.02	0.41
1:F:4:ALA:HB2	1:F:89:ILE:HD12	2.03	0.41
1:O:76:ASN:HB3	1:O:82:LEU:CD2	2.50	0.41
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.56	0.41
1:E:324:LEU:HD12	1:E:327:ILE:HD12	2.01	0.41
1:A:238:SER:HB2	1:A:311:TYR:CZ	2.54	0.41
1:O:191:ARG:HH11	1:O:191:ARG:HG3	1.82	0.41
1:D:109:ILE:HG13	1:D:116:VAL:HG23	2.01	0.41
1:H:83:PRO:HB2	1:H:86:GLU:HG2	2.03	0.41
1:G:320:ARG:NE	1:G:323:ASP:OD2	2.50	0.41
1:F:34:GLY:HA2	1:F:39:GLN:NE2	2.35	0.41
1:H:44:LEU:HB3	1:H:57:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:VAL:HG12	1:E:214:VAL:O	2.20	0.41
1:A:129:VAL:HG23	1:A:217:VAL:HG11	2.02	0.41
1:Q:221:LEU:HD12	1:Q:225:LEU:HD11	2.01	0.41
1:G:170:GLY:CA	1:G:243:VAL:O	2.67	0.41
1:E:30:ILE:CD1	1:E:71:ILE:HD12	2.50	0.41
1:F:202:ASN:HD21	1:H:281:VAL:HG12	1.85	0.41
1:E:239:VAL:HG22	1:E:240:VAL:N	2.36	0.41
1:H:115:LYS:HB2	1:H:115:LYS:HE2	1.97	0.41
1:G:39:GLN:O	1:G:40:ALA:C	2.57	0.41
1:G:291:THR:HG22	1:G:310:TRP:HB2	2.01	0.41
1:F:17:ARG:HD3	1:F:50:LEU:CD1	2.50	0.41
1:B:100:VAL:O	1:B:118:ILE:HD13	2.20	0.41
1:Q:175:THR:CG2	1:Q:232:VAL:HG11	2.50	0.41
1:F:79:PRO:HA	1:F:82:LEU:CD1	2.43	0.41
1:F:310:TRP:CZ2	1:H:205:PRO:HG2	2.55	0.41
1:C:2:LYS:HD3	1:C:28:ILE:CD1	2.50	0.41
1:B:262:SER:HB3	1:B:267:LEU:HB2	2.02	0.41
1:F:138:SER:O	1:F:139:HIS:HB3	2.19	0.41
1:B:39:GLN:HE22	1:C:188:SER:HB2	1.86	0.41
1:B:165:PHE:CB	1:B:246:VAL:HG11	2.51	0.41
1:H:216:LEU:N	1:H:216:LEU:HD12	2.35	0.41
1:G:302:ASP:HB3	4:G:651:HOH:O	2.20	0.41
1:F:117:ILE:HD11	1:F:328:VAL:HG21	2.03	0.41
1:F:319:GLN:HA	1:F:319:GLN:OE1	2.20	0.41
1:C:77:ARG:NH2	4:C:364:HOH:O	2.45	0.41
1:G:109:ILE:HA	1:G:113:ALA:O	2.20	0.41
1:O:194:ARG:CZ	1:Q:277:PRO:HA	2.51	0.41
1:H:100:VAL:HG23	1:H:101:ASP:N	2.36	0.41
1:D:6:ASN:OD1	1:D:31:ASN:ND2	2.40	0.41
1:F:114:LYS:N	1:F:114:LYS:CD	2.82	0.41
1:F:128:TYR:OH	1:F:141:GLU:OE2	2.39	0.41
1:F:114:LYS:HB2	1:F:332:TRP:HH2	1.85	0.41
1:G:177:SER:CB	1:G:234:THR:O	2.66	0.41
1:F:269:GLY:HA2	1:F:288:PHE:CE2	2.56	0.41
1:F:28:ILE:O	1:F:72:GLN:HB2	2.20	0.41
1:E:131:GLY:HA3	1:E:270:ILE:HG21	2.03	0.41
1:B:221:LEU:HD22	1:B:221:LEU:N	2.35	0.41
1:C:96:THR:HB	1:C:98:VAL:HG22	2.02	0.41
1:G:171:THR:O	1:G:242:LEU:HA	2.19	0.41
1:H:271:LEU:HD12	1:H:290:THR:O	2.21	0.41
1:F:78:ASN:CB	1:F:81:LEU:HD13	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:76:ASN:HB3	1:H:82:LEU:HD23	2.03	0.41
1:G:324:LEU:O	1:G:327:ILE:HB	2.21	0.41
1:H:118:ILE:HG22	1:H:120:ALA:H	1.86	0.41
1:C:102:ARG:HB2	1:C:125:ILE:HD11	2.01	0.41
1:A:96:THR:OG1	1:A:98:VAL:HG22	2.20	0.41
1:O:327:ILE:O	1:O:328:VAL:C	2.59	0.41
1:F:267:LEU:HD13	1:F:271:LEU:HB2	2.03	0.41
1:D:89:ILE:N	1:D:89:ILE:HD12	2.36	0.41
1:G:28:ILE:C	1:G:71:ILE:HG23	2.41	0.41
1:B:153:CYS:O	1:B:290:THR:HG21	2.21	0.41
1:H:38:LYS:CD	1:H:38:LYS:N	2.82	0.41
1:G:317:TYR:O	1:G:320:ARG:HB2	2.21	0.41
1:F:249:LYS:HZ3	1:F:302:ASP:HB2	1.86	0.41
1:H:85:LYS:CG	1:H:112:GLY:HA3	2.50	0.41
1:F:145:SER:C	1:F:147:ALA:N	2.72	0.41
1:H:41:SER:O	1:H:57:VAL:HG12	2.21	0.41
1:F:5:ILE:HD11	1:F:12:GLY:CA	2.51	0.41
1:B:154:LEU:O	1:B:155:ALA:C	2.57	0.41
1:F:333:LYS:OXT	1:F:333:LYS:HG3	2.21	0.41
1:G:207:SER:O	1:G:208:THR:HB	2.20	0.41
1:Q:142:PRO:O	1:Q:143:ILE:HD13	2.21	0.41
1:D:9:GLY:HA3	2:D:335:NAD:O5B	2.21	0.41
1:Q:90:ASP:HA	1:Q:114:LYS:CG	2.51	0.41
1:F:282:ASP:OD2	1:H:197:ARG:NH1	2.50	0.41
1:C:8:PHE:O	1:C:13:ARG:NH1	2.51	0.41
1:F:17:ARG:NH2	1:F:53:PHE:HA	2.36	0.41
1:O:190:HIS:HB3	1:O:196:ALA:HB2	2.02	0.41
1:O:271:LEU:HD23	1:O:272:ASP:N	2.36	0.41
1:Q:9:GLY:O	1:Q:10:ARG:C	2.59	0.41
1:O:141:GLU:HA	1:O:142:PRO:HD2	1.92	0.41
1:G:29:ALA:HA	1:G:72:GLN:O	2.21	0.41
1:E:168:ILE:HD11	1:E:247:SER:HB3	2.02	0.41
1:G:132:VAL:HG12	1:G:133:ASN:N	2.36	0.41
1:D:243:VAL:HG22	1:D:306:LYS:HE3	2.02	0.41
1:A:76:ASN:HD21	1:A:78:ASN:HB3	1.86	0.41
1:C:2:LYS:HD2	1:C:88:GLY:O	2.21	0.41
1:D:5:ILE:HD11	1:D:27:ILE:HD13	2.03	0.41
1:C:100:VAL:HA	1:C:118:ILE:HD13	2.03	0.41
1:H:215:ALA:O	1:H:219:PRO:HA	2.21	0.41
1:O:239:VAL:CG2	1:O:308:ILE:HG23	2.51	0.41
1:D:137:TYR:CE2	1:D:328:VAL:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:272:ASP:HB2	1:G:288:PHE:CD1	2.56	0.41
1:G:265:LYS:HD2	1:G:265:LYS:HA	1.83	0.41
1:G:173:THR:O	1:G:241:ASP:N	2.54	0.40
1:F:31:ASN:CB	1:F:74:VAL:HG13	2.43	0.40
1:B:202:ASN:O	1:B:233:PRO:HD3	2.21	0.40
1:E:178:TYR:HB2	1:E:199:ALA:HB1	2.02	0.40
1:H:41:SER:CB	1:H:59:PRO:HG3	2.50	0.40
1:Q:115:LYS:HB2	1:Q:115:LYS:HE3	1.82	0.40
1:H:79:PRO:O	1:H:80:SER:C	2.59	0.40
1:F:48:SER:OG	1:G:202:ASN:ND2	2.54	0.40
1:F:165:PHE:HD1	1:F:248:LYS:HB3	1.86	0.40
1:E:275:ASP:HA	1:E:294:SER:OG	2.20	0.40
1:F:283:PHE:N	1:F:283:PHE:CD2	2.89	0.40
1:A:154:LEU:HD22	1:A:172:MET:HE2	2.03	0.40
1:F:139:HIS:HB2	1:F:331:ASN:O	2.22	0.40
1:G:208:THR:O	1:G:210:ALA:N	2.54	0.40
1:C:64:ILE:HD13	1:C:66:VAL:HG23	2.04	0.40
1:Q:235:PRO:O	1:Q:236:ASN:HB2	2.20	0.40
1:A:139:HIS:ND1	1:A:333:LYS:HB3	2.36	0.40
1:E:146:ASN:O	1:E:146:ASN:OD1	2.39	0.40
1:D:137:TYR:CZ	1:D:328:VAL:HG22	2.57	0.40
1:C:157:PHE:HB2	1:C:259:PHE:CE1	2.56	0.40
1:B:264:GLU:O	1:B:265:LYS:HD3	2.21	0.40
1:D:142:PRO:O	1:D:143:ILE:HD13	2.21	0.40
1:G:18(A):TRP:HH2	1:G:69:LYS:HE2	1.85	0.40
1:C:333:LYS:HD2	1:C:333:LYS:HA	1.81	0.40
1:E:176:HIS:CE1	1:E:313:ASN:HD22	2.40	0.40
1:H:76:ASN:HB3	1:H:82:LEU:CD2	2.51	0.40
1:E:94:GLU:HB3	1:E:118:ILE:HG23	2.04	0.40
1:O:293:ASP:OD1	1:O:296:LEU:HG	2.21	0.40
1:O:31:ASN:HB2	1:O:74:VAL:HG22	2.03	0.40
1:D:275:ASP:HA	1:D:294:SER:OG	2.21	0.40
1:F:3:VAL:HG22	1:F:91:ILE:HG23	2.01	0.40
1:E:252:ALA:CB	1:E:298:MET:HA	2.49	0.40
1:H:194:ARG:C	1:H:196:ALA:N	2.75	0.40
1:G:232:VAL:HG23	1:G:234:THR:OG1	2.21	0.40
1:F:16:LEU:O	1:F:16:LEU:HD23	2.21	0.40
1:A:279:VAL:HG22	1:C:197:ARG:NH1	2.36	0.40
1:H:239:VAL:O	1:H:239:VAL:HG13	2.22	0.40
1:E:109:ILE:C	1:E:109:ILE:HD13	2.42	0.40
1:C:31:ASN:O	1:C:32:ASP:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:ASP:HB3	1:E:294:SER:OG	2.21	0.40
1:B:1:LEU:HD22	1:B:329:ALA:HA	2.03	0.40
1:F:91:ILE:HD11	1:F:117:ILE:HD12	2.03	0.40
1:E:27:ILE:HD11	1:E:30:ILE:HG12	2.03	0.40
1:E:242:LEU:HD21	1:E:244:VAL:CG1	2.51	0.40
1:H:154:LEU:HD21	1:H:172:MET:HG3	2.04	0.40
1:B:164:LYS:HA	1:B:164:LYS:HD2	1.90	0.40
1:H:294:SER:C	1:H:296:LEU:N	2.74	0.40
1:D:172:MET:HE3	1:D:211:ALA:HB2	2.02	0.40
1:F:240:VAL:O	1:F:240:VAL:CG2	2.70	0.40
1:D:146:ASN:HD22	1:D:321:VAL:CG2	2.34	0.40
1:Q:122(A):LYS:HD3	1:Q:122(A):LYS:HA	1.88	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ASN:OD1	1:D:331:ASN:OD1[3_656]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/337 (99%)	292 (87%)	36 (11%)	7 (2%)	9	16
1	B	335/337 (99%)	293 (88%)	34 (10%)	8 (2%)	7	13
1	C	335/337 (99%)	293 (88%)	34 (10%)	8 (2%)	7	13
1	D	334/337 (99%)	269 (80%)	52 (16%)	13 (4%)	4	5
1	E	334/337 (99%)	260 (78%)	57 (17%)	17 (5%)	2	3
1	F	334/337 (99%)	244 (73%)	67 (20%)	23 (7%)	1	1
1	G	334/337 (99%)	257 (77%)	55 (16%)	22 (7%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	333/337 (99%)	248 (74%)	61 (18%)	24 (7%)	1	1
1	O	335/337 (99%)	308 (92%)	24 (7%)	3 (1%)	21	42
1	Q	334/337 (99%)	298 (89%)	31 (9%)	5 (2%)	13	26
All	All	3343/3370 (99%)	2762 (83%)	451 (14%)	130 (4%)	4	5

