Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:45 PM GMT

PDB ID	:	4J9U
Title	:	Crystal Structure of the TrkH/TrkA potassium transport complex
Authors	:	Cao, Y.; Jin, X.; Huang, H.; Levin, E.J.; Zhou, M.; New York Consortium on Membrane Protein Structure (NYCOMPS)
Deposited on	:	2013-02-17
Resolution	:	3.80 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:

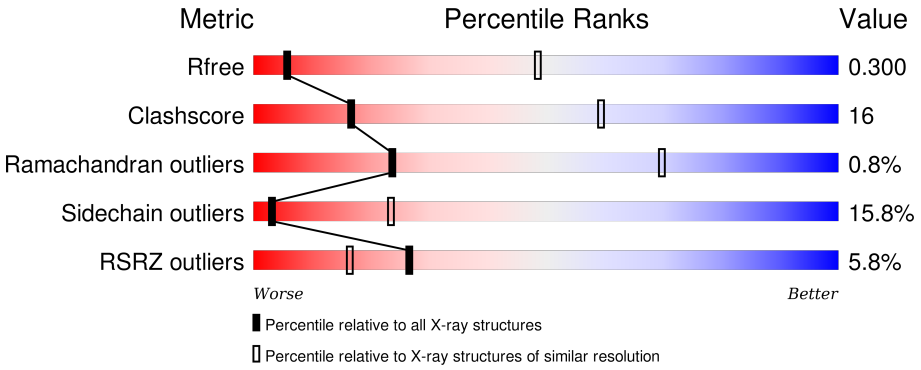
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.80 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	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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	485	5% 52% 38% 6% 5%
1	B	485	4% 53% 36% 6% 5%
1	C	485	8% 53% 36% 6% 5%
1	D	485	5% 53% 37% 5% 5%
2	E	458	6% 58% 34% 6% •

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Mol	Chain	Length	Quality of chain
2	F	458	6% 57% 34% 6%
2	G	458	4% 58% 35% 5%
2	H	458	8% 59% 34% 6%

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	TBR	A	501	-	-	-	X
3	TBR	B	501	-	-	-	X
3	TBR	C	501	-	-	-	X
3	TBR	D	501	-	-	-	X
3	TBR	D	502	-	-	-	X
3	TBR	D	503	-	-	-	X
3	TBR	E	503	-	-	-	X
3	TBR	F	503	-	-	-	X
3	TBR	G	503	-	-	-	X
3	TBR	H	503	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28567 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.

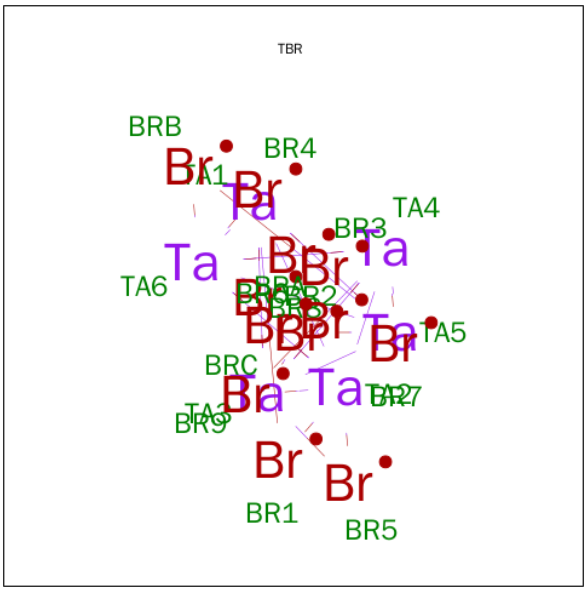
- Molecule 1 is a protein called Trk system potassium uptake protein TrkH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3569	2389	564	598	18			
1	B	462	Total	C	N	O	S	0	0	0
			3569	2389	564	598	18			
1	C	462	Total	C	N	O	S	0	0	0
			3569	2389	564	598	18			
1	D	462	Total	C	N	O	S	0	0	0
			3569	2389	564	598	18			

- Molecule 2 is a protein called Potassium uptake protein TrkA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	451	Total	C	N	O	S	0	0	0
			3454	2162	611	669	12			
2	F	444	Total	C	N	O	S	0	0	0
			3410	2138	600	660	12			
2	G	452	Total	C	N	O	S	0	0	0
			3468	2174	612	670	12			
2	H	450	Total	C	N	O	S	0	0	0
			3455	2165	610	668	12			

- Molecule 3 is HEXATANTALUM DODECABROMIDE (three-letter code: TBR) (formula: $Br_{12}Ta_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Br Ta 18 12 6	0	0
3	A	1	Total Br Ta 18 12 6	0	0
3	A	1	Total Br Ta 18 12 6	0	0
3	B	1	Total Br Ta 18 12 6	0	0
3	B	1	Total Br Ta 18 12 6	0	0
3	C	1	Total Br Ta 18 12 6	0	0
3	C	1	Total Br Ta 18 12 6	0	0
3	D	1	Total Br Ta 18 12 6	0	0
3	D	1	Total Br Ta 18 12 6	0	0
3	D	1	Total Br Ta 18 12 6	0	0
3	E	1	Total Br Ta 18 12 6	0	0
3	E	1	Total Br Ta 18 12 6	0	0
3	F	1	Total Br Ta 18 12 6	0	0
3	F	1	Total Br Ta 18 12 6	0	0

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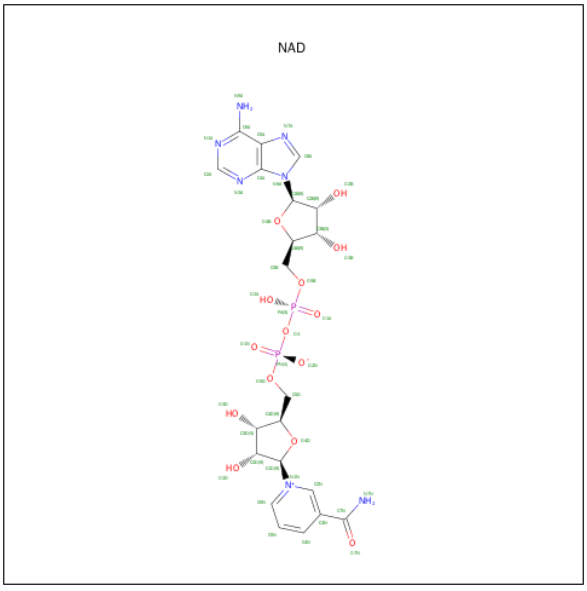
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Br Ta 18 12 6	0	0
3	G	1	Total Br Ta 18 12 6	0	0
3	H	1	Total Br Ta 18 12 6	0	0
3	H	1	Total Br Ta 18 12 6	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total K 1 1	0	0
4	A	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C N O P 44 21 7 14 2	0	0

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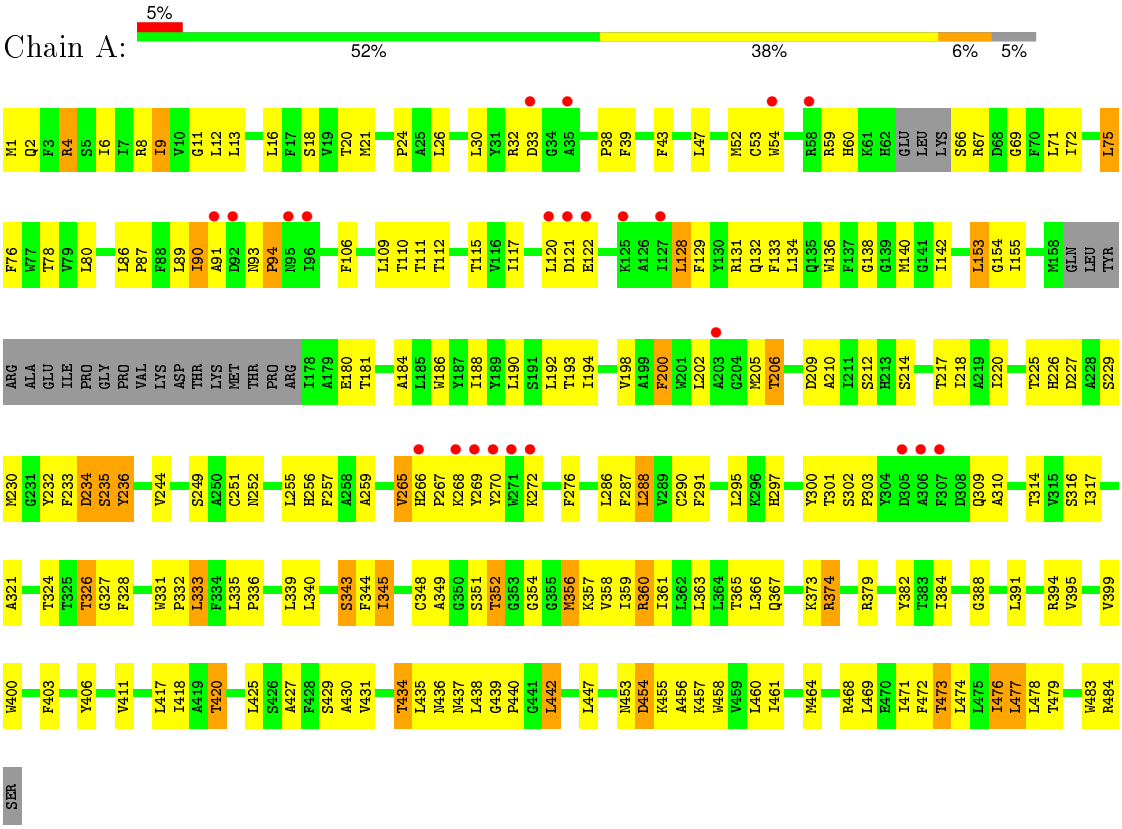
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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.

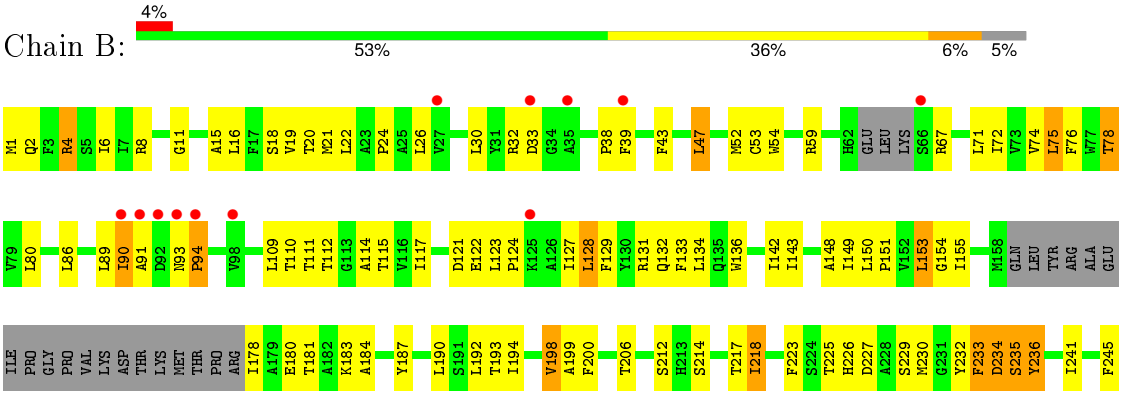
- Molecule 1: Trk system potassium uptake protein TrkH

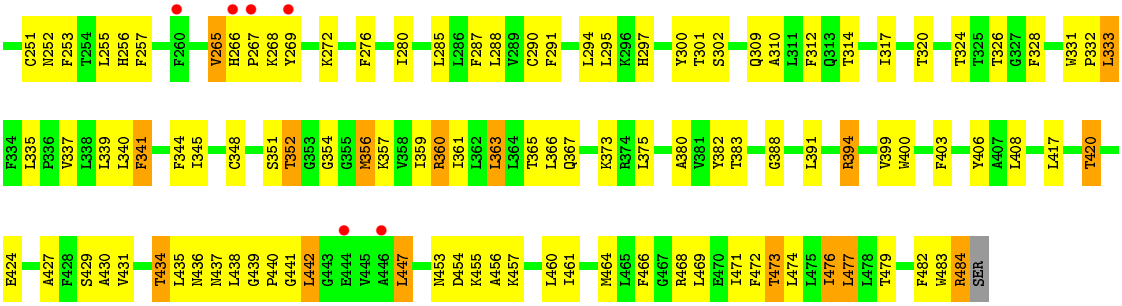
Chain A:



- Molecule 1: Trk system potassium uptake protein TrkH

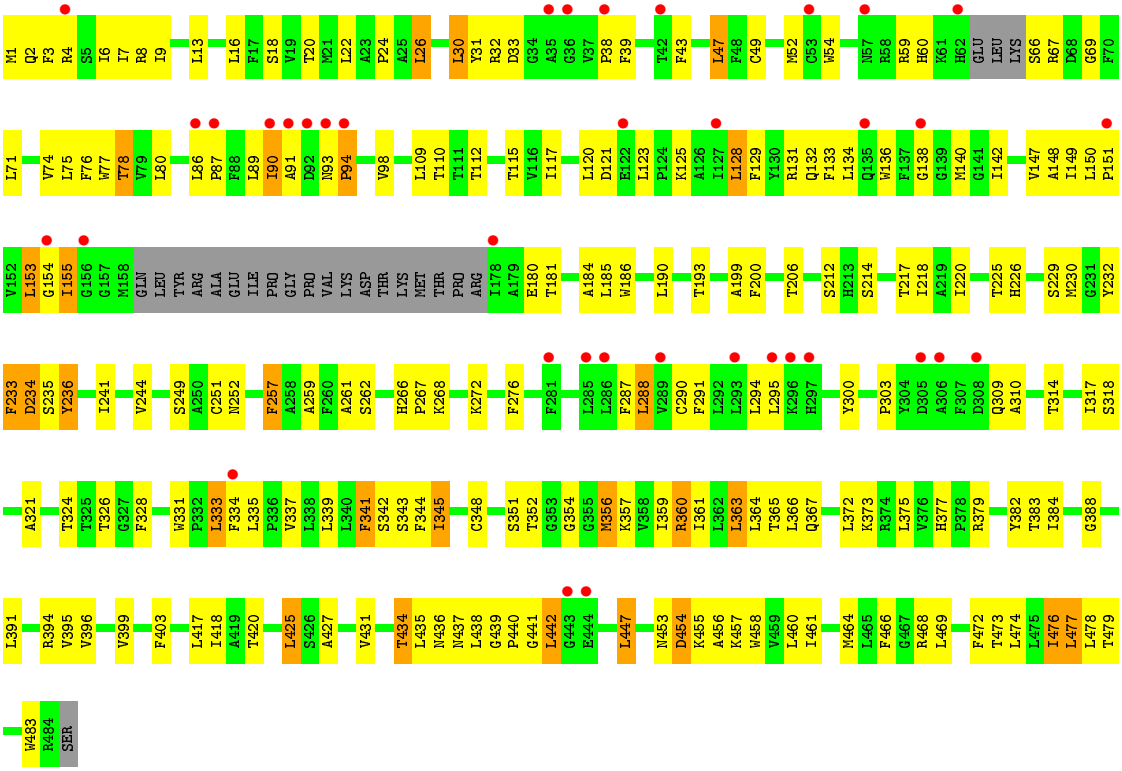
Chain B:





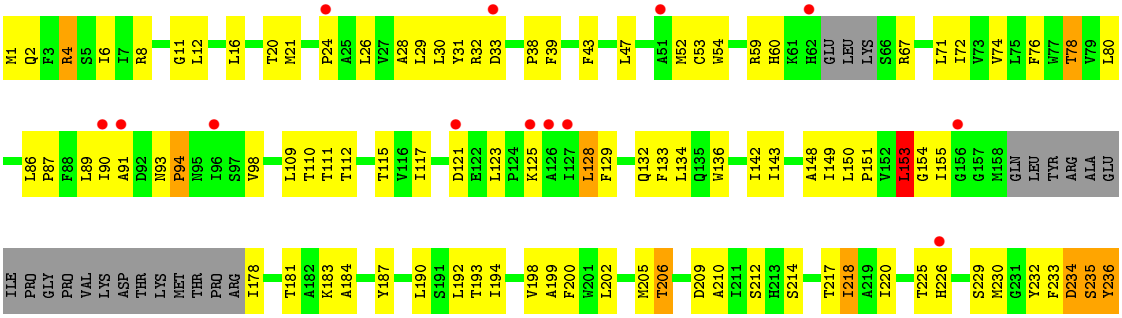
• Molecule 1: Trk system potassium uptake protein TrkH

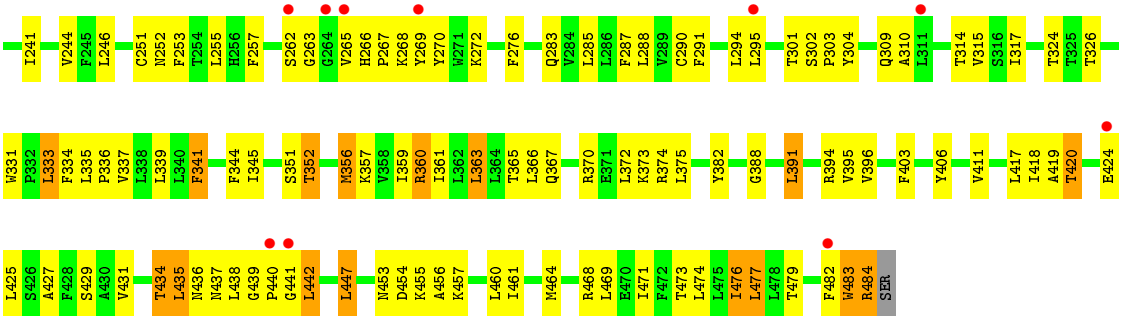
Chain C:



