Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:23 PM GMT

PDB ID	:	3X2E
Title	:	A thermophilic hydrolase
Authors	:	Zheng, Y.; Ko, T.P.; Huang, C.H.
Deposited on	:	2014-12-21
Resolution	:	2.85 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

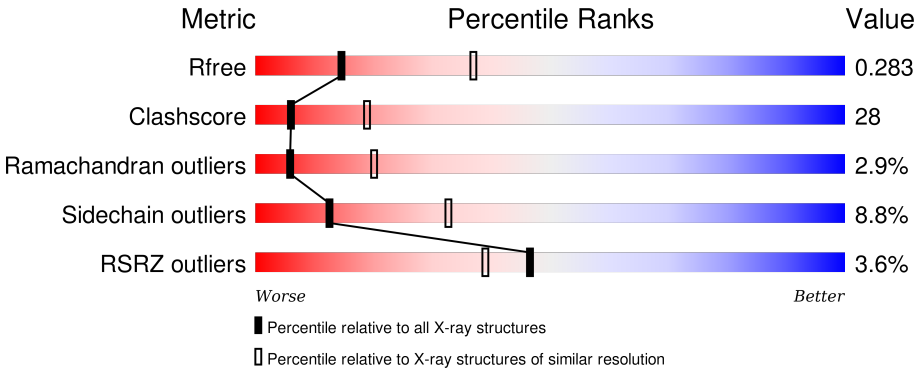
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 <=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	411	5% 50% 41% 6%
1	B	411	2% 48% 44% 6%
1	C	411	2% 52% 39% 6%
1	D	411	4% 49% 42% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12993 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 Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3116	1970	539	593	14			
1	B	401	Total	C	N	O	S	0	0	0
			3116	1970	539	593	14			
1	C	401	Total	C	N	O	S	0	0	0
			3116	1970	539	593	14			
1	D	401	Total	C	N	O	S	0	0	0
			3116	1970	539	593	14			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP O51933
A	2	ALA	-	EXPRESSION TAG	UNP O51933
A	406	HIS	-	EXPRESSION TAG	UNP O51933
A	407	HIS	-	EXPRESSION TAG	UNP O51933
A	408	HIS	-	EXPRESSION TAG	UNP O51933
A	409	HIS	-	EXPRESSION TAG	UNP O51933
A	410	HIS	-	EXPRESSION TAG	UNP O51933
A	411	HIS	-	EXPRESSION TAG	UNP O51933
B	1	MET	-	EXPRESSION TAG	UNP O51933
B	2	ALA	-	EXPRESSION TAG	UNP O51933
B	406	HIS	-	EXPRESSION TAG	UNP O51933
B	407	HIS	-	EXPRESSION TAG	UNP O51933
B	408	HIS	-	EXPRESSION TAG	UNP O51933
B	409	HIS	-	EXPRESSION TAG	UNP O51933
B	410	HIS	-	EXPRESSION TAG	UNP O51933
B	411	HIS	-	EXPRESSION TAG	UNP O51933
C	1	MET	-	EXPRESSION TAG	UNP O51933
C	2	ALA	-	EXPRESSION TAG	UNP O51933
C	406	HIS	-	EXPRESSION TAG	UNP O51933
C	407	HIS	-	EXPRESSION TAG	UNP O51933
C	408	HIS	-	EXPRESSION TAG	UNP O51933

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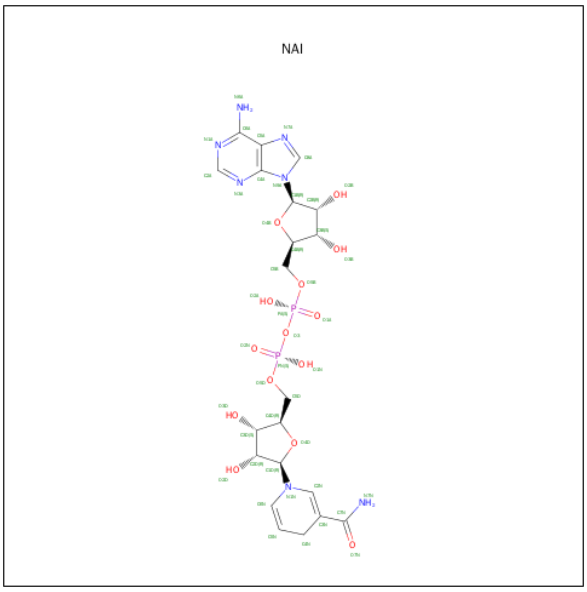
Chain	Residue	Modelled	Actual	Comment	Reference
C	409	HIS	-	EXPRESSION TAG	UNP O51933
C	410	HIS	-	EXPRESSION TAG	UNP O51933
C	411	HIS	-	EXPRESSION TAG	UNP O51933
D	1	MET	-	EXPRESSION TAG	UNP O51933
D	2	ALA	-	EXPRESSION TAG	UNP O51933
D	406	HIS	-	EXPRESSION TAG	UNP O51933
D	407	HIS	-	EXPRESSION TAG	UNP O51933
D	408	HIS	-	EXPRESSION TAG	UNP O51933
D	409	HIS	-	EXPRESSION TAG	UNP O51933
D	410	HIS	-	EXPRESSION TAG	UNP O51933
D	411	HIS	-	EXPRESSION TAG	UNP O51933

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



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		

- Molecule 3 is water.

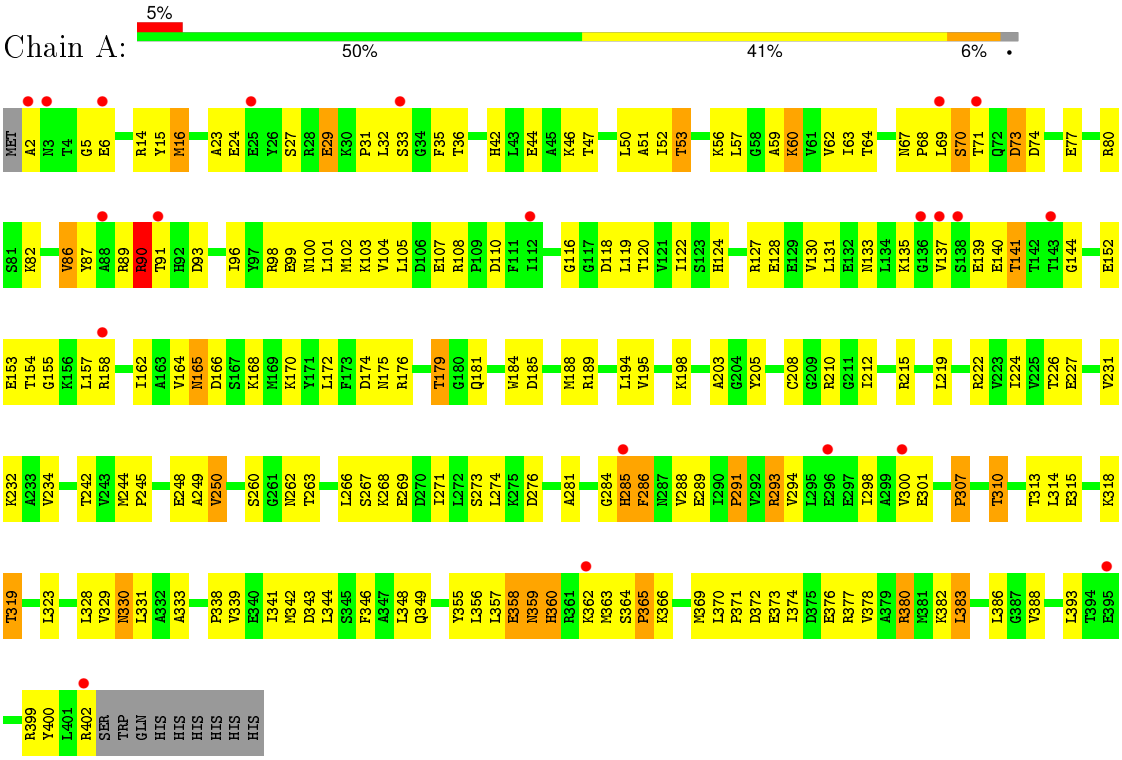
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	89	Total O 89 89	0	0
3	B	98	Total O 98 98	0	0
3	C	75	Total O 75 75	0	0
3	D	91	Total O 91 91	0	0

3 Residue-property plots (i)

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.

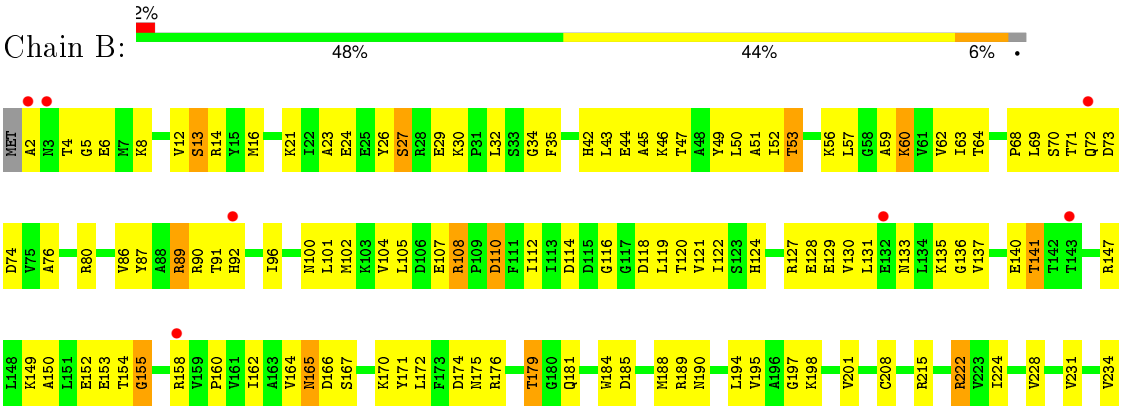
- Molecule 1: Adenosylhomocysteinase

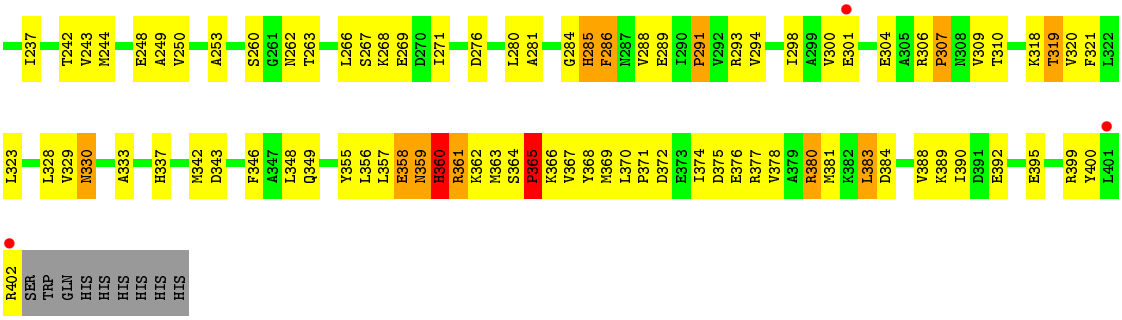
Chain A:



