Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 04:46 PM EDT

PDB ID	:	2NUT
Title	:	Crystal Structure of the human Sec23a/24a heterodimer, complexed with the SNARE protein Sec22b
Authors	:	Mancias, J.D.; Goldberg, J.
Deposited on	:	2006-11-09
Resolution	:	2.30 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

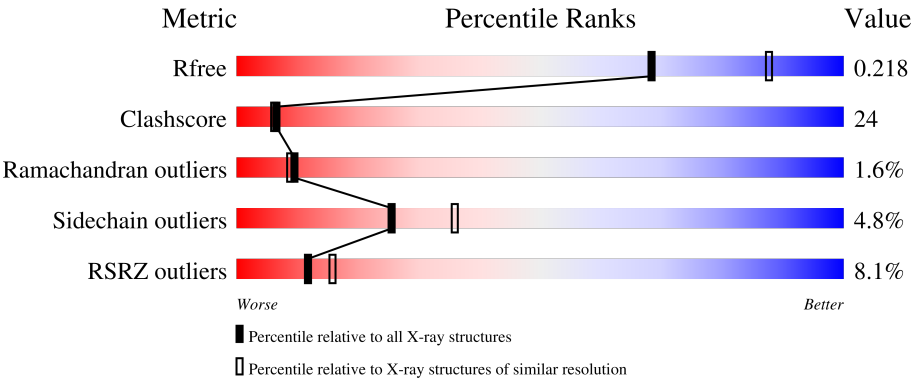
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	769	8% 55% 32% · 8%
2	B	753	6% 66% 28% · ·
3	C	196	11% 41% 25% · 31%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12778 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 Protein transport protein Sec23A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	708	5627	3585	968	1034	40	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	cloning artifact	UNP Q15436
A	-2	ALA	-	cloning artifact	UNP Q15436
A	-1	MET	-	cloning artifact	UNP Q15436
A	0	GLY	-	cloning artifact	UNP Q15436

- Molecule 2 is a protein called Protein transport protein Sec24A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	729	5761	3675	981	1071	34	0	0	0

- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	135	1087	699	177	203	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	cloning artifact	UNP O75396

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0

- Molecule 5 is water.

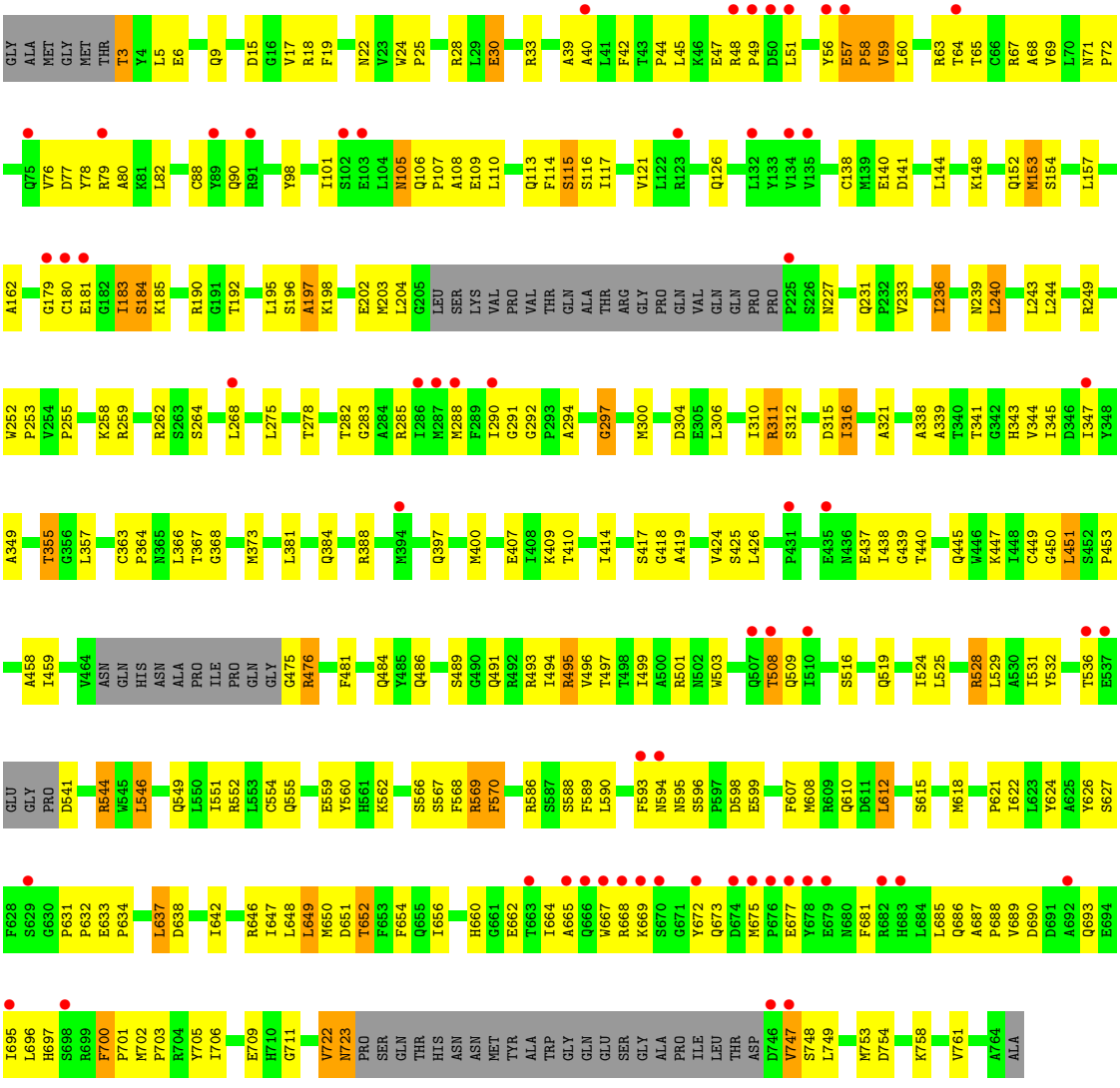
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	123	Total O 123 123	0	0
5	B	167	Total O 167 167	0	0
5	C	11	Total O 11 11	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

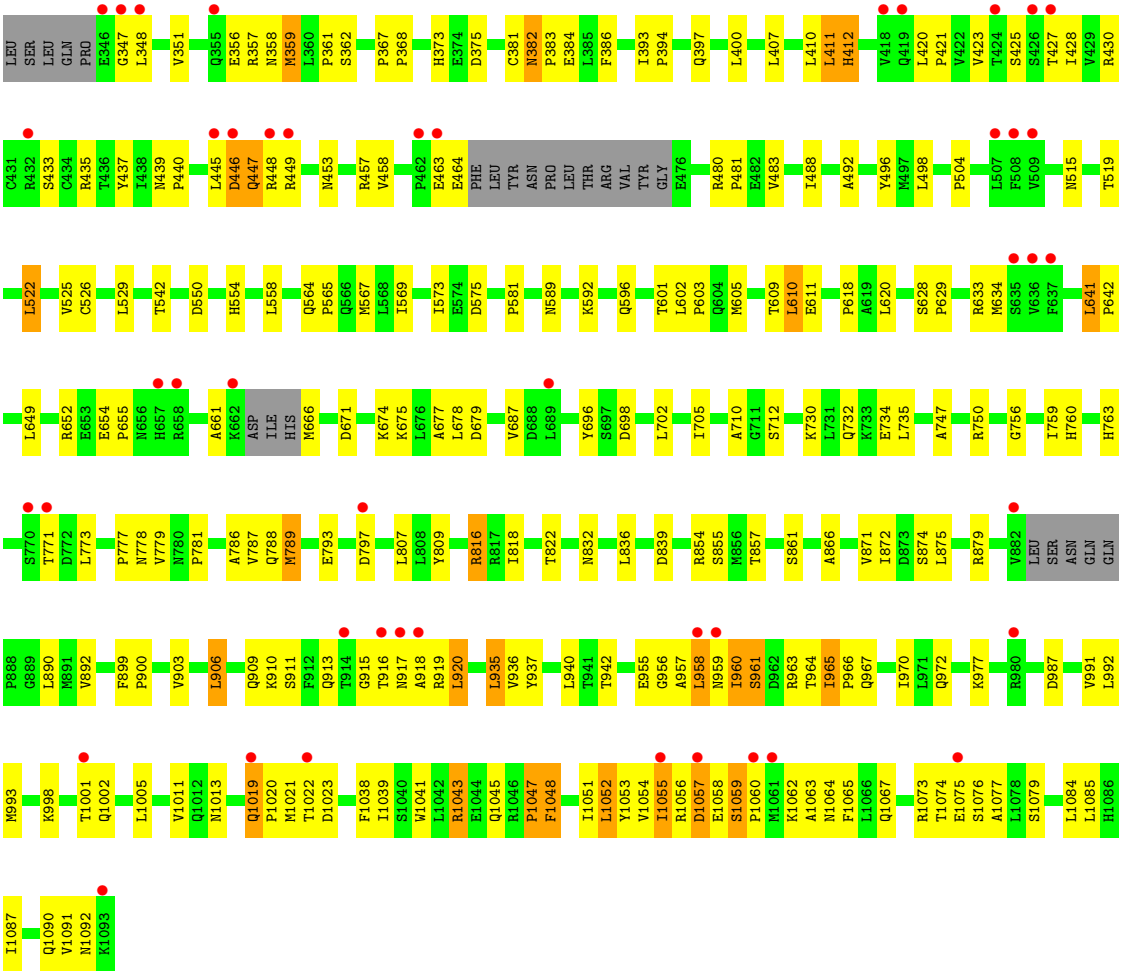
• Molecule 1: Protein transport protein Sec23A