• Molecule 1: Trk system potassium uptake protein TrkH

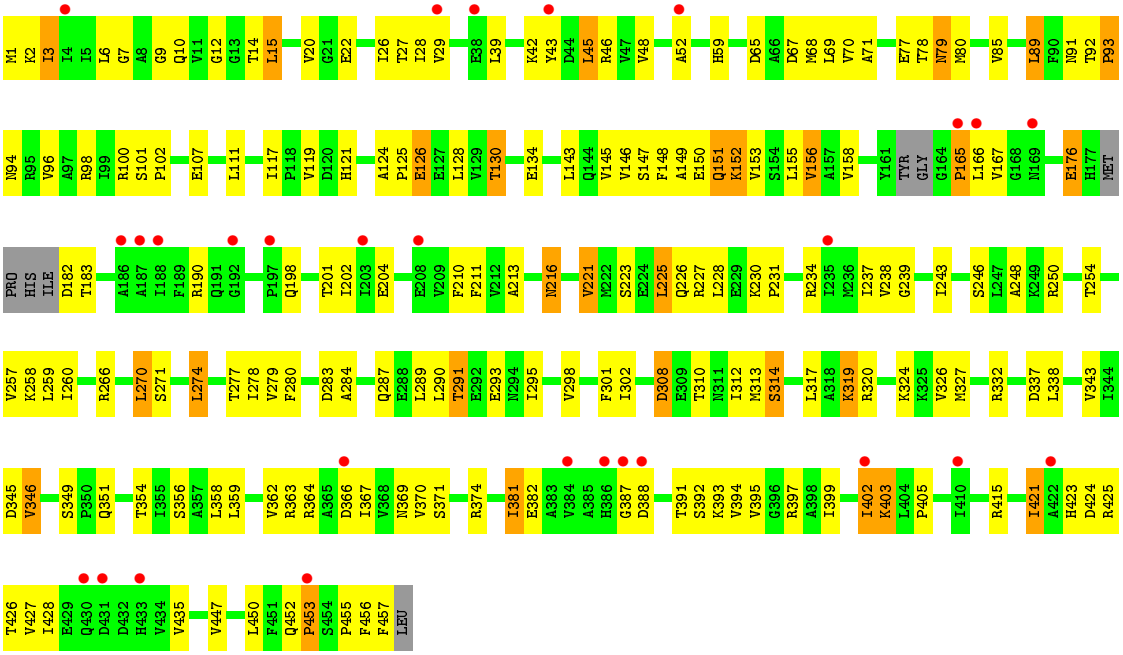
Chain D:





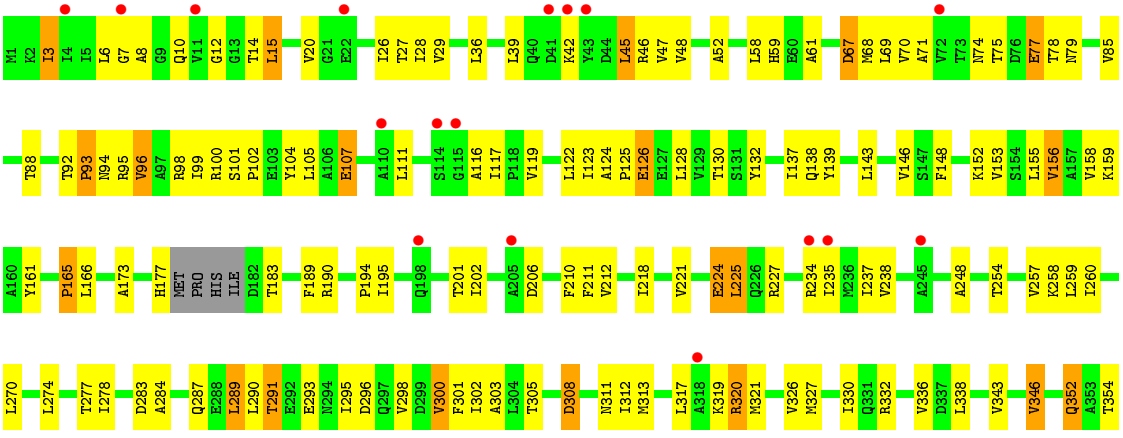
• Molecule 2: Potassium uptake protein TrkA

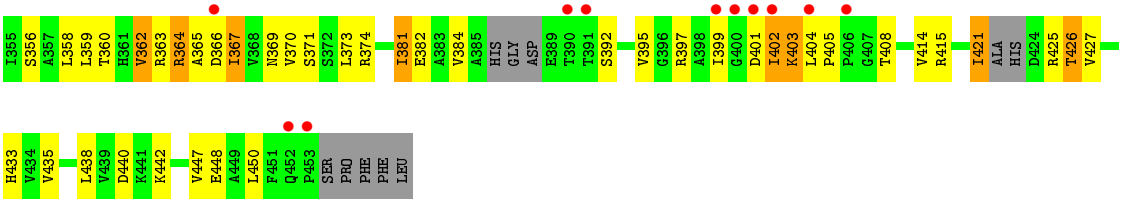
Chain E:



• Molecule 2: Potassium uptake protein TrkA

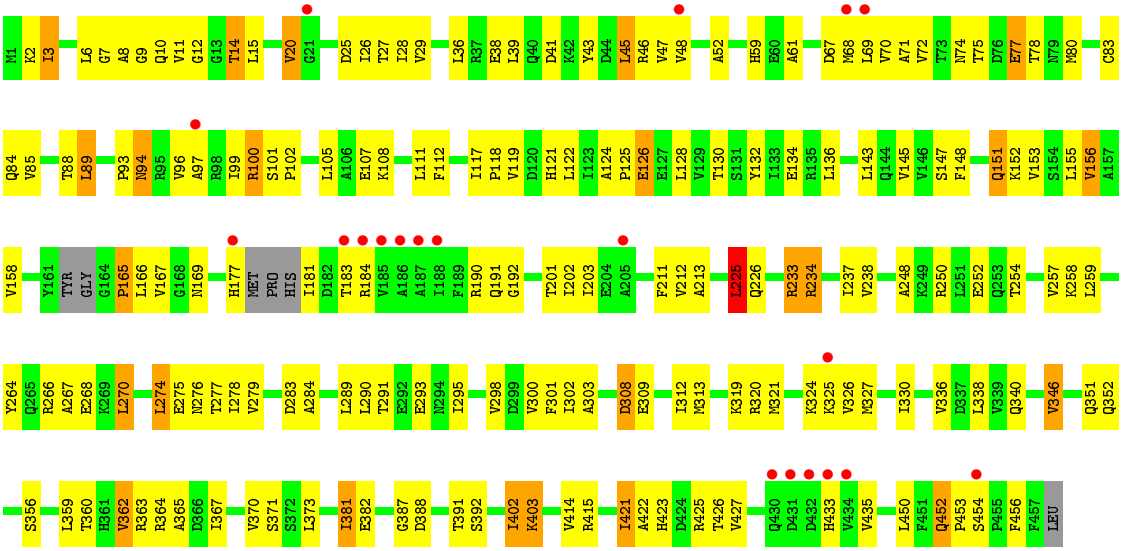
Chain F:





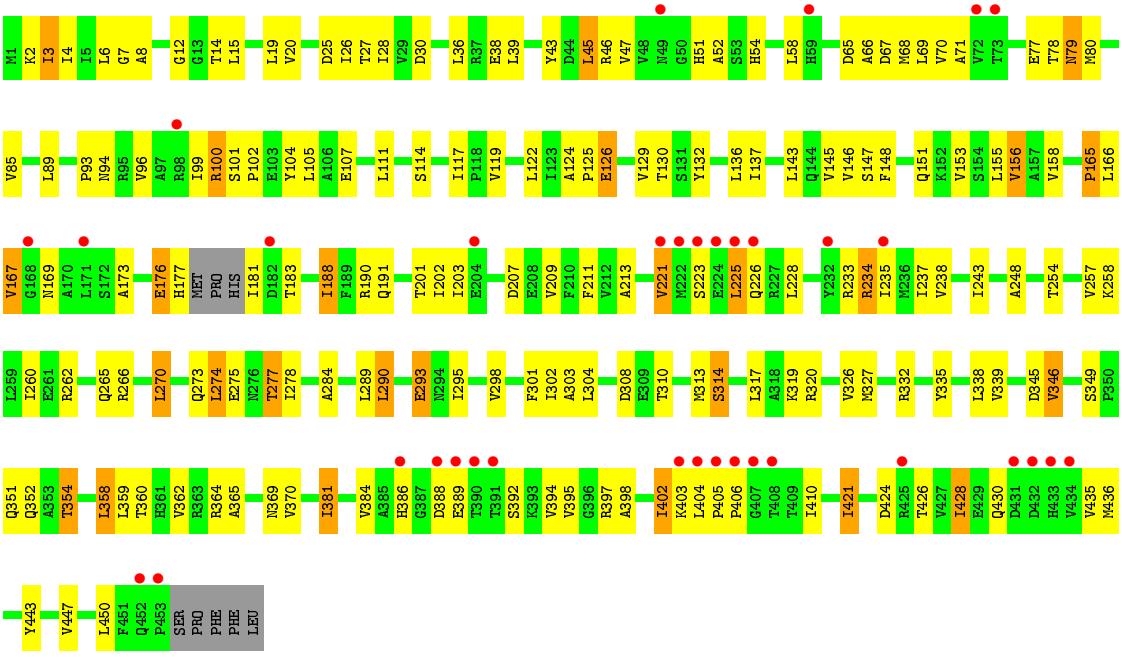
• Molecule 2: Potassium uptake protein TrkA

Chain G:



• Molecule 2: Potassium uptake protein TrkA

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	133.72Å 146.63Å 163.67Å 90.00° 99.32° 90.00°	Depositor
Resolution (Å)	49.79 – 3.80 49.79 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.79-3.80) 99.6 (49.79-3.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.52 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.232 , 0.280 0.258 , 0.300	Depositor DCC
R_{free} test set	3130 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	118.3	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	2 of 61321 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	28567	wwPDB-VP
Average B, all atoms (Å^2)	89.0	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 20.89 % 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 7.8858e-03.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: K, TBR, 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	0.30	0/3670	0.55	0/5000
1	B	0.30	0/3670	0.56	0/5000
1	C	0.30	0/3670	0.54	0/5000
1	D	0.28	0/3670	0.54	1/5000 (0.0%)
2	E	0.27	0/3498	0.54	0/4743
2	F	0.27	0/3451	0.54	0/4676
2	G	0.28	0/3513	0.54	0/4763
2	H	0.28	0/3500	0.56	0/4746
All	All	0.29	0/28642	0.55	1/38928 (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	D	153	LEU	CA-CB-CG	5.31	127.52	115.30

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	3569	0	3638	144	0
1	B	3569	0	3638	132	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3569	0	3638	132	0
1	D	3569	0	3638	129	0
2	E	3454	0	3489	105	0
2	F	3410	0	3458	110	0
2	G	3468	0	3507	113	0
2	H	3455	0	3497	108	0
3	A	54	0	0	0	0
3	B	36	0	0	0	0
3	C	36	0	0	1	0
3	D	54	0	0	2	0
3	E	36	0	0	3	0
3	F	36	0	0	2	0
3	G	36	0	0	3	0
3	H	36	0	0	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	E	44	0	26	5	0
5	F	44	0	26	3	0
5	G	44	0	26	5	0
5	H	44	0	26	5	0
All	All	28567	0	28607	941	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 16.