- Molecule 1: Adenosylhomocysteinase

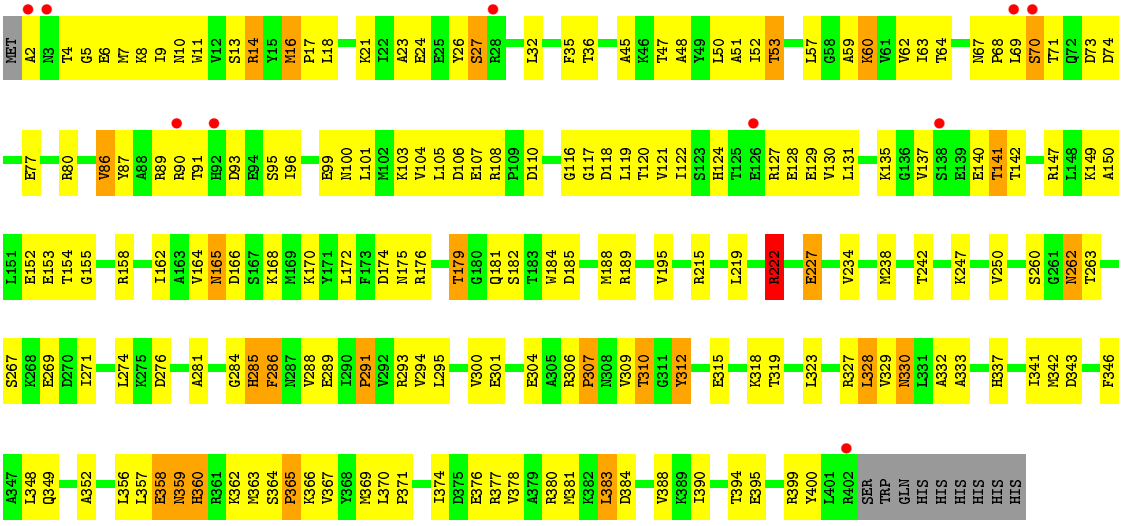
Chain B:





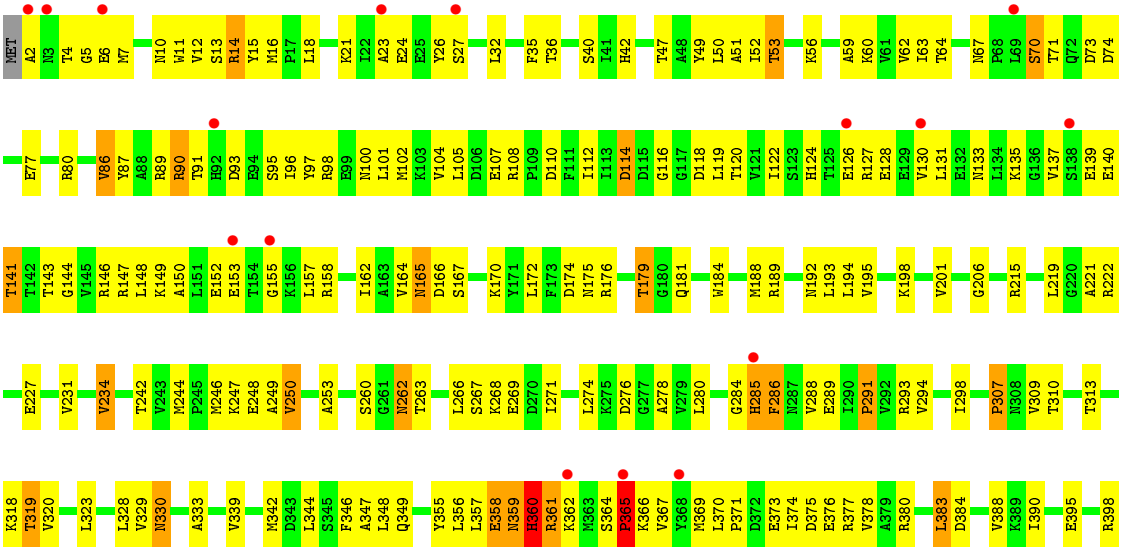
• Molecule 1: Adenosylhomocysteinase

Chain C:



• Molecule 1: Adenosylhomocysteinase

Chain D:




R399
Y400
L401
R402
SER
TRP
GLN
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	106.33Å 112.00Å 164.89Å 90.00° 103.50° 90.00°	Depositor
Resolution (Å)	25.00 – 2.85 24.80 – 2.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.85) 93.2 (24.80-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 2.84Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.229 , 0.282 0.230 , 0.283	Depositor DCC
R_{free} test set	2043 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	54.2	Xtriage
Anisotropy	0.856	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 67.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 40772 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12993	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.82 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0846e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAI

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	0.43	0/3161	0.68	0/4273
1	B	0.47	0/3161	0.72	0/4273
1	C	0.45	0/3161	0.70	1/4273 (0.0%)
1	D	0.46	0/3161	0.70	0/4273
All	All	0.46	0/12644	0.70	1/17092 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	222	ARG	N-CA-C	-5.01	97.48	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	3116	0	3190	193	0
1	B	3116	0	3190	195	0
1	C	3116	0	3190	177	0
1	D	3116	0	3190	192	0
2	A	44	0	27	2	0
2	B	44	0	27	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	44	0	27	2	0
2	D	44	0	27	2	0
3	A	89	0	0	2	0
3	B	98	0	0	4	0
3	C	75	0	0	3	0
3	D	91	0	0	1	0
All	All	12993	0	12868	724	0

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 28.

