



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 04:52 PM EDT

PDB ID : 4ADY
Title : Crystal structure of 26S proteasome subunit Rpn2
Authors : Kulkarni, K.; He, J.; Da Fonseca, P.C.A.; Krutauz, D.; Glickman, M.H.; Barford, D.; Morris, E.P.
Deposited on : 2012-01-04
Resolution : 2.70 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

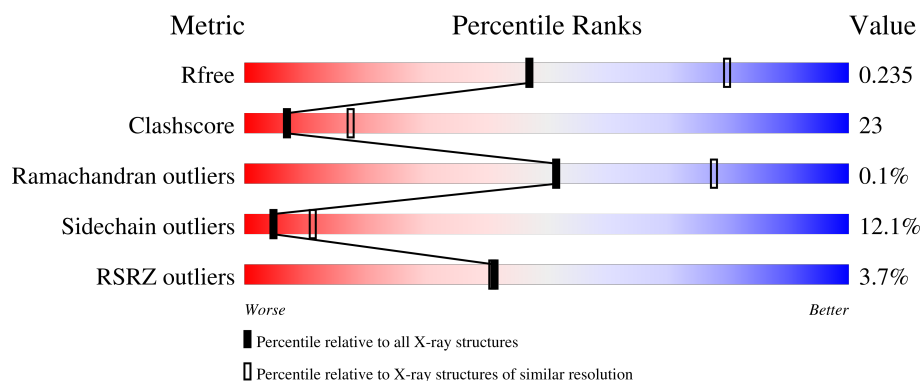
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	963	<div> <div>3%</div> <div>56%</div> <div>27%</div> <div>5%</div> <div>12%</div> </div>
1	B	963	<div> <div>4%</div> <div>50%</div> <div>28%</div> <div>6%</div> <div>17%</div> </div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 12581 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 26S PROTEASOME REGULATORY SUBUNIT RPN2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	849	Total	C	N	O	S	Se	0	0	0
			6498	4138	1076	1256	8	20			
1	B	802	Total	C	N	O	S	Se	0	0	0
			6024	3851	993	1152	8	20			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MSE	-	expression tag	UNP P32565
A	-9	ARG	-	expression tag	UNP P32565
A	-8	GLY	-	expression tag	UNP P32565
A	-7	SER	-	expression tag	UNP P32565
A	-6	HIS	-	expression tag	UNP P32565
A	-5	HIS	-	expression tag	UNP P32565