All (941) 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:B:420:THR:HG21	1:B:456:ALA:HB2	1.50	0.94
2:F:3:ILE:HG22	2:F:68:MET:HB3	1.59	0.85
1:A:420:THR:HG21	1:A:456:ALA:HB2	1.58	0.85
1:B:132:GLN:HG3	1:B:212:SER:HB2	1.57	0.84
1:D:420:THR:HG21	1:D:456:ALA:HB2	1.60	0.83
2:E:96:VAL:HG12	2:E:121:HIS:HB2	1.63	0.81
2:E:3:ILE:HG22	2:E:68:MET:HB3	1.62	0.80
1:C:132:GLN:HG3	1:C:212:SER:HB2	1.64	0.80
2:E:77:GLU:HG3	2:H:78:THR:HG22	1.62	0.80
1:A:132:GLN:HG3	1:A:212:SER:HB2	1.62	0.79
1:D:132:GLN:HG3	1:D:212:SER:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:THR:HA	1:C:184:ALA:HB3	1.63	0.79
1:B:136:TRP:HE1	1:B:193:THR:HG21	1.48	0.79
1:A:136:TRP:HE1	1:A:193:THR:HG21	1.47	0.79
2:E:190:ARG:NH2	2:E:202:ILE:O	2.16	0.78
2:E:455:PRO:O	2:E:457:PHE:N	2.16	0.78
2:G:20:VAL:HG23	2:G:26:ILE:HD12	1.64	0.78
2:G:364:ARG:HG3	2:G:365:ALA:H	1.49	0.78
1:A:112:THR:HA	1:A:437:ASN:HB3	1.65	0.77
2:F:77:GLU:HG3	2:G:78:THR:HG22	1.64	0.77
2:E:78:THR:HG22	2:H:77:GLU:HG3	1.67	0.77
1:D:136:TRP:HE1	1:D:193:THR:HG21	1.49	0.76
2:F:78:THR:HG22	2:G:77:GLU:HG3	1.66	0.76
2:H:169:ASN:HB2	2:H:203:ILE:HG12	1.68	0.76
2:H:237:ILE:HG22	2:H:302:ILE:HB	1.68	0.75
2:F:190:ARG:NH2	2:F:202:ILE:O	2.19	0.75
2:E:363:ARG:HB2	2:E:367:ILE:HD11	1.68	0.74
1:C:268:LYS:HE3	1:C:272:LYS:HE3	1.68	0.74
2:H:20:VAL:HG23	2:H:26:ILE:HD12	1.69	0.74
1:A:268:LYS:HE3	1:A:272:LYS:HE3	1.68	0.74
1:D:181:THR:HA	1:D:184:ALA:HB3	1.69	0.74
2:E:176:GLU:OE2	2:E:182:ASP:N	2.21	0.73
2:G:3:ILE:HG22	2:G:68:MET:HB3	1.69	0.73
1:B:268:LYS:HE3	1:B:272:LYS:HE3	1.71	0.73
1:D:24:PRO:HB3	1:D:129:PHE:HD2	1.54	0.72
2:G:96:VAL:HG12	2:G:121:HIS:HB2	1.69	0.72
2:E:6:LEU:HB2	2:E:71:ALA:HA	1.69	0.72
2:F:6:LEU:HD22	2:F:52:ALA:HB1	1.72	0.71
2:H:3:ILE:HG22	2:H:68:MET:HB3	1.70	0.71
2:E:20:VAL:HG23	2:E:26:ILE:HD12	1.73	0.71
2:G:156:VAL:HG12	2:G:211:PHE:HB2	1.71	0.70
2:H:156:VAL:HG12	2:H:211:PHE:HB2	1.71	0.70
2:F:237:ILE:HG22	2:F:302:ILE:HB	1.72	0.70
1:B:441:GLY:HA3	1:B:447:LEU:HA	1.74	0.70
2:H:284:ALA:H	5:H:501:NAD:H61A	1.37	0.70
2:G:10:GLN:NE2	2:G:74:ASN:OD1	2.23	0.70
2:E:301:PHE:HB3	2:E:326:VAL:HG12	1.72	0.69
2:G:370:VAL:HG23	2:G:381:ILE:HG22	1.74	0.69
1:C:440:PRO:HB2	1:C:442:LEU:HD23	1.74	0.69
2:E:284:ALA:H	5:E:501:NAD:H61A	1.39	0.69
2:H:143:LEU:HD13	2:H:158:VAL:HA	1.72	0.69
2:G:177:HIS:HA	2:G:181:ILE:HB	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ASN:HB2	1:C:94:PRO:HD3	1.75	0.69
1:C:24:PRO:HB3	1:C:129:PHE:HD2	1.58	0.69
2:E:15:LEU:HD11	2:E:358:LEU:HG	1.72	0.69
2:G:100:ARG:NH2	5:G:501:NAD:O7N	2.26	0.69
2:G:388:ASP:HB2	2:G:391:THR:HG22	1.74	0.69
2:H:20:VAL:HG11	2:H:43:TYR:HB3	1.74	0.69
1:A:214:SER:HA	1:A:217:THR:HG22	1.75	0.69
1:B:214:SER:HA	1:B:217:THR:HG22	1.75	0.68
1:D:214:SER:HA	1:D:217:THR:HG22	1.72	0.68
1:B:265:VAL:HG13	1:B:269:TYR:HE2	1.57	0.68
2:F:352:GLN:NE2	2:F:373:LEU:O	2.26	0.68
1:A:290:CYS:HA	1:A:335:LEU:HD11	1.76	0.68
1:C:214:SER:HA	1:C:217:THR:HG22	1.76	0.68
1:A:136:TRP:NE1	1:A:193:THR:HG21	2.08	0.68
1:D:93:ASN:HB2	1:D:94:PRO:HD3	1.75	0.67
1:B:128:LEU:HD11	1:B:225:THR:HA	1.75	0.67
1:A:128:LEU:HD11	1:A:225:THR:HA	1.77	0.67
2:E:22:GLU:OE2	2:E:363:ARG:NH1	2.28	0.67
2:H:100:ARG:NH2	5:H:501:NAD:O7N	2.28	0.67
1:C:420:THR:HG21	1:C:456:ALA:HB2	1.75	0.67
1:B:93:ASN:HB2	1:B:94:PRO:HD3	1.77	0.67
2:G:415:ARG:NH2	2:G:427:VAL:O	2.27	0.67
1:A:24:PRO:HB3	1:A:129:PHE:HD2	1.60	0.67
1:B:356:MET:HE1	1:B:403:PHE:HD1	1.60	0.66
2:H:6:LEU:HB2	2:H:71:ALA:HA	1.78	0.66
1:D:438:LEU:HB2	1:D:439:GLY:HA2	1.77	0.66
1:B:114:ALA:HB2	1:B:439:GLY:HA2	1.78	0.66
1:D:110:THR:O	1:D:468:ARG:NH1	2.28	0.66
1:B:136:TRP:NE1	1:B:193:THR:HG21	2.11	0.66
1:D:205:MET:HB2	1:D:210:ALA:HB2	1.78	0.66
2:E:6:LEU:HD22	2:E:52:ALA:HB1	1.78	0.66
2:E:387:GLY:HA3	2:E:392:SER:HB2	1.78	0.65
2:H:233:ARG:HH22	2:H:234:ARG:HH21	1.44	0.65
2:F:27:THR:HG22	2:F:46:ARG:HB3	1.79	0.65
2:H:332:ARG:HG3	3:H:503:TBR:BR2	2.51	0.65
1:C:230:MET:SD	1:C:232:TYR:OH	2.53	0.65
1:A:379:ARG:HD3	2:G:289:LEU:HD13	1.79	0.65
1:C:112:THR:HA	1:C:437:ASN:HB3	1.79	0.65
2:H:183:THR:HB	2:H:213:ALA:HB2	1.79	0.65
2:G:6:LEU:HD22	2:G:52:ALA:HB1	1.79	0.65
1:C:391:LEU:HD12	1:C:395:VAL:HG11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:PRO:HB3	1:B:129:PHE:HD2	1.62	0.64
2:F:258:LYS:HG2	2:F:278:ILE:HD11	1.79	0.64
2:H:238:VAL:HG12	2:H:260:ILE:HB	1.79	0.64
2:G:8:ALA:HA	2:G:28:ILE:HD11	1.78	0.64
1:D:440:PRO:HB2	1:D:442:LEU:HD23	1.78	0.64
2:H:27:THR:HG22	2:H:46:ARG:HB3	1.80	0.64
1:D:136:TRP:NE1	1:D:193:THR:HG21	2.11	0.64
1:C:112:THR:HG23	1:C:437:ASN:HA	1.79	0.64
2:G:6:LEU:HB2	2:G:71:ALA:HA	1.78	0.64
2:E:370:VAL:HG23	2:E:381:ILE:HG22	1.79	0.64
1:D:206:THR:HG23	1:D:209:ASP:HB2	1.80	0.64
1:A:93:ASN:HB2	1:A:94:PRO:HD3	1.80	0.64
2:H:145:VAL:HG22	2:H:156:VAL:HG23	1.80	0.64
2:G:295:ILE:HD12	2:G:298:VAL:HG11	1.80	0.64
2:F:284:ALA:H	5:F:501:NAD:H61A	1.45	0.64
2:E:327:MET:HG2	2:E:346:VAL:HG13	1.79	0.63
1:A:252:ASN:H	1:A:351:SER:HB3	1.63	0.63
2:H:129:VAL:HG11	2:H:243:ILE:HD13	1.81	0.63
2:H:370:VAL:HG23	2:H:381:ILE:HG22	1.81	0.63
2:E:156:VAL:HG12	2:E:211:PHE:HB2	1.80	0.63
1:A:354:GLY:HA2	1:A:357:LYS:HE3	1.81	0.63
2:F:364:ARG:HG3	2:F:365:ALA:H	1.64	0.63
1:A:234:ASP:OD2	1:A:234:ASP:N	2.31	0.63
1:A:440:PRO:HB2	1:A:442:LEU:HD23	1.81	0.63
1:C:287:PHE:HA	1:C:314:THR:HG21	1.81	0.62
1:A:38:PRO:HB3	1:A:90:ILE:HG23	1.81	0.62
2:F:107:GLU:HG3	2:G:89:LEU:HD11	1.81	0.62
2:H:99:ILE:HG13	2:H:122:LEU:HD23	1.80	0.62
2:H:15:LEU:HD11	2:H:358:LEU:HG	1.82	0.62
2:H:68:MET:HG3	2:H:94:ASN:HB3	1.81	0.62
2:G:237:ILE:HG22	2:G:302:ILE:HB	1.81	0.62
2:G:258:LYS:HG2	2:G:278:ILE:HD11	1.82	0.62
1:A:180:GLU:HG3	1:A:181:THR:HG23	1.80	0.62
2:F:221:VAL:HG13	2:F:225:LEU:HD23	1.81	0.62
2:G:20:VAL:HG11	2:G:43:TYR:HB3	1.81	0.62
1:A:38:PRO:HG2	1:A:91:ALA:HB2	1.81	0.62
2:F:235:ILE:HB	2:F:257:VAL:HG22	1.82	0.62
1:A:206:THR:HG23	1:A:209:ASP:HB2	1.82	0.62
1:B:420:THR:O	1:B:453:ASN:ND2	2.33	0.62
2:H:77:GLU:HA	2:H:80:MET:HE2	1.82	0.62
1:C:417:LEU:O	1:C:420:THR:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:14:THR:HG23	3:G:503:TBR:BRB	2.55	0.61
3:D:501:TBR:BRB	2:E:42:LYS:HA	2.55	0.61
1:D:453:ASN:OD1	1:D:454:ASP:N	2.34	0.61
2:H:221:VAL:HG13	2:H:225:LEU:HD23	1.82	0.61
1:D:2:GLN:HA	1:D:4:ARG:HH11	1.63	0.61
2:F:397:ARG:HB3	2:F:401:ASP:HB3	1.83	0.61
1:D:24:PRO:HB2	1:D:39:PHE:HE1	1.66	0.61
2:E:182:ASP:HB2	2:E:421:ILE:HD11	1.83	0.61
2:E:134:GLU:OE2	2:E:250:ARG:NH1	2.34	0.61
2:F:70:VAL:HA	2:F:96:VAL:HG23	1.81	0.61
1:B:38:PRO:HB3	1:B:90:ILE:HG23	1.83	0.61
1:A:344:PHE:HA	1:A:436:ASN:OD1	2.00	0.61
1:B:234:ASP:N	1:B:234:ASP:OD2	2.34	0.61
2:H:364:ARG:HG3	2:H:365:ALA:H	1.66	0.61
2:E:237:ILE:HG22	2:E:302:ILE:HB	1.81	0.61
1:D:287:PHE:HA	1:D:314:THR:HG21	1.83	0.60
1:A:438:LEU:HB2	1:A:439:GLY:HA2	1.83	0.60
1:B:484:ARG:HG3	2:G:234:ARG:HH12	1.65	0.60
2:G:27:THR:HG22	2:G:46:ARG:HB3	1.83	0.60
1:A:117:ILE:HG13	1:A:120:LEU:HD23	1.83	0.60
1:C:136:TRP:NE1	1:C:193:THR:HG21	2.16	0.60
2:F:392:SER:HB3	2:F:395:VAL:HG22	1.83	0.60
1:C:252:ASN:H	1:C:351:SER:HB3	1.67	0.60
1:C:110:THR:O	1:C:468:ARG:NH1	2.34	0.60
1:B:180:GLU:HG3	1:B:181:THR:HG23	1.83	0.60
1:D:252:ASN:H	1:D:351:SER:HB3	1.66	0.59
2:F:301:PHE:HB3	2:F:326:VAL:HG12	1.83	0.59
1:B:109:LEU:HD13	1:B:134:LEU:HD22	1.85	0.59
2:F:238:VAL:HG12	2:F:260:ILE:HB	1.85	0.59
1:B:420:THR:OG1	1:B:455:LYS:HB2	2.03	0.59
1:D:265:VAL:HG13	1:D:269:TYR:HE2	1.67	0.59
1:D:344:PHE:HA	1:D:436:ASN:OD1	2.03	0.59
2:E:146:VAL:HG13	2:E:155:LEU:HB3	1.85	0.59
1:D:469:LEU:HD12	1:D:474:LEU:HD12	1.85	0.59
1:C:150:LEU:HD11	3:C:502:TBR:BR5	2.58	0.59
2:F:153:VAL:HG11	2:F:435:VAL:HG21	1.85	0.59
2:H:188:ILE:HG23	2:H:209:VAL:HG22	1.84	0.59
1:B:153:LEU:HD13	1:B:154:GLY:H	1.68	0.58
2:H:258:LYS:HG2	2:H:278:ILE:HD11	1.85	0.58
2:F:6:LEU:HB2	2:F:71:ALA:HA	1.85	0.58
2:F:415:ARG:NH2	2:F:427:VAL:O	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:CYS:HA	1:C:335:LEU:HD11	1.85	0.58
2:G:301:PHE:HB3	2:G:326:VAL:HG12	1.84	0.58
2:H:310:THR:O	2:H:314:SER:HB3	2.02	0.58
1:C:372:LEU:HG	1:D:476:ILE:HG22	1.84	0.58
1:D:112:THR:HA	1:D:437:ASN:HB3	1.84	0.58
1:A:453:ASN:OD1	1:A:454:ASP:N	2.36	0.58
1:D:290:CYS:HA	1:D:335:LEU:HD11	1.84	0.58
2:E:148:PHE:HB2	2:E:153:VAL:HG13	1.86	0.58
2:F:68:MET:HG3	2:F:94:ASN:HB3	1.86	0.58
2:F:126:GLU:O	2:F:130:THR:HG23	2.04	0.58
1:C:469:LEU:HD12	1:C:474:LEU:HD12	1.86	0.58
1:B:290:CYS:HA	1:B:335:LEU:HD11	1.85	0.58
1:C:8:ARG:HD3	1:C:59:ARG:H	1.69	0.58
1:C:377:HIS:ND1	2:F:293:GLU:OE2	2.27	0.58
2:G:364:ARG:HG3	2:G:365:ALA:N	2.18	0.57
1:C:136:TRP:HE1	1:C:193:THR:HG21	1.69	0.57
1:B:344:PHE:HA	1:B:436:ASN:OD1	2.04	0.57
1:C:234:ASP:OD2	1:C:234:ASP:N	2.37	0.57
1:D:236:TYR:H	1:D:236:TYR:HD2	1.51	0.57
2:G:274:LEU:HD13	2:G:277:THR:OG1	2.04	0.57
2:G:275:GLU:O	2:G:275:GLU:HG3	2.03	0.57
1:B:112:THR:HA	1:B:437:ASN:HB3	1.86	0.57
2:F:183:THR:HA	2:F:421:ILE:HG21	1.85	0.57
2:G:184:ARG:HH21	2:G:422:ALA:HB3	1.69	0.57
1:A:420:THR:OG1	1:A:455:LYS:HB2	2.04	0.57
2:E:310:THR:O	2:E:314:SER:HB3	2.04	0.57
1:D:38:PRO:HB3	1:D:90:ILE:HG23	1.86	0.57
1:A:374:ARG:HD2	1:B:394:ARG:HH21	1.70	0.57
2:E:295:ILE:HD12	2:E:298:VAL:HG11	1.85	0.57
2:F:370:VAL:HG23	2:F:381:ILE:HG22	1.86	0.57
2:F:99:ILE:HG13	2:F:122:LEU:HD23	1.86	0.57
2:F:237:ILE:HG13	2:F:259:LEU:HG	1.86	0.57
1:C:343:SER:HB2	1:C:438:LEU:HD21	1.85	0.57
1:A:142:ILE:HG23	1:A:352:THR:HG22	1.86	0.57
1:B:287:PHE:HA	1:B:314:THR:HG21	1.85	0.57
2:F:116:ALA:HB2	2:G:88:THR:HG21	1.85	0.57
2:F:117:ILE:HG22	2:F:119:VAL:HG23	1.87	0.57
2:G:125:PRO:HB2	5:G:501:NAD:N7N	2.20	0.57
1:B:38:PRO:HG3	1:B:90:ILE:HG12	1.86	0.56
2:G:20:VAL:HG21	2:G:45:LEU:HD12	1.87	0.56
1:A:71:LEU:HD13	1:A:477:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:THR:OG1	1:C:455:LYS:HB2	2.06	0.56
1:D:262:SER:OG	1:D:263:GLY:N	2.37	0.56
2:H:395:VAL:HA	2:H:428:ILE:HB	1.87	0.56
1:B:469:LEU:HD12	1:B:474:LEU:HD12	1.88	0.56
1:C:379:ARG:HD3	2:F:289:LEU:HD22	1.87	0.56
2:F:237:ILE:HD11	2:F:248:ALA:HB2	1.88	0.56
1:A:226:HIS:CE1	1:A:232:TYR:HB3	2.41	0.56
2:G:68:MET:HG3	2:G:94:ASN:HB3	1.88	0.56
2:E:20:VAL:HG21	2:E:45:LEU:HD12	1.86	0.56
1:C:117:ILE:HD11	1:C:131:ARG:HD2	1.86	0.56
2:E:388:ASP:HB2	2:E:391:THR:HG22	1.86	0.56
1:A:427:ALA:O	1:A:431:VAL:HG22	2.06	0.56
2:E:274:LEU:HD13	2:E:277:THR:OG1	2.05	0.56
2:G:143:LEU:HD13	2:G:158:VAL:HA	1.87	0.56
2:E:415:ARG:NH2	2:E:427:VAL:O	2.33	0.56
2:H:359:LEU:HA	2:H:362:VAL:HG22	1.87	0.56
1:C:24:PRO:HB2	1:C:39:PHE:HE1	1.70	0.56
1:C:453:ASN:OD1	1:C:454:ASP:N	2.39	0.56
1:D:441:GLY:HA3	1:D:447:LEU:HA	1.87	0.56
2:H:398:ALA:O	2:H:402:ILE:HG12	2.06	0.55
1:B:20:THR:HB	1:B:133:PHE:HE1	1.71	0.55
2:E:70:VAL:HA	2:E:96:VAL:HG23	1.88	0.55
2:E:111:LEU:HD21	2:H:85:VAL:HG22	1.89	0.55
2:F:287:GLN:O	2:F:291:THR:OG1	2.24	0.55
2:F:305:THR:OG1	2:F:311:ASN:OD1	2.12	0.55
1:B:453:ASN:OD1	1:B:454:ASP:N	2.39	0.55
2:H:176:GLU:HG3	2:H:225:LEU:HD22	1.89	0.55
2:F:363:ARG:HB3	2:F:367:ILE:HD13	1.88	0.55
1:C:2:GLN:HA	1:C:4:ARG:NH1	2.22	0.55
1:D:439:GLY:N	1:D:440:PRO:HD3	2.22	0.55
1:D:11:GLY:HA3	1:D:53:CYS:HB2	1.88	0.55
2:G:117:ILE:HG22	2:G:119:VAL:HG23	1.89	0.55
1:B:117:ILE:HD11	1:B:131:ARG:HD2	1.88	0.55
1:C:38:PRO:HB3	1:C:90:ILE:HG23	1.89	0.55
2:E:221:VAL:HG13	2:E:225:LEU:HD23	1.89	0.55
1:B:440:PRO:HB2	1:B:442:LEU:HD23	1.87	0.54
1:C:309:GLN:NE2	1:C:326:THR:HG22	2.21	0.54
1:A:110:THR:O	1:A:468:ARG:NH1	2.37	0.54
2:H:397:ARG:HB2	2:H:402:ILE:HG23	1.88	0.54
1:C:266:HIS:CG	1:C:267:PRO:HD3	2.43	0.54
2:G:421:ILE:HD13	2:G:421:ILE:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:THR:HG22	2:E:46:ARG:HE	1.72	0.54
2:E:237:ILE:HD11	2:E:248:ALA:HB2	1.90	0.54
2:G:257:VAL:HB	2:G:277:THR:HG22	1.90	0.54
2:F:189:PHE:CD1	2:F:194:PRO:HB3	2.42	0.54
2:G:284:ALA:H	5:G:501:NAD:H61A	1.55	0.54
1:B:86:LEU:HD12	1:B:89:LEU:HD12	1.90	0.54
2:F:295:ILE:HD12	2:F:298:VAL:HG11	1.89	0.54
2:E:77:GLU:HA	2:E:80:MET:HE2	1.90	0.54
2:H:146:VAL:HG13	2:H:155:LEU:HB3	1.89	0.54
1:C:344:PHE:HA	1:C:436:ASN:OD1	2.08	0.54
2:G:387:GLY:HA3	2:G:392:SER:HB2	1.89	0.54
1:A:205:MET:HB2	1:A:210:ALA:HB2	1.90	0.54
2:H:167:VAL:O	2:H:203:ILE:HB	2.08	0.54
2:H:70:VAL:HA	2:H:96:VAL:HG23	1.90	0.54
1:A:420:THR:O	1:A:453:ASN:ND2	2.41	0.54
2:E:68:MET:HG3	2:E:94:ASN:HB3	1.88	0.54
2:H:137:ILE:HD11	2:H:302:ILE:HD11	1.89	0.54
2:E:42:LYS:HE3	3:E:503:TBR:BRA	2.63	0.54
1:D:226:HIS:CE1	1:D:232:TYR:HB3	2.43	0.53
1:B:457:LYS:O	1:B:461:ILE:HG13	2.08	0.53
1:D:234:ASP:OD2	1:D:234:ASP:N	2.41	0.53
1:D:420:THR:HG23	1:D:453:ASN:HD22	1.71	0.53
2:G:38:GLU:HB3	3:G:503:TBR:BR9	2.63	0.53
1:A:20:THR:HB	1:A:133:PHE:HE1	1.73	0.53
1:D:142:ILE:HG23	1:D:352:THR:HG22	1.89	0.53
2:H:233:ARG:NH2	2:H:234:ARG:HH21	2.07	0.53
1:A:117:ILE:HD11	1:A:131:ARG:HD2	1.90	0.53
1:A:349:ALA:HB2	1:A:359:ILE:HG12	1.90	0.53
2:E:223:SER:HA	2:E:228:LEU:HB2	1.90	0.53
2:F:308:ASP:O	2:F:312:ILE:HD12	2.08	0.53
1:B:38:PRO:HG2	1:B:91:ALA:HB2	1.89	0.53
1:C:427:ALA:O	1:C:431:VAL:HG22	2.09	0.53
2:E:143:LEU:HD13	2:E:158:VAL:HA	1.89	0.53
1:C:109:LEU:HD13	1:C:134:LEU:HD22	1.91	0.53
1:A:24:PRO:HB2	1:A:39:PHE:HE1	1.72	0.53
1:A:354:GLY:HA3	1:A:468:ARG:NH2	2.23	0.53
1:C:220:ILE:HG22	1:C:321:ALA:HA	1.91	0.53
1:B:252:ASN:H	1:B:351:SER:HB3	1.74	0.53
2:G:252:GLU:O	2:G:276:ASN:ND2	2.42	0.53
1:A:468:ARG:HA	1:A:468:ARG:NE	2.24	0.53
2:F:327:MET:HG2	2:F:346:VAL:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ILE:O	1:B:153:LEU:N	2.39	0.53
2:E:153:VAL:HG11	2:E:435:VAL:HG21	1.91	0.53
1:D:20:THR:HB	1:D:133:PHE:HE1	1.73	0.53
1:A:425:LEU:HD11	1:B:424:GLU:HB3	1.90	0.53
2:E:67:ASP:HA	2:E:93:PRO:HG2	1.91	0.53
2:G:352:GLN:NE2	2:G:373:LEU:O	2.41	0.52
1:A:317:ILE:HD13	1:A:442:LEU:HD11	1.92	0.52
1:D:420:THR:O	1:D:453:ASN:ND2	2.42	0.52
1:D:268:LYS:HE3	1:D:272:LYS:HE3	1.90	0.52
2:F:15:LEU:HD11	2:F:358:LEU:HG	1.89	0.52
1:D:301:THR:OG1	1:D:302:SER:N	2.43	0.52
2:G:183:THR:HB	2:G:213:ALA:HB2	1.91	0.52
2:F:139:TYR:HE1	2:F:218:ILE:HG23	1.74	0.52
1:C:181:THR:HG22	1:C:257:PHE:HE2	1.74	0.52
2:H:38:GLU:HB3	3:H:503:TBR:BR9	2.65	0.52
1:D:109:LEU:HD13	1:D:134:LEU:HD22	1.91	0.52