All (724) 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:C:67:ASN:HD22	1:C:70:SER:HB2	1.09	1.10
1:C:108:ARG:HH21	1:C:129:GLU:HB3	1.10	1.07
1:A:245:PRO:HG2	1:B:389:LYS:HE3	1.36	1.06
1:A:67:ASN:HD22	1:A:70:SER:HB2	1.22	1.00
1:B:361:ARG:HH11	1:B:361:ARG:HB3	1.25	0.99
1:D:67:ASN:HD22	1:D:70:SER:HB2	1.26	0.99
1:B:135:LYS:HB3	1:B:360:HIS:CE1	2.02	0.94
1:C:108:ARG:NH2	1:C:129:GLU:HB3	1.85	0.91
1:C:263:THR:HG22	1:C:288:VAL:CG2	2.00	0.90
1:C:116:GLY:H	1:C:141:THR:HG21	1.36	0.90
1:B:383:LEU:HD12	1:B:388:VAL:HB	1.52	0.89
1:C:87:TYR:HB3	1:C:100:ASN:HD22	1.37	0.87
1:A:67:ASN:O	1:A:71:THR:HG23	1.75	0.86
1:B:120:THR:HG21	1:B:137:VAL:HG11	1.56	0.86
1:C:108:ARG:HG2	1:C:130:VAL:HG12	1.57	0.86
1:A:90:ARG:HB3	1:A:90:ARG:HH11	1.38	0.86
1:C:165:ASN:HD22	1:C:166:ASP:N	1.74	0.85
1:B:165:ASN:HD22	1:B:166:ASP:N	1.75	0.85
1:A:348:LEU:HD23	1:A:378:VAL:HG21	1.57	0.85
1:A:181:GLN:HE22	1:C:195:VAL:H	1.24	0.85
1:D:285:HIS:CG	1:D:286:PHE:H	1.92	0.85
1:A:90:ARG:NH1	1:A:90:ARG:HB3	1.92	0.84
1:B:116:GLY:H	1:B:141:THR:HG21	1.40	0.84
1:A:371:PRO:HB2	1:A:373:GLU:CD	1.97	0.84
1:B:101:LEU:HD22	1:B:119:LEU:HD13	1.59	0.84
1:A:165:ASN:HD22	1:A:166:ASP:N	1.75	0.83
1:C:120:THR:HG21	1:C:137:VAL:HG11	1.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:LEU:HD12	1:A:388:VAL:HB	1.57	0.83
1:A:152:GLU:OE2	1:A:366:LYS:HG3	1.79	0.82
1:B:184:TRP:O	1:B:188:MET:HG2	1.80	0.81
1:B:268:LYS:NZ	1:B:298:ILE:HD11	1.95	0.81
1:C:7:MET:HG3	3:C:662:HOH:O	1.79	0.81
1:B:152:GLU:OE2	1:B:366:LYS:HG3	1.81	0.81
1:A:120:THR:HG21	1:A:137:VAL:HG11	1.62	0.81
1:C:35:PHE:HA	1:C:110:ASP:OD2	1.81	0.80
1:D:165:ASN:HD22	1:D:166:ASP:N	1.79	0.80
1:C:101:LEU:HD22	1:C:119:LEU:HD13	1.62	0.80
1:D:67:ASN:O	1:D:71:THR:HG23	1.82	0.79
1:C:276:ASP:OD2	1:C:318:LYS:HA	1.82	0.79
1:A:102:MET:HG3	1:A:127:ARG:HH11	1.48	0.78
1:D:174:ASP:O	1:D:179:THR:HG22	1.83	0.78
1:B:300:VAL:HG12	1:B:301:GLU:HG3	1.64	0.78
1:D:87:TYR:HB3	1:D:100:ASN:HD22	1.45	0.78
1:A:116:GLY:H	1:A:141:THR:HG21	1.49	0.78
1:C:140:GLU:HB2	1:C:349:GLN:HE21	1.47	0.78
1:A:135:LYS:HB3	1:A:360:HIS:NE2	1.99	0.78
1:B:263:THR:HG22	1:B:288:VAL:CG2	2.13	0.78
1:D:330:ASN:HD22	1:D:330:ASN:H	1.30	0.78
1:A:174:ASP:O	1:A:179:THR:HG22	1.83	0.77
1:B:181:GLN:HE22	1:D:195:VAL:H	1.32	0.77
1:A:89:ARG:HH11	1:A:89:ARG:HG2	1.49	0.77
1:C:348:LEU:HD23	1:C:378:VAL:HG21	1.65	0.77
1:C:152:GLU:OE1	1:C:367:VAL:HG12	1.84	0.77
1:A:189:ARG:HA	1:C:189:ARG:NH2	1.99	0.77
1:C:184:TRP:O	1:C:188:MET:HG2	1.85	0.77
1:B:361:ARG:HG2	3:B:673:HOH:O	1.82	0.77
1:D:116:GLY:H	1:D:141:THR:HG21	1.49	0.77
1:D:263:THR:HG22	1:D:288:VAL:CG2	2.15	0.77
1:A:135:LYS:HB3	1:A:360:HIS:CE1	2.19	0.77
1:A:67:ASN:HD22	1:A:70:SER:CB	1.98	0.77
1:D:139:GLU:OE2	1:D:144:GLY:HA3	1.85	0.77
1:D:62:VAL:HG12	1:D:104:VAL:HG12	1.66	0.76
1:C:131:LEU:HD23	1:C:131:LEU:O	1.84	0.76
1:D:268:LYS:NZ	1:D:298:ILE:HD11	2.00	0.76
1:D:348:LEU:HD23	1:D:378:VAL:HG21	1.67	0.76
1:B:359:ASN:HD22	1:B:359:ASN:N	1.84	0.76
1:B:101:LEU:O	1:B:104:VAL:HG22	1.84	0.75
1:A:80:ARG:HE	1:A:86:VAL:HG13	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:THR:HG22	1:C:60:LYS:HB2	1.68	0.75
1:D:108:ARG:HG2	1:D:130:VAL:HG12	1.69	0.74
1:A:195:VAL:H	1:C:181:GLN:HE22	1.33	0.74
1:D:276:ASP:OD2	1:D:318:LYS:HA	1.86	0.74
1:D:135:LYS:HB3	1:D:360:HIS:CE1	2.23	0.74
1:C:32:LEU:HD23	1:C:59:ALA:HB2	1.70	0.74
1:A:101:LEU:HD22	1:A:119:LEU:HD13	1.70	0.74
1:C:285:HIS:CG	1:C:286:PHE:H	2.06	0.73
1:A:285:HIS:CG	1:A:286:PHE:H	2.05	0.73
1:D:118:ASP:HA	1:D:147:ARG:HH22	1.54	0.73
1:D:131:LEU:O	1:D:131:LEU:HD23	1.87	0.73
1:C:263:THR:HG22	1:C:288:VAL:HG23	1.69	0.73
1:C:67:ASN:ND2	1:C:70:SER:HB2	1.95	0.73
1:B:285:HIS:CG	1:B:286:PHE:H	2.06	0.73
1:A:101:LEU:O	1:A:104:VAL:HG22	1.87	0.72
1:A:87:TYR:HB3	1:A:100:ASN:HD22	1.53	0.72
1:C:174:ASP:O	1:C:179:THR:HG22	1.89	0.72
1:D:67:ASN:HD22	1:D:70:SER:CB	2.01	0.72
1:D:35:PHE:HA	1:D:110:ASP:OD2	1.87	0.72
1:C:263:THR:HG22	1:C:288:VAL:HG21	1.71	0.72
1:C:67:ASN:O	1:C:71:THR:HG23	1.89	0.72
1:D:120:THR:HG21	1:D:137:VAL:HG11	1.71	0.71
1:A:195:VAL:H	1:C:181:GLN:NE2	1.86	0.71
1:C:149:LYS:HG2	1:C:367:VAL:HG11	1.72	0.71
1:D:101:LEU:HD22	1:D:119:LEU:HD13	1.72	0.71
1:B:281:ALA:HB2	1:B:323:LEU:HD12	1.72	0.71
1:B:402:ARG:O	3:B:668:HOH:O	2.08	0.70
1:A:371:PRO:HG2	1:A:374:ILE:HG13	1.73	0.70
1:B:121:VAL:HG11	1:B:147:ARG:NH2	2.06	0.70
1:A:108:ARG:HG2	1:A:130:VAL:HG12	1.73	0.70
1:A:32:LEU:HD23	1:A:59:ALA:HB2	1.74	0.70
1:A:73:ASP:OD1	1:A:90:ARG:NH2	2.25	0.69
1:B:32:LEU:HD23	1:B:59:ALA:HB2	1.74	0.69
1:D:101:LEU:O	1:D:104:VAL:HG22	1.92	0.69
1:A:35:PHE:HA	1:A:110:ASP:OD2	1.92	0.69
1:A:90:ARG:CB	1:A:90:ARG:HH11	2.06	0.69
1:C:135:LYS:HB3	1:C:360:HIS:CE1	2.27	0.69
1:B:135:LYS:HB3	1:B:360:HIS:NE2	2.08	0.69
1:D:135:LYS:HB3	1:D:360:HIS:NE2	2.07	0.69
1:C:371:PRO:HG2	1:C:374:ILE:HG13	1.74	0.68
1:D:383:LEU:HD12	1:D:388:VAL:HB	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ARG:HB3	1:B:361:ARG:NH1	2.05	0.68
1:A:181:GLN:HE22	1:C:195:VAL:N	1.90	0.68
1:C:383:LEU:HD12	1:C:388:VAL:HB	1.76	0.68
1:B:165:ASN:ND2	1:B:166:ASP:N	2.40	0.68
1:A:359:ASN:HD22	1:A:359:ASN:N	1.91	0.68
1:D:149:LYS:HG2	1:D:367:VAL:HG11	1.76	0.68
1:B:268:LYS:HZ2	1:B:298:ILE:HD11	1.56	0.68
1:C:135:LYS:HB3	1:C:360:HIS:NE2	2.08	0.68
1:B:380:ARG:HD3	3:B:675:HOH:O	1.93	0.68
1:A:310:THR:HG22	3:A:642:HOH:O	1.94	0.67
1:B:34:GLY:H	1:B:60:LYS:HZ1	1.40	0.67
1:A:300:VAL:HG12	1:A:301:GLU:HG3	1.74	0.67
1:D:285:HIS:CG	1:D:286:PHE:N	2.63	0.67
1:C:158:ARG:NH1	1:C:158:ARG:HB2	2.10	0.67
1:A:288:VAL:HG12	1:A:293:ARG:HH22	1.60	0.67
1:B:174:ASP:O	1:B:179:THR:HG22	1.94	0.67
1:C:89:ARG:C	1:C:91:THR:H	1.98	0.67
1:A:67:ASN:ND2	1:A:70:SER:HB2	2.05	0.67
1:A:181:GLN:NE2	1:C:195:VAL:H	1.92	0.67
1:D:263:THR:HG22	1:D:288:VAL:HG23	1.77	0.66
1:D:89:ARG:C	1:D:91:THR:H	1.97	0.66
1:A:36:THR:HG22	1:A:60:LYS:HB2	1.76	0.66
1:A:194:LEU:O	1:A:198:LYS:HD2	1.95	0.66
1:A:185:ASP:O	1:A:189:ARG:HG2	1.96	0.66
1:B:276:ASP:OD2	1:B:318:LYS:HA	1.94	0.66
1:D:359:ASN:HD22	1:D:359:ASN:N	1.93	0.66
1:A:263:THR:HG22	1:A:288:VAL:CG2	2.26	0.66
1:A:102:MET:HG3	1:A:127:ARG:NH1	2.11	0.66
1:B:364:SER:O	1:B:366:LYS:N	2.29	0.66
1:D:371:PRO:HG2	1:D:374:ILE:HG13	1.76	0.66
1:B:371:PRO:HG2	1:B:374:ILE:HG13	1.78	0.66
1:C:162:ILE:HG13	1:C:356:LEU:HD21	1.78	0.66
1:A:89:ARG:C	1:A:91:THR:H	1.97	0.65
1:A:330:ASN:H	1:A:330:ASN:HD22	1.44	0.65
1:D:158:ARG:HB2	1:D:158:ARG:NH1	2.11	0.65
1:B:162:ILE:HG13	1:B:356:LEU:HD21	1.79	0.65
1:B:222:ARG:HH12	1:C:222:ARG:NH1	1.94	0.65
1:A:131:LEU:HD23	1:A:131:LEU:O	1.96	0.65
1:B:87:TYR:HB3	1:B:100:ASN:HD22	1.62	0.65
1:C:121:VAL:HG11	1:C:147:ARG:NH2	2.12	0.65
1:B:101:LEU:HD22	1:B:119:LEU:CD1	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:ASN:N	1:C:359:ASN:HD22	1.94	0.64
1:A:16:MET:HB3	1:A:343:ASP:OD1	1.96	0.64
1:A:168:LYS:HG2	1:A:172:LEU:HD13	1.79	0.64
1:B:195:VAL:H	1:D:181:GLN:NE2	1.95	0.64
1:C:165:ASN:ND2	1:C:166:ASP:N	2.46	0.64
1:D:50:LEU:HD22	1:D:346:PHE:CD1	2.33	0.64
1:A:165:ASN:ND2	1:A:166:ASP:N	2.46	0.64
1:B:348:LEU:HD23	1:B:378:VAL:HG21	1.79	0.64
1:B:35:PHE:HD1	1:B:110:ASP:OD2	1.81	0.63
1:B:318:LYS:HZ2	1:B:318:LYS:HB2	1.63	0.63
1:B:165:ASN:HD22	1:B:166:ASP:H	1.47	0.63
1:C:300:VAL:HG12	1:C:301:GLU:HG3	1.81	0.63
1:B:2:ALA:O	1:B:6:GLU:HB2	1.99	0.63
1:A:195:VAL:N	1:C:181:GLN:HE22	1.97	0.62
1:B:131:LEU:O	1:B:131:LEU:HD23	1.99	0.62
1:D:102:MET:HG3	1:D:127:ARG:HH11	1.64	0.62
1:C:101:LEU:O	1:C:104:VAL:HG22	2.00	0.62
1:A:168:LYS:O	1:A:172:LEU:HD13	1.99	0.62
1:B:359:ASN:O	1:B:363:MET:HG3	2.00	0.62
1:D:194:LEU:O	1:D:198:LYS:HD2	1.99	0.62
1:B:120:THR:HG21	1:B:137:VAL:CG1	2.28	0.62
1:D:32:LEU:HD23	1:D:59:ALA:HB2	1.82	0.62
1:B:136:GLY:HA3	1:B:356:LEU:HD13	1.81	0.62
1:D:285:HIS:CD2	1:D:286:PHE:H	2.17	0.61
1:D:184:TRP:O	1:D:188:MET:HG2	2.01	0.61
1:A:99:GLU:HG3	1:A:103:LYS:NZ	2.15	0.61
1:C:364:SER:O	1:C:366:LYS:N	2.33	0.61