All (130) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	294	SER
1	D	1	LEU
1	D	210	ALA
1	E	75	SER
1	E	237	VAL
1	E	313	ASN
1	F	37	VAL
1	F	76	ASN
1	F	280	SER
1	G	198	ALA
1	G	202	ASN
1	G	208	THR
1	G	225	LEU
1	G	295	SER
1	H	27	ILE
1	H	28	ILE
1	H	71	ILE
1	H	87	LEU
1	H	89	ILE
1	H	133	ASN
1	Q	2	LYS
1	Q	124	ASP
1	A	237	VAL
1	B	0	LYS
1	B	166	GLY
1	B	237	VAL
1	B	302	ASP
1	C	237	VAL
1	D	36	GLY
1	D	166	GLY
1	D	180	GLY
1	D	237	VAL
1	E	55	ALA

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Mol	Chain	Res	Type
1	E	74	VAL
1	E	139	HIS
1	E	186	ASP
1	E	233	PRO
1	E	252	ALA
1	F	49	THR
1	F	69	LYS
1	F	130	VAL
1	F	146	ASN
1	F	266	GLU
1	F	297	THR
1	G	132	VAL
1	G	163	GLN
1	G	166	GLY
1	G	199	ALA
1	G	220	ASN
1	G	223	GLY
1	G	226	ASN
1	G	237	VAL
1	H	22	ASP
1	H	104	GLY
1	H	186	ASP
1	H	237	VAL
1	H	295	SER
1	O	237	VAL
1	Q	302	ASP
1	A	8	PHE
1	A	133	ASN
1	B	233	PRO
1	C	33	THR
1	C	34	GLY
1	C	198	ALA
1	D	55	ALA
1	E	56	ASP
1	F	8	PHE
1	F	132	VAL
1	F	211	ALA
1	F	237	VAL
1	G	18(B)	HIS
1	G	214	VAL
1	G	285	CYS
1	H	43	LEU