Chain A:



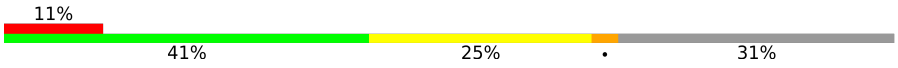
• Molecule 2: Protein transport protein Sec24A

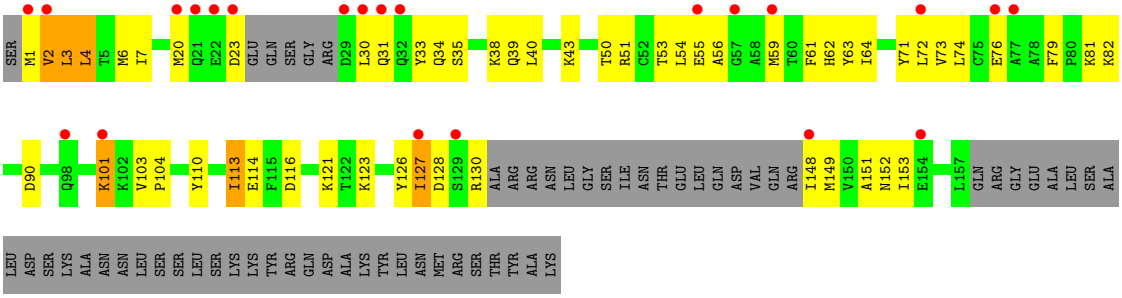
Chain B:



• Molecule 3: Vesicle-trafficking protein SEC22b

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.28Å 97.58Å 129.80Å 90.00° 90.15° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.52 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.5 (30.00-2.30) 87.3 (29.52-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.268 0.221 , 0.218	Depositor DCC
R_{free} test set	4378 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.0	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12778	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN

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	0.36	0/5758	0.66	3/7795 (0.0%)
2	B	0.37	0/5884	0.63	0/7997
3	C	0.33	0/1106	0.58	0/1489
All	All	0.36	0/12748	0.64	3/17281 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	57	GLU	N-CA-C	-8.15	88.98	111.00
1	A	115	SER	N-CA-C	-7.32	91.24	111.00
1	A	652	THR	N-CA-C	-6.56	93.29	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	5627	0	5574	280	0
2	B	5761	0	5812	247	0
3	C	1087	0	1091	75	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	123	0	0	33	0
5	B	167	0	0	29	0
5	C	11	0	0	1	0
All	All	12778	0	12477	591	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 24.