A	-4	HIS	-	expression tag	UNP P32565
A	-3	HIS	-	expression tag	UNP P32565
A	-2	HIS	-	expression tag	UNP P32565
A	-1	HIS	-	expression tag	UNP P32565
A	0	GLY	-	expression tag	UNP P32565
A	1	SER	-	expression tag	UNP P32565
A	946	LEU	-	expression tag	UNP P32565
A	947	GLN	-	expression tag	UNP P32565
A	948	PRO	-	expression tag	UNP P32565
A	949	SER	-	expression tag	UNP P32565
A	950	LEU	-	expression tag	UNP P32565
A	951	ILE	-	expression tag	UNP P32565
A	952	SER	-	expression tag	UNP P32565
B	-10	MSE	-	expression tag	UNP P32565
B	-9	ARG	-	expression tag	UNP P32565
B	-8	GLY	-	expression tag	UNP P32565
B	-7	SER	-	expression tag	UNP P32565
B	-6	HIS	-	expression tag	UNP P32565
B	-5	HIS	-	expression tag	UNP P32565

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP P32565
B	-3	HIS	-	expression tag	UNP P32565
B	-2	HIS	-	expression tag	UNP P32565
B	-1	HIS	-	expression tag	UNP P32565
B	0	GLY	-	expression tag	UNP P32565
B	1	SER	-	expression tag	UNP P32565
B	946	LEU	-	expression tag	UNP P32565
B	947	GLN	-	expression tag	UNP P32565
B	948	PRO	-	expression tag	UNP P32565
B	949	SER	-	expression tag	UNP P32565
B	950	LEU	-	expression tag	UNP P32565
B	951	ILE	-	expression tag	UNP P32565
B	952	SER	-	expression tag	UNP P32565