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Mol	Chain	Res	Type
1	H	76	ASN
1	H	140	ASP
1	Q	237	VAL
1	B	198	ALA
1	B	249	LYS
1	C	133	ASN
1	D	233	PRO
1	D	252	ALA
1	E	22	ASP
1	E	33	THR
1	E	73	VAL
1	E	193	LEU
1	E	285	CYS
1	F	186	ASP
1	F	285	CYS
1	F	294	SER
1	G	60	SER
1	G	162	ASP
1	G	190	HIS
1	G	207	SER
1	G	246	VAL
1	H	55	ALA
1	H	195	ARG
1	H	226	ASN
1	H	233	PRO
1	O	198	ALA
1	D	22	ASP
1	D	198	ALA
1	F	103	GLU
1	F	139	HIS
1	G	139	HIS
1	H	163	GLN
1	H	166	GLY
1	H	331	ASN
1	O	166	GLY
1	A	0	LYS
1	A	186	ASP
1	F	7	GLY
1	F	24	PRO
1	H	79	PRO
1	E	24	PRO
1	E	279	VAL

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Mol	Chain	Res	Type
1	F	66	VAL
1	B	104	GLY
1	C	83	PRO
1	D	219	PRO
1	F	281	VAL
1	A	166	GLY
1	C	233	PRO
1	D	156	PRO
1	F	219	PRO
1	H	74	VAL
1	A	37	VAL
1	H	142	PRO
1	Q	34	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/279 (100%)	264 (95%)	15 (5%)	27	52
1	B	279/279 (100%)	268 (96%)	11 (4%)	39	68
1	C	279/279 (100%)	265 (95%)	14 (5%)	30	56
1	D	279/279 (100%)	272 (98%)	7 (2%)	55	81
1	E	278/279 (100%)	260 (94%)	18 (6%)	21	42
1	F	279/279 (100%)	264 (95%)	15 (5%)	27	52
1	G	279/279 (100%)	259 (93%)	20 (7%)	18	35
1	H	278/279 (100%)	261 (94%)	17 (6%)	23	46
1	O	279/279 (100%)	266 (95%)	13 (5%)	32	59
1	Q	279/279 (100%)	263 (94%)	16 (6%)	25	49
All	All	2788/2790 (100%)	2642 (95%)	146 (5%)	29	54

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	VAL
1	A	84	TRP
1	A	85	LYS
1	A	91	ILE
1	A	133	ASN
1	A	163	GLN
1	A	164	LYS
1	A	172	MET
1	A	191	ARG
1	A	240	VAL
1	A	265	LYS
1	A	266	GLU
1	A	276	GLU
1	A	290	THR
1	A	333	LYS
1	B	16	LEU
1	B	38	LYS
1	B	58	LYS
1	B	84	TRP
1	B	107	LYS
1	B	124	ASP
1	B	133	ASN
1	B	140	ASP
1	B	246	VAL
1	B	271	LEU
1	B	290	THR
1	C	14	ASN
1	C	21	LYS
1	C	58	LYS
1	C	76	ASN
1	C	84	TRP
1	C	86	GLU
1	C	135	ASP
1	C	169	LYS
1	C	172	MET
1	C	191	ARG
1	C	226	ASN
1	C	261	ASP
1	C	290	THR
1	C	333	LYS
1	D	8	PHE
1	D	56	ASP
1	D	58	LYS

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Mol	Chain	Res	Type
1	D	84	TRP
1	D	133	ASN
1	D	228	ILE
1	D	290	THR
1	E	8	PHE
1	E	14	ASN
1	E	17	ARG
1	E	56	ASP
1	E	58	LYS
1	E	67	ASP
1	E	70	ILE
1	E	71	ILE
1	E	84	TRP
1	E	109	ILE
1	E	133	ASN
1	E	172	MET
1	E	183	ARG
1	E	191	ARG
1	E	202	ASN
1	E	228	ILE
1	E	233	PRO
1	E	290	THR
1	F	11	ILE
1	F	14	ASN
1	F	25	LEU
1	F	62	THR
1	F	85	LYS
1	F	91	ILE
1	F	115	LYS
1	F	121	PRO
1	F	124	ASP
1	F	133	ASN
1	F	174	THR
1	F	191	ARG
1	F	228	ILE
1	F	290	THR
1	F	300	MET
1	G	0	LYS
1	G	72	GLN
1	G	84	TRP
1	G	85	LYS
1	G	103	GLU

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Mol	Chain	Res	Type
1	G	115	LYS
1	G	130	VAL
1	G	133	ASN
1	G	138	SER
1	G	149	CYS
1	G	150	THR
1	G	178	TYR
1	G	191	ARG
1	G	228	ILE
1	G	234	THR
1	G	253	GLU
1	G	256	ASN
1	G	265	LYS
1	G	279	VAL
1	G	300	MET
1	H	38	LYS
1	H	67	ASP
1	H	72	GLN
1	H	76	ASN
1	H	84	TRP
1	H	90	ASP
1	H	91	ILE
1	H	124	ASP
1	H	133	ASN
1	H	164	LYS
1	H	178	TYR
1	H	181	ASP
1	H	186	ASP
1	H	228	ILE
1	H	290	THR
1	H	300	MET
1	H	311	TYR
1	O	3	VAL
1	O	16	LEU
1	O	17	ARG
1	O	39	GLN
1	O	72	GLN
1	O	84	TRP
1	O	94	GLU
1	O	124	ASP
1	O	133	ASN
1	O	138	SER

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Mol	Chain	Res	Type
1	O	177	SER
1	O	178	TYR
1	O	264	GLU
1	Q	8	PHE
1	Q	38	LYS
1	Q	39	GLN
1	Q	56	ASP
1	Q	76	ASN
1	Q	84	TRP
1	Q	103	GLU
1	Q	114	LYS
1	Q	133	ASN
1	Q	135	ASP
1	Q	140	ASP
1	Q	172	MET
1	Q	178	TYR
1	Q	191	ARG
1	Q	276	GLU
1	Q	290	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	78	ASN
1	A	133	ASN
1	A	152	ASN
1	A	163	GLN
1	A	202	ASN
1	A	245	GLN
1	A	256	ASN
1	A	330	ASN
1	B	18(B)	HIS
1	B	39	GLN
1	B	133	ASN
1	B	152	ASN
1	B	163	GLN
1	B	226	ASN
1	B	256	ASN
1	B	330	ASN
1	C	39	GLN
1	C	42	HIS

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Mol	Chain	Res	Type
1	C	72	GLN
1	C	76	ASN
1	C	133	ASN
1	C	152	ASN
1	C	202	ASN
1	C	226	ASN
1	C	256	ASN
1	C	330	ASN
1	D	72	GLN
1	D	133	ASN
1	D	139	HIS
1	D	146	ASN
1	D	202	ASN
1	D	226	ASN
1	D	256	ASN
1	D	330	ASN
1	E	18(B)	HIS
1	E	42	HIS
1	E	108	HIS
1	E	133	ASN
1	E	146	ASN
1	E	152	ASN
1	E	202	ASN
1	E	226	ASN
1	E	245	GLN
1	E	256	ASN
1	E	330	ASN
1	F	42	HIS
1	F	133	ASN
1	F	139	HIS
1	F	152	ASN
1	F	202	ASN
1	F	256	ASN
1	F	330	ASN
1	G	72	GLN
1	G	133	ASN
1	G	152	ASN
1	G	202	ASN
1	G	256	ASN
1	G	330	ASN
1	G	331	ASN
1	H	42	HIS