All (591) 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)
3:C:54:LEU:HD13	3:C:153:ILE:HD13	1.20	1.20
1:A:48:ARG:HB2	1:A:49:PRO:HD2	1.26	1.11
2:B:629:PRO:HG3	3:C:23:ASP:HB2	1.38	1.03
2:B:879:ARG:HH12	2:B:1092:ASN:HD22	1.04	0.98
2:B:874:SER:HB3	5:B:249:HOH:O	1.64	0.95
2:B:872:ILE:HD12	2:B:1090:GLN:HB2	1.51	0.91
1:A:290:ILE:HB	5:A:910:HOH:O	1.69	0.91
2:B:382:ASN:ND2	2:B:384:GLU:H	1.70	0.90
2:B:879:ARG:NH1	2:B:1092:ASN:HD22	1.69	0.89
1:A:3:THR:HG22	1:A:6:GLU:H	1.37	0.88
2:B:1021:MET:H	2:B:1055:ILE:HG12	1.37	0.88
2:B:872:ILE:HD13	2:B:1087:ILE:HG23	1.56	0.88
2:B:633:ARG:HB2	2:B:778:ASN:HD21	1.40	0.87
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.55	0.87
1:A:48:ARG:HB2	1:A:49:PRO:CD	2.04	0.86
2:B:573:ILE:HA	5:B:128:HOH:O	1.74	0.86
1:A:140:GLU:HA	1:A:249:ARG:HH21	1.39	0.86
3:C:123:LYS:O	3:C:127:ILE:HD13	1.75	0.85
1:A:283:GLY:H	1:A:486:GLN:HE22	1.20	0.84
2:B:854:ARG:HH12	2:B:866:ALA:HB2	1.41	0.84
3:C:35:SER:O	3:C:39:GLN:HG2	1.77	0.83
2:B:358:ASN:HA	2:B:972:GLN:HE22	1.40	0.83
2:B:818:ILE:HD13	5:B:109:HOH:O	1.78	0.83
2:B:620:LEU:HD22	2:B:634:MET:HE3	1.61	0.82
1:A:384:GLN:O	1:A:388:ARG:HG2	1.79	0.82
2:B:916:THR:HG22	2:B:917:ASN:H	1.45	0.81
2:B:567:MET:HG2	2:B:569:ILE:HD11	1.62	0.80
2:B:958:LEU:HA	2:B:964:THR:HA	1.62	0.80
2:B:1019:GLN:HB3	2:B:1020:PRO:CD	2.11	0.80
2:B:916:THR:HB	5:B:281:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:THR:HB	5:A:892:HOH:O	1.83	0.78
2:B:1064:ASN:HA	5:B:274:HOH:O	1.83	0.77
2:B:351:VAL:HG23	5:B:240:HOH:O	1.83	0.77
2:B:960:ILE:HG21	2:B:963:ARG:HH12	1.47	0.77
2:B:382:ASN:HD22	2:B:384:GLU:H	1.31	0.77
1:A:121:VAL:HG12	5:A:900:HOH:O	1.85	0.77
1:A:297:GLY:H	1:A:300:MET:HE2	1.49	0.76
2:B:433:SER:OG	2:B:457:ARG:HD3	1.85	0.76
2:B:872:ILE:HD11	2:B:1087:ILE:HA	1.66	0.76
2:B:609:THR:HG21	5:B:5:HOH:O	1.85	0.76
2:B:609:THR:HG22	2:B:611:GLU:H	1.49	0.76
1:A:45:LEU:HA	1:A:495:ARG:NH1	2.01	0.76
1:A:459:ILE:HD13	1:A:481:PHE:HE2	1.50	0.76
1:A:310:ILE:HD12	1:A:310:ILE:H	1.50	0.76
2:B:916:THR:HG22	2:B:917:ASN:N	2.00	0.76
1:A:627:SER:HB3	1:A:646:ARG:HG3	1.67	0.75
1:A:493:ARG:C	1:A:494:ILE:HD12	2.06	0.75
1:A:33:ARG:HB3	5:A:923:HOH:O	1.85	0.75
2:B:759:ILE:HG23	2:B:787:VAL:HG13	1.67	0.74
1:A:647:ILE:HD11	1:A:664:ILE:HG21	1.68	0.74
1:A:259:ARG:NH1	1:A:306:LEU:HD23	2.03	0.74
1:A:622:ILE:HD13	1:A:624:TYR:CE1	2.23	0.73
1:A:28:ARG:HH11	1:A:28:ARG:HB3	1.51	0.73
1:A:312:SER:O	1:A:316:ILE:HD13	1.89	0.73
2:B:634:MET:HE2	2:B:687:VAL:HG13	1.71	0.72
1:A:297:GLY:H	1:A:300:MET:CE	2.01	0.72
3:C:113:ILE:O	3:C:116:ASP:HB2	1.90	0.72
3:C:54:LEU:CD1	3:C:153:ILE:HD13	2.11	0.72
1:A:562:LYS:NZ	1:A:562:LYS:HB3	2.05	0.72
1:A:593:PHE:O	1:A:594:ASN:HB2	1.89	0.71
2:B:1059:SER:H	2:B:1060:PRO:HD3	1.55	0.71
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.05	0.71
1:A:311:ARG:HB2	1:A:316:ILE:HD11	1.71	0.71
1:A:240:LEU:HD22	1:A:244:LEU:HG	1.72	0.71
1:A:673:GLN:HG2	1:A:685:LEU:HD12	1.73	0.71
1:A:449:CYS:HB2	5:A:831:HOH:O	1.91	0.71
2:B:760:HIS:CE1	2:B:788:GLN:HG2	2.26	0.71
3:C:113:ILE:HD13	3:C:113:ILE:H	1.56	0.71
1:A:115:SER:O	1:A:116:SER:HB3	1.89	0.70
1:A:283:GLY:N	1:A:486:GLN:HE22	1.88	0.70
1:A:44:PRO:O	1:A:495:ARG:NH1	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:THR:HG21	5:A:909:HOH:O	1.90	0.70
2:B:504:PRO:HG2	2:B:542:THR:HA	1.74	0.70
1:A:183:ILE:HD12	2:B:565:PRO:HG2	1.74	0.69
1:A:541:ASP:HB3	1:A:544:ARG:HD2	1.74	0.69
1:A:63:ARG:HD2	1:A:88:CYS:SG	2.33	0.69
2:B:1019:GLN:CB	2:B:1020:PRO:HD3	2.22	0.69
2:B:412:HIS:HE1	2:B:781:PRO:O	1.76	0.68
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.74	0.68
1:A:484:GLN:HG2	1:A:494:ILE:HG13	1.74	0.68
2:B:915:GLY:HA3	2:B:1076:SER:HB2	1.76	0.68
1:A:76:VAL:HG12	1:A:77:ASP:H	1.58	0.68
1:A:419:ALA:HB3	5:A:892:HOH:O	1.94	0.68
1:A:622:ILE:HD13	1:A:624:TYR:HE1	1.57	0.68
2:B:382:ASN:HD22	2:B:382:ASN:C	1.97	0.67
2:B:641:LEU:CD2	2:B:649:LEU:HB2	2.23	0.67
2:B:1063:ALA:C	2:B:1065:PHE:H	1.96	0.67
2:B:1074:THR:HG22	2:B:1077:ALA:HB3	1.76	0.67
2:B:1074:THR:HG23	2:B:1076:SER:H	1.59	0.67
2:B:654:GLU:OE2	2:B:919:ARG:HB3	1.95	0.67
2:B:496:TYR:HE1	5:B:109:HOH:O	1.76	0.66
2:B:879:ARG:NH1	2:B:1092:ASN:HB3	2.10	0.66
2:B:1021:MET:N	2:B:1055:ILE:HG12	2.09	0.66
1:A:686:GLN:HG2	1:A:690:ASP:OD1	1.96	0.66
1:A:722:VAL:O	1:A:723:ASN:HB2	1.96	0.66
2:B:671:ASP:OD2	2:B:675:LYS:HE3	1.95	0.66
2:B:879:ARG:HH12	2:B:1092:ASN:ND2	1.88	0.66
2:B:1020:PRO:HA	2:B:1055:ILE:HG12	1.78	0.66
2:B:641:LEU:HD21	2:B:649:LEU:HB2	1.78	0.65
1:A:283:GLY:H	1:A:486:GLN:NE2	1.94	0.65
1:A:649:LEU:HD12	1:A:650:MET:N	2.11	0.65
1:A:60:LEU:HG	5:A:846:HOH:O	1.96	0.64
1:A:494:ILE:HD12	1:A:494:ILE:N	2.11	0.64
2:B:955:GLU:OE1	2:B:955:GLU:N	2.31	0.64
1:A:749:LEU:O	1:A:753:MET:HG2	1.97	0.64
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.80	0.64
1:A:5:LEU:O	1:A:9:GLN:HG3	1.97	0.64
1:A:106:GLN:HB2	1:A:107:PRO:HD2	1.80	0.64
3:C:110:TYR:HB3	3:C:113:ILE:CG2	2.28	0.64
1:A:185:LYS:HB3	2:B:567:MET:HB3	1.80	0.64
2:B:779:VAL:HG21	2:B:807:LEU:HD21	1.79	0.64
1:A:121:VAL:HG23	1:A:494:ILE:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:525:VAL:HG22	2:B:735:LEU:HD11	1.80	0.64
2:B:1054:VAL:O	2:B:1056:ARG:N	2.30	0.64
1:A:126:GLN:HE22	1:A:491:GLN:HG2	1.62	0.63
2:B:915:GLY:HA3	2:B:1076:SER:CB	2.28	0.63
2:B:916:THR:CG2	2:B:917:ASN:H	2.10	0.63
2:B:1067:GLN:HG3	5:B:274:HOH:O	1.97	0.63
1:A:28:ARG:HB3	1:A:28:ARG:NH1	2.12	0.63
1:A:311:ARG:HB2	1:A:316:ILE:CD1	2.28	0.63
2:B:906:LEU:HD13	2:B:942:THR:HG21	1.80	0.63
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.81	0.63
2:B:567:MET:HE2	2:B:569:ILE:HD11	1.81	0.63
1:A:345:ILE:HD13	1:A:367:THR:HG21	1.81	0.63
2:B:1048:PHE:HB2	5:B:154:HOH:O	1.99	0.63
1:A:116:SER:HA	1:A:496:VAL:O	1.99	0.62
1:A:610:GLN:HG3	1:A:618:MET:HE3	1.81	0.62
2:B:641:LEU:HD23	2:B:642:PRO:HD2	1.81	0.62
1:A:76:VAL:HG12	1:A:77:ASP:N	2.13	0.62
3:C:110:TYR:O	3:C:113:ILE:HG23	1.98	0.62
3:C:127:ILE:N	3:C:127:ILE:HD12	2.14	0.62
2:B:439:ASN:HB2	2:B:440:PRO:CD	2.29	0.62
1:A:624:TYR:CE2	1:A:634:PRO:HG3	2.35	0.62
1:A:282:THR:HG22	5:A:810:HOH:O	1.99	0.62
2:B:382:ASN:HD22	2:B:383:PRO:N	1.98	0.62
2:B:879:ARG:CZ	2:B:1092:ASN:HB3	2.29	0.62
1:A:58:PRO:O	1:A:59:VAL:HB	2.00	0.62
2:B:361:PRO:HG2	5:B:250:HOH:O	1.99	0.62
2:B:1020:PRO:HG3	2:B:1062:LYS:NZ	2.15	0.61
3:C:56:ALA:HB2	3:C:153:ILE:HG21	1.82	0.61
1:A:596:SER:OG	1:A:599:GLU:HG3	2.00	0.61
1:A:414:ILE:HD11	1:A:503:TRP:HH2	1.66	0.61
3:C:2:VAL:HG12	3:C:3:LEU:H	1.66	0.61
2:B:909:GLN:HG2	2:B:911:SER:H	1.65	0.61
1:A:63:ARG:HB2	1:A:90:GLN:HG2	1.83	0.61
1:A:696:LEU:CD1	1:A:703:PRO:HG2	2.29	0.61