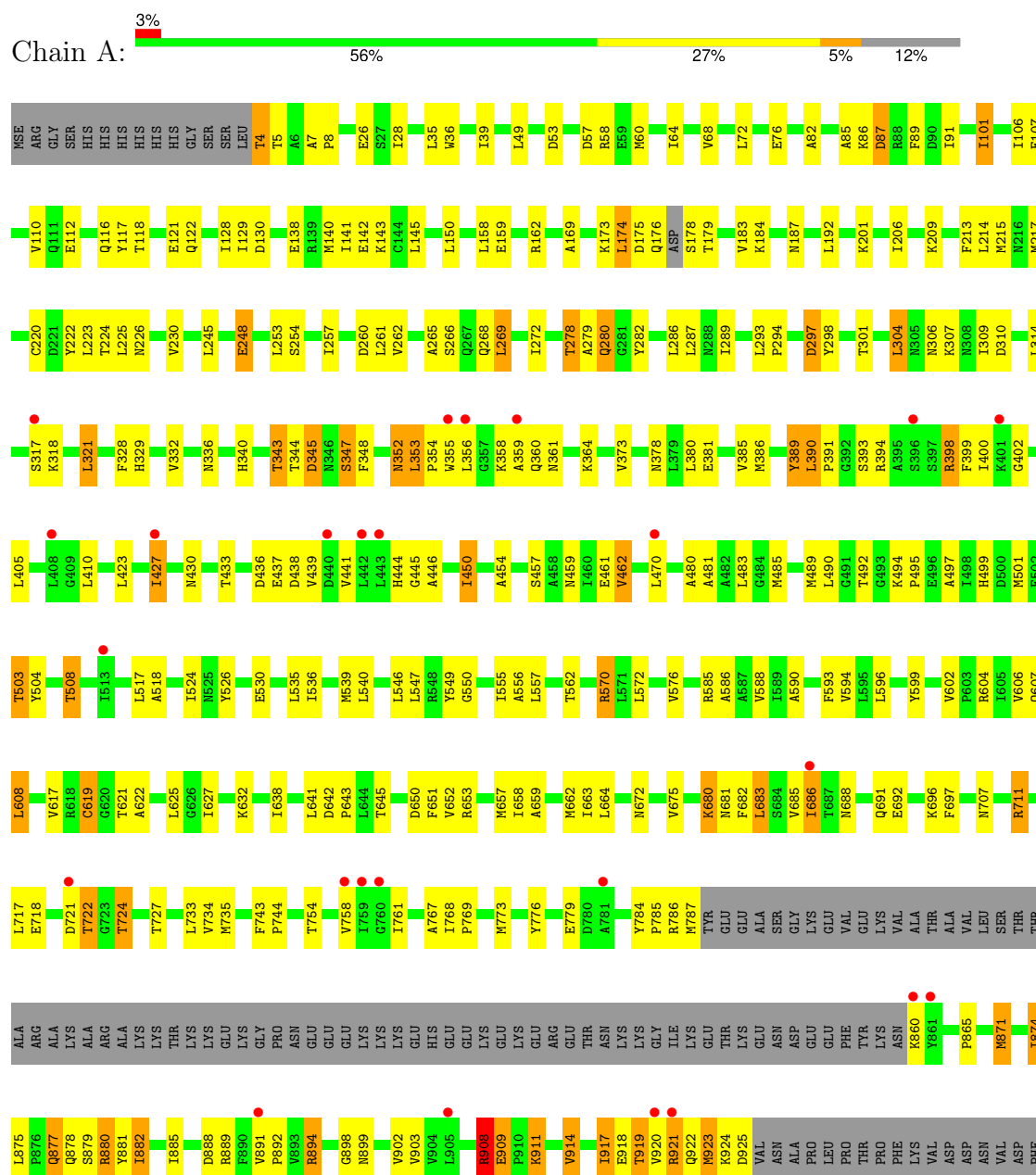
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	30	Total O 30 30	0	0

3 Residue-property plots

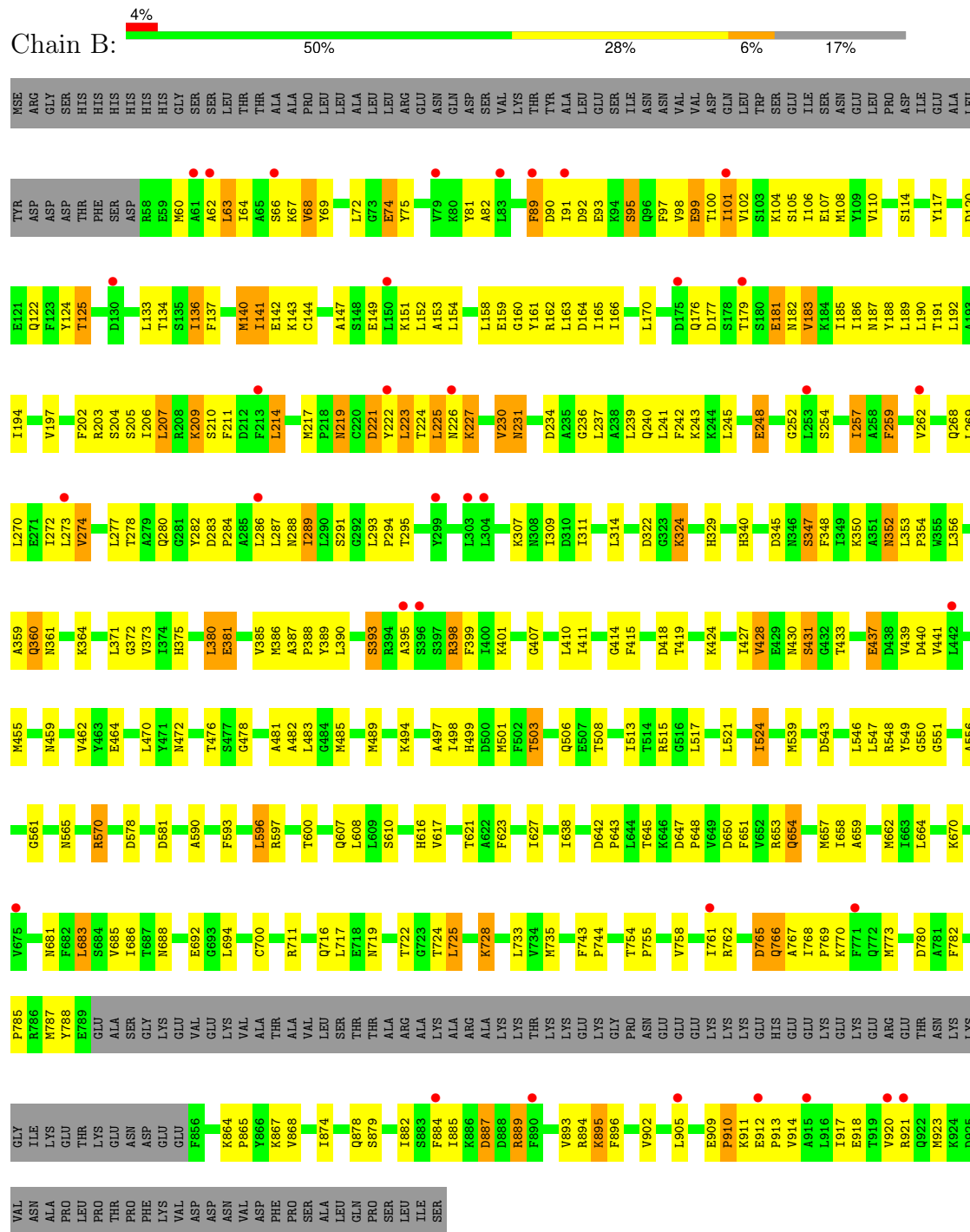
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 26S PROTEASOME REGULATORY SUBUNIT RPN2



PRO
SER
ALA
LEU
GLN
PRO
SER
LEU
ILE
SER

● Molecule 1: 26S PROTEASOME REGULATORY SUBUNIT RPN2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.96Å 148.66Å 114.03Å 90.00° 107.39° 90.00°	Depositor
Resolution (Å)	70.58 – 2.70 74.33 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (70.58-2.70) 99.9 (74.33-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.183 , 0.240 0.183 , 0.235	Depositor DCC
R_{free} test set	1323 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12581	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/6586	0.60	0/8893
1	B	0.41	0/6106	0.59	0/8252
All	All	0.42	0/12692	0.60	0/17145

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	GLU	Peptide
1	A	908	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	6498	0	6471	249	0
1	B	6024	0	5933	323	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	29	0	0	2	0
2	B	30	0	0	1	0
All	All	12581	0	12404	570	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 23.