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Mol	Chain	Res	Type
1	H	72	GLN
1	H	76	ASN
1	H	133	ASN
1	H	146	ASN
1	H	152	ASN
1	H	202	ASN
1	H	220	ASN
1	H	256	ASN
1	H	330	ASN
1	H	331	ASN
1	O	18(B)	HIS
1	O	72	GLN
1	O	78	ASN
1	O	133	ASN
1	O	152	ASN
1	O	202	ASN
1	O	256	ASN
1	Q	133	ASN
1	Q	152	ASN
1	Q	163	GLN
1	Q	202	ASN
1	Q	245	GLN
1	Q	256	ASN
1	Q	330	ASN
1	Q	331	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

55 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	SO4	A	334	-	4,4,4	0.23	0	6,6,6	0.14	0
2	NAD	A	335	-	38,48,48	1.41	7 (18%)	47,73,73	1.80	13 (27%)
3	SO4	A	336	-	4,4,4	0.20	0	6,6,6	0.09	0
3	SO4	A	337	-	4,4,4	0.30	0	6,6,6	0.13	0
3	SO4	A	338	-	4,4,4	0.20	0	6,6,6	0.12	0
3	SO4	A	339	-	4,4,4	0.19	0	6,6,6	0.09	0
3	SO4	A	340	-	4,4,4	0.14	0	6,6,6	0.12	0
3	SO4	A	341	-	4,4,4	0.20	0	6,6,6	0.08	0
3	SO4	B	334	-	4,4,4	0.31	0	6,6,6	0.08	0
2	NAD	B	335	-	38,48,48	1.42	6 (15%)	47,73,73	1.80	12 (25%)
3	SO4	B	336	-	4,4,4	0.27	0	6,6,6	0.11	0
3	SO4	B	337	-	4,4,4	0.19	0	6,6,6	0.13	0
3	SO4	B	338	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	B	339	-	4,4,4	0.21	0	6,6,6	0.11	0
3	SO4	C	334	-	4,4,4	0.22	0	6,6,6	0.08	0
2	NAD	C	335	-	38,48,48	1.61	6 (15%)	47,73,73	1.71	11 (23%)
3	SO4	C	336	-	4,4,4	0.28	0	6,6,6	0.14	0
3	SO4	C	337	-	4,4,4	0.21	0	6,6,6	0.09	0
3	SO4	C	338	-	4,4,4	0.18	0	6,6,6	0.10	0
3	SO4	D	334	-	4,4,4	0.19	0	6,6,6	0.17	0
2	NAD	D	335	-	38,48,48	1.51	6 (15%)	47,73,73	1.79	14 (29%)
3	SO4	D	336	-	4,4,4	0.28	0	6,6,6	0.15	0
3	SO4	D	337	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	E	334	-	4,4,4	0.23	0	6,6,6	0.18	0
2	NAD	E	335	-	38,48,48	1.46	6 (15%)	47,73,73	1.92	13 (27%)
3	SO4	E	336	-	4,4,4	0.29	0	6,6,6	0.08	0
3	SO4	E	337	-	4,4,4	0.19	0	6,6,6	0.10	0
3	SO4	E	338	-	4,4,4	0.25	0	6,6,6	0.12	0
3	SO4	F	334	-	4,4,4	0.19	0	6,6,6	0.11	0
2	NAD	F	335	-	38,48,48	1.54	5 (13%)	47,73,73	1.84	14 (29%)
3	SO4	F	336	-	4,4,4	0.22	0	6,6,6	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	F	337	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	G	334	-	4,4,4	0.28	0	6,6,6	0.11	0
2	NAD	G	335	-	38,48,48	1.52	5 (13%)	47,73,73	1.87	16 (34%)
3	SO4	G	336	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	G	337	-	4,4,4	0.25	0	6,6,6	0.06	0
3	SO4	G	338	-	4,4,4	0.22	0	6,6,6	0.08	0
3	SO4	G	339	-	4,4,4	0.21	0	6,6,6	0.10	0
3	SO4	H	334	-	4,4,4	0.21	0	6,6,6	0.13	0
2	NAD	H	335	-	38,48,48	1.56	6 (15%)	47,73,73	1.87	14 (29%)
3	SO4	H	336	-	4,4,4	0.30	0	6,6,6	0.13	0
3	SO4	H	337	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	O	334	-	4,4,4	0.24	0	6,6,6	0.14	0
2	NAD	O	335	-	38,48,48	1.36	5 (13%)	47,73,73	1.83	16 (34%)
3	SO4	O	336	-	4,4,4	0.24	0	6,6,6	0.20	0
3	SO4	O	337	-	4,4,4	0.26	0	6,6,6	0.18	0
3	SO4	O	338	-	4,4,4	0.23	0	6,6,6	0.06	0
3	SO4	O	339	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	O	340	-	4,4,4	0.23	0	6,6,6	0.17	0
3	SO4	Q	334	-	4,4,4	0.23	0	6,6,6	0.14	0
2	NAD	Q	335	-	38,48,48	1.61	8 (21%)	47,73,73	1.71	10 (21%)
3	SO4	Q	336	-	4,4,4	0.33	0	6,6,6	0.24	0
3	SO4	Q	337	-	4,4,4	0.19	0	6,6,6	0.07	0
3	SO4	Q	338	-	4,4,4	0.18	0	6,6,6	0.16	0
3	SO4	Q	339	-	4,4,4	0.26	0	6,6,6	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	334	-	-	0/0/0/0	0/0/0/0
2	NAD	A	335	-	-	0/22/62/62	0/5/5/5
3	SO4	A	336	-	-	0/0/0/0	0/0/0/0
3	SO4	A	337	-	-	0/0/0/0	0/0/0/0
3	SO4	A	338	-	-	0/0/0/0	0/0/0/0
3	SO4	A	339	-	-	0/0/0/0	0/0/0/0
3	SO4	A	340	-	-	0/0/0/0	0/0/0/0
3	SO4	A	341	-	-	0/0/0/0	0/0/0/0
3	SO4	B	334	-	-	0/0/0/0	0/0/0/0
2	NAD	B	335	-	-	0/22/62/62	0/5/5/5
3	SO4	B	336	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	337	-	-	0/0/0/0	0/0/0/0
3	SO4	B	338	-	-	0/0/0/0	0/0/0/0
3	SO4	B	339	-	-	0/0/0/0	0/0/0/0
3	SO4	C	334	-	-	0/0/0/0	0/0/0/0
2	NAD	C	335	-	-	0/22/62/62	0/5/5/5
3	SO4	C	336	-	-	0/0/0/0	0/0/0/0
3	SO4	C	337	-	-	0/0/0/0	0/0/0/0
3	SO4	C	338	-	-	0/0/0/0	0/0/0/0
3	SO4	D	334	-	-	0/0/0/0	0/0/0/0
2	NAD	D	335	-	-	0/22/62/62	0/5/5/5
3	SO4	D	336	-	-	0/0/0/0	0/0/0/0
3	SO4	D	337	-	-	0/0/0/0	0/0/0/0
3	SO4	E	334	-	-	0/0/0/0	0/0/0/0
2	NAD	E	335	-	-	0/22/62/62	0/5/5/5
3	SO4	E	336	-	-	0/0/0/0	0/0/0/0
3	SO4	E	337	-	-	0/0/0/0	0/0/0/0
3	SO4	E	338	-	-	0/0/0/0	0/0/0/0
3	SO4	F	334	-	-	0/0/0/0	0/0/0/0
2	NAD	F	335	-	-	0/22/62/62	0/5/5/5
3	SO4	F	336	-	-	0/0/0/0	0/0/0/0
3	SO4	F	337	-	-	0/0/0/0	0/0/0/0
3	SO4	G	334	-	-	0/0/0/0	0/0/0/0
2	NAD	G	335	-	-	0/22/62/62	0/5/5/5
3	SO4	G	336	-	-	0/0/0/0	0/0/0/0
3	SO4	G	337	-	-	0/0/0/0	0/0/0/0
3	SO4	G	338	-	-	0/0/0/0	0/0/0/0
3	SO4	G	339	-	-	0/0/0/0	0/0/0/0
3	SO4	H	334	-	-	0/0/0/0	0/0/0/0
2	NAD	H	335	-	-	0/22/62/62	0/5/5/5
3	SO4	H	336	-	-	0/0/0/0	0/0/0/0
3	SO4	H	337	-	-	0/0/0/0	0/0/0/0
3	SO4	O	334	-	-	0/0/0/0	0/0/0/0
2	NAD	O	335	-	-	0/22/62/62	0/5/5/5
3	SO4	O	336	-	-	0/0/0/0	0/0/0/0
3	SO4	O	337	-	-	0/0/0/0	0/0/0/0
3	SO4	O	338	-	-	0/0/0/0	0/0/0/0
3	SO4	O	339	-	-	0/0/0/0	0/0/0/0
3	SO4	O	340	-	-	0/0/0/0	0/0/0/0
3	SO4	Q	334	-	-	0/0/0/0	0/0/0/0
2	NAD	Q	335	-	-	0/22/62/62	0/5/5/5
3	SO4	Q	336	-	-	0/0/0/0	0/0/0/0
3	SO4	Q	337	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	Q	338	-	-	0/0/0/0	0/0/0/0
3	SO4	Q	339	-	-	0/0/0/0	0/0/0/0