1:A:475:GLY:O	1:A:476:ARG:HB2	2.00	0.61
2:B:1059:SER:H	2:B:1060:PRO:CD	2.14	0.61
2:B:832:ASN:O	2:B:836:LEU:HG	2.00	0.61
2:B:633:ARG:HB2	2:B:778:ASN:ND2	2.14	0.60
1:A:349:ALA:HB1	1:A:355:THR:HG21	1.81	0.60
1:A:259:ARG:NE	5:A:847:HOH:O	2.35	0.60
2:B:654:GLU:OE1	2:B:920:LEU:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:992:LEU:O	2:B:1052:LEU:HD12	2.02	0.59
1:A:414:ILE:HD11	1:A:503:TRP:CH2	2.37	0.59
2:B:991:VAL:HG22	5:B:149:HOH:O	2.02	0.59
1:A:536:THR:HB	5:A:919:HOH:O	2.03	0.59
1:A:80:ALA:O	1:A:82:LEU:HG	2.02	0.59
1:A:42:PHE:HB3	1:A:459:ILE:HD11	1.84	0.59
1:A:665:ALA:O	1:A:669:LYS:HG3	2.02	0.59
3:C:113:ILE:HD13	3:C:113:ILE:N	2.16	0.59
1:A:183:ILE:HG23	1:A:184:SER:N	2.17	0.58
1:A:116:SER:HA	1:A:497:THR:HA	1.84	0.58
2:B:987:ASP:HA	2:B:992:LEU:HD23	1.84	0.58
3:C:127:ILE:HG22	3:C:127:ILE:O	2.03	0.58
2:B:1073:ARG:HB3	2:B:1079:SER:HB3	1.85	0.58
3:C:2:VAL:HG12	3:C:3:LEU:N	2.18	0.58
2:B:1011:VAL:HG12	2:B:1013:ASN:H	1.68	0.58
1:A:67:ARG:HG2	5:A:906:HOH:O	2.03	0.58
1:A:622:ILE:HD12	1:A:622:ILE:O	2.04	0.58
2:B:760:HIS:NE2	2:B:788:GLN:HG2	2.18	0.58
1:A:562:LYS:HB3	1:A:562:LYS:HZ2	1.69	0.58
2:B:605:MET:SD	5:B:220:HOH:O	2.57	0.58
1:A:368:GLY:N	5:A:831:HOH:O	2.26	0.58
2:B:909:GLN:HG2	2:B:910:LYS:N	2.19	0.58
3:C:148:ILE:N	3:C:148:ILE:HD12	2.19	0.57
1:A:227:ASN:HD21	1:A:278:THR:HB	1.68	0.57
2:B:347:GLY:HA3	5:B:130:HOH:O	2.03	0.57
2:B:1064:ASN:HA	5:B:78:HOH:O	2.04	0.57
3:C:1:MET:H2	3:C:76:GLU:H	1.50	0.57
1:A:524:ILE:HD12	1:A:615:SER:HB3	1.86	0.57
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.86	0.57
1:A:338:ALA:HB1	1:A:345:ILE:HD11	1.86	0.57
2:B:960:ILE:HG21	2:B:963:ARG:NH1	2.18	0.57
1:A:711:GLY:HA2	5:A:889:HOH:O	2.04	0.57
1:A:297:GLY:CA	1:A:300:MET:HB2	2.34	0.57
1:A:338:ALA:CB	1:A:345:ILE:HD11	2.34	0.57
1:A:642:ILE:HD13	1:A:648:LEU:CD1	2.34	0.57
2:B:872:ILE:HD11	2:B:1087:ILE:HD13	1.87	0.57
3:C:127:ILE:N	3:C:127:ILE:CD1	2.66	0.57
1:A:439:GLY:HA2	1:A:532:TYR:CE2	2.39	0.56
2:B:958:LEU:HD23	2:B:958:LEU:O	2.06	0.56
1:A:607:PHE:HD2	1:A:608:MET:HE3	1.69	0.56
2:B:446:ASP:HB2	2:B:449:ARG:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:696:TYR:CE1	2:B:920:LEU:HD23	2.41	0.56
1:A:311:ARG:CG	1:A:316:ILE:HD11	2.35	0.56
1:A:621:PRO:HD2	1:A:637:LEU:HD11	1.87	0.56
1:A:747:VAL:HG12	1:A:748:SER:N	2.21	0.56
2:B:958:LEU:H	2:B:958:LEU:HD22	1.71	0.56
1:A:240:LEU:CD2	1:A:244:LEU:HG	2.36	0.56
1:A:647:ILE:HD12	1:A:660:HIS:ND1	2.20	0.56
2:B:1052:LEU:HG	2:B:1053:TYR:N	2.20	0.56
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.87	0.56
2:B:554:HIS:CD2	2:B:569:ILE:HD12	2.41	0.56
2:B:411:LEU:N	2:B:411:LEU:HD23	2.21	0.56
2:B:620:LEU:CD2	2:B:634:MET:HE3	2.35	0.55
1:A:311:ARG:CB	1:A:316:ILE:HD11	2.36	0.55
2:B:750:ARG:HD2	5:B:44:HOH:O	2.07	0.55
2:B:1059:SER:N	2:B:1060:PRO:CD	2.70	0.55
3:C:61:PHE:CZ	3:C:74:LEU:HD13	2.41	0.55
2:B:1019:GLN:CB	2:B:1020:PRO:CD	2.83	0.55
1:A:15:ASP:OD1	1:A:116:SER:HB2	2.06	0.55
1:A:185:LYS:CB	2:B:567:MET:HB3	2.36	0.55
1:A:345:ILE:HD12	1:A:345:ILE:N	2.21	0.55
1:A:647:ILE:HD11	1:A:664:ILE:CG2	2.36	0.55
3:C:6:MET:O	3:C:7:ILE:HD13	2.07	0.55
2:B:854:ARG:NH1	2:B:866:ALA:HB2	2.19	0.54
2:B:601:THR:C	2:B:605:MET:HE3	2.26	0.54
1:A:180:CYS:HB3	5:A:857:HOH:O	2.07	0.54
2:B:963:ARG:HB3	2:B:965:ILE:HD11	1.88	0.54
2:B:1051:ILE:N	2:B:1051:ILE:HD12	2.23	0.54
1:A:297:GLY:N	1:A:300:MET:HE2	2.22	0.54
2:B:1022:THR:O	2:B:1023:ASP:HB2	2.08	0.54
1:A:24:TRP:HB3	1:A:25:PRO:HD2	1.90	0.54
1:A:626:TYR:CD2	1:A:632:PRO:HG3	2.43	0.54
2:B:359:MET:HE3	2:B:359:MET:H	1.73	0.54
1:A:162:ALA:O	1:A:233:VAL:HG23	2.08	0.53
1:A:344:VAL:C	1:A:345:ILE:HD12	2.28	0.53
1:A:364:PRO:O	1:A:367:THR:O	2.27	0.53
1:A:647:ILE:HD12	1:A:660:HIS:HA	1.91	0.53
3:C:30:LEU:O	3:C:34:GLN:HB2	2.08	0.53
1:A:121:VAL:CG2	1:A:494:ILE:HD13	2.39	0.53
1:A:438:ILE:HG21	1:A:529:LEU:HD21	1.90	0.53
1:A:673:GLN:HG2	1:A:685:LEU:CD1	2.37	0.53
2:B:710:ALA:HB3	2:B:777:PRO:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1039:ILE:O	2:B:1043:ARG:HG2	2.07	0.53
1:A:519:GLN:HG2	5:A:812:HOH:O	2.07	0.53
1:A:642:ILE:HD13	1:A:648:LEU:HD11	1.89	0.53
1:A:622:ILE:HD12	1:A:622:ILE:C	2.29	0.53
2:B:351:VAL:HG13	2:B:356:GLU:HG3	1.90	0.53
3:C:33:TYR:CE2	3:C:59:MET:HG3	2.43	0.53
2:B:1087:ILE:O	2:B:1091:VAL:HG23	2.09	0.53
2:B:966:PRO:HG2	2:B:1038:PHE:HB2	1.90	0.53
3:C:50:THR:O	3:C:51:ARG:HG2	2.09	0.53
1:A:316:ILE:HD12	1:A:321:ALA:HB2	1.91	0.53
2:B:430:ARG:HD3	2:B:435:ARG:NH2	2.23	0.53
2:B:875:LEU:HD22	2:B:892:VAL:HG12	1.90	0.53
3:C:110:TYR:HB3	3:C:113:ILE:HG23	1.91	0.53
1:A:310:ILE:HD12	1:A:310:ILE:N	2.23	0.52
1:A:310:ILE:HG22	1:A:311:ARG:HD3	1.90	0.52
2:B:359:MET:H	2:B:359:MET:CE	2.21	0.52
2:B:620:LEU:HD22	2:B:634:MET:CE	2.37	0.52
2:B:879:ARG:NH1	5:B:232:HOH:O	2.41	0.52
3:C:101:LYS:HE3	3:C:101:LYS:HA	1.91	0.52
2:B:666:MET:HE2	2:B:855:SER:HB3	1.91	0.52
1:A:687:ALA:N	1:A:688:PRO:HD2	2.24	0.52
2:B:958:LEU:HB3	2:B:964:THR:HG23	1.91	0.52
3:C:39:GLN:HE21	3:C:39:GLN:HA	1.74	0.52
3:C:61:PHE:CE2	3:C:74:LEU:HD13	2.45	0.52
1:A:153:MET:HE1	1:A:154:SER:HA	1.91	0.52
1:A:649:LEU:HD12	1:A:649:LEU:C	2.28	0.52
2:B:872:ILE:CD1	2:B:1087:ILE:HA	2.38	0.52
1:A:311:ARG:HG3	1:A:316:ILE:HD11	1.92	0.52
1:A:696:LEU:HD13	1:A:703:PRO:HG2	1.92	0.52
1:A:722:VAL:HG13	1:A:723:ASN:N	2.24	0.52
2:B:428:ILE:HD12	2:B:428:ILE:N	2.25	0.52
3:C:1:MET:N	3:C:76:GLU:HB2	2.24	0.52
1:A:297:GLY:N	1:A:300:MET:HB2	2.25	0.52
1:A:344:VAL:HG22	5:A:831:HOH:O	2.10	0.52
2:B:381:CYS:HB2	2:B:822:THR:O	2.09	0.52
2:B:641:LEU:HD23	2:B:642:PRO:CD	2.40	0.52
3:C:63:TYR:HB3	3:C:72:LEU:HD12	1.92	0.52
1:A:407:GLU:HG3	1:A:445:GLN:HG2	1.91	0.52
3:C:4:LEU:HD12	3:C:20:MET:HG2	1.91	0.51
1:A:316:ILE:CD1	1:A:316:ILE:N	2.73	0.51
1:A:349:ALA:CB	1:A:355:THR:HG21	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:HIS:HD2	5:B:10:HOH:O	1.93	0.51
2:B:936:VAL:O	2:B:940:LEU:HD23	2.11	0.51
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.91	0.51
3:C:148:ILE:HG22	3:C:149:MET:N	2.25	0.51
1:A:262:ARG:NH1	5:A:860:HOH:O	2.41	0.51
2:B:423:VAL:HG23	2:B:488:ILE:HD11	1.92	0.51
2:B:425:SER:HB3	2:B:427:THR:O	2.11	0.51
2:B:558:LEU:HD23	2:B:565:PRO:HB3	1.92	0.51
2:B:1057:ASP:H	2:B:1060:PRO:HG3	1.75	0.51
3:C:2:VAL:HG12	3:C:3:LEU:HD23	1.92	0.51
1:A:275:LEU:HB3	1:A:343:HIS:CE1	2.46	0.51
1:A:355:THR:HG22	1:A:357:LEU:HG	1.93	0.51
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.46	0.51
1:A:652:THR:HG22	1:A:654:PHE:H	1.76	0.51
2:B:1063:ALA:C	2:B:1065:PHE:N	2.63	0.51
2:B:437:TYR:HE1	5:B:109:HOH:O	1.93	0.51
2:B:993:MET:CE	2:B:1065:PHE:HA	2.41	0.51
3:C:54:LEU:HB3	3:C:153:ILE:HB	1.93	0.50