All (570) 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:A:918:GLU:CD	1:A:923:MSE:SE	2.38	1.12
1:A:398:ARG:HD3	1:A:438:ASP:HA	1.25	1.11
1:A:919:THR:HG22	1:A:922:GLN:H	1.08	1.09
1:B:371:LEU:HB3	1:B:386:MSE:HE1	1.33	1.08
1:A:570:ARG:HG3	1:A:570:ARG:HH11	1.21	1.05
1:B:570:ARG:HG3	1:B:570:ARG:HH11	1.20	1.05
1:B:659:ALA:HA	1:B:662:MSE:HE3	1.38	1.04
1:B:63:LEU:HG	1:B:67:LYS:HZ1	1.22	1.04
1:A:501:MSE:HG2	1:A:517:LEU:HD22	1.39	1.03
1:A:908:ARG:NH1	1:A:908:ARG:HG3	1.74	1.00
1:A:918:GLU:OE1	1:A:923:MSE:SE	2.30	0.99
1:A:918:GLU:OE2	1:A:923:MSE:SE	2.30	0.99
1:B:909:GLU:O	1:B:909:GLU:HG2	1.65	0.94
1:B:658:ILE:HG22	1:B:662:MSE:HE2	1.47	0.94
1:B:722:THR:HG23	1:B:724:THR:H	1.33	0.94
1:B:895:LYS:HD3	1:B:896:PHE:H	1.33	0.92
1:A:588:VAL:HG11	1:A:621:THR:HG22	1.53	0.91
1:B:63:LEU:HD23	1:B:67:LYS:HZ3	1.35	0.91
1:B:895:LYS:HD3	1:B:896:PHE:N	1.86	0.91
1:B:63:LEU:CG	1:B:67:LYS:HZ1	1.84	0.90
1:A:398:ARG:HH11	1:A:398:ARG:CG	1.86	0.89
1:B:617:VAL:O	1:B:621:THR:HG23	1.74	0.87
1:A:919:THR:HG22	1:A:922:GLN:N	1.88	0.86
1:B:497:ALA:HB1	1:B:501:MSE:HE2	1.58	0.85
1:B:259:PHE:O	1:B:262:VAL:HG12	1.76	0.84
1:A:657:MSE:HE1	1:A:685:VAL:HG21	1.60	0.83
1:A:329:HIS:CE1	1:A:359:ALA:HB2	2.16	0.81
1:A:398:ARG:HH11	1:A:398:ARG:HG2	1.46	0.81
1:B:499:HIS:O	1:B:503:THR:HG23	1.80	0.81
1:A:599:TYR:CZ	1:A:632:LYS:HG2	2.15	0.81
1:A:501:MSE:HG2	1:A:517:LEU:CD2	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:911:LYS:C	1:B:913:PRO:HD2	2.02	0.80
1:B:241:LEU:HD12	1:B:241:LEU:O	1.82	0.79
1:A:908:ARG:HG3	1:A:908:ARG:HH11	1.47	0.79
1:A:632:LYS:HD2	1:A:632:LYS:N	1.96	0.79
1:A:680:LYS:O	1:A:680:LYS:HD3	1.83	0.79
1:B:909:GLU:O	1:B:909:GLU:CG	2.30	0.78
1:B:570:ARG:HH11	1:B:570:ARG:CG	1.94	0.78
1:B:248:GLU:OE1	1:B:248:GLU:HA	1.82	0.78
1:B:245:LEU:HD11	1:B:257:ILE:HG12	1.65	0.77
1:B:556:ALA:HB2	1:B:590:ALA:HB1	1.67	0.77
1:B:329:HIS:CE1	1:B:359:ALA:HB2	2.19	0.77
1:B:657:MSE:HE2	1:B:681:ASN:ND2	1.99	0.76
1:B:719:ASN:HB3	1:B:722:THR:HG22	1.66	0.76
1:A:459:ASN:OD1	1:A:462:VAL:HG12	1.85	0.76
1:B:63:LEU:HG	1:B:67:LYS:NZ	1.99	0.76
1:B:154:LEU:HD22	1:B:166:ILE:HG23	1.67	0.76
1:A:642:ASP:HB3	1:A:643:PRO:HD3	1.68	0.75
1:A:767:ALA:O	1:A:769:PRO:HD3	1.86	0.75
1:B:361:ASN:HA	1:B:399:PHE:CE2	2.20	0.75