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	335	NAD	O5B-C5B	2.02	1.53	1.44
2	A	335	NAD	O3D-C3D	2.02	1.47	1.43
2	E	335	NAD	O5B-C5B	2.05	1.53	1.44
2	H	335	NAD	O5B-C5B	2.06	1.53	1.44
2	Q	335	NAD	C2A-N3A	2.06	1.35	1.32
2	Q	335	NAD	O3D-C3D	2.07	1.47	1.43
2	B	335	NAD	O5B-C5B	2.09	1.53	1.44
2	B	335	NAD	C4A-N3A	2.09	1.38	1.35
2	O	335	NAD	C2A-N3A	2.12	1.36	1.32
2	D	335	NAD	O3D-C3D	2.13	1.48	1.43
2	C	335	NAD	C2A-N3A	2.14	1.36	1.32
2	F	335	NAD	C4A-N3A	2.21	1.38	1.35
2	A	335	NAD	C5N-C4N	2.21	1.43	1.38
2	A	335	NAD	C4A-N3A	2.28	1.39	1.35
2	H	335	NAD	C4A-N3A	2.32	1.39	1.35
2	E	335	NAD	O4B-C1B	2.32	1.44	1.41
2	C	335	NAD	O3D-C3D	2.33	1.48	1.43
2	E	335	NAD	C4A-N3A	2.35	1.39	1.35
2	D	335	NAD	O4B-C1B	2.35	1.44	1.41
2	D	335	NAD	C4A-N3A	2.59	1.39	1.35
2	B	335	NAD	C4N-C3N	2.62	1.43	1.39
2	G	335	NAD	C4A-N3A	2.62	1.39	1.35
2	A	335	NAD	C3N-C7N	2.64	1.54	1.50
2	Q	335	NAD	C4A-N3A	2.66	1.39	1.35
2	O	335	NAD	C4N-C3N	2.71	1.43	1.39
2	G	335	NAD	C4N-C3N	2.74	1.44	1.39
2	F	335	NAD	O4B-C1B	2.80	1.44	1.41
2	H	335	NAD	C4N-C3N	2.81	1.44	1.39
2	A	335	NAD	C4N-C3N	2.96	1.44	1.39
2	E	335	NAD	C4N-C3N	2.97	1.44	1.39
2	G	335	NAD	O4B-C1B	3.03	1.45	1.41
2	O	335	NAD	O4B-C1B	3.07	1.45	1.41
2	A	335	NAD	O4B-C1B	3.08	1.45	1.41
2	O	335	NAD	C6N-N1N	3.18	1.44	1.35
2	D	335	NAD	C4N-C3N	3.18	1.44	1.39
2	B	335	NAD	C3N-C7N	3.20	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	335	NAD	O4B-C1B	3.22	1.45	1.41
2	A	335	NAD	C6N-N1N	3.31	1.44	1.35
2	F	335	NAD	C4N-C3N	3.31	1.45	1.39
2	O	335	NAD	C3N-C7N	3.34	1.55	1.50
2	G	335	NAD	C6N-N1N	3.35	1.44	1.35
2	C	335	NAD	C6N-N1N	3.36	1.44	1.35
2	C	335	NAD	C4N-C3N	3.38	1.45	1.39
2	Q	335	NAD	C4N-C3N	3.40	1.45	1.39
2	H	335	NAD	O4B-C1B	3.43	1.45	1.41
2	C	335	NAD	O4B-C1B	3.44	1.45	1.41
2	H	335	NAD	C6N-N1N	3.44	1.44	1.35
2	Q	335	NAD	C6N-N1N	3.48	1.44	1.35
2	E	335	NAD	C6N-N1N	3.48	1.44	1.35
2	Q	335	NAD	O4B-C1B	3.48	1.45	1.41
2	B	335	NAD	C6N-N1N	3.50	1.44	1.35
2	F	335	NAD	C6N-N1N	3.60	1.45	1.35
2	D	335	NAD	C6N-N1N	3.63	1.45	1.35
2	E	335	NAD	C3N-C7N	4.13	1.57	1.50
2	D	335	NAD	C3N-C7N	4.29	1.57	1.50
2	Q	335	NAD	C3N-C7N	4.55	1.57	1.50
2	C	335	NAD	C3N-C7N	4.55	1.57	1.50
2	H	335	NAD	C3N-C7N	4.62	1.57	1.50
2	G	335	NAD	C3N-C7N	4.71	1.58	1.50
2	F	335	NAD	C3N-C7N	4.80	1.58	1.50