2:H:301:PHE:HB3	2:H:326:VAL:HG12	1.91	0.52
1:B:363:LEU:HD12	1:B:399:VAL:HG21	1.91	0.52
1:D:345:ILE:HG12	1:D:361:ILE:HG13	1.91	0.52
2:H:125:PRO:HB2	5:H:501:NAD:N7N	2.24	0.52
2:F:146:VAL:HG13	2:F:155:LEU:HB3	1.91	0.52
1:D:441:GLY:H	1:D:447:LEU:HB3	1.74	0.52
2:F:126:GLU:N	5:F:501:NAD:H72N	2.07	0.52
1:A:373:LYS:HD2	1:A:382:TYR:CE1	2.45	0.52
2:H:3:ILE:HD11	2:H:26:ILE:HG12	1.91	0.52
2:F:137:ILE:HD11	2:F:302:ILE:HD11	1.91	0.52
1:A:2:GLN:HA	1:A:4:ARG:HH11	1.74	0.52
1:B:354:GLY:HA2	1:B:357:LYS:HE3	1.92	0.52
2:E:319:LYS:NZ	2:E:345:ASP:OD2	2.41	0.52
1:B:71:LEU:HD13	1:B:477:LEU:HD11	1.91	0.52
2:E:126:GLU:N	5:E:501:NAD:H72N	2.07	0.52
1:A:357:LYS:HD2	1:A:357:LYS:H	1.74	0.52
1:A:439:GLY:N	1:A:440:PRO:HD3	2.25	0.52
1:C:310:ALA:O	1:C:314:THR:HG23	2.10	0.52
1:A:430:ALA:HB1	1:A:460:LEU:HD21	1.90	0.52
1:D:153:LEU:HD22	1:D:154:GLY:H	1.73	0.52
2:H:100:ARG:NE	2:H:126:GLU:HG3	2.24	0.52
1:B:15:ALA:O	1:B:19:VAL:HG23	2.09	0.52
2:F:367:ILE:HD11	2:F:448:GLU:HG3	1.91	0.51
2:E:190:ARG:NH2	2:E:201:THR:HG22	2.25	0.51
1:D:184:ALA:HB1	1:D:257:PHE:HE1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:GLY:H	1:C:447:LEU:HB3	1.74	0.51
1:C:24:PRO:HB2	1:C:39:PHE:CE1	2.46	0.51
1:C:420:THR:O	1:C:453:ASN:ND2	2.43	0.51
1:A:266:HIS:N	1:A:267:PRO:HD2	2.26	0.51
1:D:2:GLN:HA	1:D:4:ARG:NH1	2.24	0.51
1:A:265:VAL:HG13	1:A:269:TYR:HE2	1.76	0.51
1:C:457:LYS:O	1:C:461:ILE:HG13	2.10	0.51
2:E:152:LYS:HE3	2:E:216:ASN:HD21	1.76	0.51
1:D:370:ARG:HD3	1:D:374:ARG:CZ	2.41	0.51
2:G:70:VAL:HA	2:G:96:VAL:HG23	1.93	0.51
2:F:414:VAL:HB	2:F:433:HIS:HB2	1.92	0.51
1:B:427:ALA:O	1:B:431:VAL:HG22	2.10	0.51
2:E:20:VAL:HG11	2:E:43:TYR:HB3	1.92	0.51
1:D:94:PRO:HG3	1:D:123:LEU:HD13	1.93	0.51
1:A:106:PHE:O	1:A:110:THR:OG1	2.23	0.51
1:C:142:ILE:HG23	1:C:352:THR:HG22	1.93	0.51
1:B:357:LYS:O	1:B:360:ARG:HB2	2.10	0.51
2:F:440:ASP:OD2	2:F:442:LYS:HB2	2.11	0.51
1:A:8:ARG:HD3	1:A:59:ARG:H	1.76	0.51
1:B:74:VAL:HG12	1:B:469:LEU:HD13	1.93	0.50
1:D:309:GLN:NE2	1:D:326:THR:HG22	2.25	0.50
1:A:438:LEU:CB	1:A:439:GLY:HA2	2.41	0.50
2:E:27:THR:HG22	2:E:46:ARG:HB3	1.94	0.50
1:B:110:THR:O	1:B:468:ARG:NH1	2.44	0.50
1:A:434:THR:HG22	1:A:464:MET:HB3	1.93	0.50
2:H:404:LEU:HD21	2:H:410:ILE:HG12	1.93	0.50
2:H:8:ALA:HA	2:H:28:ILE:HD11	1.93	0.50
1:C:117:ILE:HG13	1:C:120:LEU:HD23	1.93	0.50
2:F:111:LEU:HD21	2:G:85:VAL:HG22	1.92	0.50
2:F:143:LEU:HD21	2:F:159:LYS:HG2	1.93	0.50
1:C:476:ILE:HG22	1:D:372:LEU:HG	1.94	0.50
1:C:74:VAL:HG12	1:C:469:LEU:HD13	1.93	0.50
1:D:8:ARG:HD3	1:D:59:ARG:H	1.76	0.50
1:D:438:LEU:CB	1:D:439:GLY:HA2	2.38	0.50
2:E:290:LEU:HD12	2:E:295:ILE:HD13	1.94	0.50
1:C:472:PHE:O	1:C:476:ILE:HG23	2.12	0.50
1:D:89:LEU:HD21	1:D:98:VAL:HA	1.93	0.50
1:D:24:PRO:HB2	1:D:39:PHE:CE1	2.46	0.50
2:H:85:VAL:O	2:H:89:LEU:HB2	2.11	0.50
1:D:71:LEU:HD13	1:D:477:LEU:HD11	1.94	0.50
2:E:89:LEU:HD12	2:H:111:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:GLY:HA2	1:C:357:LYS:HE3	1.93	0.50
1:C:334:PHE:HD2	1:C:335:LEU:HD22	1.77	0.50
2:H:8:ALA:N	2:H:30:ASP:OD2	2.35	0.50
2:E:117:ILE:HG22	2:E:119:VAL:HG23	1.94	0.50
1:A:309:GLN:NE2	1:A:326:THR:HG22	2.27	0.50
1:B:373:LYS:HD2	1:B:382:TYR:CE1	2.47	0.50
2:H:221:VAL:O	2:H:225:LEU:HB2	2.12	0.50
2:E:221:VAL:O	2:E:225:LEU:HB2	2.12	0.50
2:F:155:LEU:HD11	2:F:210:PHE:HD2	1.76	0.50
2:H:136:LEU:HD13	2:H:346:VAL:HG21	1.92	0.50
2:F:369:ASN:HB2	2:F:382:GLU:HB3	1.94	0.50
2:E:183:THR:HB	2:E:213:ALA:HB2	1.92	0.50
2:H:100:ARG:HE	2:H:126:GLU:HG3	1.77	0.49
2:E:145:VAL:HG22	2:E:156:VAL:HG23	1.93	0.49
2:E:364:ARG:HB3	2:E:366:ASP:OD1	2.12	0.49
1:C:86:LEU:HD12	1:C:89:LEU:HD12	1.93	0.49
1:A:476:ILE:HA	1:A:479:THR:HG23	1.92	0.49
1:B:441:GLY:H	1:B:447:LEU:HB3	1.76	0.49
2:F:124:ALA:O	2:F:128:LEU:HG	2.13	0.49
1:A:142:ILE:HD12	1:A:468:ARG:CZ	2.41	0.49
1:D:356:MET:HE1	1:D:403:PHE:HD1	1.77	0.49
2:E:359:LEU:HA	2:E:362:VAL:HG22	1.93	0.49
1:A:112:THR:HG23	1:A:437:ASN:HA	1.95	0.49
1:A:24:PRO:HB2	1:A:39:PHE:CE1	2.47	0.49
1:B:438:LEU:HB3	1:B:440:PRO:HD2	1.94	0.49
2:E:287:GLN:O	2:E:291:THR:OG1	2.31	0.49
2:E:266:ARG:O	2:E:270:LEU:HB2	2.13	0.49
1:D:434:THR:HG22	1:D:464:MET:HB3	1.93	0.49
1:B:468:ARG:HA	1:B:468:ARG:NE	2.27	0.49
2:G:300:VAL:HG12	2:G:325:LYS:HB2	1.94	0.49
2:F:101:SER:HB3	2:F:104:TYR:HD2	1.76	0.49
1:A:39:PHE:CE2	1:A:87:PRO:HB3	2.48	0.49
1:C:226:HIS:CE1	1:C:232:TYR:HB3	2.47	0.49
1:A:430:ALA:O	1:A:434:THR:OG1	2.31	0.49
1:D:373:LYS:HD2	1:D:382:TYR:CE1	2.46	0.49
1:B:94:PRO:HG3	1:B:123:LEU:HD13	1.93	0.49
1:D:74:VAL:HG12	1:D:469:LEU:HD13	1.94	0.49
2:E:258:LYS:HG2	2:E:278:ILE:HD11	1.94	0.49
1:B:472:PHE:O	1:B:476:ILE:HG23	2.12	0.49
1:B:11:GLY:HA3	1:B:53:CYS:HB2	1.94	0.49
2:G:126:GLU:O	2:G:130:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:327:MET:HG2	2:G:346:VAL:HG13	1.94	0.49
1:C:294:LEU:HD12	1:C:310:ALA:HB2	1.94	0.49
1:D:149:ILE:O	1:D:153:LEU:N	2.41	0.49
2:G:153:VAL:HG11	2:G:435:VAL:HG21	1.94	0.49
1:D:391:LEU:HD12	1:D:395:VAL:HG11	1.95	0.49
1:D:427:ALA:O	1:D:431:VAL:HG22	2.12	0.49
2:E:7:GLY:O	2:E:12:GLY:HA3	2.13	0.49
2:G:29:VAL:HG22	2:G:48:VAL:HB	1.95	0.49
1:A:406:TYR:HA	1:A:471:ILE:HD13	1.94	0.49
2:H:237:ILE:HD11	2:H:248:ALA:HB2	1.93	0.49
2:F:27:THR:HG22	2:F:46:ARG:HE	1.77	0.49
2:F:258:LYS:HD3	2:F:293:GLU:HG3	1.94	0.49
1:B:112:THR:HG23	1:B:437:ASN:HA	1.94	0.49
1:B:476:ILE:HA	1:B:479:THR:HG23	1.95	0.49
2:G:169:ASN:ND2	2:G:203:ILE:HD11	2.28	0.48
2:H:388:ASP:HA	2:H:430:GLN:HG2	1.95	0.48
1:A:236:TYR:H	1:A:236:TYR:HD2	1.59	0.48
1:C:417:LEU:HD11	1:C:460:LEU:HD21	1.95	0.48
2:E:308:ASP:O	2:E:312:ILE:HD12	2.13	0.48
1:C:356:MET:HE1	1:C:403:PHE:HD1	1.77	0.48
2:F:330:ILE:HB	2:F:336:VAL:HG22	1.95	0.48
2:H:2:LYS:HB3	2:H:25:ASP:HB3	1.96	0.48
2:H:2:LYS:HD2	2:H:65:ASP:O	2.13	0.48
1:B:434:THR:HG22	1:B:464:MET:HB3	1.95	0.48
2:F:85:VAL:HG22	2:G:111:LEU:HD21	1.95	0.48
2:G:283:ASP:OD2	5:G:501:NAD:N6A	2.46	0.48
2:G:147:SER:HB2	2:G:151:GLN:HA	1.95	0.48
2:E:399:ILE:HB	2:E:424:ASP:HA	1.95	0.48
2:H:6:LEU:HD22	2:H:52:ALA:HB1	1.94	0.48
1:C:142:ILE:HD12	1:C:468:ARG:CZ	2.43	0.48
1:D:112:THR:HG23	1:D:437:ASN:HA	1.96	0.48
1:B:294:LEU:HD12	1:B:310:ALA:HB2	1.94	0.48
1:B:143:ILE:HG21	1:B:253:PHE:CD2	2.49	0.48
1:C:149:ILE:O	1:C:153:LEU:N	2.44	0.48
1:A:460:LEU:O	1:A:464:MET:HG2	2.13	0.48
1:A:361:ILE:O	1:A:365:THR:HG23	2.13	0.48
2:F:36:LEU:HD22	2:F:47:VAL:HG13	1.96	0.48
1:B:251:CYS:SG	1:B:276:PHE:HD1	2.36	0.48
2:H:36:LEU:HD22	2:H:47:VAL:HG13	1.96	0.48
2:H:2:LYS:HG3	2:H:66:ALA:HA	1.96	0.48
1:C:153:LEU:HD22	1:C:154:GLY:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:238:VAL:HG23	2:G:303:ALA:HA	1.96	0.48
1:C:20:THR:HB	1:C:133:PHE:HE1	1.78	0.48
1:B:2:GLN:HA	1:B:4:ARG:HH11	1.79	0.48
2:G:258:LYS:HE2	2:G:278:ILE:HD11	1.96	0.48
1:B:181:THR:HA	1:B:184:ALA:HB3	1.96	0.48
2:E:257:VAL:HB	2:E:277:THR:HG22	1.95	0.48
2:F:8:ALA:HA	2:F:28:ILE:HD11	1.95	0.48
2:G:134:GLU:OE2	2:G:250:ARG:NH1	2.46	0.48
1:A:181:THR:HA	1:A:184:ALA:HB3	1.96	0.48
1:B:142:ILE:HD12	1:B:468:ARG:CZ	2.44	0.48
1:A:233:PHE:C	1:A:235:SER:H	2.17	0.48
1:A:301:THR:OG1	1:A:302:SER:N	2.47	0.48
1:D:406:TYR:HA	1:D:471:ILE:HD13	1.95	0.48
1:D:183:LYS:HE3	1:D:187:TYR:HE2	1.78	0.48
1:C:38:PRO:HG2	1:C:91:ALA:HB2	1.94	0.47
1:A:140:MET:HE2	1:A:186:TRP:HB2	1.96	0.47
1:A:11:GLY:HA3	1:A:53:CYS:HB2	1.94	0.47
1:D:468:ARG:HA	1:D:468:ARG:NE	2.29	0.47
2:G:290:LEU:HD12	2:G:295:ILE:HD13	1.96	0.47
1:C:300:TYR:CZ	1:C:309:GLN:HG3	2.48	0.47
2:G:99:ILE:HG13	2:G:122:LEU:HD23	1.95	0.47
2:H:26:ILE:O	2:H:45:LEU:HB2	2.14	0.47
2:H:126:GLU:O	2:H:130:THR:HG23	2.14	0.47
2:H:148:PHE:HB2	2:H:153:VAL:HG13	1.95	0.47
1:A:109:LEU:HD13	1:A:134:LEU:HD22	1.95	0.47
2:E:237:ILE:HG13	2:E:259:LEU:HG	1.96	0.47
1:C:76:PHE:O	1:C:80:LEU:HB2	2.13	0.47
2:F:332:ARG:HA	3:F:503:TBR:BR2	2.69	0.47
1:A:86:LEU:HD12	1:A:89:LEU:HD12	1.96	0.47
2:G:283:ASP:OD2	2:G:284:ALA:N	2.47	0.47
2:G:237:ILE:HD11	2:G:248:ALA:HB2	1.96	0.47
1:C:468:ARG:NE	1:C:468:ARG:HA	2.29	0.47
2:H:266:ARG:O	2:H:270:LEU:HB2	2.14	0.47
1:B:184:ALA:HB1	1:B:257:PHE:HE1	1.79	0.47
2:F:111:LEU:HD11	2:G:85:VAL:HG22	1.97	0.47
2:E:258:LYS:HE2	2:E:278:ILE:HD11	1.97	0.47
1:D:233:PHE:C	1:D:235:SER:H	2.18	0.47
1:B:420:THR:HG23	1:B:453:ASN:HD22	1.80	0.47
1:C:77:TRP:CD1	1:C:469:LEU:HD21	2.50	0.47
1:C:153:LEU:HD13	1:C:154:GLY:H	1.79	0.47
1:B:226:HIS:CE1	1:B:232:TYR:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:PHE:C	1:C:235:SER:H	2.18	0.47
1:A:194:ILE:O	1:A:198:VAL:HG12	2.15	0.47
1:B:300:TYR:CZ	1:B:309:GLN:HG3	2.50	0.47
2:G:7:GLY:O	2:G:12:GLY:HA3	2.15	0.47
1:A:384:ILE:HG22	1:A:391:LEU:HD23	1.97	0.47
1:B:24:PRO:HB2	1:B:39:PHE:CE1	2.49	0.47
1:A:357:LYS:O	1:A:360:ARG:HB2	2.14	0.47
2:F:138:GLN:HG3	2:F:139:TYR:CD2	2.50	0.47
1:A:220:ILE:HG22	1:A:321:ALA:HA	1.96	0.47
2:F:10:GLN:HE21	2:F:98:ARG:HH12	1.63	0.47
1:C:251:CYS:SG	1:C:276:PHE:HD1	2.37	0.47
1:C:439:GLY:N	1:C:440:PRO:HD3	2.29	0.47
2:G:126:GLU:N	5:G:501:NAD:H72N	2.13	0.47
1:A:438:LEU:HB3	1:A:440:PRO:HD2	1.95	0.47
2:F:235:ILE:HG12	2:F:300:VAL:HG23	1.97	0.47
2:F:360:THR:CG2	2:F:370:VAL:HG12	2.45	0.47
2:H:153:VAL:HG11	2:H:435:VAL:HG21	1.97	0.47
1:A:153:LEU:HD22	1:A:154:GLY:H	1.78	0.47
1:D:457:LYS:O	1:D:461:ILE:HG13	2.14	0.47
2:E:392:SER:HB3	2:E:395:VAL:HG22	1.97	0.47
2:F:125:PRO:HB3	2:F:354:THR:CG2	2.44	0.47
1:D:361:ILE:O	1:D:365:THR:HG23	2.15	0.47
1:B:357:LYS:H	1:B:357:LYS:HD2	1.79	0.47
2:F:143:LEU:HD13	2:F:158:VAL:HA	1.97	0.47
1:A:472:PHE:O	1:A:476:ILE:HG23	2.14	0.47
2:E:271:SER:HA	2:E:279:VAL:HG21	1.97	0.47
1:A:417:LEU:O	1:A:420:THR:HG22	2.15	0.46
2:H:238:VAL:HG23	2:H:303:ALA:HA	1.98	0.46
2:H:258:LYS:HD3	2:H:293:GLU:HG3	1.98	0.46
1:B:8:ARG:HD3	1:B:59:ARG:H	1.79	0.46
1:C:128:LEU:HD11	1:C:225:THR:HA	1.97	0.46
2:F:364:ARG:HG3	2:F:365:ALA:N	2.30	0.46
1:D:38:PRO:HG2	1:D:91:ALA:HB2	1.96	0.46
1:C:2:GLN:HA	1:C:4:ARG:HH11	1.80	0.46
2:G:117:ILE:O	2:G:119:VAL:N	2.45	0.46
2:G:48:VAL:HG21	2:G:61:ALA:HA	1.97	0.46
1:B:76:PHE:O	1:B:80:LEU:HB2	2.15	0.46
1:B:74:VAL:O	1:B:78:THR:HB	2.15	0.46
1:B:430:ALA:O	1:B:434:THR:OG1	2.34	0.46
1:B:333:LEU:HD22	1:B:337:VAL:HG23	1.96	0.46
1:D:294:LEU:HD11	1:D:331:TRP:CZ2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:36:LEU:HD22	2:G:47:VAL:HG13	1.98	0.46
1:D:148:ALA:O	1:D:151:PRO:HD2	2.14	0.46
1:D:229:SER:OG	1:D:230:MET:N	2.48	0.46
1:D:291:PHE:CZ	1:D:295:LEU:HD11	2.51	0.46
1:C:31:TYR:HD1	1:C:125:LYS:HG3	1.80	0.46
1:B:124:PRO:HG2	1:B:127:ILE:HD12	1.98	0.46
1:D:142:ILE:HD12	1:D:468:ARG:CZ	2.45	0.46
1:C:384:ILE:HG22	1:C:391:LEU:HD23	1.97	0.46
1:B:24:PRO:HB2	1:B:39:PHE:HE1	1.80	0.46
2:H:4:ILE:HG12	2:H:27:THR:OG1	2.15	0.46
2:H:243:ILE:HG22	2:H:304:LEU:HD13	1.97	0.46
1:D:236:TYR:CD2	1:D:236:TYR:N	2.83	0.46
1:B:233:PHE:C	1:B:235:SER:H	2.19	0.46
1:C:148:ALA:O	1:C:151:PRO:HD2	2.14	0.46
1:A:80:LEU:HB3	1:A:109:LEU:HD21	1.97	0.46
1:A:286:LEU:HD22	1:A:314:THR:HB	1.98	0.46
1:D:442:LEU:H	1:D:447:LEU:HD22	1.81	0.46
1:A:343:SER:HB2	1:A:438:LEU:HD11	1.97	0.46
2:G:258:LYS:HD3	2:G:293:GLU:HG3	1.97	0.46
1:D:476:ILE:HA	1:D:479:THR:HG23	1.97	0.46
1:C:259:ALA:HA	1:C:266:HIS:HB3	1.98	0.46
2:E:67:ASP:O	2:E:93:PRO:HB2	2.15	0.46
1:B:142:ILE:HD13	1:B:352:THR:HA	1.96	0.46
1:C:89:LEU:HD21	1:C:98:VAL:HA	1.96	0.46
1:A:153:LEU:HD13	1:A:154:GLY:H	1.80	0.46
2:H:421:ILE:HG12	2:H:421:ILE:H	1.47	0.46
2:E:402:ILE:H	2:E:402:ILE:HG13	1.42	0.46
1:C:140:MET:HE2	1:C:186:TRP:HB2	1.97	0.46
1:B:236:TYR:N	1:B:236:TYR:CD2	2.84	0.46
2:G:359:LEU:HD13	2:G:363:ARG:HH21	1.80	0.46
2:E:403:LYS:HG3	2:E:403:LYS:H	1.58	0.46
1:A:326:THR:OG1	1:A:327:GLY:N	2.47	0.46
2:G:29:VAL:HA	2:G:48:VAL:O	2.16	0.46
1:A:345:ILE:HG21	1:A:361:ILE:HD12	1.99	0.46
2:E:356:SER:HB3	2:E:371:SER:HA	1.98	0.46
2:G:308:ASP:O	2:G:312:ILE:HD12	2.16	0.46
2:G:148:PHE:HB3	2:G:382:GLU:OE2	2.16	0.45
2:E:238:VAL:HG12	2:E:260:ILE:HB	1.97	0.45
1:A:192:LEU:HD23	1:A:192:LEU:HA	1.74	0.45
1:D:420:THR:OG1	1:D:455:LYS:HB2	2.17	0.45
2:F:238:VAL:HG23	2:F:303:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:SER:OG	1:A:230:MET:N	2.48	0.45
1:A:72:ILE:HA	1:A:72:ILE:HD13	1.82	0.45
1:D:72:ILE:HA	1:D:72:ILE:HD13	1.80	0.45
1:A:310:ALA:O	1:A:314:THR:HG23	2.17	0.45
2:H:274:LEU:HD13	2:H:277:THR:OG1	2.16	0.45
2:G:136:LEU:HD13	2:G:346:VAL:HG21	1.97	0.45
1:A:418:ILE:HD12	1:B:337:VAL:HG11	1.98	0.45
1:A:287:PHE:HA	1:A:314:THR:HG21	1.99	0.45
2:H:335:TYR:O	2:H:339:VAL:HG22	2.16	0.45
2:G:360:THR:HG22	2:G:370:VAL:H	1.80	0.45
2:H:188:ILE:HG22	2:H:207:ASP:HB3	1.98	0.45
1:C:476:ILE:HA	1:C:479:THR:HG23	1.97	0.45
1:A:317:ILE:HG21	1:A:339:LEU:HB3	1.98	0.45
1:A:76:PHE:O	1:A:80:LEU:HB2	2.16	0.45
1:A:297:HIS:CG	1:A:332:PRO:HG3	2.52	0.45
1:C:226:HIS:ND1	1:C:232:TYR:HB3	2.32	0.45
1:A:477:LEU:HD13	1:A:477:LEU:HA	1.75	0.45
2:F:384:VAL:HG22	2:F:433:HIS:ND1	2.32	0.45
2:H:410:ILE:HD13	2:H:436:MET:HB3	1.98	0.45
1:A:328:PHE:HA	1:A:331:TRP:CD1	2.51	0.45
1:D:178:ILE:HB	3:D:502:TBR:BRA	2.72	0.45
2:E:283:ASP:OD2	5:E:501:NAD:N6A	2.49	0.45
2:G:233:ARG:NH2	2:G:234:ARG:HH21	2.15	0.45
1:A:406:TYR:HA	1:A:471:ILE:CD1	2.47	0.45
2:G:330:ILE:HB	2:G:336:VAL:HG22	1.98	0.45
1:B:230:MET:HG3	1:B:312:PHE:HZ	1.80	0.45
1:B:21:MET:HB2	1:B:43:PHE:HB2	1.99	0.45
2:H:79:ASN:HA	2:H:79:ASN:HD22	1.59	0.45
1:D:86:LEU:HD12	1:D:86:LEU:HA	1.82	0.45
2:G:26:ILE:O	2:G:45:LEU:HB2	2.16	0.45
1:A:473:THR:HA	1:A:476:ILE:HD12	1.99	0.45
1:C:71:LEU:HD13	1:C:477:LEU:HD11	1.98	0.45
2:H:173:ALA:HB1	2:H:177:HIS:NE2	2.32	0.45
1:D:417:LEU:O	1:D:420:THR:HG22	2.17	0.44
1:D:39:PHE:N	1:D:39:PHE:CD2	2.85	0.44
1:B:94:PRO:HG2	1:B:127:ILE:HG21	1.99	0.44
2:F:27:THR:HA	2:F:46:ARG:O	2.17	0.44
1:D:230:MET:SD	1:D:232:TYR:OH	2.67	0.44
1:A:418:ILE:HD13	1:B:337:VAL:HG21	1.98	0.44
2:F:359:LEU:HA	2:F:362:VAL:HG23	1.99	0.44
2:E:2:LYS:HD2	2:E:65:ASP:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:LEU:HD11	1:D:424:GLU:HB3	1.98	0.44
1:A:66:SER:O	1:A:69:GLY:N	2.49	0.44
2:G:145:VAL:HG22	2:G:156:VAL:HG23	1.99	0.44
1:C:94:PRO:HG3	1:C:123:LEU:HD13	1.99	0.44
2:F:10:GLN:NE2	2:F:74:ASN:OD1	2.43	0.44
2:H:223:SER:HA	2:H:228:LEU:HB2	1.99	0.44
1:A:469:LEU:HD12	1:A:474:LEU:HD12	1.99	0.44