1:D:40:SER:HG	1:D:97:TYR:HH	1.48	0.61
1:B:175:ASN:O	1:B:179:THR:CG2	2.49	0.61
1:D:23:ALA:O	1:D:27:SER:HB2	2.00	0.61
1:D:105:LEU:HD22	1:D:130:VAL:HG21	1.83	0.61
1:D:364:SER:O	1:D:366:LYS:N	2.34	0.61
1:C:185:ASP:O	1:C:189:ARG:HG2	2.00	0.60
1:D:374:ILE:O	1:D:378:VAL:HG23	2.02	0.60
1:C:327:ARG:NH2	1:C:332:ALA:HB1	2.16	0.60
1:A:172:LEU:O	1:A:176:ARG:HB3	2.01	0.60
1:A:101:LEU:HD22	1:A:119:LEU:CD1	2.32	0.60
1:C:140:GLU:HB2	1:C:349:GLN:NE2	2.17	0.60
1:A:23:ALA:O	1:A:27:SER:HB2	2.02	0.60
1:A:120:THR:HG21	1:A:137:VAL:CG1	2.29	0.59
1:B:263:THR:HG22	1:B:288:VAL:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ASP:HB3	1:D:135:LYS:HD2	1.84	0.59
1:C:175:ASN:O	1:C:179:THR:HG23	2.02	0.59
1:D:170:LYS:HG2	1:D:348:LEU:CD1	2.32	0.59
1:B:175:ASN:O	1:B:179:THR:HG23	2.01	0.59
1:D:91:THR:C	1:D:93:ASP:H	2.05	0.59
1:B:330:ASN:HD22	1:B:330:ASN:H	1.49	0.59
1:B:267:SER:O	1:B:271:ILE:HG13	2.02	0.59
1:D:140:GLU:HB2	1:D:349:GLN:NE2	2.18	0.59
1:D:36:THR:HG22	1:D:60:LYS:HB2	1.84	0.59
1:A:118:ASP:O	1:A:122:ILE:HG12	2.02	0.59
1:C:120:THR:HG21	1:C:137:VAL:CG1	2.31	0.59
1:A:364:SER:O	1:A:366:LYS:N	2.36	0.59
1:B:195:VAL:H	1:D:181:GLN:HE22	1.49	0.59
1:B:194:LEU:O	1:B:198:LYS:HD2	2.03	0.59
1:C:172:LEU:O	1:C:176:ARG:HB3	2.02	0.58
1:C:131:LEU:HD11	1:C:158:ARG:HH12	1.69	0.58
1:C:394:THR:HG22	3:C:648:HOH:O	2.04	0.58
1:C:260:SER:O	1:C:289:GLU:OE2	2.22	0.58
1:C:165:ASN:HD22	1:C:166:ASP:H	1.52	0.58
1:A:62:VAL:HG12	1:A:104:VAL:HG12	1.86	0.58
1:A:288:VAL:HG12	1:A:293:ARG:NH2	2.18	0.58
1:B:222:ARG:NH1	1:C:222:ARG:NH1	2.52	0.58
1:A:128:GLU:HA	1:A:131:LEU:HB2	1.86	0.58
1:C:2:ALA:O	1:C:6:GLU:HB2	2.04	0.58
1:D:51:ALA:CB	1:D:63:ILE:HD11	2.33	0.58
1:D:73:ASP:O	1:D:77:GLU:HG2	2.03	0.58
1:D:165:ASN:ND2	1:D:166:ASP:N	2.50	0.58
1:B:23:ALA:O	1:B:27:SER:HB2	2.04	0.58
1:B:383:LEU:HD12	1:B:388:VAL:CB	2.31	0.58
1:B:118:ASP:O	1:B:122:ILE:HG12	2.04	0.58
1:B:268:LYS:HZ3	1:B:298:ILE:HD11	1.67	0.57
1:A:260:SER:O	1:A:289:GLU:OE1	2.21	0.57
1:A:80:ARG:NE	1:A:86:VAL:HG13	2.19	0.57
1:C:91:THR:C	1:C:93:ASP:H	2.07	0.57
1:C:158:ARG:HH11	1:C:158:ARG:HB2	1.69	0.57
1:C:118:ASP:O	1:C:122:ILE:HG12	2.04	0.57
1:B:280:LEU:HD11	1:B:320:VAL:HG11	1.87	0.57
1:C:267:SER:OG	1:C:269:GLU:HB2	2.04	0.57
1:A:276:ASP:OD2	1:A:318:LYS:HA	2.05	0.57
1:D:263:THR:HG22	1:D:288:VAL:HG21	1.85	0.57
1:C:135:LYS:HD3	1:C:360:HIS:NE2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:NH1	1:A:89:ARG:HG2	2.17	0.56
1:A:108:ARG:CG	1:A:130:VAL:HG12	2.34	0.56
1:D:285:HIS:CD2	1:D:286:PHE:N	2.72	0.56
1:A:285:HIS:CG	1:A:286:PHE:N	2.73	0.56
1:B:23:ALA:HB2	1:B:53:THR:HG22	1.85	0.56
1:C:51:ALA:CB	1:C:63:ILE:HD11	2.35	0.56
1:C:164:VAL:O	1:C:170:LYS:HG3	2.05	0.56
1:A:184:TRP:O	1:A:188:MET:HG2	2.04	0.56
1:A:91:THR:C	1:A:93:ASP:H	2.09	0.56
1:D:152:GLU:OE2	1:D:366:LYS:HG3	2.06	0.56
1:D:158:ARG:HH11	1:D:158:ARG:HB2	1.70	0.56
1:A:285:HIS:CD2	1:A:286:PHE:H	2.24	0.56
1:C:175:ASN:O	1:C:179:THR:CG2	2.53	0.56
1:A:371:PRO:HB2	1:A:373:GLU:OE1	2.05	0.56
1:D:120:THR:HG21	1:D:137:VAL:CG1	2.36	0.56
1:A:263:THR:HG23	1:B:400:TYR:CE2	2.41	0.56
1:A:348:LEU:CD2	1:A:378:VAL:HG21	2.32	0.55
1:A:266:LEU:O	1:A:291:PRO:HG3	2.06	0.55
1:B:267:SER:OG	1:B:269:GLU:HB2	2.07	0.55
1:B:185:ASP:O	1:B:189:ARG:HG2	2.06	0.55
1:A:63:ILE:HG22	1:A:64:THR:N	2.22	0.55
1:C:185:ASP:OD2	1:C:189:ARG:NH2	2.39	0.55
1:A:2:ALA:O	1:A:6:GLU:HB2	2.07	0.55
1:C:23:ALA:O	1:C:27:SER:HB2	2.06	0.55
1:A:162:ILE:HD11	1:A:355:TYR:HD2	1.72	0.55
1:D:2:ALA:O	1:D:6:GLU:HB2	2.06	0.55
1:B:284:GLY:HA3	1:B:289:GLU:OE2	2.07	0.55
1:D:67:ASN:ND2	1:D:70:SER:HB2	2.10	0.55
1:C:260:SER:O	1:C:289:GLU:CD	2.45	0.55
1:C:17:PRO:HG2	1:C:18:LEU:H	1.72	0.55
1:A:260:SER:O	1:A:289:GLU:CD	2.46	0.55
1:C:168:LYS:O	1:C:172:LEU:HD13	2.07	0.54
1:B:108:ARG:HG3	1:B:130:VAL:HG12	1.89	0.54
1:D:87:TYR:CB	1:D:100:ASN:HD22	2.18	0.54
1:D:330:ASN:HD21	2:D:500:NAI:H72N	1.55	0.54
1:C:89:ARG:O	1:C:91:THR:HG23	2.06	0.54
1:C:285:HIS:CD2	1:C:286:PHE:H	2.25	0.54
1:A:52:ILE:O	1:A:56:LYS:HG3	2.07	0.54
1:A:158:ARG:HA	1:A:365:PRO:HB3	1.90	0.54
1:A:400:TYR:CE2	1:B:263:THR:HG23	2.43	0.54
1:B:189:ARG:HA	1:D:189:ARG:NH2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:ARG:HD3	1:D:90:ARG:NH1	2.23	0.54
1:A:315:GLU:H	1:A:315:GLU:CD	2.10	0.54
1:A:89:ARG:O	1:A:91:THR:HG23	2.07	0.53
1:B:285:HIS:CG	1:B:286:PHE:N	2.76	0.53
1:B:128:GLU:HA	1:B:131:LEU:HB2	1.90	0.53
1:B:21:LYS:NZ	1:B:384:ASP:HB3	2.23	0.53
1:A:319:THR:HG21	1:C:14:ARG:NH2	2.23	0.53
1:D:4:THR:HA	1:D:7:MET:HE2	1.89	0.53
1:C:62:VAL:HG12	1:C:104:VAL:HG12	1.89	0.53
1:B:263:THR:HG22	1:B:288:VAL:HG21	1.90	0.53
1:D:158:ARG:HA	1:D:365:PRO:HB3	1.90	0.53
1:D:152:GLU:OE2	1:D:367:VAL:HG12	2.08	0.53
1:A:165:ASN:C	1:A:165:ASN:ND2	2.61	0.53
1:A:32:LEU:HD12	1:A:357:LEU:HD22	1.90	0.53
1:B:133:ASN:O	1:B:135:LYS:HG3	2.09	0.53
1:B:165:ASN:C	1:B:165:ASN:ND2	2.62	0.53
1:A:383:LEU:HD12	1:A:388:VAL:CB	2.33	0.53
1:D:87:TYR:HB3	1:D:100:ASN:ND2	2.20	0.53
1:C:168:LYS:HG2	1:C:172:LEU:HD13	1.91	0.53
1:A:80:ARG:HG3	1:A:86:VAL:CG1	2.39	0.53
1:B:285:HIS:CD2	1:B:286:PHE:H	2.26	0.53
1:D:42:HIS:O	1:D:47:THR:HG21	2.08	0.52
1:B:121:VAL:HG11	1:B:147:ARG:HH22	1.74	0.52
1:C:80:ARG:HG3	1:C:86:VAL:CG1	2.39	0.52
1:B:116:GLY:H	1:B:141:THR:CG2	2.17	0.52
1:D:105:LEU:C	1:D:107:GLU:H	2.13	0.52
1:B:370:LEU:HD12	1:B:371:PRO:HD2	1.91	0.52
1:C:400:TYR:CE2	1:D:263:THR:HG23	2.44	0.52
1:B:91:THR:HG21	1:B:96:ILE:HG12	1.92	0.52
1:B:105:LEU:C	1:B:107:GLU:H	2.13	0.52
1:C:285:HIS:CG	1:C:286:PHE:N	2.77	0.52
1:A:268:LYS:HE3	1:A:298:ILE:CD1	2.40	0.52
1:B:358:GLU:HG3	1:B:359:ASN:HD22	1.74	0.52
1:D:165:ASN:HD22	1:D:166:ASP:H	1.56	0.52
1:A:285:HIS:CD2	1:A:286:PHE:N	2.78	0.52
1:D:89:ARG:HB3	1:D:91:THR:CG2	2.40	0.52
1:D:102:MET:HG3	1:D:127:ARG:NH1	2.24	0.52
1:B:231:VAL:O	1:B:234:VAL:HG12	2.10	0.52
1:B:158:ARG:HA	1:B:365:PRO:HB3	1.90	0.52
1:C:158:ARG:HA	1:C:365:PRO:HB3	1.91	0.52
1:B:363:MET:HB3	1:B:368:TYR:HE2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASN:C	1:A:165:ASN:HD22	2.12	0.52
1:C:93:ASP:OD2	1:C:95:SER:HB2	2.10	0.52
1:A:164:VAL:O	1:A:170:LYS:HG3	2.10	0.52
1:C:128:GLU:HA	1:C:131:LEU:HB2	1.91	0.52
1:D:5:GLY:HA3	1:D:74:ASP:O	2.10	0.52
1:D:268:LYS:CE	1:D:298:ILE:HD11	2.41	0.51
1:B:35:PHE:HA	1:B:110:ASP:OD2	2.11	0.51
1:D:118:ASP:O	1:D:122:ILE:HG12	2.10	0.51
1:A:105:LEU:C	1:A:107:GLU:H	2.13	0.51
1:D:23:ALA:HB2	1:D:53:THR:HG22	1.91	0.51
1:B:293:ARG:HG3	1:B:293:ARG:NH1	2.25	0.51
1:A:263:THR:HG22	1:A:288:VAL:HG23	1.91	0.51
1:A:267:SER:OG	1:A:269:GLU:HB2	2.10	0.51
1:A:329:VAL:O	1:A:333:ALA:HB3	2.09	0.51
1:C:16:MET:HB3	1:C:343:ASP:OD1	2.10	0.51
1:B:304:GLU:HA	1:B:304:GLU:OE2	2.10	0.51
1:D:188:MET:HE1	1:D:219:LEU:HD13	1.93	0.51
1:B:361:ARG:HH11	1:B:361:ARG:CB	2.12	0.51
1:A:140:GLU:HA	1:A:164:VAL:HG22	1.92	0.51
1:A:376:GLU:OE1	1:A:380:ARG:NH1	2.44	0.51
1:D:293:ARG:HG3	1:D:293:ARG:HH11	1.76	0.51
1:C:68:PRO:HG2	1:C:69:LEU:HG	1.93	0.51
1:A:51:ALA:CB	1:A:63:ILE:HD11	2.41	0.51
1:D:358:GLU:C	1:D:360:HIS:H	2.14	0.51
1:D:309:VAL:HG22	1:D:323:LEU:HD23	1.93	0.51
1:D:80:ARG:HG3	1:D:86:VAL:CG1	2.41	0.51
1:A:382:LYS:HE3	1:A:386:LEU:HD11	1.93	0.51
1:D:395:GLU:OE1	1:D:395:GLU:HA	2.10	0.51
1:C:165:ASN:C	1:C:165:ASN:ND2	2.64	0.50
1:C:170:LYS:HG2	1:C:348:LEU:CD1	2.42	0.50
1:A:110:ASP:HB3	1:A:135:LYS:HD2	1.93	0.50
1:D:149:LYS:HZ1	1:D:367:VAL:HG13	1.77	0.50
1:C:105:LEU:C	1:C:107:GLU:H	2.14	0.50
1:D:124:HIS:NE2	1:D:157:LEU:HD12	2.27	0.50
1:A:203:ALA:HA	1:A:226:THR:OG1	2.10	0.50
1:C:304:GLU:HA	1:C:304:GLU:OE2	2.11	0.50
1:B:164:VAL:O	1:B:170:LYS:HG3	2.12	0.50
1:B:152:GLU:OE1	1:B:367:VAL:HG12	2.12	0.50
1:D:359:ASN:N	1:D:359:ASN:ND2	2.59	0.50
1:B:359:ASN:ND2	1:B:359:ASN:N	2.54	0.50
1:B:195:VAL:N	1:D:181:GLN:HE22	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ASN:O	1:D:179:THR:HG23	2.11	0.50
1:A:358:GLU:C	1:A:360:HIS:H	2.14	0.50
1:B:51:ALA:CB	1:B:63:ILE:HD11	2.41	0.50