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	335	NAD	C5N-C6N-N1N	-4.69	112.35	120.47
2	B	335	NAD	C5N-C6N-N1N	-4.62	112.48	120.47
2	O	335	NAD	C5N-C6N-N1N	-4.53	112.63	120.47
2	G	335	NAD	C5N-C6N-N1N	-4.52	112.66	120.47
2	D	335	NAD	C5N-C6N-N1N	-4.52	112.66	120.47
2	Q	335	NAD	C5N-C6N-N1N	-4.48	112.72	120.47
2	E	335	NAD	C5N-C6N-N1N	-4.47	112.74	120.47
2	F	335	NAD	C5N-C6N-N1N	-4.46	112.76	120.47
2	H	335	NAD	C5N-C6N-N1N	-4.40	112.87	120.47
2	C	335	NAD	C5N-C6N-N1N	-4.37	112.92	120.47
2	H	335	NAD	C4N-C3N-C7N	-4.20	109.99	121.09
2	E	335	NAD	C4N-C3N-C7N	-4.19	110.01	121.09
2	C	335	NAD	C4N-C3N-C7N	-4.06	110.36	121.09
2	G	335	NAD	C4N-C3N-C7N	-3.96	110.64	121.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	335	NAD	C4N-C3N-C7N	-3.79	111.07	121.09
2	A	335	NAD	C4N-C3N-C7N	-3.68	111.35	121.09
2	B	335	NAD	C4N-C3N-C7N	-3.68	111.36	121.09
2	D	335	NAD	C4N-C3N-C7N	-3.60	111.58	121.09
2	O	335	NAD	C4N-C3N-C7N	-3.57	111.65	121.09
2	Q	335	NAD	C4N-C3N-C7N	-3.57	111.66	121.09
2	C	335	NAD	C3N-C2N-N1N	-3.38	116.46	120.36
2	D	335	NAD	C1B-N9A-C4A	-3.21	122.10	126.94
2	O	335	NAD	C5N-C4N-C3N	-3.20	116.31	120.33
2	G	335	NAD	N3A-C2A-N1A	-3.04	126.56	128.89
2	B	335	NAD	C5N-C4N-C3N	-3.04	116.51	120.33
2	A	335	NAD	C5N-C4N-C3N	-2.95	116.62	120.33
2	E	335	NAD	C3N-C2N-N1N	-2.94	116.98	120.36
2	F	335	NAD	C3N-C2N-N1N	-2.92	117.00	120.36
2	B	335	NAD	O3D-C3D-C4D	-2.85	102.50	111.05
2	H	335	NAD	C3N-C2N-N1N	-2.80	117.14	120.36
2	H	335	NAD	C5N-C4N-C3N	-2.78	116.84	120.33
2	G	335	NAD	C3N-C2N-N1N	-2.78	117.16	120.36
2	E	335	NAD	C5N-C4N-C3N	-2.77	116.85	120.33
2	A	335	NAD	C1B-N9A-C4A	-2.76	122.77	126.94
2	Q	335	NAD	C3N-C2N-N1N	-2.73	117.21	120.36
2	O	335	NAD	N3A-C2A-N1A	-2.73	126.80	128.89
2	F	335	NAD	C1B-N9A-C4A	-2.72	122.83	126.94
2	E	335	NAD	C1B-N9A-C4A	-2.72	122.84	126.94
2	B	335	NAD	C1B-N9A-C4A	-2.70	122.86	126.94
2	D	335	NAD	N3A-C2A-N1A	-2.70	126.82	128.89
2	Q	335	NAD	N3A-C2A-N1A	-2.70	126.83	128.89
2	A	335	NAD	N3A-C2A-N1A	-2.69	126.83	128.89
2	D	335	NAD	C5N-C4N-C3N	-2.69	116.95	120.33
2	A	335	NAD	C3N-C2N-N1N	-2.69	117.27	120.36
2	F	335	NAD	N3A-C2A-N1A	-2.68	126.84	128.89
2	O	335	NAD	O4B-C1B-N9A	-2.67	102.52	108.10
2	C	335	NAD	O3D-C3D-C4D	-2.64	103.14	111.05
2	D	335	NAD	C3N-C2N-N1N	-2.63	117.33	120.36
2	Q	335	NAD	C5N-C4N-C3N	-2.61	117.05	120.33
2	E	335	NAD	O7N-C7N-C3N	-2.60	116.75	119.59
2	O	335	NAD	C1B-N9A-C4A	-2.56	123.07	126.94
2	H	335	NAD	O7N-C7N-C3N	-2.55	116.81	119.59
2	E	335	NAD	N3A-C2A-N1A	-2.54	126.95	128.89
2	G	335	NAD	C5N-C4N-C3N	-2.52	117.17	120.33
2	A	335	NAD	O5B-C5B-C4B	-2.48	99.98	109.12
2	B	335	NAD	C3N-C2N-N1N	-2.46	117.53	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	335	NAD	O3D-C3D-C4D	-2.46	103.68	111.05
2	F	335	NAD	C5N-C4N-C3N	-2.44	117.27	120.33
2	H	335	NAD	N3A-C2A-N1A	-2.44	127.03	128.89
2	E	335	NAD	O3D-C3D-C4D	-2.44	103.74	111.05
2	O	335	NAD	O3D-C3D-C4D	-2.42	103.78	111.05
2	B	335	NAD	N3A-C2A-N1A	-2.42	127.04	128.89
2	Q	335	NAD	O3D-C3D-C4D	-2.32	104.10	111.05
2	O	335	NAD	O5B-C5B-C4B	-2.30	100.64	109.12
2	O	335	NAD	O7N-C7N-C3N	-2.28	117.10	119.59
2	O	335	NAD	C3N-C2N-N1N	-2.27	117.75	120.36
2	A	335	NAD	O3D-C3D-C4D	-2.25	104.30	111.05
2	F	335	NAD	O3D-C3D-C4D	-2.25	104.30	111.05
2	C	335	NAD	N3A-C2A-N1A	-2.23	127.19	128.89
2	G	335	NAD	O5B-C5B-C4B	-2.14	101.24	109.12
2	C	335	NAD	C5N-C4N-C3N	-2.13	117.65	120.33
2	H	335	NAD	O3D-C3D-C4D	-2.13	104.68	111.05
2	H	335	NAD	O4B-C1B-N9A	-2.11	103.69	108.10
2	B	335	NAD	O7N-C7N-C3N	-2.10	117.29	119.59
2	G	335	NAD	C1B-N9A-C4A	-2.09	123.80	126.94
2	H	335	NAD	C1B-N9A-C4A	-2.07	123.81	126.94
2	D	335	NAD	O4B-C1B-N9A	-2.07	103.77	108.10
2	A	335	NAD	O7N-C7N-C3N	-2.06	117.33	119.59
2	F	335	NAD	O5B-C5B-C4B	-2.06	101.52	109.12
2	D	335	NAD	O3D-C3D-C4D	-2.04	104.93	111.05
2	C	335	NAD	C1B-N9A-C4A	-2.04	123.87	126.94
2	G	335	NAD	O7N-C7N-C3N	-2.03	117.37	119.59
2	F	335	NAD	O7N-C7N-C3N	-2.02	117.38	119.59
2	D	335	NAD	C4D-O4D-C1D	2.06	111.98	109.72
2	F	335	NAD	O4D-C1D-N1N	2.07	110.41	108.13
2	G	335	NAD	O2A-PA-O3	2.10	114.61	105.09
2	O	335	NAD	O2A-PA-O3	2.11	114.66	105.09
2	O	335	NAD	C2B-C1B-N9A	2.13	117.55	114.29
2	G	335	NAD	PN-O3-PA	2.18	138.84	132.73
2	D	335	NAD	C2B-C1B-N9A	2.33	117.85	114.29
2	G	335	NAD	C4D-O4D-C1D	2.37	112.32	109.72
2	H	335	NAD	C4D-O4D-C1D	2.49	112.46	109.72
2	O	335	NAD	C2N-C3N-C7N	2.50	126.56	119.31
2	F	335	NAD	C2N-C3N-C4N	2.57	121.15	118.29
2	E	335	NAD	C2B-C3B-C4B	2.57	107.89	102.61