1:B:470:LEU:HB2	1:B:485:MSE:HE1	1.69	0.75
1:A:722:THR:HB	1:A:724:THR:OG1	1.87	0.74
1:B:89:PHE:HE1	1:B:98:VAL:HG23	1.51	0.74
1:A:657:MSE:CE	1:A:681:ASN:ND2	2.51	0.74
1:B:920:VAL:O	1:B:921:ARG:HB3	1.87	0.73
1:B:63:LEU:HD23	1:B:67:LYS:NZ	2.03	0.73
1:A:570:ARG:HG3	1:A:570:ARG:NH1	1.99	0.73
1:B:761:ILE:HD11	1:B:766:GLN:HA	1.68	0.73
1:A:680:LYS:HD3	1:A:680:LYS:C	2.09	0.72
1:B:455:MSE:CE	1:B:728:LYS:HG2	2.18	0.72
1:A:657:MSE:HE3	1:A:681:ASN:ND2	2.04	0.72
1:B:181:GLU:HA	1:B:181:GLU:OE1	1.88	0.72
1:B:570:ARG:HG3	1:B:570:ARG:NH1	2.01	0.72
1:A:658:ILE:HG22	1:A:662:MSE:HE3	1.71	0.72
1:B:162:ARG:HB3	1:B:165:ILE:HG13	1.72	0.71
1:B:259:PHE:CZ	1:B:289:ILE:HD13	2.25	0.71
1:B:717:LEU:HD11	1:B:733:LEU:HD12	1.71	0.71
1:A:570:ARG:HH11	1:A:570:ARG:CG	2.03	0.70
1:A:87:ASP:OD1	1:A:87:ASP:C	2.30	0.70
1:A:390:LEU:HD13	1:A:391:PRO:HD2	1.73	0.70
1:B:657:MSE:HE1	1:B:685:VAL:HG21	1.72	0.70
1:A:877:GLN:O	1:A:880:ARG:HD3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:909:GLU:C	1:B:911:LYS:H	1.95	0.70
1:A:398:ARG:HD3	1:A:438:ASP:CA	2.16	0.70
1:A:682:PHE:O	1:A:686:ILE:HG13	1.92	0.69
1:A:889:ARG:NH2	1:A:914:VAL:HG22	2.07	0.69
1:A:36:TRP:CZ3	1:A:72:LEU:HD23	2.27	0.69
1:A:53:ASP:HA	1:A:58:ARG:NH1	2.06	0.69
1:B:63:LEU:CD2	1:B:67:LYS:NZ	2.56	0.69
1:A:121:GLU:CD	1:A:201:LYS:HE3	2.13	0.68
1:A:35:LEU:O	1:A:39:ILE:HG13	1.94	0.68
1:A:121:GLU:OE2	1:A:201:LYS:HE3	1.94	0.68
1:B:882:ILE:HG22	1:B:896:PHE:CE2	2.29	0.68
1:B:506:GLN:HE21	1:B:547:LEU:HD11	1.57	0.68
1:B:63:LEU:CD2	1:B:67:LYS:HZ3	2.07	0.67
1:B:375:HIS:O	1:B:411:ILE:HG23	1.95	0.67
1:B:64:ILE:O	1:B:68:VAL:HG12	1.94	0.67
1:A:398:ARG:CD	1:A:438:ASP:HA	2.13	0.67
1:A:879:SER:HB3	1:A:899:ASN:HA	1.76	0.67
1:A:918:GLU:OE2	1:A:923:MSE:CG	2.42	0.67
1:B:190:LEU:HD23	1:B:207:LEU:HD12	1.77	0.67
1:B:231:ASN:N	1:B:231:ASN:HD22	1.93	0.66
1:B:596:LEU:HD23	1:B:725:LEU:HD11	1.77	0.66
1:A:924:LYS:O	1:A:925:ASP:CB	2.43	0.66
1:B:105:SER:OG	1:B:136:ILE:HG21	1.94	0.66
1:B:89:PHE:CE1	1:B:98:VAL:HG23	2.29	0.66
1:B:912:GLU:N	1:B:913:PRO:CD	2.58	0.66
1:A:657:MSE:HE3	1:A:681:ASN:HD21	1.56	0.66
1:B:63:LEU:CG	1:B:67:LYS:NZ	2.56	0.66
1:B:221:ASP:OD1	1:B:223:LEU:HG	1.96	0.66
1:A:7:ALA:N	1:A:8:PRO:HD2	2.11	0.65
1:B:556:ALA:HB2	1:B:590:ALA:CB	2.26	0.65