1:A:196:SER:O	1:A:197:ALA:HB2	2.12	0.50
1:A:410:THR:HB	1:A:414:ILE:HB	1.92	0.50
1:A:184:SER:HA	5:A:857:HOH:O	2.10	0.50
1:A:190:ARG:NH1	2:B:575:ASP:OD2	2.44	0.50
2:B:1019:GLN:CG	2:B:1020:PRO:HD3	2.41	0.50
1:A:664:ILE:HD13	1:A:667:TRP:CE3	2.47	0.50
1:A:114:PHE:HB3	1:A:117:ILE:HD12	1.93	0.50
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.94	0.50
1:A:528:ARG:HD2	5:A:876:HOH:O	2.12	0.50
1:A:673:GLN:HG3	1:A:681:PHE:CE2	2.47	0.50
1:A:426:LEU:HD12	1:A:445:GLN:HB3	1.94	0.50
2:B:445:LEU:C	2:B:447:GLN:H	2.15	0.50
1:A:180:CYS:SG	1:A:185:LYS:HE2	2.52	0.49
1:A:610:GLN:HG3	1:A:618:MET:CE	2.42	0.49
2:B:348:LEU:HG	2:B:348:LEU:O	2.11	0.49
3:C:38:LYS:NZ	5:C:203:HOH:O	2.45	0.49
1:A:18:ARG:CZ	1:A:612:LEU:HD22	2.41	0.49
1:A:183:ILE:O	2:B:565:PRO:O	2.30	0.49
1:A:586:ARG:HB2	1:A:586:ARG:NH1	2.27	0.49
2:B:351:VAL:CG1	2:B:356:GLU:HG3	2.42	0.49
2:B:958:LEU:HD11	5:B:107:HOH:O	2.12	0.49
1:A:138:CYS:HB2	1:A:262:ARG:HH11	1.76	0.49
1:A:183:ILE:HG23	1:A:184:SER:H	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:618:PRO:HB3	5:B:128:HOH:O	2.12	0.49
2:B:1055:ILE:CG2	2:B:1062:LYS:HD2	2.42	0.49
2:B:1054:VAL:C	2:B:1056:ARG:N	2.62	0.49
1:A:695:ILE:C	1:A:697:HIS:H	2.16	0.49
1:A:19:PHE:CE1	1:A:499:ILE:HD12	2.47	0.48
1:A:259:ARG:CZ	5:A:847:HOH:O	2.61	0.48
2:B:439:ASN:HB2	2:B:440:PRO:HD2	1.94	0.48
3:C:39:GLN:O	3:C:43:LYS:HG2	2.13	0.48
1:A:397:GLN:HE22	1:A:489:SER:CB	2.26	0.48
3:C:7:ILE:HD12	3:C:71:TYR:CD2	2.47	0.48
2:B:446:ASP:O	2:B:448:ARG:N	2.46	0.48
1:A:668:ARG:HA	1:A:673:GLN:NE2	2.28	0.48
2:B:446:ASP:C	2:B:448:ARG:H	2.14	0.48
2:B:483:VAL:HG12	2:B:483:VAL:O	2.13	0.48
2:B:854:ARG:HH12	2:B:866:ALA:CB	2.19	0.48
2:B:410:LEU:HD22	2:B:935:LEU:HG	1.93	0.48
1:A:495:ARG:NE	5:A:840:HOH:O	2.47	0.48
1:A:651:ASP:HA	1:A:656:ILE:HD13	1.95	0.48
2:B:652:ARG:HB2	2:B:696:TYR:CE2	2.49	0.48
3:C:33:TYR:HB3	3:C:74:LEU:HD22	1.96	0.48
1:A:180:CYS:CB	5:A:857:HOH:O	2.61	0.48
1:A:115:SER:O	1:A:116:SER:CB	2.56	0.48
1:A:249:ARG:NH1	3:C:130:ARG:HB2	2.29	0.48
1:A:459:ILE:HD13	1:A:481:PHE:CE2	2.41	0.48
1:A:560:TYR:CD1	1:A:761:VAL:HG12	2.49	0.48
2:B:779:VAL:HA	5:B:52:HOH:O	2.14	0.48
3:C:55:GLU:O	3:C:152:ASN:ND2	2.46	0.48
2:B:956:GLY:HA2	2:B:967:GLN:HG2	1.96	0.47
1:A:179:GLY:HA2	1:A:239:ASN:HD22	1.78	0.47
1:A:259:ARG:HH11	1:A:306:LEU:HD23	1.76	0.47
1:A:531:ILE:HD13	1:A:590:LEU:CD2	2.44	0.47
2:B:936:VAL:HG13	2:B:937:TYR:N	2.29	0.47
2:B:958:LEU:HD22	2:B:958:LEU:N	2.29	0.47
1:A:148:LYS:O	1:A:152:GLN:HG3	2.14	0.47
2:B:677:ALA:HB2	2:B:705:ILE:HA	1.97	0.47
2:B:913:GLN:NE2	2:B:918:ALA:HB2	2.30	0.47
1:A:647:ILE:CD1	1:A:660:HIS:HA	2.45	0.47
2:B:734:GLU:HA	2:B:1048:PHE:HE2	1.79	0.47
1:A:42:PHE:CB	1:A:459:ILE:HD11	2.44	0.47
1:A:71:ASN:HB2	1:A:72:PRO:CD	2.44	0.47
2:B:602:LEU:HB2	2:B:603:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:872:ILE:HD12	2:B:1090:GLN:CB	2.33	0.47
1:A:417:SER:O	1:A:437:GLU:HA	2.15	0.47
1:A:622:ILE:HG13	1:A:651:ASP:HB3	1.97	0.47
2:B:382:ASN:HD22	2:B:384:GLU:N	2.06	0.47
2:B:1053:TYR:CD1	2:B:1055:ILE:HD12	2.50	0.47
2:B:964:THR:C	2:B:965:ILE:HD12	2.35	0.47
1:A:76:VAL:C	5:A:882:HOH:O	2.53	0.47
2:B:965:ILE:HD12	2:B:965:ILE:N	2.30	0.47
1:A:56:TYR:CE1	1:A:98:TYR:OH	2.64	0.47
2:B:759:ILE:HD12	2:B:759:ILE:N	2.30	0.47
1:A:554:CYS:HA	1:A:570:PHE:CZ	2.49	0.47
3:C:114:GLU:C	3:C:116:ASP:H	2.16	0.46
1:A:30:GLU:OE1	1:A:30:GLU:HA	2.15	0.46
1:A:559:GLU:O	1:A:568:PHE:HA	2.16	0.46
2:B:1047:PRO:HD2	5:B:154:HOH:O	2.14	0.46
1:A:528:ARG:N	5:A:876:HOH:O	2.48	0.46
2:B:373:HIS:CD2	2:B:375:ASP:H	2.33	0.46
2:B:730:LYS:HD3	5:B:257:HOH:O	2.15	0.46
1:A:316:ILE:HD13	1:A:316:ILE:N	2.31	0.46
2:B:871:VAL:CG2	2:B:903:VAL:HG21	2.45	0.46
1:A:528:ARG:CD	5:A:876:HOH:O	2.63	0.46
1:A:549:GLN:HE22	1:A:552:ARG:HH11	1.63	0.46
2:B:439:ASN:ND2	2:B:822:THR:HG21	2.30	0.46
2:B:957:ALA:C	2:B:959:ASN:H	2.18	0.46
3:C:113:ILE:H	3:C:113:ILE:CD1	2.26	0.46
1:A:291:GLY:N	5:A:910:HOH:O	2.48	0.46
1:A:638:ASP:C	1:A:722:VAL:HG22	2.36	0.46
2:B:771:THR:O	2:B:771:THR:HG22	2.16	0.46
1:A:425:SER:HB2	1:A:440:THR:HG22	1.98	0.46
1:A:536:THR:HG22	1:A:536:THR:O	2.16	0.46
3:C:1:MET:HA	3:C:79:PHE:HB2	1.97	0.46
2:B:1005:LEU:HD13	2:B:1013:ASN:HA	1.96	0.46
2:B:1053:TYR:HB2	2:B:1055:ILE:HG13	1.96	0.46
1:A:259:ARG:HH11	1:A:259:ARG:HG2	1.81	0.46
1:A:476:ARG:HA	1:A:501:ARG:O	2.16	0.46
1:A:195:LEU:HD13	1:A:203:MET:HE1	1.97	0.46
1:A:249:ARG:HH12	3:C:130:ARG:HB2	1.81	0.46
1:A:588:SER:OG	1:A:595:ASN:ND2	2.49	0.45
3:C:3:LEU:O	3:C:4:LEU:HB2	2.16	0.45
3:C:4:LEU:HD13	3:C:30:LEU:HD11	1.97	0.45
1:A:368:GLY:HA3	1:A:450:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:GLN:HE22	2:B:400:LEU:HD23	1.81	0.45
2:B:609:THR:HG22	2:B:610:LEU:N	2.30	0.45
2:B:890:LEU:HD23	2:B:1084:LEU:HD22	1.98	0.45
2:B:916:THR:CG2	2:B:917:ASN:N	2.67	0.45
2:B:956:GLY:HA3	2:B:965:ILE:O	2.16	0.45
1:A:140:GLU:CD	1:A:249:ARG:NH2	2.70	0.45
1:A:79:ARG:HG3	1:A:79:ARG:HH11	1.81	0.45
1:A:153:MET:CE	1:A:157:LEU:HD12	2.46	0.45
1:A:754:ASP:O	1:A:758:LYS:HG3	2.16	0.45
2:B:959:ASN:O	2:B:961:SER:N	2.48	0.45
2:B:1041:TRP:O	2:B:1045:GLN:HG2	2.17	0.45
2:B:730:LYS:HE2	2:B:734:GLU:OE2	2.17	0.45
2:B:998:LYS:HB2	2:B:1058:GLU:OE1	2.16	0.45
2:B:1074:THR:CG2	2:B:1077:ALA:HB3	2.45	0.45
1:A:672:TYR:N	5:A:921:HOH:O	2.50	0.45
2:B:368:PRO:HD2	2:B:839:ASP:OD2	2.16	0.45
2:B:410:LEU:CD2	2:B:935:LEU:HG	2.47	0.45
3:C:110:TYR:HB3	3:C:113:ILE:HG22	1.96	0.45
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.98	0.45
2:B:977:LYS:HE3	5:B:284:HOH:O	2.16	0.45
1:A:494:ILE:N	1:A:494:ILE:CD1	2.79	0.45
2:B:666:MET:CE	2:B:855:SER:HB3	2.47	0.45
1:A:108:ALA:HB1	1:A:114:PHE:CD1	2.52	0.45
2:B:1060:PRO:O	2:B:1062:LYS:HG3	2.17	0.45
3:C:50:THR:C	3:C:51:ARG:HG2	2.36	0.45
1:A:59:VAL:N	5:A:846:HOH:O	2.50	0.44
2:B:362:SER:O	2:B:970:ILE:HD13	2.16	0.44
2:B:642:PRO:HG2	2:B:702:LEU:HD21	1.98	0.44
1:A:631:PRO:O	1:A:633:GLU:HG3	2.16	0.44
1:A:153:MET:HE3	1:A:157:LEU:HD12	2.00	0.44
2:B:423:VAL:CG2	2:B:488:ILE:HD11	2.47	0.44
2:B:970:ILE:HD12	2:B:970:ILE:N	2.32	0.44
3:C:51:ARG:HD3	3:C:64:ILE:HG22	1.99	0.44
1:A:153:MET:HE3	1:A:157:LEU:CD1	2.47	0.44
2:B:382:ASN:ND2	2:B:382:ASN:C	2.69	0.44
2:B:1054:VAL:C	2:B:1056:ARG:H	2.20	0.44
1:A:47:GLU:HG3	1:A:453:PRO:HB3	1.99	0.44
1:A:204:LEU:HA	5:A:841:HOH:O	2.18	0.44
2:B:661:ALA:HB3	2:B:861:SER:OG	2.18	0.44
1:A:19:PHE:HE1	1:A:499:ILE:HD12	1.82	0.44
1:A:28:ARG:HH11	1:A:28:ARG:CB	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:MET:C	3:C:7:ILE:HD13	2.38	0.44
1:A:560:TYR:CD2	1:A:560:TYR:N	2.85	0.44
2:B:601:THR:HB	2:B:605:MET:CE	2.47	0.44
3:C:4:LEU:CD1	3:C:20:MET:HG2	2.48	0.44
3:C:81:LYS:HE3	3:C:148:ILE:HG21	2.00	0.44