2	B	335	NAD	C2N-C3N-C7N	2.60	126.85	119.31
2	G	335	NAD	C2N-C3N-C4N	2.62	121.20	118.29
2	D	335	NAD	C2N-C3N-C7N	2.63	126.96	119.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	335	NAD	C2N-C3N-C7N	2.66	127.03	119.31
2	Q	335	NAD	C2N-C3N-C7N	2.67	127.07	119.31
2	Q	335	NAD	C2N-C3N-C4N	2.67	121.27	118.29
2	C	335	NAD	C2N-C3N-C4N	2.68	121.27	118.29
2	C	335	NAD	C3N-C7N-N7N	2.84	120.92	117.82
2	D	335	NAD	C2N-C3N-C4N	2.85	121.46	118.29
2	Q	335	NAD	C3N-C7N-N7N	2.85	120.94	117.82
2	H	335	NAD	C2N-C3N-C4N	2.88	121.50	118.29
2	F	335	NAD	C2N-C3N-C7N	2.92	127.78	119.31
2	A	335	NAD	C3N-C7N-N7N	2.94	121.03	117.82
2	D	335	NAD	C3N-C7N-N7N	2.95	121.04	117.82
2	A	335	NAD	C2N-C3N-C4N	2.99	121.62	118.29
2	O	335	NAD	C3N-C7N-N7N	3.03	121.13	117.82
2	E	335	NAD	C2N-C3N-C4N	3.04	121.68	118.29
2	G	335	NAD	C2N-C3N-C7N	3.05	128.16	119.31
2	E	335	NAD	C2N-C3N-C7N	3.10	128.31	119.31
2	C	335	NAD	C2N-C3N-C7N	3.12	128.36	119.31
2	B	335	NAD	C3N-C7N-N7N	3.13	121.24	117.82
2	O	335	NAD	C2N-C3N-C4N	3.14	121.79	118.29
2	B	335	NAD	C2N-C3N-C4N	3.15	121.80	118.29
2	H	335	NAD	C2N-C3N-C7N	3.17	128.51	119.31
2	C	335	NAD	C6N-C5N-C4N	3.55	124.81	119.44
2	O	335	NAD	C6N-C5N-C4N	3.72	125.07	119.44
2	D	335	NAD	C6N-C5N-C4N	3.74	125.10	119.44
2	F	335	NAD	C3N-C7N-N7N	3.75	121.92	117.82
2	Q	335	NAD	C6N-C5N-C4N	3.76	125.12	119.44
2	F	335	NAD	C6N-C5N-C4N	3.78	125.16	119.44
2	E	335	NAD	C6N-C5N-C4N	3.85	125.27	119.44
2	E	335	NAD	C3N-C7N-N7N	3.86	122.04	117.82
2	G	335	NAD	C3N-C7N-N7N	3.86	122.04	117.82
2	A	335	NAD	C6N-C5N-C4N	3.87	125.30	119.44
2	G	335	NAD	C6N-C5N-C4N	3.98	125.45	119.44
2	H	335	NAD	C6N-C5N-C4N	4.00	125.49	119.44
2	B	335	NAD	C6N-C5N-C4N	4.01	125.51	119.44
2	H	335	NAD	C3N-C7N-N7N	4.11	122.31	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	335	NAD	1	0
2	B	335	NAD	1	0
2	D	335	NAD	3	0
3	E	334	SO4	1	0
2	E	335	NAD	5	0
3	E	337	SO4	1	0
3	E	338	SO4	1	0
2	F	335	NAD	2	0
2	G	335	NAD	1	0
2	H	335	NAD	2	0
2	O	335	NAD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	337/337 (100%)	-0.08	1 (0%) 94 93	29, 42, 59, 80	0
1	B	337/337 (100%)	-0.06	2 (0%) 90 88	31, 46, 63, 71	0
1	C	337/337 (100%)	0.01	2 (0%) 90 88	31, 48, 69, 81	0
1	D	336/337 (99%)	0.03	2 (0%) 90 88	35, 62, 79, 96	0
1	E	336/337 (99%)	1.49	93 (27%) 1 0	55, 87, 108, 114	0
1	F	336/337 (99%)	0.85	50 (14%) 3 2	43, 88, 105, 113	0
1	G	336/337 (99%)	0.67	29 (8%) 13 8	34, 69, 91, 101	0
1	H	335/337 (99%)	0.51	23 (6%) 20 14	48, 83, 103, 114	0
1	O	337/337 (100%)	-0.03	0 100 100	19, 31, 45, 56	0
1	Q	336/337 (99%)	-0.06	1 (0%) 94 93	21, 39, 58, 81	0
All	All	3363/3370 (99%)	0.33	203 (6%) 25 18	19, 56, 99, 114	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	187	ALA	7.7
1	E	29	ALA	7.0
1	E	25	LEU	6.7
1	E	270	ILE	6.1
1	E	228	ILE	6.1
1	E	28	ILE	5.7
1	F	214	VAL	5.5
1	E	15	PHE	5.4
1	E	79	PRO	5.3
1	E	0(A)	ALA	5.3
1	E	116	VAL	5.1
1	E	66	VAL	5.1
1	F	119	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	273	VAL	4.7
1	G	269	GLY	4.7
1	E	255	VAL	4.6
1	E	328	VAL	4.6
1	E	129	VAL	4.6
1	E	92	VAL	4.4
1	E	32	ASP	4.4
1	E	267	LEU	4.3
1	C	0(A)	ALA	4.3
1	F	128	TYR	4.3
1	E	1	LEU	4.1
1	E	64	ILE	4.1
1	F	84	TRP	4.0
1	F	108	HIS	4.0
1	E	53	PHE	4.0
1	G	244	VAL	4.0
1	F	87	LEU	4.0
1	E	63	ALA	4.0
1	E	72	GLN	4.0
1	E	84	TRP	3.9
1	H	332	TRP	3.9
1	H	191	ARG	3.9
1	H	193	LEU	3.8
1	C	332	TRP	3.8
1	F	89	ILE	3.8
1	E	100	VAL	3.7
1	F	263	ALA	3.7
1	F	131	GLY	3.6
1	E	18(A)	TRP	3.5
1	E	55	ALA	3.5
1	F	46	TYR	3.5
1	E	271	LEU	3.5
1	G	290	THR	3.4
1	E	98	VAL	3.4
1	E	44	LEU	3.4
1	F	155	ALA	3.4
1	E	316	GLY	3.4
1	F	74	VAL	3.4
1	F	322	VAL	3.3
1	F	259	PHE	3.3
1	G	156	PRO	3.3
1	E	62	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	215	ALA	3.2
1	Q	333	LYS	3.2
1	F	268	LYS	3.2
1	F	5	ILE	3.1
1	F	288	PHE	3.1
1	E	300	MET	3.1
1	E	24	PRO	3.1
1	E	321	VAL	3.1
1	E	23	SER	3.1
1	G	160	VAL	3.1
1	E	292	ILE	3.1
1	E	330	ASN	3.0
1	F	52	ILE	3.0
1	E	259	PHE	3.0
1	G	130	VAL	3.0
1	E	22	ASP	3.0
1	G	273	VAL	3.0
1	F	14	ASN	3.0
1	F	217	VAL	2.9
1	E	108	HIS	2.9
1	E	209	GLY	2.9
1	E	327	ILE	2.9
1	E	322	VAL	2.9
1	F	82	LEU	2.8
1	G	254	GLU	2.8
1	E	67	ASP	2.8
1	E	74	VAL	2.8
1	E	16	LEU	2.8
1	F	32	ASP	2.8
1	E	154	LEU	2.8
1	E	324	LEU	2.8
1	H	46	TYR	2.8
1	E	91	ILE	2.8
1	E	325	ALA	2.8
1	E	114	LYS	2.7
1	F	225	LEU	2.7
1	H	221	LEU	2.7
1	E	70	ILE	2.7
1	G	152	ASN	2.7
1	F	278	LEU	2.7
1	G	225	LEU	2.7
1	F	61	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	305	VAL	2.7
1	G	330	ASN	2.7
1	F	27	ILE	2.7
1	G	217	VAL	2.7
1	H	92	VAL	2.7