1:A:622:ALA:HA	1:A:641:LEU:HD21	1.78	0.65
1:B:211:PHE:CE2	1:B:237:LEU:HG	2.32	0.65
1:B:765:ASP:N	1:B:765:ASP:OD1	2.30	0.65
1:A:36:TRP:HZ3	1:A:72:LEU:HD23	1.61	0.65
1:A:353:LEU:N	1:A:354:PRO:HD2	2.11	0.65
1:B:64:ILE:HA	1:B:67:LYS:HZ2	1.62	0.65
1:A:911:LYS:H	1:A:911:LYS:HD2	1.62	0.64
1:B:133:LEU:O	1:B:136:ILE:HG22	1.96	0.64
1:B:270:LEU:O	1:B:274:VAL:HG22	1.97	0.64
1:B:398:ARG:NH1	1:B:437:GLU:HG3	2.12	0.64
1:B:909:GLU:O	1:B:911:LYS:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:ARG:NH1	1:A:908:ARG:CG	2.58	0.64
1:B:548:ARG:HD2	1:B:578:ASP:OD2	1.98	0.64
1:A:150:LEU:HD13	1:A:173:LYS:HG3	1.78	0.64
1:B:226:ASN:O	1:B:230:VAL:HG23	1.97	0.64
1:A:874:ILE:HA	1:A:878:GLN:OE1	1.97	0.63
1:B:596:LEU:HD11	1:B:717:LEU:HD23	1.78	0.63
1:A:919:THR:HG21	1:A:921:ARG:HE	1.64	0.63
1:B:911:LYS:C	1:B:913:PRO:CD	2.67	0.63
1:A:593:PHE:CE2	1:A:627:ILE:HD13	2.33	0.63
1:B:106:ILE:HD11	1:B:140:MSE:HG3	1.81	0.63
1:B:395:ALA:O	1:B:401:LYS:HE3	1.99	0.62
1:B:638:ILE:HD11	1:B:664:LEU:HD21	1.81	0.62
1:B:455:MSE:HE2	1:B:728:LYS:HG2	1.82	0.62
1:B:911:LYS:O	1:B:913:PRO:HD2	1.99	0.62
1:A:518:ALA:HB1	1:A:550:GLY:HA3	1.80	0.62
1:A:318:LYS:NZ	1:A:352:ASN:HB3	2.14	0.62
1:B:190:LEU:O	1:B:194:ILE:HG22	2.00	0.62
1:B:222:TYR:HD2	1:B:241:LEU:HD11	1.63	0.62
1:A:138:GLU:OE2	1:A:162:ARG:NH2	2.33	0.62
1:B:62:ALA:O	1:B:81:TYR:HB3	1.99	0.62
1:B:482:ALA:HA	1:B:485:MSE:HE3	1.82	0.62
1:B:190:LEU:CD2	1:B:207:LEU:HD12	2.30	0.62
1:A:304:LEU:HD12	1:A:304:LEU:O	2.00	0.62
1:B:381:GLU:O	1:B:385:VAL:HG23	2.00	0.61
1:A:268:GLN:O	1:A:272:ILE:HG13	1.99	0.61
1:A:919:THR:HG21	1:A:921:ARG:NE	2.16	0.61
1:A:685:VAL:HG13	1:A:691:GLN:HG2	1.81	0.61
1:A:158:LEU:HD11	1:A:206:ILE:CD1	2.30	0.61
1:B:63:LEU:C	1:B:67:LYS:NZ	2.54	0.61
1:B:104:LYS:O	1:B:108:MSE:HG3	2.00	0.61
1:B:282:TYR:HE1	1:B:286:LEU:HD12	1.65	0.61
1:B:309:ILE:HD13	1:B:340:HIS:CD2	2.35	0.60
1:A:91:ILE:HD12	1:A:143:LYS:HD2	1.83	0.60
1:A:321:LEU:HD21	1:A:686:ILE:HG23	1.84	0.60
1:A:632:LYS:HD2	1:A:632:LYS:H	1.63	0.60
1:A:76:GLU:H	1:A:76:GLU:CD	2.05	0.60
1:A:309:ILE:HD13	1:A:340:HIS:CE1	2.37	0.60
1:A:650:ASP:HA	1:A:653:ARG:NH2	2.17	0.60
1:A:402:GLY:O	1:A:445:GLY:HA3	2.02	0.59
1:A:588:VAL:HG11	1:A:621:THR:CG2	2.30	0.59