2:H:190:ARG:NH2	2:H:202:ILE:O	2.51	0.44
2:E:190:ARG:HH22	2:E:201:THR:HG22	1.82	0.44
2:H:360:THR:HG23	2:H:370:VAL:HG12	2.00	0.44
2:H:364:ARG:HD2	2:H:364:ARG:HA	1.80	0.44
2:G:112:PHE:CD1	2:G:122:LEU:HD21	2.52	0.44
1:D:220:ILE:HD12	1:D:352:THR:C	2.38	0.44
1:A:252:ASN:HB2	1:A:348:CYS:HB3	2.00	0.44
2:G:309:GLU:HG2	2:H:310:THR:HA	2.00	0.44
1:A:358:VAL:O	1:A:361:ILE:HG22	2.17	0.44
2:H:319:LYS:NZ	2:H:345:ASP:OD2	2.51	0.44
1:C:199:ALA:HB1	1:C:241:ILE:HD13	1.99	0.44
1:B:266:HIS:N	1:B:267:PRO:HD2	2.32	0.44
2:F:408:THR:HG23	2:F:438:LEU:HD13	2.00	0.44
1:D:246:LEU:HA	1:D:246:LEU:HD23	1.87	0.44
2:H:117:ILE:HG22	2:H:119:VAL:HG23	1.99	0.44
2:G:11:VAL:HG11	2:G:72:VAL:HG21	2.00	0.44
2:H:360:THR:CG2	2:H:370:VAL:HG12	2.47	0.44
1:A:345:ILE:HG21	1:A:361:ILE:HB	1.99	0.44
1:C:418:ILE:HD13	1:D:337:VAL:HG21	1.99	0.44
2:E:125:PRO:HB2	5:E:501:NAD:N7N	2.33	0.44
1:C:39:PHE:N	1:C:39:PHE:CD2	2.86	0.44
1:A:39:PHE:CD2	1:A:39:PHE:N	2.84	0.44
2:F:125:PRO:HB2	5:F:501:NAD:N7N	2.32	0.44
2:H:136:LEU:HA	2:H:136:LEU:HD23	1.82	0.44
2:H:327:MET:HG2	2:H:346:VAL:HG13	1.99	0.44
2:G:108:LYS:HG3	2:G:122:LEU:HD13	1.99	0.44
2:E:369:ASN:HB2	2:E:382:GLU:HB3	2.00	0.44
1:C:236:TYR:HD2	1:C:236:TYR:H	1.65	0.44
2:G:237:ILE:HG13	2:G:259:LEU:HG	2.00	0.44
1:D:310:ALA:O	1:D:314:THR:HG23	2.18	0.44
2:G:233:ARG:HB3	2:G:234:ARG:HG2	2.00	0.44
2:E:149:ALA:O	2:E:152:LYS:HB2	2.18	0.44
2:G:359:LEU:HA	2:G:362:VAL:HG23	2.00	0.44
1:B:22:LEU:HD21	1:B:43:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:406:PRO:HB2	2:H:443:TYR:CE2	2.53	0.44
2:E:59:HIS:CE1	3:H:502:TBR:BRC	3.26	0.44
2:G:391:THR:HA	2:G:456:PHE:CD2	2.53	0.44
1:C:477:LEU:HD13	1:C:477:LEU:HA	1.87	0.44
2:G:155:LEU:HD13	2:G:212:VAL:HG22	1.99	0.44
2:F:48:VAL:HG21	2:F:61:ALA:HA	2.00	0.44
1:C:185:LEU:HA	1:C:185:LEU:HD23	1.87	0.44
1:A:357:LYS:CD	1:A:357:LYS:H	2.31	0.43
1:C:150:LEU:HB2	1:C:151:PRO:HD3	1.98	0.43
1:C:149:ILE:HD11	1:C:155:ILE:HD12	2.00	0.43
2:G:266:ARG:O	2:G:270:LEU:HB2	2.18	0.43
2:G:124:ALA:O	2:G:128:LEU:HG	2.18	0.43
1:A:458:TRP:CE3	1:A:461:ILE:HD12	2.53	0.43
1:C:229:SER:OG	1:C:230:MET:N	2.49	0.43
1:C:334:PHE:CD1	1:D:419:ALA:HB2	2.54	0.43
2:E:92:THR:HA	2:E:93:PRO:HD3	1.86	0.43
1:B:476:ILE:HG12	1:B:482:PHE:CD1	2.53	0.43
1:B:236:TYR:HD2	1:B:236:TYR:N	2.16	0.43
1:B:148:ALA:O	1:B:151:PRO:HD2	2.18	0.43
2:E:190:ARG:HD3	2:E:204:GLU:CD	2.38	0.43
2:E:283:ASP:OD2	2:E:284:ALA:N	2.51	0.43
1:B:192:LEU:HA	1:B:192:LEU:HD23	1.87	0.43
1:A:468:ARG:HA	1:A:468:ARG:HE	1.83	0.43
1:C:74:VAL:O	1:C:78:THR:HB	2.19	0.43
1:D:435:LEU:HD21	1:D:471:ILE:HD11	1.99	0.43
2:F:165:PRO:HB2	2:F:166:LEU:H	1.47	0.43
2:F:399:ILE:HG12	2:F:426:THR:O	2.18	0.43
1:C:49:CYS:O	1:C:52:MET:HG2	2.18	0.43
1:D:341:PHE:HA	1:D:341:PHE:HD1	1.74	0.43
2:F:75:THR:HG22	2:F:77:GLU:HG2	1.98	0.43
1:C:438:LEU:HB3	1:C:440:PRO:HD2	2.00	0.43
2:F:283:ASP:OD2	2:F:284:ALA:N	2.51	0.43
1:D:80:LEU:HB3	1:D:109:LEU:HD21	2.00	0.43
2:G:165:PRO:HB2	2:G:166:LEU:H	1.57	0.43
2:F:356:SER:HB3	2:F:371:SER:HA	2.00	0.43
1:D:317:ILE:HG21	1:D:339:LEU:HB3	2.01	0.43
1:D:4:ARG:H	1:D:4:ARG:HG2	1.53	0.43
1:D:74:VAL:O	1:D:78:THR:HB	2.19	0.43
1:C:466:PHE:HE1	1:C:474:LEU:HD22	1.83	0.43
1:B:253:PHE:CD1	1:B:256:HIS:HD2	2.36	0.43
1:A:333:LEU:O	1:A:336:PRO:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:LEU:HA	1:D:192:LEU:HD23	1.74	0.43
1:A:39:PHE:HD2	1:A:39:PHE:N	2.17	0.43
2:H:176:GLU:O	2:H:176:GLU:HG2	2.19	0.43
1:A:411:VAL:HG13	1:B:341:PHE:CE2	2.53	0.43
1:B:406:TYR:HA	1:B:471:ILE:HD13	2.00	0.43
2:F:173:ALA:O	2:F:177:HIS:ND1	2.52	0.43
1:A:356:MET:HE1	1:A:403:PHE:HD1	1.84	0.43
1:C:43:PHE:O	1:C:47:LEU:HB2	2.19	0.43
2:F:405:PRO:HG2	2:F:447:VAL:HG23	2.01	0.43
2:H:290:LEU:HD12	2:H:295:ILE:HD13	2.00	0.43
1:A:13:LEU:HA	1:A:13:LEU:HD23	1.76	0.43
2:F:92:THR:O	2:F:95:ARG:NH1	2.52	0.43
2:E:29:VAL:HA	2:E:48:VAL:O	2.19	0.43
2:F:189:PHE:HD2	2:F:374:ARG:HE	1.66	0.43
1:B:297:HIS:CD2	1:B:332:PRO:HG3	2.54	0.43
1:C:288:LEU:HA	1:C:288:LEU:HD22	1.83	0.43
2:F:403:LYS:H	2:F:403:LYS:HG3	1.59	0.43
1:B:473:THR:HA	1:B:476:ILE:HD12	2.01	0.43
3:F:502:TBR:BRC	2:G:59:HIS:CG	3.27	0.43
1:C:328:PHE:HA	1:C:331:TRP:CD1	2.54	0.43
1:C:333:LEU:HD22	1:C:337:VAL:HG23	1.99	0.43
1:D:255:LEU:HD22	1:D:270:TYR:CD1	2.54	0.43
1:B:75:LEU:HA	1:B:75:LEU:HD12	1.78	0.43
1:B:178:ILE:C	1:B:180:GLU:H	2.20	0.43
2:H:428:ILE:HG12	2:H:428:ILE:H	1.57	0.43
1:B:4:ARG:H	1:B:4:ARG:HG2	1.42	0.43
2:F:29:VAL:HA	2:F:48:VAL:O	2.18	0.43
1:A:457:LYS:O	1:A:461:ILE:HG13	2.18	0.43
2:H:295:ILE:HD12	2:H:298:VAL:HG11	2.01	0.43
1:D:128:LEU:HD11	1:D:225:THR:HA	2.00	0.43
2:H:165:PRO:HB2	2:H:166:LEU:H	1.51	0.43
2:H:101:SER:HB3	2:H:104:TYR:HD2	1.83	0.43
1:A:9:ILE:H	1:A:9:ILE:HG12	1.56	0.43
1:C:138:GLY:O	1:C:142:ILE:HG22	2.18	0.42
1:D:476:ILE:HG12	1:D:482:PHE:CD1	2.53	0.42
1:C:134:LEU:HA	1:C:134:LEU:HD23	1.81	0.42
1:D:76:PHE:O	1:D:80:LEU:HB2	2.18	0.42
2:H:406:PRO:HB2	2:H:443:TYR:HE2	1.83	0.42
1:C:361:ILE:O	1:C:365:THR:HG23	2.19	0.42
1:C:13:LEU:HA	1:C:13:LEU:HD23	1.79	0.42
2:G:77:GLU:HA	2:G:80:MET:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:43:TYR:HE2	3:E:503:TBR:BR7	2.56	0.42
1:D:438:LEU:HB3	1:D:440:PRO:HD2	2.01	0.42
2:G:452:GLN:O	2:G:454:SER:N	2.52	0.42
1:D:31:TYR:HD1	1:D:125:LYS:HG3	1.84	0.42
2:H:124:ALA:HA	2:H:125:PRO:HD3	1.86	0.42
2:H:262:ARG:HB2	5:H:501:NAD:N7A	2.33	0.42
2:F:235:ILE:O	2:F:257:VAL:HA	2.19	0.42
2:E:393:LYS:O	2:E:397:ARG:HD2	2.19	0.42
1:B:194:ILE:O	1:B:198:VAL:HG12	2.18	0.42
1:C:39:PHE:CE2	1:C:87:PRO:HB3	2.55	0.42
1:C:252:ASN:N	1:C:348:CYS:HB2	2.34	0.42
1:B:142:ILE:HG23	1:B:352:THR:HG22	2.00	0.42
1:B:150:LEU:HB2	1:B:151:PRO:HD3	2.01	0.42
1:B:406:TYR:HA	1:B:471:ILE:CD1	2.49	0.42
1:A:21:MET:HB2	1:A:43:PHE:HB2	2.00	0.42
1:C:341:PHE:CE2	1:D:411:VAL:HG13	2.54	0.42
1:A:291:PHE:CZ	1:A:295:LEU:HD11	2.54	0.42
1:C:357:LYS:O	1:C:360:ARG:HB2	2.20	0.42
2:H:2:LYS:CB	2:H:25:ASP:HB3	2.49	0.42
2:E:452:GLN:HA	2:E:453:PRO:HD2	1.74	0.42
1:A:251:CYS:SG	1:A:276:PHE:HD1	2.43	0.42
2:H:405:PRO:HG2	2:H:447:VAL:HG23	2.00	0.42
1:B:18:SER:HB2	1:B:47:LEU:HD23	2.00	0.42
2:F:152:LYS:HD2	2:F:152:LYS:HA	1.79	0.42
1:D:317:ILE:HD13	1:D:442:LEU:HD11	2.01	0.42
1:B:309:GLN:NE2	1:B:326:THR:HG22	2.33	0.42
1:B:361:ILE:O	1:B:365:THR:HG23	2.19	0.42
2:G:403:LYS:H	2:G:403:LYS:HG3	1.59	0.42
1:B:72:ILE:HA	1:B:72:ILE:HD13	1.84	0.42
1:B:340:LEU:HD13	1:B:442:LEU:HB3	2.00	0.42
2:F:295:ILE:O	2:F:298:VAL:HG12	2.19	0.42
1:A:316:SER:O	1:A:321:ALA:HB3	2.19	0.42
1:B:218:ILE:HD11	1:B:245:PHE:HD1	1.85	0.42
2:H:235:ILE:HB	2:H:257:VAL:HG22	2.01	0.42
2:E:332:ARG:HG3	3:E:503:TBR:BR2	2.75	0.42
2:F:360:THR:HG23	2:F:370:VAL:HG12	2.01	0.42
2:E:85:VAL:O	2:E:89:LEU:HB2	2.19	0.42
2:F:101:SER:HA	2:F:102:PRO:HD3	1.76	0.42
1:D:28:ALA:O	1:D:29:LEU:HD23	2.20	0.42
2:E:130:THR:HG21	2:E:246:SER:OG	2.19	0.42
2:H:125:PRO:HB3	2:H:354:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:PHE:CD2	1:B:39:PHE:N	2.87	0.42
1:B:466:PHE:HE1	1:B:474:LEU:HD22	1.85	0.42
2:F:155:LEU:HD13	2:F:212:VAL:HG22	2.00	0.42
1:B:354:GLY:HA3	1:B:468:ARG:NH2	2.35	0.42
2:E:85:VAL:HG22	2:H:111:LEU:HD21	2.02	0.42
1:D:460:LEU:O	1:D:464:MET:HG2	2.20	0.42
1:D:150:LEU:HB2	1:D:151:PRO:HD3	2.02	0.42
1:D:333:LEU:O	1:D:336:PRO:HD2	2.19	0.42
2:E:405:PRO:HG2	2:E:447:VAL:HG23	2.00	0.42
1:B:252:ASN:HB2	1:B:348:CYS:CB	2.50	0.42
1:A:300:TYR:CZ	1:A:309:GLN:HG3	2.55	0.42
1:C:18:SER:HB2	1:C:47:LEU:HD23	2.02	0.42
2:H:101:SER:HA	2:H:102:PRO:HD3	1.78	0.42
1:C:342:SER:HA	1:C:345:ILE:HD12	2.01	0.42
1:D:134:LEU:HD23	1:D:134:LEU:HA	1.78	0.41
1:B:232:TYR:HD2	1:B:233:PHE:HB2	1.84	0.41
2:G:101:SER:HA	2:G:102:PRO:HD3	1.81	0.41
2:E:147:SER:HB2	2:E:151:GLN:HA	2.02	0.41
1:A:200:PHE:HD1	1:A:200:PHE:HA	1.76	0.41
1:D:217:THR:HG23	1:D:218:ILE:HD13	2.01	0.41
1:A:142:ILE:CG2	1:A:352:THR:HG22	2.49	0.41
2:F:158:VAL:HG21	2:F:227:ARG:HD3	2.02	0.41
1:B:301:THR:OG1	1:B:302:SER:N	2.53	0.41
1:D:266:HIS:N	1:D:267:PRO:HD2	2.35	0.41
2:G:356:SER:HB3	2:G:371:SER:HA	2.01	0.41
1:B:380:ALA:HB2	2:E:280:PHE:CE1	2.56	0.41
1:A:75:LEU:HA	1:A:75:LEU:HD12	1.80	0.41
2:H:126:GLU:N	5:H:501:NAD:H72N	2.17	0.41
2:G:295:ILE:O	2:G:298:VAL:HG12	2.20	0.41
2:H:36:LEU:HB3	2:H:47:VAL:HG11	2.02	0.41
2:G:83:CYS:SG	2:G:97:ALA:HB2	2.60	0.41
1:C:363:LEU:HD12	1:C:399:VAL:HG21	2.01	0.41
2:F:195:ILE:HD12	2:F:195:ILE:HA	1.91	0.41
2:G:225:LEU:HB3	2:G:226:GLN:H	1.61	0.41
2:F:59:HIS:CE1	3:G:502:TBR:BRC	3.28	0.41
2:G:10:GLN:HG2	2:G:11:VAL:H	1.85	0.41
1:A:184:ALA:O	1:A:188:ILE:HG13	2.20	0.41
1:D:334:PHE:HD2	1:D:335:LEU:HD22	1.84	0.41
1:A:86:LEU:HA	1:A:86:LEU:HD12	1.86	0.41
1:B:328:PHE:HB3	1:B:331:TRP:HB2	2.00	0.41
1:C:317:ILE:HG21	1:C:339:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LEU:O	1:C:30:LEU:HB2	2.21	0.41
2:E:98:ARG:HG3	2:E:125:PRO:HD3	2.02	0.41
2:E:155:LEU:HD11	2:E:210:PHE:HB3	2.03	0.41
2:F:148:PHE:HB2	2:F:153:VAL:HG13	2.02	0.41
1:B:199:ALA:HB1	1:B:241:ILE:HD13	2.02	0.41
1:D:251:CYS:SG	1:D:276:PHE:HD1	2.43	0.41
2:F:156:VAL:HG12	2:F:211:PHE:HB2	2.03	0.41
1:A:317:ILE:HD12	1:A:339:LEU:HD23	2.03	0.41
1:D:302:SER:C	1:D:304:TYR:H	2.23	0.41
2:G:112:PHE:CE1	2:G:122:LEU:HD21	2.56	0.41
2:E:394:VAL:HG12	2:E:428:ILE:HG21	2.02	0.41
1:D:39:PHE:CE2	1:D:87:PRO:HB3	2.56	0.41
1:A:184:ALA:HB1	1:A:257:PHE:HE1	1.84	0.41
1:C:142:ILE:HD13	1:C:352:THR:HA	2.03	0.41
1:B:317:ILE:HG21	1:B:339:LEU:HB3	2.03	0.41
1:A:134:LEU:HA	1:A:134:LEU:HD23	1.84	0.41
1:C:66:SER:O	1:C:69:GLY:N	2.54	0.41
1:D:21:MET:HB2	1:D:43:PHE:HB2	2.02	0.41
1:D:143:ILE:HG21	1:D:253:PHE:CD2	2.55	0.41
1:B:183:LYS:HE3	1:B:187:TYR:HE2	1.85	0.41
1:C:367:GLN:OE1	1:C:396:VAL:HG13	2.19	0.41
1:C:373:LYS:HD2	1:C:382:TYR:CE1	2.56	0.41
1:C:147:VAL:HG11	1:C:181:THR:OG1	2.20	0.41
2:E:239:GLY:HA2	5:E:501:NAD:C8A	2.50	0.41
1:C:460:LEU:O	1:C:464:MET:HG2	2.20	0.41
1:A:257:PHE:C	1:A:259:ALA:H	2.23	0.41
1:B:310:ALA:O	1:B:314:THR:HG23	2.20	0.41
1:C:86:LEU:HA	1:C:86:LEU:HD12	1.81	0.41
2:G:36:LEU:HB3	2:G:47:VAL:HG11	2.02	0.41
1:D:483:TRP:HA	1:D:484:ARG:HA	1.85	0.41
2:G:414:VAL:HB	2:G:433:HIS:HB2	2.03	0.41
2:H:7:GLY:O	2:H:12:GLY:HA3	2.20	0.41
2:F:320:ARG:NE	2:F:320:ARG:HA	2.35	0.41
1:D:39:PHE:N	1:D:39:PHE:HD2	2.18	0.41
2:G:10:GLN:HG2	2:G:11:VAL:N	2.36	0.41
1:A:252:ASN:HB2	1:A:348:CYS:CB	2.51	0.41
1:A:438:LEU:HB3	1:A:440:PRO:CD	2.51	0.41
1:A:259:ALA:HA	1:A:266:HIS:NE2	2.35	0.41
1:B:134:LEU:HD23	1:B:134:LEU:HA	1.81	0.41
2:E:295:ILE:O	2:E:298:VAL:HG12	2.21	0.41
2:F:360:THR:HG22	2:F:370:VAL:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:LEU:HB3	1:B:367:GLN:HE21	1.84	0.41
2:G:148:PHE:HB2	2:G:153:VAL:HG13	2.02	0.41
1:A:297:HIS:CD2	1:A:332:PRO:HG3	2.55	0.41
1:C:71:LEU:HA	1:C:71:LEU:HD12	1.91	0.41
1:C:418:ILE:HD12	1:D:337:VAL:HG11	2.01	0.41
2:G:191:GLN:HB3	2:G:192:GLY:H	1.79	0.41
2:E:124:ALA:O	2:E:128:LEU:HG	2.20	0.41
2:E:79:ASN:HD22	2:E:79:ASN:HA	1.58	0.41
1:D:199:ALA:HB1	1:D:241:ILE:HD13	2.03	0.41
2:F:224:GLU:HG2	2:F:224:GLU:H	1.54	0.41
2:G:75:THR:HG21	2:G:78:THR:HG23	2.03	0.41
2:F:124:ALA:HA	2:F:125:PRO:HD3	1.79	0.41
1:A:354:GLY:HA3	1:A:468:ARG:HH22	1.86	0.41
2:F:107:GLU:H	2:F:107:GLU:HG2	1.71	0.41
1:A:230:MET:SD	1:A:232:TYR:OH	2.73	0.41
1:B:229:SER:OG	1:B:230:MET:N	2.53	0.41
2:E:101:SER:HA	2:E:102:PRO:HD3	1.77	0.41
2:G:267:ALA:O	2:G:279:VAL:HG11	2.21	0.41
2:G:190:ARG:NH2	2:G:202:ILE:O	2.54	0.41
1:B:291:PHE:CZ	1:B:295:LEU:HD11	2.56	0.41
2:G:402:ILE:HG13	2:G:402:ILE:H	1.50	0.41
1:D:357:LYS:O	1:D:360:ARG:HB2	2.21	0.41
1:C:438:LEU:HB2	1:C:439:GLY:HA2	2.02	0.40
2:E:10:GLN:CG	2:E:98:ARG:HH22	2.34	0.40
1:C:434:THR:OG1	1:C:460:LEU:HD22	2.21	0.40
1:A:138:GLY:O	1:A:142:ILE:HG22	2.21	0.40
2:F:364:ARG:HB3	2:F:366:ASP:OD1	2.21	0.40
1:A:363:LEU:O	1:A:367:GLN:HG3	2.22	0.40
1:A:395:VAL:O	1:A:399:VAL:HG23	2.21	0.40
1:D:367:GLN:OE1	1:D:396:VAL:HG13	2.20	0.40
1:A:38:PRO:HG3	1:A:90:ILE:HG12	2.02	0.40
1:C:142:ILE:CG2	1:C:352:THR:HG22	2.50	0.40
1:B:466:PHE:CE1	1:B:474:LEU:HD22	2.56	0.40
1:B:317:ILE:HD11	1:B:442:LEU:HD21	2.03	0.40
1:B:442:LEU:HD22	1:B:442:LEU:HA	1.87	0.40
1:C:458:TRP:CE3	1:C:461:ILE:HD12	2.56	0.40
1:C:337:VAL:HG11	1:D:418:ILE:HD12	2.02	0.40
2:F:26:ILE:O	2:F:45:LEU:HB2	2.20	0.40
1:A:256:HIS:HD2	1:A:270:TYR:OH	2.03	0.40
2:G:84:GLN:HA	2:G:118:PRO:CG	2.51	0.40
1:C:291:PHE:CZ	1:C:295:LEU:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:GLU:HG3	1:C:181:THR:HG23	2.02	0.40
2:H:169:ASN:HB3	2:H:201:THR:O	2.22	0.40
2:H:19:LEU:HB2	2:H:26:ILE:HD11	2.02	0.40
1:A:374:ARG:HD2	1:B:394:ARG:NH2	2.35	0.40
1:B:121:ASP:OD1	1:B:226:HIS:HA	2.22	0.40
1:C:22:LEU:HD21	1:C:43:PHE:CD2	2.56	0.40
1:A:18:SER:O	1:A:43:PHE:HD1	2.05	0.40
2:F:7:GLY:O	2:F:12:GLY:HA3	2.21	0.40
2:E:230:LYS:HA	2:E:231:PRO:HD3	1.91	0.40
2:E:165:PRO:HB2	2:E:166:LEU:H	1.57	0.40
2:F:67:ASP:HA	2:F:93:PRO:HG2	2.01	0.40
1:D:218:ILE:HA	1:D:218:ILE:HD12	1.88	0.40
2:F:125:PRO:HB3	2:F:354:THR:HG22	2.03	0.40
1:B:340:LEU:HB2	1:B:442:LEU:HD12	2.02	0.40
1:B:142:ILE:CG2	1:B:352:THR:HG22	2.50	0.40
1:A:287:PHE:CD2	1:A:288:LEU:HD23	2.56	0.40
1:A:363:LEU:HA	1:A:363:LEU:HD23	1.77	0.40
2:G:2:LYS:CB	2:G:25:ASP:HB3	2.52	0.40
2:H:51:HIS:HD2	2:H:54:HIS:NE2	2.20	0.40
2:F:397:ARG:HH11	2:F:402:ILE:HG23	1.86	0.40
1:D:71:LEU:HD12	1:D:71:LEU:HA	1.86	0.40
1:A:236:TYR:N	1:A:236:TYR:CD2	2.88	0.40
1:D:406:TYR:HA	1:D:471:ILE:CD1	2.52	0.40
1:D:363:LEU:HB3	1:D:367:GLN:HE21	1.87	0.40
1:D:283:GLN:HE21	1:D:315:VAL:HA	1.86	0.40
1:B:417:LEU:HD11	1:B:460:LEU:HD21	2.03	0.40
1:B:320:THR:HG22	1:B:320:THR:O	2.21	0.40
1:C:3:PHE:O	1:C:7:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	456/485 (94%)	386 (85%)	66 (14%)	4 (1%)	21	68
1	B	456/485 (94%)	385 (84%)	68 (15%)	3 (1%)	26	72
1	C	456/485 (94%)	385 (84%)	66 (14%)	5 (1%)	17	65
1	D	456/485 (94%)	387 (85%)	66 (14%)	3 (1%)	26	72
2	E	445/458 (97%)	395 (89%)	45 (10%)	5 (1%)	17	65
2	F	436/458 (95%)	393 (90%)	41 (9%)	2 (0%)	34	77
2	G	446/458 (97%)	391 (88%)	50 (11%)	5 (1%)	17	65
2	H	446/458 (97%)	401 (90%)	42 (9%)	3 (1%)	26	72
All	All	3597/3772 (95%)	3123 (87%)	444 (12%)	30 (1%)	24	70