2:B:393:ILE:HA	2:B:394:PRO:HD3	1.91	0.44
2:B:958:LEU:HD23	2:B:958:LEU:C	2.38	0.44
2:B:367:PRO:HA	2:B:368:PRO:HD3	1.91	0.43
3:C:126:TYR:C	3:C:127:ILE:HD12	2.39	0.43
1:A:101:ILE:O	1:A:101:ILE:HG13	2.19	0.43
1:A:705:TYR:O	1:A:706:ILE:HD13	2.16	0.43
1:A:198:LYS:O	1:A:202:GLU:HG3	2.17	0.43
2:B:358:ASN:HA	2:B:972:GLN:NE2	2.19	0.43
2:B:763:HIS:HB2	2:B:786:ALA:HB3	1.99	0.43
1:A:536:THR:CB	5:A:919:HOH:O	2.64	0.43
2:B:1051:ILE:HD12	2:B:1051:ILE:H	1.82	0.43
1:A:60:LEU:CD2	1:A:69:VAL:HG22	2.49	0.43
1:A:153:MET:CE	1:A:154:SER:HA	2.48	0.43
1:A:607:PHE:HD2	1:A:608:MET:CE	2.31	0.43
2:B:457:ARG:HG3	2:B:458:VAL:N	2.32	0.43
2:B:498:LEU:CD1	2:B:498:LEU:N	2.82	0.43
3:C:63:TYR:CD1	3:C:63:TYR:C	2.91	0.43
1:A:567:SER:O	1:A:569:ARG:HG3	2.18	0.43
2:B:747:ALA:HB2	2:B:809:TYR:CB	2.48	0.43
1:A:113:GLN:H	1:A:113:GLN:HG3	1.53	0.43
2:B:567:MET:HG2	2:B:569:ILE:CD1	2.42	0.43
3:C:3:LEU:HD13	3:C:123:LYS:HD3	2.00	0.43
3:C:4:LEU:HD11	3:C:20:MET:SD	2.58	0.43
1:A:419:ALA:HA	1:A:458:ALA:O	2.19	0.43
3:C:1:MET:H1	3:C:76:GLU:HB2	1.84	0.43
3:C:53:THR:HG23	3:C:62:HIS:CE1	2.54	0.43
3:C:62:HIS:HB2	3:C:73:VAL:CG1	2.49	0.43
1:A:373:MET:HE1	1:A:598:ASP:HB3	1.99	0.43
3:C:103:VAL:N	3:C:104:PRO:HD2	2.34	0.43
1:A:262:ARG:NH2	1:A:292:GLY:HA3	2.34	0.42
2:B:463:GLU:O	2:B:464:GLU:HG3	2.19	0.42
2:B:611:GLU:HG3	5:B:5:HOH:O	2.19	0.42
3:C:4:LEU:HD13	3:C:30:LEU:CD1	2.48	0.42
3:C:153:ILE:HD12	3:C:153:ILE:O	2.18	0.42
1:A:357:LEU:HD12	1:A:373:MET:CE	2.49	0.42
2:B:629:PRO:CG	3:C:23:ASP:HB2	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:THR:CG2	1:A:6:GLU:HG3	2.50	0.42
1:A:39:ALA:HB3	1:A:525:LEU:HD13	2.01	0.42
1:A:78:TYR:HD1	1:A:78:TYR:H	1.66	0.42
1:A:288:MET:HB3	1:A:347:ILE:HD13	2.00	0.42
1:A:316:ILE:HD12	1:A:321:ALA:CB	2.50	0.42
1:A:700:PHE:CB	1:A:701:PRO:HD3	2.49	0.42
1:A:363:CYS:HB2	1:A:364:PRO:CD	2.49	0.42
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.84	0.42
1:A:622:ILE:HD11	1:A:651:ASP:HB3	2.02	0.42
2:B:357:ARG:C	2:B:359:MET:HE2	2.39	0.42
2:B:480:ARG:HG3	2:B:481:PRO:HD2	2.02	0.42
1:A:68:ALA:HA	1:A:409:LYS:HZ2	1.83	0.42
1:A:107:PRO:HG2	1:A:110:LEU:HD12	2.01	0.42
2:B:567:MET:CE	2:B:569:ILE:HD11	2.49	0.42
2:B:1055:ILE:HG22	2:B:1062:LYS:HD2	2.01	0.42
1:A:252:TRP:CE2	2:B:581:PRO:HD3	2.54	0.42
1:A:546:LEU:HD12	1:A:546:LEU:HA	1.90	0.42
1:A:675:MET:HB3	1:A:677:GLU:OE2	2.20	0.42
2:B:522:LEU:HD22	2:B:526:CYS:SG	2.60	0.42
2:B:1055:ILE:HG13	2:B:1055:ILE:H	1.70	0.42
3:C:7:ILE:HD12	3:C:71:TYR:HA	2.00	0.42
3:C:64:ILE:C	3:C:64:ILE:HD12	2.40	0.42
3:C:114:GLU:C	3:C:116:ASP:N	2.73	0.42
1:A:67:ARG:C	1:A:409:LYS:HZ3	2.23	0.42
1:A:183:ILE:O	1:A:184:SER:CB	2.68	0.42
1:A:341:THR:HG22	1:A:341:THR:O	2.19	0.42
1:A:76:VAL:CG1	1:A:77:ASP:N	2.82	0.42
1:A:418:GLY:HA3	1:A:438:ILE:O	2.20	0.42
2:B:446:ASP:C	2:B:448:ARG:N	2.73	0.42
2:B:634:MET:HE2	2:B:687:VAL:CG1	2.45	0.42
3:C:54:LEU:HA	3:C:151:ALA:O	2.20	0.42
1:A:56:TYR:HE1	1:A:109:GLU:OE1	2.02	0.42
2:B:674:LYS:O	2:B:678:LEU:HG	2.19	0.42
1:A:231:GLN:HB2	1:A:236:ILE:HG13	2.01	0.41
1:A:367:THR:HB	5:A:831:HOH:O	2.20	0.41
2:B:439:ASN:HD21	2:B:453:ASN:ND2	2.17	0.41
2:B:447:GLN:O	2:B:447:GLN:HG2	2.20	0.41
2:B:564:GLN:HB2	2:B:565:PRO:HD2	2.02	0.41
3:C:4:LEU:HB3	3:C:74:LEU:HB3	2.01	0.41
3:C:39:GLN:HA	3:C:39:GLN:NE2	2.35	0.41
1:A:19:PHE:CE2	1:A:40:ALA:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:LEU:HD12	1:A:703:PRO:HG2	2.00	0.41
1:A:258:LYS:HA	1:A:304:ASP:O	2.20	0.41
1:A:339:ALA:HB1	1:A:424:VAL:HG21	2.02	0.41
1:A:381:LEU:HA	1:A:702:MET:HE1	2.02	0.41
1:A:700:PHE:O	1:A:702:MET:N	2.53	0.41
2:B:348:LEU:O	2:B:348:LEU:CG	2.68	0.41
2:B:654:GLU:HA	2:B:655:PRO:HD3	1.91	0.41
2:B:1062:LYS:C	2:B:1064:ASN:H	2.24	0.41
3:C:20:MET:SD	3:C:30:LEU:HD21	2.60	0.41
1:A:22:ASN:HB2	1:A:516:SER:HB2	2.02	0.41
1:A:195:LEU:HD22	1:A:203:MET:CE	2.51	0.41
1:A:689:VAL:O	1:A:693:GLN:HG2	2.20	0.41
1:A:722:VAL:O	1:A:723:ASN:CB	2.64	0.41
1:A:78:TYR:CD1	1:A:78:TYR:N	2.88	0.41
1:A:297:GLY:H	1:A:300:MET:HB2	1.85	0.41
1:A:312:SER:H	1:A:315:ASP:HB2	1.84	0.41
1:A:637:LEU:HD22	1:A:722:VAL:HA	2.02	0.41
2:B:358:ASN:CA	2:B:972:GLN:HE22	2.20	0.41
2:B:529:LEU:HD23	2:B:529:LEU:HA	1.88	0.41
2:B:567:MET:HE2	2:B:569:ILE:CD1	2.49	0.41
2:B:628:SER:HB3	2:B:629:PRO:HD3	2.02	0.41
3:C:4:LEU:HD12	3:C:4:LEU:HA	1.70	0.41
3:C:82:LYS:H	3:C:82:LYS:HG2	1.68	0.41
1:A:140:GLU:OE2	1:A:249:ARG:NH2	2.54	0.41
1:A:310:ILE:H	1:A:310:ILE:CD1	2.26	0.41
1:A:339:ALA:O	1:A:447:LYS:HE3	2.21	0.41
2:B:515:ASN:O	2:B:519:THR:HG23	2.21	0.41
2:B:573:ILE:HG22	5:B:106:HOH:O	2.20	0.41
2:B:854:ARG:HH11	2:B:854:ARG:HG2	1.84	0.41
1:A:48:ARG:CZ	1:A:51:LEU:HD11	2.51	0.41
1:A:144:LEU:O	1:A:148:LYS:HG3	2.21	0.41
2:B:498:LEU:N	2:B:498:LEU:HD12	2.36	0.41
2:B:1053:TYR:HD1	2:B:1055:ILE:HB	1.85	0.41
3:C:40:LEU:HD23	3:C:72:LEU:HD13	2.03	0.41
1:A:3:THR:HG23	1:A:5:LEU:H	1.86	0.41
1:A:63:ARG:O	1:A:65:THR:N	2.53	0.41
1:A:190:ARG:NH1	2:B:575:ASP:CG	2.74	0.41
1:A:252:TRP:HA	1:A:253:PRO:HD3	1.92	0.41
1:A:531:ILE:HD13	1:A:590:LEU:HD21	2.03	0.41
1:A:662:GLU:O	1:A:665:ALA:HB3	2.21	0.41
2:B:407:LEU:HG	2:B:789:MET:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:592:LYS:O	2:B:596:GLN:HG3	2.21	0.41
3:C:62:HIS:O	3:C:73:VAL:HG12	2.21	0.41
1:A:63:ARG:HB2	1:A:90:GLN:CG	2.50	0.41
1:A:660:HIS:HB2	1:A:709:GLU:HB3	2.02	0.41
2:B:573:ILE:HD13	5:B:128:HOH:O	2.21	0.41
2:B:756:GLY:HA2	2:B:793:GLU:HB2	2.02	0.41
2:B:958:LEU:CA	2:B:964:THR:HA	2.42	0.41
3:C:54:LEU:HB2	3:C:61:PHE:HB2	2.03	0.41
1:A:747:VAL:HG12	1:A:748:SER:H	1.86	0.40
2:B:963:ARG:HB3	2:B:965:ILE:CD1	2.50	0.40
2:B:1021:MET:H	2:B:1055:ILE:CG1	2.20	0.40
3:C:128:ASP:OD1	3:C:130:ARG:HG2	2.21	0.40
1:A:283:GLY:CA	1:A:486:GLN:HE22	2.33	0.40
1:A:531:ILE:CD1	1:A:589:PHE:HB3	2.50	0.40
2:B:633:ARG:CB	2:B:778:ASN:HD21	2.19	0.40
2:B:641:LEU:HA	2:B:642:PRO:HD3	1.96	0.40
1:A:140:GLU:HB3	5:A:881:HOH:O	2.21	0.40
1:A:551:ILE:O	1:A:555:GLN:HG3	2.21	0.40
1:A:559:GLU:O	1:A:560:TYR:HB3	2.21	0.40
2:B:420:LEU:HA	2:B:421:PRO:HD3	1.96	0.40
1:A:586:ARG:CB	1:A:586:ARG:HH11	2.35	0.40
1:A:656:ILE:HD13	1:A:656:ILE:HA	1.92	0.40
1:A:700:PHE:O	1:A:701:PRO:C	2.53	0.40
2:B:747:ALA:HB2	2:B:809:TYR:HB3	2.03	0.40
1:A:183:ILE:CG2	1:A:184:SER:N	2.84	0.40
1:A:297:GLY:HA3	1:A:300:MET:HB2	2.02	0.40
2:B:732:GLN:NE2	5:B:126:HOH:O	2.55	0.40
2:B:1054:VAL:O	2:B:1054:VAL:HG12	2.21	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	698/769 (91%)	638 (91%)	46 (7%)	14 (2%)	7 6
2	B	721/753 (96%)	666 (92%)	46 (6%)	9 (1%)	13 14
3	C	129/196 (66%)	113 (88%)	14 (11%)	2 (2%)	9 9
All	All	1548/1718 (90%)	1417 (92%)	106 (7%)	25 (2%)	9 9