1	F	156	PRO	2.7
1	F	267	LEU	2.6
1	E	37	VAL	2.6
1	E	193	LEU	2.6
1	H	84	TRP	2.6
1	E	144	ILE	2.6
1	F	264	GLU	2.6
1	E	139	HIS	2.6
1	G	283	PHE	2.6
1	E	249	LYS	2.5
1	E	171	THR	2.5
1	E	206	THR	2.5
1	E	138	SER	2.5
1	F	299	VAL	2.5
1	G	27	ILE	2.5
1	E	283	PHE	2.5
1	E	21	LYS	2.5
1	E	143	ILE	2.5
1	F	48	SER	2.5
1	H	188	SER	2.5
1	E	231	ARG	2.5
1	F	164	LYS	2.5
1	G	266	GLU	2.5
1	E	258	ALA	2.5
1	H	105	ALA	2.5
1	A	333	LYS	2.5
1	G	333	LYS	2.5
1	G	143	ILE	2.5
1	F	83	PRO	2.5
1	F	274	CYS	2.4
1	E	111	ALA	2.4
1	F	37	VAL	2.4
1	E	57	VAL	2.4
1	G	331	ASN	2.4
1	E	317	TYR	2.4
1	E	153	CYS	2.4
1	F	269	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	115	LYS	2.4
1	H	128	TYR	2.4
1	F	146	ASN	2.4
1	H	132	VAL	2.4
1	E	81	LEU	2.3
1	F	242	LEU	2.3
1	G	304	MET	2.3
1	E	263	ALA	2.3
1	E	121	PRO	2.3
1	F	319	GLN	2.3
1	E	252	ALA	2.3
1	H	7	GLY	2.3
1	E	54	ASP	2.3
1	E	18	CYS	2.3
1	E	329	ALA	2.3
1	H	187	ALA	2.3
1	E	194	ARG	2.3
1	G	278	LEU	2.3
1	H	116	VAL	2.3
1	E	203	ILE	2.3
1	E	308	ILE	2.3
1	F	68	GLY	2.3
1	F	56	ASP	2.2
1	F	219	PRO	2.2
1	B	262	SER	2.2
1	F	130	VAL	2.2
1	H	57	VAL	2.2
1	E	33	THR	2.2
1	E	250	THR	2.2
1	E	46	TYR	2.2
1	H	25	LEU	2.2
1	F	31	ASN	2.2
1	H	190	HIS	2.2
1	G	25	LEU	2.2
1	E	191	ARG	2.2
1	E	140	ASP	2.2
1	F	265	LYS	2.2
1	E	204	VAL	2.2
1	G	226	ASN	2.2
1	E	279	VAL	2.2
1	G	193	LEU	2.1
1	G	247	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	165	PHE	2.1
1	G	164	LYS	2.1
1	D	188	SER	2.1
1	F	160	VAL	2.1
1	H	44	LEU	2.1
1	G	167	ILE	2.1
1	H	113	ALA	2.1
1	G	275	ASP	2.1
1	E	170	GLY	2.1
1	F	333	LYS	2.1
1	H	27	ILE	2.1
1	H	99	PHE	2.1
1	B	249	LYS	2.1
1	F	325	ALA	2.1
1	F	43	LEU	2.0
1	D	305	VAL	2.0
1	F	10	ARG	2.0
1	G	332	TRP	2.0
1	H	328	VAL	2.0
1	E	142	PRO	2.0
1	E	40	ALA	2.0
1	E	59	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	O	337	5/5	0.89	0.32	4.84	72,74,75,75	5
3	SO4	O	340	5/5	0.88	0.23	3.29	68,68,69,70	5
3	SO4	H	334	5/5	0.88	0.21	2.05	79,80,80,81	5
3	SO4	A	337	5/5	0.97	0.19	1.81	64,65,66,68	0
3	SO4	O	334	5/5	0.84	0.19	1.80	74,74,75,77	5
3	SO4	G	334	5/5	0.85	0.34	1.63	87,87,88,89	5
3	SO4	O	339	5/5	0.90	0.22	1.40	87,87,88,88	5
3	SO4	G	337	5/5	0.88	0.24	1.31	101,102,102,102	5
3	SO4	Q	337	5/5	0.98	0.19	1.27	58,58,59,59	5
3	SO4	Q	334	5/5	0.92	0.21	1.17	73,75,75,75	5
3	SO4	B	337	5/5	0.97	0.17	0.69	59,60,61,61	5
2	NAD	B	335	44/44	0.96	0.17	0.46	36,44,50,51	0
3	SO4	F	337	5/5	0.91	0.18	0.38	85,86,86,87	5
2	NAD	Q	335	44/44	0.95	0.16	0.22	41,48,50,51	0
3	SO4	B	339	5/5	0.95	0.18	0.08	69,70,71,71	5
2	NAD	H	335	44/44	0.92	0.21	0.06	83,87,95,96	0
3	SO4	C	338	5/5	0.94	0.18	0.03	62,63,64,65	5
2	NAD	O	335	44/44	0.98	0.17	-0.03	19,23,26,29	0
3	SO4	D	334	5/5	0.94	0.17	-0.03	75,76,76,76	5
2	NAD	A	335	44/44	0.97	0.17	-0.06	37,41,47,50	0
2	NAD	D	335	44/44	0.95	0.17	-0.10	50,53,55,56	0
2	NAD	C	335	44/44	0.97	0.16	-0.11	40,45,50,51	0
2	NAD	G	335	44/44	0.96	0.18	-0.13	43,47,51,52	0
3	SO4	C	337	5/5	0.99	0.15	-0.32	49,49,50,50	0
2	NAD	E	335	44/44	0.90	0.23	-0.44	87,97,102,104	0
3	SO4	Q	339	5/5	0.90	0.15	-0.48	88,88,90,90	5
2	NAD	F	335	44/44	0.91	0.19	-0.57	67,73,81,81	0
3	SO4	E	337	5/5	0.81	0.20	-0.63	116,117,117,117	5
3	SO4	Q	338	5/5	0.99	0.18	-0.65	46,47,48,51	0
3	SO4	D	337	5/5	0.90	0.15	-0.76	89,90,90,90	5
3	SO4	A	340	5/5	0.98	0.16	-0.77	59,59,61,62	0
3	SO4	H	337	5/5	0.91	0.14	-0.81	80,81,82,82	5
3	SO4	E	338	5/5	0.94	0.15	-0.94	87,87,88,88	5
3	SO4	B	338	5/5	0.93	0.14	-1.16	75,75,76,76	5
3	SO4	A	338	5/5	0.98	0.14	-1.57	55,56,57,58	5
3	SO4	E	334	5/5	0.96	0.14	-1.86	60,60,61,62	5
3	SO4	G	339	5/5	0.85	0.17	-1.86	114,114,114,114	5
3	SO4	A	336	5/5	0.99	0.14	-	50,50,52,52	0
3	SO4	F	334	5/5	0.86	0.14	-	111,111,111,112	0
3	SO4	D	336	5/5	0.78	0.28	-	84,84,85,86	5
3	SO4	A	341	5/5	0.74	0.23	-	108,108,109,109	5
3	SO4	C	336	5/5	0.97	0.15	-	67,67,68,68	0
3	SO4	Q	336	5/5	0.97	0.15	-	69,71,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	O	336	5/5	0.97	0.16	-	60,62,63,63	0
3	SO4	H	336	5/5	0.87	0.21	-	77,77,78,78	5
3	SO4	O	338	5/5	0.89	0.23	-	88,89,90,90	5
3	SO4	C	334	5/5	0.94	0.17	-	79,80,80,80	5
3	SO4	A	334	5/5	0.87	0.20	-	79,79,80,81	5
3	SO4	F	336	5/5	0.91	0.19	-	56,56,59,59	5
3	SO4	E	336	5/5	0.91	0.14	-	78,79,79,80	5
3	SO4	B	336	5/5	0.96	0.17	-	52,53,53,53	5
3	SO4	G	336	5/5	0.95	0.14	-	67,68,68,69	5
3	SO4	B	334	5/5	0.84	0.19	-	91,91,92,92	5
3	SO4	G	338	5/5	0.89	0.19	-	96,96,97,97	5
3	SO4	A	339	5/5	0.87	0.28	-	104,104,105,106	5

6.5 Other polymers [i](#)

There are no such residues in this entry.