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	456	PHE
2	F	165	PRO
1	C	262	SER
2	E	93	PRO
2	E	165	PRO
2	G	9	GLY
2	G	165	PRO
2	G	225	LEU
2	H	93	PRO
2	H	165	PRO
2	E	453	PRO
2	F	93	PRO
2	G	93	PRO
2	G	453	PRO
2	H	226	GLN
1	A	388	GLY
1	B	388	GLY
1	A	303	PRO
1	C	261	ALA
1	C	388	GLY
1	A	94	PRO
1	B	94	PRO
1	C	94	PRO
1	D	303	PRO
1	D	388	GLY
1	C	303	PRO
1	D	94	PRO

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Mol	Chain	Res	Type
1	A	265	VAL
1	B	265	VAL
2	E	9	GLY

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	374/395 (95%)	310 (83%)	64 (17%)	2	19
1	B	374/395 (95%)	311 (83%)	63 (17%)	2	19
1	C	374/395 (95%)	318 (85%)	56 (15%)	3	26
1	D	374/395 (95%)	315 (84%)	59 (16%)	3	23
2	E	370/378 (98%)	312 (84%)	58 (16%)	3	24
2	F	366/378 (97%)	309 (84%)	57 (16%)	3	24
2	G	372/378 (98%)	320 (86%)	52 (14%)	4	29
2	H	370/378 (98%)	309 (84%)	61 (16%)	3	20
All	All	2974/3092 (96%)	2504 (84%)	470 (16%)	3	23