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	THR
1	A	197	ALA
1	A	508	THR
1	A	509	GLN
2	B	1019	GLN
3	C	4	LEU
1	A	105	ASN
1	A	181	GLU
2	B	447	GLN
2	B	961	SER
2	B	1055	ILE
1	A	58	PRO
2	B	1059	SER
1	A	183	ILE
1	A	747	VAL
2	B	446	ASP
1	A	59	VAL
1	A	476	ARG
1	A	700	PHE
3	C	2	VAL
1	A	184	SER
2	B	960	ILE
2	B	965	ILE
1	A	297	GLY
2	B	1047	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	619/667 (93%)	588 (95%)	31 (5%)	24	34
2	B	660/684 (96%)	631 (96%)	29 (4%)	28	39
3	C	119/171 (70%)	112 (94%)	7 (6%)	19	27
All	All	1398/1522 (92%)	1331 (95%)	67 (5%)	25	36

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	17	VAL
1	A	30	GLU
1	A	57	GLU
1	A	105	ASN
1	A	141	ASP
1	A	153	MET
1	A	192	THR
1	A	236	ILE
1	A	240	LEU
1	A	243	LEU
1	A	268	LEU
1	A	285	ARG
1	A	311	ARG
1	A	316	ILE
1	A	355	THR
1	A	400	MET
1	A	451	LEU
1	A	495	ARG
1	A	508	THR
1	A	528	ARG
1	A	544	ARG
1	A	546	LEU
1	A	566	SER
1	A	569	ARG
1	A	570	PHE
1	A	612	LEU
1	A	637	LEU
1	A	649	LEU
1	A	722	VAL
1	A	723	ASN
2	B	359	MET
2	B	382	ASN
2	B	386	PHE