1:B:358:GLU:C	1:B:360:HIS:H	2.15	0.50
1:D:284:GLY:HA3	1:D:289:GLU:OE2	2.12	0.50
1:A:73:ASP:CG	1:A:90:ARG:NH2	2.64	0.50
1:C:281:ALA:HB2	1:C:323:LEU:HD12	1.92	0.50
1:C:108:ARG:CG	1:C:130:VAL:HG12	2.36	0.50
1:B:149:LYS:HG2	1:B:367:VAL:HG11	1.93	0.50
1:D:32:LEU:HD12	1:D:357:LEU:HD22	1.94	0.50
1:D:267:SER:OG	1:D:269:GLU:HB2	2.12	0.50
1:C:89:ARG:HB3	1:C:91:THR:CG2	2.42	0.50
1:A:53:THR:O	1:A:57:LEU:HG	2.12	0.50
1:B:197:GLY:HA3	1:C:238:MET:CE	2.42	0.50
1:D:266:LEU:O	1:D:291:PRO:HG3	2.12	0.49
1:A:245:PRO:CG	1:B:389:LYS:HG3	2.42	0.49
1:D:356:LEU:O	1:D:360:HIS:HA	2.11	0.49
1:C:291:PRO:HB2	1:C:294:VAL:CG2	2.42	0.49
1:A:281:ALA:HB2	1:A:323:LEU:HD12	1.94	0.49
1:A:170:LYS:HG2	1:A:348:LEU:CD1	2.42	0.49
1:C:68:PRO:HG2	1:C:69:LEU:H	1.77	0.49
1:D:313:THR:HA	1:D:319:THR:HB	1.94	0.49
1:D:172:LEU:O	1:D:176:ARG:HB3	2.11	0.49
1:C:358:GLU:C	1:C:360:HIS:H	2.15	0.49
1:B:34:GLY:N	1:B:60:LYS:HZ1	2.07	0.49
1:B:266:LEU:O	1:B:291:PRO:HG3	2.12	0.49
1:C:47:THR:O	1:C:50:LEU:HB3	2.13	0.49
1:B:34:GLY:H	1:B:60:LYS:NZ	2.10	0.49
1:A:268:LYS:HE3	1:A:298:ILE:HD11	1.94	0.49
1:A:139:GLU:OE1	1:A:139:GLU:HA	2.13	0.49
1:A:175:ASN:O	1:A:179:THR:HG23	2.12	0.49
1:C:150:ALA:O	1:C:154:THR:HG23	2.12	0.49
1:C:330:ASN:N	1:C:330:ASN:HD22	2.11	0.49
1:D:128:GLU:HA	1:D:131:LEU:HB2	1.93	0.49
1:D:89:ARG:C	1:D:91:THR:N	2.66	0.49
1:D:260:SER:O	1:D:289:GLU:CD	2.51	0.49
1:A:107:GLU:HA	1:A:107:GLU:OE1	2.12	0.49
1:B:395:GLU:O	1:B:399:ARG:HB2	2.13	0.49
1:C:377:ARG:O	1:C:381:MET:HG3	2.13	0.49
1:C:140:GLU:HA	1:C:164:VAL:HG22	1.95	0.48
1:D:63:ILE:HG22	1:D:64:THR:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:LYS:HB2	1:C:318:LYS:HZ2	1.78	0.48
1:D:47:THR:O	1:D:50:LEU:HB3	2.13	0.48
1:B:90:ARG:HH11	1:B:90:ARG:HG2	1.78	0.48
1:B:127:ARG:HA	1:B:129:GLU:OE2	2.14	0.48
1:D:140:GLU:HA	1:D:164:VAL:HG22	1.94	0.48
1:D:11:TRP:O	1:D:14:ARG:HG2	2.13	0.48
1:A:89:ARG:C	1:A:91:THR:N	2.66	0.48
1:C:9:ILE:O	1:C:13:SER:HB3	2.13	0.48
1:A:96:ILE:O	1:A:100:ASN:OD1	2.32	0.48
1:B:370:LEU:HD11	1:B:374:ILE:HD12	1.96	0.48
1:A:139:GLU:OE2	1:A:144:GLY:HA3	2.14	0.48
1:A:68:PRO:HG2	1:A:69:LEU:H	1.79	0.48
1:D:133:ASN:O	1:D:135:LYS:HG3	2.13	0.48
1:D:10:ASN:O	1:D:14:ARG:HD2	2.13	0.48
1:C:153:GLU:HG3	1:C:154:THR:HG23	1.96	0.48
1:C:250:VAL:HG22	1:C:274:LEU:HG	1.96	0.48
1:C:32:LEU:HB3	1:C:59:ALA:HB2	1.95	0.48
1:C:330:ASN:H	1:C:330:ASN:HD22	1.61	0.48
1:B:43:LEU:HD23	1:B:69:LEU:CD1	2.43	0.48
1:A:231:VAL:O	1:A:234:VAL:HG12	2.14	0.48
1:B:358:GLU:HG3	1:B:359:ASN:ND2	2.29	0.47
1:B:356:LEU:O	1:B:360:HIS:HA	2.14	0.47
1:B:35:PHE:CD1	1:B:110:ASP:OD2	2.64	0.47
1:D:165:ASN:C	1:D:165:ASN:ND2	2.67	0.47
1:D:330:ASN:ND2	1:D:330:ASN:H	2.06	0.47
1:D:268:LYS:HZ2	1:D:298:ILE:HD11	1.79	0.47
1:B:16:MET:HB3	1:B:343:ASP:OD1	2.14	0.47
1:A:42:HIS:HD2	1:A:44:GLU:CG	2.27	0.47
1:B:52:ILE:O	1:B:56:LYS:HG3	2.14	0.47
1:A:227:GLU:O	1:B:390:ILE:HB	2.14	0.47
1:B:160:PRO:HB2	1:B:363:MET:HE3	1.96	0.47
1:A:87:TYR:CE2	1:A:103:LYS:HB3	2.49	0.47
1:C:89:ARG:C	1:C:91:THR:N	2.67	0.47
1:C:91:THR:HB	1:C:96:ILE:HB	1.95	0.47
1:A:244:MET:HG3	1:A:249:ALA:HB2	1.97	0.47
1:B:318:LYS:HB2	1:B:318:LYS:NZ	2.29	0.47
1:B:189:ARG:HG3	1:B:190:ASN:ND2	2.29	0.47
1:A:47:THR:O	1:A:50:LEU:HB3	2.15	0.47
1:D:329:VAL:O	1:D:333:ALA:HB3	2.14	0.47
1:B:361:ARG:O	1:B:363:MET:N	2.48	0.47
1:C:263:THR:HG23	1:D:400:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASN:HD22	1:A:166:ASP:H	1.58	0.47
1:A:356:LEU:O	1:A:360:HIS:HA	2.15	0.47
1:D:124:HIS:HA	1:D:131:LEU:HD12	1.97	0.47
1:C:359:ASN:O	1:C:363:MET:HG3	2.14	0.47
1:D:293:ARG:HG3	1:D:293:ARG:NH1	2.28	0.47
1:C:21:LYS:NZ	1:C:384:ASP:HB3	2.29	0.47
1:C:104:VAL:HG21	1:C:119:LEU:HD21	1.96	0.47
1:C:370:LEU:HD12	1:C:371:PRO:HD2	1.97	0.47
1:A:89:ARG:HB3	1:A:91:THR:CG2	2.45	0.47
1:B:44:GLU:OE2	1:B:46:LYS:HB2	2.15	0.47
1:D:89:ARG:O	1:D:91:THR:HG23	2.15	0.46
1:A:284:GLY:HA3	1:A:289:GLU:OE2	2.15	0.46
1:B:71:THR:HG22	1:B:90:ARG:HD3	1.97	0.46
1:C:395:GLU:HB3	1:C:399:ARG:NH2	2.30	0.46
1:C:395:GLU:HA	1:C:395:GLU:OE2	2.14	0.46
1:C:306:ARG:HB2	1:C:309:VAL:CG2	2.45	0.46
1:B:110:ASP:OD1	1:B:110:ASP:N	2.48	0.46
1:B:140:GLU:OE2	1:B:170:LYS:NZ	2.38	0.46
1:D:118:ASP:HA	1:D:147:ARG:NH2	2.28	0.46
1:B:189:ARG:NH2	1:D:189:ARG:HA	2.29	0.46
1:A:393:LEU:HD13	1:B:228:VAL:HG11	1.97	0.46
1:A:67:ASN:ND2	1:A:70:SER:C	2.69	0.46
1:D:165:ASN:C	1:D:165:ASN:HD22	2.17	0.46
1:A:116:GLY:H	1:A:141:THR:CG2	2.26	0.46
1:B:285:HIS:CD2	1:B:286:PHE:N	2.84	0.46
1:A:359:ASN:O	1:A:363:MET:HG3	2.16	0.46
1:A:5:GLY:HA3	1:A:74:ASP:O	2.16	0.46
1:A:124:HIS:NE2	1:A:157:LEU:HD12	2.31	0.46
1:D:98:ARG:NH2	1:D:126:GLU:OE1	2.46	0.46
1:D:32:LEU:HB3	1:D:59:ALA:HB2	1.97	0.46
1:A:330:ASN:N	1:A:330:ASN:HD22	2.11	0.46
1:B:291:PRO:HB2	1:B:294:VAL:CG2	2.45	0.46
1:D:51:ALA:HB2	1:D:63:ILE:HD11	1.96	0.46
1:C:63:ILE:HG22	1:C:64:THR:N	2.31	0.46
1:B:377:ARG:O	1:B:381:MET:HG3	2.16	0.46
1:D:91:THR:HB	1:D:96:ILE:HB	1.97	0.46
1:D:15:TYR:HB2	1:D:339:VAL:HG11	1.97	0.46
1:B:380:ARG:NH2	1:B:392:GLU:OE2	2.49	0.46
1:A:42:HIS:CD2	1:A:44:GLU:HG2	2.50	0.46
1:C:51:ALA:HB2	1:C:63:ILE:HD11	1.97	0.46
1:B:319:THR:HG21	1:D:14:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:GLU:HG3	1:B:154:THR:HG23	1.97	0.46
1:C:352:ALA:O	1:C:356:LEU:HG	2.15	0.46
1:A:359:ASN:N	1:A:359:ASN:ND2	2.60	0.45
1:B:171:TYR:O	1:B:175:ASN:HB2	2.15	0.45
1:A:128:GLU:OE1	1:A:128:GLU:N	2.49	0.45
1:C:16:MET:HE2	1:C:343:ASP:HB2	1.98	0.45
1:A:29:GLU:OE1	1:A:31:PRO:HB3	2.16	0.45
1:A:399:ARG:CG	1:A:402:ARG:NH1	2.80	0.45
1:D:268:LYS:HE3	1:D:298:ILE:HD11	1.98	0.45
1:A:188:MET:HE1	1:A:219:LEU:HD13	1.98	0.45
1:B:293:ARG:HG3	1:B:293:ARG:HH11	1.81	0.45
1:A:42:HIS:O	1:A:47:THR:HG21	2.16	0.45
1:C:99:GLU:OE2	1:C:103:LYS:NZ	2.32	0.45
1:D:67:ASN:HB2	1:D:70:SER:OG	2.16	0.45
1:C:188:MET:HE1	1:C:219:LEU:HD13	1.99	0.45
1:B:63:ILE:HG22	1:B:64:THR:N	2.31	0.45
1:A:42:HIS:HD2	1:A:44:GLU:HG2	1.81	0.45
1:D:206:GLY:HA3	2:D:500:NAI:O5B	2.17	0.45
1:D:162:ILE:HD11	1:D:355:TYR:HD2	1.81	0.45
1:C:32:LEU:HD23	1:C:59:ALA:CB	2.44	0.45
1:B:158:ARG:HB2	1:B:158:ARG:NH1	2.30	0.45
1:B:150:ALA:O	1:B:154:THR:HG23	2.16	0.45
1:B:76:ALA:O	1:B:80:ARG:HG3	2.16	0.45
1:C:101:LEU:HD22	1:C:119:LEU:CD1	2.39	0.45
1:B:357:LEU:O	1:B:360:HIS:HB2	2.16	0.45
1:A:189:ARG:HA	1:C:189:ARG:HH21	1.77	0.45
1:D:139:GLU:HA	1:D:139:GLU:OE1	2.17	0.45
1:D:246:MET:SD	1:D:266:LEU:HD21	2.56	0.45
1:C:284:GLY:O	1:C:328:LEU:HD13	2.16	0.45
1:B:167:SER:HB2	1:B:375:ASP:OD1	2.17	0.45
1:C:5:GLY:HA3	1:C:74:ASP:O	2.17	0.45
1:B:162:ILE:HD11	1:B:355:TYR:HD2	1.82	0.45
1:A:260:SER:O	1:A:289:GLU:OE2	2.34	0.45
1:B:237:ILE:HD11	1:B:243:VAL:HB	1.99	0.45
1:C:306:ARG:HB2	1:C:309:VAL:HG23	1.98	0.45
1:C:4:THR:HG22	1:C:8:LYS:HE3	1.97	0.45
1:A:89:ARG:CG	1:A:89:ARG:NH1	2.80	0.45
1:D:97:TYR:OH	1:D:101:LEU:HD21	2.17	0.45
1:D:89:ARG:HB3	1:D:91:THR:HG23	1.98	0.45
1:C:23:ALA:HB2	1:C:53:THR:HG22	1.97	0.45
1:C:285:HIS:CD2	1:C:286:PHE:N	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ILE:HD11	1:A:291:PRO:HG2	1.99	0.44
1:A:68:PRO:HG2	1:A:69:LEU:HG	1.98	0.44
1:C:390:ILE:HB	1:D:227:GLU:O	2.17	0.44
1:A:87:TYR:CZ	1:A:103:LYS:HB3	2.53	0.44
1:D:371:PRO:HB2	1:D:373:GLU:HG2	1.99	0.44
1:B:68:PRO:HA	1:B:89:ARG:HG3	1.98	0.44
1:C:7:MET:CG	3:C:662:HOH:O	2.53	0.44
1:C:47:THR:HA	1:C:346:PHE:CZ	2.51	0.44
1:B:90:ARG:NH1	1:B:90:ARG:HG2	2.31	0.44
1:D:26:TYR:OH	1:D:377:ARG:NH1	2.51	0.44
1:B:363:MET:HB2	1:B:363:MET:HE2	1.70	0.44
1:C:116:GLY:H	1:C:141:THR:CG2	2.18	0.44
1:B:164:VAL:HG12	1:B:370:LEU:HD13	2.00	0.44
1:B:370:LEU:CD1	1:B:374:ILE:HD12	2.47	0.44
1:B:179:THR:HG21	1:B:208:CYS:SG	2.56	0.44
1:D:193:LEU:HB3	1:D:198:LYS:NZ	2.32	0.44
1:A:346:PHE:O	1:A:349:GLN:N	2.51	0.44
1:D:298:ILE:HA	1:D:298:ILE:HD13	1.77	0.44
1:A:128:GLU:HG3	1:A:131:LEU:HD13	2.00	0.44
1:D:36:THR:HG22	1:D:60:LYS:HD3	2.00	0.44
1:A:52:ILE:HG22	1:A:56:LYS:HE3	1.98	0.44
1:D:116:GLY:H	1:D:141:THR:CG2	2.26	0.44