1:B:356:LEU:O	1:B:356:LEU:HD12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:ASN:HB3	1:A:675:VAL:HG23	1.83	0.59
1:A:889:ARG:HH22	1:A:914:VAL:HG22	1.66	0.59
1:B:67:LYS:CD	1:B:67:LYS:H	2.16	0.59
1:B:269:LEU:C	1:B:269:LEU:HD23	2.24	0.59
1:A:398:ARG:HH11	1:A:398:ARG:HG3	1.67	0.58
1:A:112:GLU:O	1:A:116:GLN:HG2	2.03	0.58
1:A:919:THR:HG23	1:A:921:ARG:H	1.67	0.58
1:A:470:LEU:HD22	1:A:485:MSE:HE1	1.84	0.58
1:A:658:ILE:HG22	1:A:662:MSE:CE	2.32	0.58
1:A:405:LEU:HD22	1:A:423:LEU:CD2	2.34	0.58
1:A:483:LEU:HD22	1:A:735:MSE:HE1	1.85	0.58
1:A:562:THR:O	1:A:594:VAL:O	2.21	0.58
1:A:645:THR:O	1:A:653:ARG:HG2	2.04	0.58
1:B:89:PHE:CE2	1:B:101:ILE:HG21	2.38	0.58
1:A:318:LYS:HZ2	1:A:352:ASN:HB3	1.69	0.58
1:A:602:VAL:HG12	1:A:625:LEU:HD23	1.86	0.58
1:B:273:LEU:O	1:B:277:LEU:HG	2.04	0.58
1:B:371:LEU:HB3	1:B:386:MSE:CE	2.22	0.58
1:B:398:ARG:HH11	1:B:437:GLU:HG3	1.69	0.58
1:B:189:LEU:C	1:B:189:LEU:HD23	2.24	0.57
1:B:570:ARG:CG	1:B:570:ARG:NH1	2.59	0.57
1:A:556:ALA:HB2	1:A:590:ALA:CB	2.33	0.57
1:B:909:GLU:N	1:B:910:PRO:HD3	2.19	0.57
1:A:260:ASP:OD2	1:A:894:ARG:NH2	2.38	0.57
1:B:224:THR:O	1:B:227:LYS:HB3	2.05	0.57
1:A:213:PHE:O	1:A:217:MSE:HG3	2.05	0.57
1:B:407:GLY:O	1:B:411:ILE:HG13	2.05	0.57
1:B:427:ILE:O	1:B:431:SER:HB3	2.04	0.57
1:A:352:ASN:HD22	1:A:352:ASN:H	1.53	0.57
1:A:60:MSE:HE3	1:A:64:ILE:HG12	1.87	0.56
1:A:314:LEU:HD11	1:A:336:ASN:HA	1.86	0.56
1:A:911:LYS:HD2	1:A:911:LYS:N	2.19	0.56
1:B:107:GLU:O	1:B:110:VAL:HG22	2.05	0.56
1:B:288:ASN:O	1:B:291:SER:OG	2.22	0.56
1:A:535:LEU:O	1:A:539:MSE:HG3	2.04	0.56
1:A:588:VAL:CG1	1:A:621:THR:HG22	2.28	0.56
1:B:716:GLN:HG3	1:B:716:GLN:O	2.05	0.56
1:B:64:ILE:O	1:B:68:VAL:CG1	2.53	0.56
1:B:183:VAL:HG23	1:B:217:MSE:HE1	1.88	0.56
1:B:722:THR:HG23	1:B:724:THR:N	2.12	0.56
1:A:470:LEU:HB2	1:A:485:MSE:HE1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LYS:H	1:B:67:LYS:HD2	1.71	0.56
1:B:353:LEU:N	1:B:354:PRO:CD	2.68	0.56
1:B:918:GLU:CB	1:B:923:MSE:HE3	2.36	0.56
1:A:427:ILE:HD11	1:A:446:ALA:HB1	1.88	0.56
1:B:642:ASP:HB3	1:B:643:PRO:HD3	1.87	0.56
1:B:225:LEU:HD23	1:B:225:LEU:N	2.21	0.56
1:A:436:ASP:O	1:A:439:VAL:HG12	2.06	0.55
1:B:75:TYR:HE2	1:B:100:THR:HG21	1.71	0.55
1:A:352:ASN:H	1:A:352:ASN:ND2	2.04	0.55
1:A:599:TYR:CE1	1:A:632:LYS:HG2	2.42	0.55