All (470) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	ARG
1	A	6	ILE
1	A	9	ILE
1	A	12	LEU
1	A	16	LEU
1	A	26	LEU
1	A	30	LEU
1	A	32	ARG
1	A	33	ASP
1	A	47	LEU
1	A	52	MET

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Mol	Chain	Res	Type
1	A	54	TRP
1	A	60	HIS
1	A	67	ARG
1	A	75	LEU
1	A	78	THR
1	A	90	ILE
1	A	111	THR
1	A	115	THR
1	A	121	ASP
1	A	122	GLU
1	A	128	LEU
1	A	153	LEU
1	A	155	ILE
1	A	190	LEU
1	A	200	PHE
1	A	202	LEU
1	A	206	THR
1	A	218	ILE
1	A	227	ASP
1	A	234	ASP
1	A	235	SER
1	A	236	TYR
1	A	244	VAL
1	A	249	SER
1	A	255	LEU
1	A	288	LEU
1	A	324	THR
1	A	326	THR
1	A	333	LEU
1	A	340	LEU
1	A	343	SER
1	A	345	ILE
1	A	352	THR
1	A	356	MET
1	A	360	ARG
1	A	366	LEU
1	A	374	ARG
1	A	394	ARG
1	A	400	TRP
1	A	420	THR
1	A	429	SER
1	A	434	THR

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Mol	Chain	Res	Type
1	A	435	LEU
1	A	442	LEU
1	A	447	LEU
1	A	454	ASP
1	A	473	THR
1	A	476	ILE
1	A	477	LEU
1	A	478	LEU
1	A	483	TRP
1	A	484	ARG
1	B	1	MET
1	B	4	ARG
1	B	6	ILE
1	B	16	LEU
1	B	26	LEU
1	B	30	LEU
1	B	32	ARG
1	B	33	ASP
1	B	47	LEU
1	B	52	MET
1	B	54	TRP
1	B	67	ARG
1	B	75	LEU
1	B	78	THR
1	B	90	ILE
1	B	111	THR
1	B	115	THR
1	B	122	GLU
1	B	128	LEU
1	B	153	LEU
1	B	155	ILE
1	B	190	LEU
1	B	198	VAL
1	B	200	PHE
1	B	206	THR
1	B	218	ILE
1	B	223	PHE
1	B	227	ASP
1	B	233	PHE
1	B	234	ASP
1	B	235	SER
1	B	236	TYR

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Mol	Chain	Res	Type
1	B	255	LEU
1	B	280	ILE
1	B	285	LEU
1	B	288	LEU
1	B	324	THR
1	B	333	LEU
1	B	341	PHE
1	B	345	ILE
1	B	352	THR
1	B	356	MET
1	B	359	ILE
1	B	360	ARG
1	B	363	LEU
1	B	366	LEU
1	B	375	LEU
1	B	383	THR
1	B	391	LEU
1	B	394	ARG
1	B	400	TRP
1	B	408	LEU
1	B	420	THR
1	B	429	SER
1	B	434	THR
1	B	435	LEU
1	B	442	LEU
1	B	447	LEU
1	B	473	THR
1	B	476	ILE
1	B	477	LEU
1	B	483	TRP
1	B	484	ARG
1	C	1	MET
1	C	6	ILE
1	C	9	ILE
1	C	16	LEU
1	C	26	LEU
1	C	30	LEU
1	C	32	ARG
1	C	33	ASP
1	C	47	LEU
1	C	54	TRP
1	C	60	HIS

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Mol	Chain	Res	Type
1	C	67	ARG
1	C	75	LEU
1	C	78	THR
1	C	90	ILE
1	C	115	THR
1	C	121	ASP
1	C	128	LEU
1	C	153	LEU
1	C	155	ILE
1	C	190	LEU
1	C	200	PHE
1	C	206	THR
1	C	218	ILE
1	C	233	PHE
1	C	234	ASP
1	C	236	TYR
1	C	244	VAL
1	C	249	SER
1	C	257	PHE
1	C	288	LEU
1	C	318	SER
1	C	324	THR
1	C	333	LEU
1	C	341	PHE
1	C	345	ILE
1	C	356	MET
1	C	359	ILE
1	C	360	ARG
1	C	363	LEU
1	C	364	LEU
1	C	366	LEU
1	C	375	LEU
1	C	383	THR
1	C	394	ARG
1	C	425	LEU
1	C	434	THR
1	C	435	LEU
1	C	442	LEU
1	C	447	LEU
1	C	454	ASP
1	C	473	THR
1	C	476	ILE

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Mol	Chain	Res	Type
1	C	477	LEU
1	C	478	LEU
1	C	483	TRP
1	D	1	MET
1	D	4	ARG
1	D	6	ILE
1	D	12	LEU
1	D	16	LEU
1	D	26	LEU
1	D	30	LEU
1	D	32	ARG
1	D	33	ASP
1	D	47	LEU
1	D	52	MET
1	D	54	TRP
1	D	60	HIS
1	D	67	ARG
1	D	78	THR
1	D	111	THR
1	D	115	THR
1	D	117	ILE
1	D	121	ASP
1	D	128	LEU
1	D	153	LEU
1	D	155	ILE
1	D	190	LEU
1	D	194	ILE
1	D	198	VAL
1	D	200	PHE
1	D	202	LEU
1	D	206	THR
1	D	218	ILE
1	D	234	ASP
1	D	235	SER
1	D	236	TYR
1	D	244	VAL
1	D	285	LEU
1	D	288	LEU
1	D	324	THR
1	D	333	LEU
1	D	341	PHE
1	D	352	THR

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Mol	Chain	Res	Type
1	D	356	MET
1	D	359	ILE
1	D	360	ARG
1	D	363	LEU
1	D	366	LEU
1	D	375	LEU
1	D	391	LEU
1	D	394	ARG
1	D	420	THR
1	D	425	LEU
1	D	429	SER
1	D	434	THR
1	D	435	LEU
1	D	442	LEU
1	D	447	LEU
1	D	473	THR
1	D	476	ILE
1	D	477	LEU
1	D	483	TRP
1	D	484	ARG
2	E	1	MET
2	E	3	ILE
2	E	14	THR
2	E	15	LEU
2	E	28	ILE
2	E	39	LEU
2	E	45	LEU
2	E	69	LEU
2	E	79	ASN
2	E	89	LEU
2	E	91	ASN
2	E	100	ARG
2	E	107	GLU
2	E	126	GLU
2	E	130	THR
2	E	150	GLU
2	E	151	GLN
2	E	152	LYS
2	E	156	VAL
2	E	167	VAL
2	E	176	GLU
2	E	198	GLN

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Mol	Chain	Res	Type
2	E	216	ASN
2	E	221	VAL
2	E	225	LEU
2	E	226	GLN
2	E	227	ARG
2	E	234	ARG
2	E	243	ILE
2	E	254	THR
2	E	270	LEU
2	E	274	LEU
2	E	289	LEU
2	E	291	THR
2	E	293	GLU
2	E	308	ASP
2	E	313	MET
2	E	314	SER
2	E	317	LEU
2	E	319	LYS
2	E	320	ARG
2	E	324	LYS
2	E	337	ASP
2	E	338	LEU
2	E	343	VAL
2	E	346	VAL
2	E	349	SER
2	E	351	GLN
2	E	354	THR
2	E	374	ARG
2	E	381	ILE
2	E	402	ILE
2	E	403	LYS
2	E	421	ILE
2	E	423	HIS
2	E	425	ARG
2	E	426	THR
2	E	450	LEU
2	F	3	ILE
2	F	14	THR
2	F	15	LEU
2	F	20	VAL
2	F	39	LEU
2	F	42	LYS

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Mol	Chain	Res	Type
2	F	45	LEU
2	F	58	LEU
2	F	67	ASP
2	F	69	LEU
2	F	77	GLU
2	F	79	ASN
2	F	88	THR
2	F	96	VAL
2	F	100	ARG
2	F	105	LEU
2	F	107	GLU
2	F	123	ILE
2	F	126	GLU
2	F	132	TYR
2	F	156	VAL
2	F	161	TYR
2	F	201	THR
2	F	206	ASP
2	F	224	GLU
2	F	225	LEU
2	F	234	ARG
2	F	254	THR
2	F	270	LEU
2	F	274	LEU
2	F	277	THR
2	F	289	LEU
2	F	290	LEU
2	F	291	THR
2	F	296	ASP
2	F	300	VAL
2	F	308	ASP
2	F	313	MET
2	F	317	LEU
2	F	319	LYS
2	F	320	ARG
2	F	321	MET
2	F	338	LEU
2	F	343	VAL
2	F	346	VAL
2	F	352	GLN
2	F	362	VAL
2	F	364	ARG

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Mol	Chain	Res	Type
2	F	367	ILE
2	F	381	ILE
2	F	402	ILE
2	F	403	LYS
2	F	404	LEU
2	F	421	ILE
2	F	425	ARG
2	F	426	THR
2	F	450	LEU
2	G	3	ILE
2	G	14	THR
2	G	15	LEU
2	G	20	VAL
2	G	39	LEU
2	G	41	ASP
2	G	45	LEU
2	G	67	ASP
2	G	69	LEU
2	G	77	GLU
2	G	89	LEU
2	G	94	ASN
2	G	100	ARG
2	G	105	LEU
2	G	107	GLU
2	G	126	GLU
2	G	132	TYR
2	G	151	GLN
2	G	152	LYS
2	G	156	VAL
2	G	167	VAL
2	G	201	THR
2	G	225	LEU
2	G	233	ARG
2	G	234	ARG
2	G	254	THR
2	G	264	TYR
2	G	268	GLU
2	G	270	LEU
2	G	274	LEU
2	G	291	THR
2	G	308	ASP
2	G	313	MET

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Mol	Chain	Res	Type
2	G	319	LYS
2	G	320	ARG
2	G	321	MET
2	G	324	LYS
2	G	338	LEU
2	G	340	GLN
2	G	346	VAL
2	G	351	GLN
2	G	362	VAL
2	G	367	ILE
2	G	381	ILE
2	G	402	ILE
2	G	403	LYS
2	G	421	ILE
2	G	423	HIS
2	G	425	ARG
2	G	426	THR
2	G	450	LEU
2	G	452	GLN
2	H	3	ILE
2	H	14	THR
2	H	39	LEU
2	H	45	LEU
2	H	58	LEU
2	H	67	ASP
2	H	69	LEU
2	H	79	ASN
2	H	100	ARG
2	H	105	LEU
2	H	107	GLU
2	H	114	SER
2	H	126	GLU
2	H	132	TYR
2	H	147	SER
2	H	151	GLN
2	H	156	VAL
2	H	167	VAL
2	H	176	GLU
2	H	181	ILE
2	H	188	ILE
2	H	191	GLN
2	H	221	VAL

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Mol	Chain	Res	Type
2	H	225	LEU
2	H	234	ARG
2	H	254	THR
2	H	265	GLN
2	H	270	LEU
2	H	273	GLN
2	H	274	LEU
2	H	275	GLU
2	H	277	THR
2	H	289	LEU
2	H	290	LEU
2	H	293	GLU
2	H	308	ASP
2	H	313	MET
2	H	314	SER
2	H	317	LEU
2	H	320	ARG
2	H	338	LEU
2	H	346	VAL
2	H	349	SER
2	H	351	GLN
2	H	352	GLN
2	H	354	THR
2	H	358	LEU
2	H	369	ASN
2	H	381	ILE
2	H	384	VAL
2	H	386	HIS
2	H	389	GLU
2	H	392	SER
2	H	394	VAL
2	H	402	ILE
2	H	403	LYS
2	H	421	ILE
2	H	424	ASP
2	H	426	THR
2	H	428	ILE
2	H	450	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	239	ASN
1	A	256	HIS
1	B	239	ASN
1	B	367	GLN
1	C	239	ASN
1	C	367	GLN
1	D	239	ASN
2	E	297	GLN
2	F	51	HIS
2	F	144	GLN
2	G	265	GLN
2	G	297	GLN
2	G	352	GLN
2	H	51	HIS

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

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 for Mogul analysis.