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Mol	Chain	Res	Type
2	B	411	LEU
2	B	412	HIS
2	B	522	LEU
2	B	550	ASP
2	B	589	ASN
2	B	610	LEU
2	B	641	LEU
2	B	679	ASP
2	B	712	SER
2	B	773	LEU
2	B	789	MET
2	B	797	ASP
2	B	816	ARG
2	B	857	THR
2	B	906	LEU
2	B	920	LEU
2	B	935	LEU
2	B	958	LEU
2	B	1001	THR
2	B	1002	GLN
2	B	1043	ARG
2	B	1048	PHE
2	B	1052	LEU
2	B	1057	ASP
2	B	1075	GLU
2	B	1085	LEU
3	C	3	LEU
3	C	31	GLN
3	C	90	ASP
3	C	101	LYS
3	C	113	ILE
3	C	121	LYS
3	C	127	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	105	ASN
1	A	126	GLN
1	A	174	GLN
1	A	227	ASN

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Mol	Chain	Res	Type
1	A	296	GLN
1	A	320	ASN
1	A	330	HIS
1	A	397	GLN
1	A	436	ASN
1	A	486	GLN
1	A	549	GLN
1	A	579	GLN
1	A	583	HIS
1	A	595	ASN
1	A	620	GLN
1	A	673	GLN
1	A	710	HIS
1	A	714	GLN
1	A	723	ASN
2	B	355	GLN
2	B	373	HIS
2	B	382	ASN
2	B	412	HIS
2	B	439	ASN
2	B	502	GLN
2	B	566	GLN
2	B	589	ASN
2	B	683	GLN
2	B	732	GLN
2	B	760	HIS
2	B	778	ASN
2	B	913	GLN
2	B	1088	GLN
2	B	1092	ASN
3	C	39	GLN
3	C	47	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	708/769 (92%)	0.33	60 (8%) 10 14	22, 44, 85, 115	0
2	B	729/753 (96%)	0.16	46 (6%) 20 25	20, 37, 80, 112	0
3	C	135/196 (68%)	0.92	22 (16%) 1 2	36, 66, 101, 122	0
All	All	1572/1718 (91%)	0.30	128 (8%) 12 16	20, 42, 86, 122	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1055	ILE	7.8
3	C	1	MET	7.6
1	A	672	TYR	6.7
2	B	346	GLU	6.3
1	A	674	ASP	6.2
1	A	675	MET	5.8
1	A	49	PRO	5.5
1	A	678	TYR	5.5
1	A	670	SER	5.3
2	B	446	ASP	5.1
3	C	23	ASP	5.1
2	B	771	THR	4.9
2	B	426	SER	4.9
1	A	507	GLN	4.9
2	B	424	THR	4.9
3	C	148	ILE	4.8
2	B	348	LEU	4.7
3	C	32	GLN	4.6
2	B	1061	MET	4.5
3	C	101	LYS	4.5
1	A	123	ARG	4.4
3	C	22	GLU	4.4
1	A	50	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	180	CYS	3.9
1	A	667	TRP	3.9
1	A	181	GLU	3.9
1	A	682	ARG	3.9
1	A	679	GLU	3.8
2	B	658	ARG	3.6
2	B	449	ARG	3.6
2	B	662	LYS	3.6
1	A	75	GLN	3.5
2	B	427	THR	3.5
1	A	669	LYS	3.5
2	B	509	VAL	3.5
1	A	64	THR	3.5
3	C	2	VAL	3.4
1	A	508	THR	3.4
1	A	593	PHE	3.4
1	A	431	PRO	3.4
2	B	463	GLU	3.3
1	A	536	THR	3.3
3	C	154	GLU	3.3
1	A	695	ILE	3.3
2	B	636	VAL	3.3
2	B	462	PRO	3.2
1	A	79	ARG	3.2
1	A	394	MET	3.2
2	B	1093	LYS	3.2
3	C	77	ALA	3.1
1	A	103	GLU	3.1
2	B	432	ARG	3.1
2	B	958	LEU	3.1
2	B	445	LEU	3.0
1	A	676	PRO	3.0
1	A	56	TYR	2.9
1	A	134	VAL	2.9
1	A	668	ARG	2.9
3	C	76	GLU	2.8
1	A	288	MET	2.8
3	C	129	SER	2.8
1	A	746	ASP	2.8
3	C	31	GLN	2.8
1	A	57	GLU	2.8
1	A	629	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	635	SER	2.8
2	B	637	PHE	2.7
2	B	508	PHE	2.7
1	A	698	SER	2.7
3	C	98	GLN	2.7
1	A	286	ILE	2.6
2	B	507	LEU	2.6
1	A	132	LEU	2.6
2	B	418	VAL	2.5
2	B	959	ASN	2.5
1	A	347	ILE	2.5
1	A	663	THR	2.5
1	A	747	VAL	2.5
3	C	59	MET	2.5
1	A	665	ALA	2.5
1	A	683	HIS	2.5
2	B	347	GLY	2.5
2	B	914	THR	2.4
2	B	657	HIS	2.4
1	A	225	PRO	2.4
2	B	1060	PRO	2.4
1	A	692	ALA	2.4
3	C	21	GLN	2.4
2	B	1022	THR	2.4
3	C	57	GLY	2.4
2	B	770	SER	2.4
3	C	30	LEU	2.4
2	B	918	ALA	2.4
1	A	102	SER	2.4
1	A	268	LEU	2.3
1	A	287	MET	2.3
2	B	917	ASN	2.3
2	B	689	LEU	2.3
1	A	179	GLY	2.3
2	B	1019	GLN	2.3
1	A	91	ARG	2.2
1	A	89	TYR	2.2
2	B	797	ASP	2.2
3	C	20	MET	2.2
2	B	980	ARG	2.2
1	A	594	ASN	2.2
1	A	537	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	666	GLN	2.2
2	B	355	GLN	2.2
2	B	916	THR	2.2
3	C	55	GLU	2.2
3	C	29	ASP	2.1
2	B	419	GLN	2.1
1	A	48	ARG	2.1
1	A	677	GLU	2.1
3	C	127	ILE	2.1
2	B	448	ARG	2.1
1	A	290	ILE	2.1
2	B	1075	GLU	2.1
3	C	72	LEU	2.1
2	B	882	VAL	2.1
1	A	435	GLU	2.1
2	B	1001	THR	2.1
1	A	135	VAL	2.1
1	A	51	LEU	2.1
1	A	510	ILE	2.0
2	B	1057	ASP	2.0
1	A	40	ALA	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
4	ZN	A	800	1/1	0.97	0.07	54,54,54,54	0
4	ZN	B	1100	1/1	0.99	0.06	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.