1:D:170:LYS:HG2	1:D:348:LEU:HD12	1.99	0.44
1:C:359:ASN:N	1:C:359:ASN:ND2	2.64	0.44
1:C:284:GLY:O	1:C:328:LEU:CD1	2.66	0.44
1:C:310:THR:HG1	1:C:312:TYR:HE1	1.63	0.44
1:D:164:VAL:O	1:D:170:LYS:HG3	2.17	0.44
1:B:185:ASP:OD2	1:B:189:ARG:NH2	2.46	0.44
1:D:291:PRO:HB2	1:D:294:VAL:HB	2.00	0.44
1:D:15:TYR:O	1:D:339:VAL:HG12	2.18	0.44
1:A:250:VAL:HG13	1:A:273:SER:HB2	1.99	0.44
1:D:93:ASP:OD2	1:D:95:SER:HB2	2.17	0.44
1:B:124:HIS:HA	1:B:131:LEU:HD12	2.00	0.44
1:B:329:VAL:O	1:B:333:ALA:HB3	2.18	0.44
1:C:35:PHE:CA	1:C:110:ASP:OD2	2.59	0.44
1:A:32:LEU:HB3	1:A:59:ALA:HB2	2.00	0.44
1:C:356:LEU:O	1:C:360:HIS:HA	2.17	0.44
1:A:291:PRO:HB2	1:A:294:VAL:HB	2.00	0.44
1:D:271:ILE:HD11	1:D:291:PRO:HG2	1.99	0.44
1:D:201:VAL:CG2	1:D:253:ALA:HB2	2.48	0.44
2:A:500:NAI:H2D	2:A:500:NAI:H6N	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:ARG:HA	1:D:101:LEU:HD12	1.99	0.43
1:D:369:MET:O	1:D:370:LEU:C	2.56	0.43
1:A:77:GLU:OE2	1:A:80:ARG:NH1	2.51	0.43
1:B:124:HIS:HA	1:B:131:LEU:CD1	2.48	0.43
1:A:338:PRO:HB2	1:A:341:ILE:HG12	2.00	0.43
1:A:313:THR:HA	1:A:319:THR:HB	2.00	0.43
1:C:329:VAL:O	1:C:333:ALA:HB3	2.18	0.43
1:D:361:ARG:HG2	1:D:361:ARG:H	1.39	0.43
1:A:153:GLU:HG3	1:A:154:THR:HG23	1.99	0.43
1:B:32:LEU:HD12	1:B:357:LEU:HD22	1.99	0.43
1:B:120:THR:CG2	1:B:137:VAL:HG21	2.48	0.43
1:B:13:SER:HB2	1:B:49:TYR:CE1	2.52	0.43
1:D:167:SER:HB2	1:D:375:ASP:OD1	2.18	0.43
1:D:18:LEU:HD12	1:D:344:LEU:HA	1.99	0.43
1:D:21:LYS:NZ	1:D:384:ASP:HB3	2.33	0.43
1:B:244:MET:HG3	1:B:249:ALA:HB2	1.99	0.43
1:B:330:ASN:HD21	2:B:500:NAI:H72N	1.65	0.43
1:D:231:VAL:O	1:D:234:VAL:HG12	2.18	0.43
1:B:42:HIS:O	1:B:47:THR:HG21	2.18	0.43
1:B:5:GLY:HA3	1:B:74:ASP:O	2.18	0.43
1:D:52:ILE:O	1:D:56:LYS:HG3	2.19	0.43
1:A:91:THR:HB	1:A:96:ILE:HB	2.00	0.43
1:C:117:GLY:O	1:C:121:VAL:HG23	2.18	0.43
1:C:369:MET:O	1:C:370:LEU:C	2.57	0.43
1:D:91:THR:C	1:D:93:ASP:N	2.72	0.43
1:B:69:LEU:HD22	1:B:73:ASP:OD1	2.19	0.43
1:C:8:LYS:O	1:C:45:ALA:HB1	2.19	0.43
1:D:278:ALA:O	1:D:320:VAL:HG13	2.19	0.43
1:D:12:VAL:CG1	1:D:16:MET:HE3	2.48	0.43
1:D:112:ILE:CG2	1:D:114:ASP:HB3	2.48	0.43
1:D:148:LEU:HD23	1:D:148:LEU:N	2.33	0.43
1:B:49:TYR:O	1:B:53:THR:OG1	2.36	0.43
1:B:260:SER:O	1:B:289:GLU:CD	2.57	0.43
1:B:102:MET:HG3	1:B:127:ARG:NH1	2.34	0.43
1:D:280:LEU:HD11	1:D:320:VAL:HG11	2.01	0.43
1:D:383:LEU:HD13	1:D:383:LEU:HA	1.89	0.42
1:A:399:ARG:HG2	1:A:402:ARG:NH1	2.34	0.42
1:A:357:LEU:O	1:A:360:HIS:HB2	2.18	0.42
1:D:4:THR:HA	1:D:7:MET:CE	2.48	0.42
1:D:398:ARG:O	1:D:402:ARG:HG3	2.20	0.42
1:C:337:HIS:HB2	1:C:342:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ARG:HH11	1:B:307:PRO:HD2	1.84	0.42
1:B:135:LYS:HD3	1:B:360:HIS:NE2	2.34	0.42
1:C:285:HIS:CE1	1:D:400:TYR:OH	2.72	0.42
1:A:104:VAL:HG21	1:A:119:LEU:HD21	2.01	0.42
1:A:298:ILE:HG22	1:A:314:LEU:HD22	2.01	0.42
1:D:260:SER:O	1:D:289:GLU:OE1	2.37	0.42
1:D:291:PRO:HB2	1:D:294:VAL:CG2	2.49	0.42
1:B:112:ILE:CG2	1:B:114:ASP:HB3	2.49	0.42
1:A:369:MET:O	1:A:370:LEU:C	2.57	0.42
1:A:51:ALA:HB2	1:A:63:ILE:HD11	2.02	0.42
1:D:250:VAL:HG22	1:D:274:LEU:HG	2.01	0.42
1:C:107:GLU:O	1:C:108:ARG:C	2.57	0.42
1:C:116:GLY:N	1:C:141:THR:HG21	2.19	0.42
1:B:271:ILE:HD11	1:B:291:PRO:HG2	2.01	0.42
1:B:69:LEU:HB3	1:B:70:SER:H	1.64	0.42
1:B:47:THR:O	1:B:50:LEU:HB3	2.20	0.42
1:B:309:VAL:CG1	1:B:321:PHE:HB3	2.49	0.42
1:B:201:VAL:CG2	1:B:253:ALA:HB2	2.48	0.42
1:B:136:GLY:CA	1:B:356:LEU:HD13	2.49	0.42
1:C:166:ASP:HB3	1:C:369:MET:HE2	2.02	0.42
1:D:346:PHE:O	1:D:349:GLN:N	2.52	0.42
1:D:96:ILE:HG22	1:D:96:ILE:O	2.20	0.42
1:D:150:ALA:O	1:D:153:GLU:HG2	2.19	0.42
1:A:98:ARG:HA	1:A:101:LEU:HD12	2.01	0.42
1:A:263:THR:HG23	1:B:400:TYR:CD2	2.55	0.42
1:B:43:LEU:HD23	1:B:69:LEU:HD12	2.01	0.42
1:D:149:LYS:NZ	1:D:367:VAL:HG13	2.34	0.42
1:B:91:THR:OG1	1:B:92:HIS:N	2.53	0.42
1:A:232:LYS:NZ	2:A:500:NAI:O3B	2.52	0.42
1:B:62:VAL:HG12	1:B:104:VAL:HG12	2.02	0.42
1:A:263:THR:HG22	1:A:288:VAL:HG21	1.99	0.42
1:B:291:PRO:HB2	1:B:294:VAL:HB	2.02	0.42
1:C:227:GLU:OE1	2:C:500:NAI:H1B	2.19	0.42
1:B:140:GLU:O	1:B:141:THR:O	2.38	0.42
1:A:383:LEU:HD13	1:A:383:LEU:HA	1.82	0.42
1:B:96:ILE:O	1:B:100:ASN:OD1	2.38	0.42
1:D:377:ARG:NH2	1:D:377:ARG:HG2	2.34	0.42
1:B:26:TYR:HB3	1:B:57:LEU:HD22	2.02	0.42
1:D:67:ASN:ND2	1:D:70:SER:C	2.73	0.41
1:A:400:TYR:CZ	1:B:263:THR:HG23	2.54	0.41
1:A:91:THR:HG22	1:A:96:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:LYS:HZ1	1:D:298:ILE:HD11	1.81	0.41
1:D:370:LEU:HD12	1:D:371:PRO:HD2	2.02	0.41
1:D:108:ARG:CG	1:D:130:VAL:HG12	2.47	0.41
1:C:267:SER:O	1:C:271:ILE:HG13	2.19	0.41
1:B:319:THR:CG2	3:D:657:HOH:O	2.67	0.41
1:C:73:ASP:O	1:C:77:GLU:HG2	2.19	0.41
1:A:164:VAL:HG12	1:A:370:LEU:HD13	2.02	0.41
1:B:285:HIS:O	1:B:286:PHE:O	2.37	0.41
1:A:224:ILE:HG12	1:A:244:MET:HE3	2.02	0.41
1:D:143:THR:O	1:D:146:ARG:HB3	2.20	0.41
1:B:174:ASP:OD1	1:B:337:HIS:HE1	2.03	0.41
1:C:227:GLU:O	1:D:390:ILE:HB	2.19	0.41
1:B:140:GLU:HA	1:B:164:VAL:HG22	2.02	0.41
1:B:369:MET:O	1:B:370:LEU:C	2.59	0.41
1:A:32:LEU:HD23	1:A:59:ALA:CB	2.48	0.41
1:D:330:ASN:N	1:D:330:ASN:HD22	2.05	0.41
1:C:182:SER:HB2	1:C:330:ASN:HB2	2.02	0.41
1:A:344:LEU:O	1:A:344:LEU:HD23	2.19	0.41
1:D:195:VAL:HG12	1:D:221:ALA:HB2	2.03	0.41
1:C:262:ASN:O	1:C:289:GLU:HG2	2.21	0.41
1:C:17:PRO:HG2	1:C:18:LEU:N	2.35	0.41
1:C:295:LEU:HB3	1:C:312:TYR:CD2	2.55	0.41
1:B:361:ARG:HG2	1:B:361:ARG:H	1.58	0.41
1:A:80:ARG:C	1:A:82:LYS:H	2.23	0.41
1:C:11:TRP:O	1:C:14:ARG:HG2	2.20	0.41
1:C:295:LEU:HB3	1:C:312:TYR:CE2	2.55	0.41
1:B:346:PHE:O	1:B:349:GLN:N	2.53	0.41
1:C:285:HIS:O	1:C:286:PHE:O	2.39	0.41
1:A:64:THR:HG23	1:A:100:ASN:HB3	2.00	0.41
1:B:155:GLY:HA2	3:B:660:HOH:O	2.21	0.41
1:C:26:TYR:HB3	1:C:57:LEU:HD22	2.02	0.41
1:B:188:MET:HE3	1:B:195:VAL:HG21	2.01	0.41
1:A:63:ILE:CG2	1:A:64:THR:N	2.83	0.41
1:C:357:LEU:O	1:C:360:HIS:HB2	2.21	0.41
1:D:91:THR:O	1:D:93:ASP:N	2.51	0.41
1:D:271:ILE:HA	1:D:274:LEU:HD12	2.02	0.41
2:C:500:NAI:H2D	2:C:500:NAI:H6N	1.91	0.41
1:D:192:ASN:CG	1:D:192:ASN:O	2.59	0.41
1:C:346:PHE:O	1:C:349:GLN:N	2.53	0.41
1:A:175:ASN:O	1:A:179:THR:CG2	2.69	0.41
1:C:124:HIS:HA	1:C:131:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:ILE:HG13	1:D:356:LEU:HD21	2.03	0.41
1:B:330:ASN:ND2	2:B:500:NAI:H72N	2.19	0.41
1:B:27:SER:O	1:B:30:LYS:HG3	2.21	0.41
1:B:319:THR:HG21	1:D:14:ARG:HH21	1.86	0.41
1:D:262:ASN:HD22	1:D:262:ASN:HA	1.67	0.41
1:A:208:CYS:O	1:A:212:ILE:HG13	2.21	0.41
1:B:8:LYS:O	1:B:45:ALA:HB1	2.20	0.41
1:C:106:ASP:OD1	1:C:127:ARG:NH1	2.54	0.41
1:D:13:SER:HB2	1:D:49:TYR:CE1	2.56	0.41
1:C:7:MET:CE	1:C:10:ASN:HD22	2.33	0.41
1:A:33:SER:C	1:A:35:PHE:H	2.23	0.41
1:A:91:THR:C	1:A:93:ASP:N	2.74	0.41
1:C:91:THR:C	1:C:93:ASP:N	2.74	0.41
1:B:222:ARG:NE	1:B:224:ILE:HD11	2.36	0.41
1:B:105:LEU:C	1:B:107:GLU:N	2.74	0.41
1:C:48:ALA:O	1:C:52:ILE:HG13	2.21	0.41
1:B:35:PHE:CE2	1:B:357:LEU:HD11	2.56	0.40
1:B:4:THR:HG22	1:B:8:LYS:HE3	2.02	0.40
1:A:15:TYR:HB2	1:A:339:VAL:HG11	2.03	0.40
1:A:107:GLU:O	1:A:108:ARG:C	2.59	0.40
1:B:172:LEU:O	1:B:176:ARG:HB3	2.20	0.40
1:A:205:TYR:CE2	1:A:210:ARG:HG2	2.56	0.40
1:D:244:MET:HG3	1:D:249:ALA:HB2	2.02	0.40
1:A:133:ASN:O	1:A:135:LYS:HG3	2.20	0.40
1:C:104:VAL:O	1:C:107:GLU:HB2	2.21	0.40
1:C:121:VAL:HG11	1:C:147:ARG:HH21	1.84	0.40
1:D:348:LEU:CD2	1:D:378:VAL:HG21	2.44	0.40
1:D:35:PHE:CA	1:D:110:ASP:OD2	2.63	0.40
1:A:194:LEU:HD13	1:C:341:ILE:HG12	2.03	0.40
1:C:359:ASN:O	1:C:363:MET:HE2	2.21	0.40
1:B:12:VAL:HG13	1:B:16:MET:HE2	2.02	0.40
1:B:52:ILE:HG22	1:B:56:LYS:HE3	2.04	0.40
1:A:250:VAL:HG22	1:A:274:LEU:CD2	2.52	0.40
1:A:46:LYS:NZ	3:A:688:HOH:O	2.54	0.40
1:C:105:LEU:HD22	1:C:130:VAL:HG21	2.04	0.40
1:C:285:HIS:CE1	1:D:400:TYR:HH	2.39	0.40
1:C:116:GLY:O	1:C:147:ARG:HD3	2.21	0.40
1:D:346:PHE:O	1:D:347:ALA:C	2.60	0.40
1:D:357:LEU:O	1:D:360:HIS:HB2	2.21	0.40
1:A:105:LEU:C	1:A:107:GLU:N	2.75	0.40
1:A:331:LEU:C	1:A:331:LEU:HD13	2.41	0.40