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	TBR	A	501	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	A	502	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	A	503	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	B	501	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	B	502	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	C	501	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	C	502	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	D	501	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	D	502	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	D	503	-	0,36,36	0.00	-	0,180,180	0.00	-
5	NAD	E	501	-	38,48,48	0.92	2 (5%)	47,73,73	1.76	7 (14%)
3	TBR	E	502	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	E	503	-	0,36,36	0.00	-	0,180,180	0.00	-
5	NAD	F	501	-	38,48,48	0.93	2 (5%)	47,73,73	1.56	7 (14%)
3	TBR	F	502	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	F	503	-	0,36,36	0.00	-	0,180,180	0.00	-
5	NAD	G	501	-	38,48,48	0.89	1 (2%)	47,73,73	1.59	7 (14%)
3	TBR	G	502	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	G	503	-	0,36,36	0.00	-	0,180,180	0.00	-
5	NAD	H	501	-	38,48,48	0.89	1 (2%)	47,73,73	1.66	7 (14%)
3	TBR	H	502	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	H	503	-	0,36,36	0.00	-	0,180,180	0.00	-

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	TBR	A	501	-	-	0/0/696/696	0/0/19/19
3	TBR	A	502	-	-	0/0/696/696	0/0/19/19
3	TBR	A	503	-	-	0/0/696/696	0/0/19/19
3	TBR	B	501	-	-	0/0/696/696	0/0/19/19
3	TBR	B	502	-	-	0/0/696/696	0/0/19/19
3	TBR	C	501	-	-	0/0/696/696	0/0/19/19
3	TBR	C	502	-	-	0/0/696/696	0/0/19/19
3	TBR	D	501	-	-	0/0/696/696	0/0/19/19
3	TBR	D	502	-	-	0/0/696/696	0/0/19/19
3	TBR	D	503	-	-	0/0/696/696	0/0/19/19
5	NAD	E	501	-	-	0/22/62/62	0/5/5/5
3	TBR	E	502	-	-	0/0/696/696	0/0/19/19
3	TBR	E	503	-	-	0/0/696/696	0/0/19/19

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAD	F	501	-	-	0/22/62/62	0/5/5/5
3	TBR	F	502	-	-	0/0/696/696	0/0/19/19
3	TBR	F	503	-	-	0/0/696/696	0/0/19/19
5	NAD	G	501	-	-	0/22/62/62	0/5/5/5
3	TBR	G	502	-	-	0/0/696/696	0/0/19/19
3	TBR	G	503	-	-	0/0/696/696	0/0/19/19
5	NAD	H	501	-	-	0/22/62/62	0/5/5/5
3	TBR	H	502	-	-	0/0/696/696	0/0/19/19
3	TBR	H	503	-	-	0/0/696/696	0/0/19/19

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	501	NAD	O4B-C1B	2.07	1.43	1.41
5	F	501	NAD	O4B-C1B	2.21	1.44	1.41
5	H	501	NAD	C5A-C4A	3.28	1.47	1.40
5	G	501	NAD	C5A-C4A	3.30	1.47	1.40
5	E	501	NAD	C5A-C4A	3.39	1.48	1.40
5	F	501	NAD	C5A-C4A	3.42	1.48	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	501	NAD	N3A-C2A-N1A	-5.90	124.37	128.89
5	F	501	NAD	N3A-C2A-N1A	-5.88	124.39	128.89
5	G	501	NAD	N3A-C2A-N1A	-5.69	124.54	128.89
5	E	501	NAD	N3A-C2A-N1A	-5.59	124.62	128.89
5	E	501	NAD	C4B-O4B-C1B	-5.13	104.09	109.72
5	H	501	NAD	C4B-O4B-C1B	-4.52	104.75	109.72
5	G	501	NAD	C4B-O4B-C1B	-4.22	105.08	109.72
5	E	501	NAD	PN-O3-PA	-3.86	121.90	132.73
5	G	501	NAD	PN-O3-PA	-3.79	122.09	132.73
5	F	501	NAD	PN-O3-PA	-3.69	122.37	132.73
5	H	501	NAD	PN-O3-PA	-3.25	123.60	132.73
5	F	501	NAD	C4B-O4B-C1B	-2.69	106.76	109.72
5	F	501	NAD	C4A-C5A-N7A	-2.42	107.25	109.48
5	G	501	NAD	C4A-C5A-N7A	-2.16	107.49	109.48
5	G	501	NAD	C2N-C3N-C4N	2.12	120.64	118.29
5	G	501	NAD	C1B-N9A-C4A	2.13	130.15	126.94
5	E	501	NAD	C2N-C3N-C4N	2.15	120.68	118.29
5	F	501	NAD	C2B-C1B-N9A	2.40	117.95	114.29
5	F	501	NAD	C1B-N9A-C4A	2.53	130.75	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	501	NAD	O4D-C1D-N1N	2.53	110.92	108.13
5	H	501	NAD	C2B-C1B-N9A	2.61	118.28	114.29
5	H	501	NAD	C1B-N9A-C4A	2.79	131.15	126.94
5	E	501	NAD	C2B-C1B-N9A	3.14	119.09	114.29
5	E	501	NAD	C1B-N9A-C4A	3.20	131.77	126.94
5	H	501	NAD	O4B-C1B-N9A	3.32	115.06	108.10
5	F	501	NAD	O4B-C1B-N9A	3.41	115.23	108.10
5	G	501	NAD	O4B-C1B-N9A	3.62	115.67	108.10
5	E	501	NAD	O4B-C1B-N9A	4.35	117.21	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	TBR	1	0
3	D	501	TBR	1	0
3	D	502	TBR	1	0
5	E	501	NAD	5	0
3	E	503	TBR	3	0
5	F	501	NAD	3	0
3	F	502	TBR	1	0
3	F	503	TBR	1	0
5	G	501	NAD	5	0
3	G	502	TBR	1	0
3	G	503	TBR	2	0
5	H	501	NAD	5	0
3	H	502	TBR	1	0
3	H	503	TBR	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	462/485 (95%)	0.03	23 (4%)	32	21	31, 70, 118, 155	0
1	B	462/485 (95%)	0.08	18 (3%)	43	29	29, 75, 127, 165	0
1	C	462/485 (95%)	0.27	37 (8%)	15	9	39, 94, 142, 173	0
1	D	462/485 (95%)	0.14	23 (4%)	32	21	41, 87, 139, 163	0
2	E	451/458 (98%)	0.21	28 (6%)	24	14	39, 84, 158, 186	0
2	F	444/458 (96%)	0.21	28 (6%)	23	14	43, 80, 132, 161	0
2	G	452/458 (98%)	0.15	20 (4%)	38	25	43, 89, 158, 181	0
2	H	450/458 (98%)	0.30	35 (7%)	16	9	43, 88, 158, 183	0
All	All	3645/3772 (96%)	0.17	212 (5%)	26	16	29, 83, 146, 186	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	ASP	7.2
2	H	390	THR	5.7
1	C	93	ASN	5.5
1	B	266	HIS	5.1
2	H	171	LEU	5.0
2	H	225	LEU	5.0
1	C	92	ASP	4.9
2	H	431	ASP	4.9
2	E	453	PRO	4.8
2	H	405	PRO	4.7
2	E	430	GLN	4.5
2	F	402	ILE	4.4
2	H	408	THR	4.4
1	A	58	ARG	4.4
2	E	166	LEU	4.4
1	C	57	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
2	H	404	LEU	4.2
1	B	91	ALA	4.2
1	A	33	ASP	4.1
1	C	53	CYS	4.1
2	H	407	GLY	4.1
1	A	91	ALA	4.1
2	H	388	ASP	4.0
2	H	432	ASP	4.0
2	E	431	ASP	3.9
2	E	4	ILE	3.9
2	E	208	GLU	3.9
1	C	94	PRO	3.9
1	B	90	ILE	3.9
2	F	400	GLY	3.8
2	F	453	PRO	3.8
1	D	125	LYS	3.8
1	C	90	ILE	3.8
1	C	305	ASP	3.8
1	C	443	GLY	3.7
1	D	126	ALA	3.7
1	B	93	ASN	3.7
1	A	306	ALA	3.7
2	E	197	PRO	3.7
1	A	203	ALA	3.7
2	F	391	THR	3.7
1	D	33	ASP	3.7
2	H	226	GLN	3.6
2	E	188	ILE	3.6
1	C	297	HIS	3.5
2	H	224	GLU	3.5
2	H	403	LYS	3.5
2	F	22	GLU	3.5
2	F	406	PRO	3.4
1	A	125	LYS	3.4
2	G	188	ILE	3.4
1	C	285	LEU	3.4
1	C	42	THR	3.3
1	A	92	ASP	3.3
1	C	444	GLU	3.3
1	A	269	TYR	3.3
2	F	390	THR	3.3
2	F	115	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	452	GLN	3.2
2	E	386	HIS	3.1
1	B	94	PRO	3.1
2	F	114	SER	3.1
2	F	401	ASP	3.1
1	C	91	ALA	3.1
2	H	222	MET	3.1
1	D	51	ALA	3.1
1	B	125	LYS	3.1
1	C	289	VAL	3.1
1	B	92	ASP	3.0
1	D	265	VAL	3.0
2	F	43	TYR	3.0
1	B	35	ALA	3.0
1	C	135	GLN	2.9
2	H	391	THR	2.9
1	D	226	HIS	2.9
2	E	187	ALA	2.9
1	A	307	PHE	2.9
1	D	264	GLY	2.9
2	E	43	TYR	2.9
2	F	42	LYS	2.9
2	G	69	LEU	2.9
1	C	178	ILE	2.9
2	E	203	ILE	2.9
2	G	186	ALA	2.9
2	H	235	ILE	2.8
2	F	4	ILE	2.8
2	H	425	ARG	2.8
1	C	87	PRO	2.8
1	D	295	LEU	2.8
1	A	95	ASN	2.8
1	C	296	LYS	2.8
1	A	271	TRP	2.8
1	D	482	PHE	2.8
2	H	389	GLU	2.7
2	E	52	ALA	2.7
2	E	366	ASP	2.7
2	F	404	LEU	2.7
2	H	221	VAL	2.7
2	E	433	HIS	2.6
1	D	121	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	41	ASP	2.6
1	D	96	ILE	2.6
1	A	96	ILE	2.6
2	H	232	TYR	2.6
2	E	388	ASP	2.6
2	H	49	ASN	2.6
2	H	453	PRO	2.6
2	G	48	VAL	2.6
1	D	440	PRO	2.6
2	H	386	HIS	2.6
1	C	306	ALA	2.6
1	D	62	HIS	2.5
1	A	305	ASP	2.5
2	E	387	GLY	2.5
2	G	97	ALA	2.5
1	D	156	GLY	2.5
2	E	186	ALA	2.5
2	F	235	ILE	2.5
2	G	431	ASP	2.5
2	H	182	ASP	2.5
1	A	266	HIS	2.5
2	F	7	GLY	2.5
2	G	454	SER	2.5
2	G	187	ALA	2.5
1	D	269	TYR	2.5
2	E	422	ALA	2.5
1	B	269	TYR	2.4
1	C	293	LEU	2.4
1	A	127	ILE	2.4
1	A	121	ASP	2.4
2	H	73	THR	2.4
1	C	151	PRO	2.4
1	D	24	PRO	2.4
1	C	286	LEU	2.4
2	E	29	VAL	2.4
2	E	402	ILE	2.4
1	C	122	GLU	2.4
1	A	268	LYS	2.4
2	F	318	ALA	2.4
1	A	272	LYS	2.4
1	C	38	PRO	2.4
2	G	325	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	452	GLN	2.4
2	G	432	ASP	2.4
2	F	366	ASP	2.4
1	C	86	LEU	2.3
1	C	308	ASP	2.3
2	F	110	ALA	2.3
2	H	168	GLY	2.3
2	F	11	VAL	2.3
1	C	35	ALA	2.3
1	C	295	LEU	2.3
2	G	434	VAL	2.3
1	D	91	ALA	2.3
1	B	444	GLU	2.3
1	D	424	GLU	2.3
2	H	59	HIS	2.3
1	C	127	ILE	2.3
1	C	156	GLY	2.3
2	G	183	THR	2.3
2	F	205	ALA	2.3
1	B	267	PRO	2.3
1	C	138	GLY	2.2
2	G	430	GLN	2.2
1	C	36	GLY	2.2
1	C	62	HIS	2.2
1	B	446	ALA	2.2
2	E	410	ILE	2.2
1	B	39	PHE	2.2
2	G	433	HIS	2.2
2	H	223	SER	2.2
1	A	54	TRP	2.2
2	F	399	ILE	2.2
1	A	122	GLU	2.2
1	C	281	PHE	2.2
2	E	384	VAL	2.2
2	H	434	VAL	2.2
2	E	165	PRO	2.2
1	D	311	LEU	2.2
1	D	441	GLY	2.2
2	E	169	ASN	2.2
2	H	433	HIS	2.2
1	A	35	ALA	2.2
1	B	27	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	127	ILE	2.2
2	G	68	MET	2.2
2	H	98	ARG	2.1
1	B	66	SER	2.1
1	A	120	LEU	2.1
2	F	234	ARG	2.1
2	E	235	ILE	2.1
1	C	154	GLY	2.1
1	C	334	PHE	2.1
2	G	205	ALA	2.1
2	E	38	GLU	2.1
2	G	184	ARG	2.1
1	D	90	ILE	2.1
1	B	260	PHE	2.1
2	G	21	GLY	2.1
2	F	72	VAL	2.1
2	H	72	VAL	2.1
2	F	245	ALA	2.1
2	H	406	PRO	2.1
1	D	262	SER	2.0
1	A	270	TYR	2.0
1	B	98	VAL	2.0
2	G	185	VAL	2.0
2	E	192	GLY	2.0
2	H	204	GLU	2.0
1	C	4	ARG	2.0
2	G	177	HIS	2.0
2	F	198	GLN	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
3	TBR	G	503	18/18	0.88	0.47	1.64	53,122,192,197	18
3	TBR	B	501	18/18	0.96	0.51	1.62	41,95,161,539	18
3	TBR	D	503	18/18	0.54	0.53	1.48	73,128,323,367	18
3	TBR	D	502	18/18	0.94	0.45	1.25	45,104,211,261	18
3	TBR	A	502	18/18	0.97	0.36	1.12	86,125,275,297	18
3	TBR	H	503	18/18	0.93	0.40	0.99	52,92,184,211	18
3	TBR	A	501	18/18	0.97	0.53	0.91	86,145,324,330	18
3	TBR	C	501	18/18	0.98	0.50	0.87	50,93,125,189	18
3	TBR	G	502	18/18	0.86	0.34	0.57	70,139,259,285	18
3	TBR	D	501	18/18	0.97	0.47	0.56	31,77,99,170	18
4	K	D	504	1/1	0.93	0.22	0.54	119,119,119,119	0
3	TBR	F	503	18/18	0.88	0.46	0.53	49,80,197,198	18
3	TBR	E	503	18/18	0.90	0.43	0.42	48,100,209,232	18
3	TBR	C	502	18/18	0.97	0.37	0.12	81,131,298,309	18
5	NAD	G	501	44/44	0.92	0.21	-0.15	36,58,82,115	0
5	NAD	H	501	44/44	0.93	0.24	-0.18	41,62,102,117	0
5	NAD	E	501	44/44	0.92	0.20	-0.24	33,54,84,122	0
3	TBR	B	502	18/18	0.97	0.33	-0.33	74,116,217,295	18
5	NAD	F	501	44/44	0.95	0.21	-0.39	40,70,92,125	0
3	TBR	A	503	18/18	0.77	0.28	-0.61	99,160,345,346	18
4	K	C	503	1/1	0.76	0.08	-2.05	103,103,103,103	0
3	TBR	F	502	18/18	0.86	0.13	-2.05	81,118,256,309	18
4	K	B	503	1/1	0.92	0.11	-2.22	73,73,73,73	0
4	K	A	504	1/1	0.98	0.12	-2.59	66,66,66,66	0
3	TBR	H	502	18/18	0.90	0.17	-	83,180,334,361	18
3	TBR	E	502	18/18	0.81	0.33	-	59,128,282,314	18

6.5 Other polymers (i)

There are no such residues in this entry.