There are no symmetry-related clashes.

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	399/411 (97%)	345 (86%)	41 (10%)	13 (3%)	5	17
1	B	399/411 (97%)	350 (88%)	39 (10%)	10 (2%)	7	24
1	C	399/411 (97%)	348 (87%)	39 (10%)	12 (3%)	5	19
1	D	399/411 (97%)	346 (87%)	41 (10%)	12 (3%)	5	19
All	All	1596/1644 (97%)	1389 (87%)	160 (10%)	47 (3%)	6	20

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	THR
1	A	285	HIS
1	A	286	PHE
1	A	365	PRO
1	B	141	THR
1	B	285	HIS
1	B	286	PHE
1	B	365	PRO
1	C	141	THR
1	C	285	HIS
1	C	286	PHE
1	C	365	PRO
1	D	141	THR
1	D	285	HIS
1	D	286	PHE
1	D	365	PRO
1	A	328	LEU
1	B	362	LYS
1	C	328	LEU
1	A	360	HIS

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Mol	Chain	Res	Type
1	B	155	GLY
1	B	328	LEU
1	B	360	HIS
1	C	358	GLU
1	C	360	HIS
1	D	328	LEU
1	D	358	GLU
1	D	360	HIS
1	A	155	GLY
1	A	358	GLU
1	A	362	LYS
1	B	358	GLU
1	C	155	GLY
1	C	362	LYS
1	D	362	LYS
1	A	73	ASP
1	C	90	ARG
1	D	90	ARG
1	D	291	PRO
1	A	90	ARG
1	D	155	GLY
1	B	291	PRO
1	D	307	PRO
1	A	291	PRO
1	A	307	PRO
1	C	307	PRO
1	C	291	PRO

5.3.2 Protein sidechains (i)

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	337/347 (97%)	309 (92%)	28 (8%)	14	36
1	B	337/347 (97%)	304 (90%)	33 (10%)	10	27
1	C	337/347 (97%)	308 (91%)	29 (9%)	13	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	337/347 (97%)	309 (92%)	28 (8%)	14 36
All	All	1348/1388 (97%)	1230 (91%)	118 (9%)	12 33

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	16	MET
1	A	24	GLU
1	A	29	GLU
1	A	53	THR
1	A	60	LYS
1	A	70	SER
1	A	86	VAL
1	A	90	ARG
1	A	165	ASN
1	A	179	THR
1	A	215	ARG
1	A	222	ARG
1	A	242	THR
1	A	248	GLU
1	A	250	VAL
1	A	262	ASN
1	A	293	ARG
1	A	307	PRO
1	A	310	THR
1	A	319	THR
1	A	330	ASN
1	A	342	MET
1	A	359	ASN
1	A	372	ASP
1	A	377	ARG
1	A	380	ARG
1	A	383	LEU
1	B	13	SER
1	B	14	ARG
1	B	24	GLU
1	B	27	SER
1	B	29	GLU
1	B	53	THR
1	B	60	LYS
1	B	72	GLN

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Mol	Chain	Res	Type
1	B	86	VAL
1	B	89	ARG
1	B	108	ARG
1	B	110	ASP
1	B	165	ASN
1	B	179	THR
1	B	215	ARG
1	B	222	ARG
1	B	242	THR
1	B	248	GLU
1	B	250	VAL
1	B	262	ASN
1	B	307	PRO
1	B	310	THR
1	B	319	THR
1	B	330	ASN
1	B	342	MET
1	B	359	ASN
1	B	360	HIS
1	B	361	ARG
1	B	365	PRO
1	B	372	ASP
1	B	376	GLU
1	B	380	ARG
1	B	383	LEU
1	C	14	ARG
1	C	16	MET
1	C	24	GLU
1	C	27	SER
1	C	53	THR
1	C	60	LYS
1	C	70	SER
1	C	86	VAL
1	C	142	THR
1	C	165	ASN
1	C	179	THR
1	C	215	ARG
1	C	222	ARG
1	C	227	GLU
1	C	234	VAL
1	C	242	THR
1	C	247	LYS

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Mol	Chain	Res	Type
1	C	262	ASN
1	C	293	ARG
1	C	307	PRO
1	C	310	THR
1	C	312	TYR
1	C	315	GLU
1	C	319	THR
1	C	330	ASN
1	C	359	ASN
1	C	376	GLU
1	C	380	ARG
1	C	383	LEU
1	D	14	ARG
1	D	24	GLU
1	D	53	THR
1	D	70	SER
1	D	86	VAL
1	D	114	ASP
1	D	165	ASN
1	D	179	THR
1	D	215	ARG
1	D	222	ARG
1	D	234	VAL
1	D	242	THR
1	D	247	LYS
1	D	248	GLU
1	D	250	VAL
1	D	262	ASN
1	D	307	PRO
1	D	310	THR
1	D	319	THR
1	D	330	ASN
1	D	342	MET
1	D	359	ASN
1	D	360	HIS
1	D	361	ARG
1	D	365	PRO
1	D	376	GLU
1	D	380	ARG
1	D	383	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	100	ASN
1	A	165	ASN
1	A	181	GLN
1	A	330	ASN
1	A	337	HIS
1	A	349	GLN
1	B	10	ASN
1	B	100	ASN
1	B	165	ASN
1	B	181	GLN
1	B	330	ASN
1	B	337	HIS
1	B	349	GLN
1	B	359	ASN
1	C	10	ASN
1	C	100	ASN
1	C	165	ASN
1	C	181	GLN
1	C	285	HIS
1	C	330	ASN
1	C	337	HIS
1	C	349	GLN
1	C	359	ASN
1	D	10	ASN
1	D	72	GLN
1	D	100	ASN
1	D	165	ASN
1	D	181	GLN
1	D	192	ASN
1	D	330	ASN
1	D	349	GLN
1	D	359	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
2	NAI	A	500	-	38,48,48	1.01	1 (2%)	48,73,73	1.97	6 (12%)
2	NAI	B	500	-	38,48,48	1.07	2 (5%)	48,73,73	1.96	6 (12%)
2	NAI	C	500	-	38,48,48	1.01	2 (5%)	48,73,73	2.10	7 (14%)
2	NAI	D	500	-	38,48,48	1.01	2 (5%)	48,73,73	2.09	7 (14%)

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
2	NAI	A	500	-	-	0/25/72/72	0/5/5/5
2	NAI	B	500	-	-	0/25/72/72	0/5/5/5
2	NAI	C	500	-	-	0/25/72/72	0/5/5/5
2	NAI	D	500	-	-	0/25/72/72	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	NAI	C8A-N7A	-2.12	1.30	1.34
2	C	500	NAI	C8A-N7A	-2.02	1.30	1.34
2	A	500	NAI	O4B-C1B	2.05	1.43	1.41
2	B	500	NAI	C4N-C5N	2.12	1.53	1.49
2	C	500	NAI	O4B-C1B	2.48	1.44	1.41
2	D	500	NAI	O4B-C1B	2.90	1.44	1.41
2	B	500	NAI	O4B-C1B	3.18	1.45	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	NAI	N3A-C2A-N1A	-9.88	121.33	128.89
2	C	500	NAI	N3A-C2A-N1A	-9.88	121.33	128.89
2	B	500	NAI	N3A-C2A-N1A	-9.39	121.71	128.89
2	A	500	NAI	N3A-C2A-N1A	-9.25	121.81	128.89
2	C	500	NAI	PN-O3-PA	-7.59	111.41	132.73
2	D	500	NAI	PN-O3-PA	-7.53	111.58	132.73
2	B	500	NAI	PN-O3-PA	-6.95	113.22	132.73
2	A	500	NAI	PN-O3-PA	-6.89	113.39	132.73
2	D	500	NAI	C4B-O4B-C1B	-3.78	105.56	109.72
2	C	500	NAI	C4B-O4B-C1B	-3.48	105.89	109.72
2	B	500	NAI	C4A-C5A-N7A	-3.02	106.70	109.48
2	A	500	NAI	C4B-O4B-C1B	-2.96	106.47	109.72
2	A	500	NAI	C4A-C5A-N7A	-2.74	106.95	109.48
2	C	500	NAI	C4A-C5A-N7A	-2.70	106.99	109.48
2	D	500	NAI	C4A-C5A-N7A	-2.38	107.29	109.48
2	B	500	NAI	C1D-N1N-C2N	-2.13	117.20	120.91
2	C	500	NAI	C1D-N1N-C2N	-2.08	117.28	120.91
2	D	500	NAI	C1D-N1N-C2N	-2.05	117.33	120.91
2	C	500	NAI	O3-PN-O5D	2.12	108.55	102.94
2	D	500	NAI	O3-PN-O5D	2.22	108.81	102.94
2	D	500	NAI	O3-PA-O5B	2.37	109.23	102.94
2	B	500	NAI	O3-PA-O5B	2.38	109.25	102.94
2	B	500	NAI	O3-PN-O5D	2.39	109.28	102.94
2	A	500	NAI	O3-PN-O5D	2.48	109.51	102.94
2	A	500	NAI	O3-PA-O5B	2.50	109.57	102.94
2	C	500	NAI	O3-PA-O5B	2.52	109.63	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	NAI	2	0
2	B	500	NAI	2	0
2	C	500	NAI	2	0
2	D	500	NAI	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	401/411 (97%)	0.17	21 (5%)	31	24	29, 83, 127, 140	0
1	B	401/411 (97%)	-0.05	10 (2%)	61	56	32, 68, 100, 120	0
1	C	401/411 (97%)	0.06	10 (2%)	61	56	38, 80, 121, 135	0
1	D	401/411 (97%)	0.01	16 (3%)	42	34	35, 74, 112, 121	0
All	All	1604/1644 (97%)	0.05	57 (3%)	46	39	29, 76, 118, 140	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	10.8
1	C	70	SER	6.3
1	B	2	ALA	5.1
1	A	137	VAL	5.1
1	C	92	HIS	4.8
1	D	2	ALA	4.8
1	C	2	ALA	4.7
1	A	91	THR	4.5
1	B	402	ARG	4.2
1	B	401	LEU	4.2
1	A	362	LYS	4.1
1	A	3	ASN	4.0
1	D	365	PRO	3.9
1	C	69	LEU	3.9
1	A	285	HIS	3.8
1	A	71	THR	3.7
1	A	138	SER	3.4
1	D	23	ALA	3.2
1	A	112	ILE	3.1
1	B	92	HIS	3.1
1	D	92	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	143	THR	3.0
1	A	69	LEU	3.0
1	A	88	ALA	2.9
1	B	143	THR	2.9
1	C	90	ARG	2.9
1	A	395	GLU	2.8
1	D	138	SER	2.8
1	B	3	ASN	2.8
1	A	136	GLY	2.8
1	A	296	GLU	2.7
1	B	72	GLN	2.7
1	D	362	LYS	2.7
1	C	402	ARG	2.6
1	A	158	ARG	2.6
1	B	158	ARG	2.6
1	D	285	HIS	2.5
1	C	138	SER	2.5
1	D	130	VAL	2.4
1	C	3	ASN	2.4
1	D	368	TYR	2.4
1	C	28	ARG	2.3
1	C	126	GLU	2.3
1	D	27	SER	2.3
1	B	132	GLU	2.3
1	B	301	GLU	2.3
1	A	25	GLU	2.2
1	D	126	GLU	2.2
1	D	155	GLY	2.2
1	D	69	LEU	2.2
1	A	402	ARG	2.1
1	A	6	GLU	2.1
1	D	6	GLU	2.1
1	D	153	GLU	2.1
1	A	33	SER	2.1
1	A	300	VAL	2.1
1	D	3	ASN	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, 95^{th} 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(Å^2)	Q<0.9
2	NAI	A	500	44/44	0.96	0.14	-0.63	58,75,86,86	0
2	NAI	C	500	44/44	0.96	0.15	-0.76	55,74,88,94	0
2	NAI	B	500	44/44	0.96	0.14	-0.90	65,72,86,89	0
2	NAI	D	500	44/44	0.95	0.14	-0.91	58,69,78,81	0

6.5 Other polymers (i)

There are no such residues in this entry.