1:A:918:GLU:OE2	1:A:923:MSE:CA	2.54	0.55
1:B:348:PHE:O	1:B:352:ASN:ND2	2.39	0.55
1:B:455:MSE:HE1	1:B:728:LYS:HG2	1.89	0.54
1:A:82:ALA:O	1:A:85:ALA:HB3	2.06	0.54
1:B:501:MSE:HE1	1:B:524:ILE:CD1	2.38	0.54
1:B:414:GLY:O	1:B:415:PHE:CD1	2.59	0.54
1:A:398:ARG:HD2	1:A:441:VAL:CG2	2.38	0.54
1:B:227:LYS:HE2	1:B:722:THR:O	2.08	0.54
1:A:784:TYR:HB3	1:A:785:PRO:HD2	1.89	0.54
1:A:386:MSE:O	1:A:390:LEU:HD23	2.07	0.54
1:B:430:ASN:HB3	1:B:439:VAL:HG13	1.88	0.54
1:A:318:LYS:HE3	1:A:355:TRP:HB2	1.90	0.54
1:B:647:ASP:CG	1:B:648:PRO:HD2	2.28	0.54
1:A:226:ASN:O	1:A:230:VAL:HG23	2.08	0.54
1:A:352:ASN:ND2	1:A:352:ASN:N	2.56	0.54
1:A:436:ASP:HB3	1:A:439:VAL:HG12	1.91	0.53
1:A:918:GLU:OE2	1:A:923:MSE:CB	2.56	0.53
1:B:89:PHE:HE1	1:B:98:VAL:CG2	2.20	0.53
1:B:360:GLN:HA	1:B:364:LYS:HD2	1.90	0.53
1:B:483:LEU:HD13	1:B:735:MSE:HE1	1.89	0.53
1:B:593:PHE:CE2	1:B:627:ILE:HD13	2.43	0.53
1:A:504:TYR:CE1	1:A:508:THR:HB	2.44	0.53
1:A:556:ALA:HB2	1:A:590:ALA:HB1	1.91	0.53
1:B:154:LEU:CD2	1:B:166:ILE:HG23	2.36	0.53
1:B:501:MSE:HB3	1:B:517:LEU:HD22	1.91	0.53
1:B:345:ASP:OD1	1:B:347:SER:HB3	2.09	0.53
1:B:657:MSE:HE2	1:B:681:ASN:HD21	1.71	0.53
1:B:909:GLU:C	1:B:911:LYS:N	2.63	0.53
1:A:345:ASP:OD1	1:A:347:SER:HB3	2.09	0.52
1:B:187:ASN:O	1:B:191:THR:HG23	2.09	0.52
1:A:497:ALA:O	1:A:501:MSE:HE3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:PHE:HE2	1:B:101:ILE:HG21	1.73	0.52
1:A:536:ILE:HD13	1:A:555:ILE:HG12	1.90	0.52
1:A:298:TYR:CD1	1:A:768:ILE:HD11	2.45	0.52
1:A:908:ARG:HH11	1:A:908:ARG:CG	2.19	0.52
1:A:501:MSE:CG	1:A:517:LEU:HD22	2.26	0.52
1:B:102:VAL:HG22	1:B:136:ILE:HD11	1.90	0.52
1:B:654:GLN:NE2	1:B:694:LEU:O	2.38	0.52
1:B:361:ASN:HA	1:B:399:PHE:CD2	2.45	0.52
1:B:72:LEU:HB3	1:B:74:GLU:OE2	2.11	0.52
1:B:151:LYS:HB2	1:B:188:TYR:HE2	1.74	0.52
1:B:782:PHE:CZ	1:B:878:GLN:HB2	2.44	0.52
1:B:407:GLY:HA2	1:B:410:LEU:HD12	1.92	0.51
1:B:864:LYS:HD2	1:B:865:PRO:HD2	1.92	0.51
1:A:717:LEU:HD11	1:A:733:LEU:HD12	1.92	0.51
1:B:506:GLN:NE2	1:B:547:LEU:HD11	2.24	0.51
1:A:489:MSE:HE3	1:A:492:THR:HG21	1.93	0.51
1:B:188:TYR:CZ	1:B:192:LEU:HD13	2.45	0.51
1:A:310:ASP:OD2	1:A:787:MSE:HB2	2.11	0.51
1:B:154:LEU:O	1:B:158:LEU:HB2	2.11	0.51
1:B:440:ASP:HB3	1:B:476:THR:HB	1.93	0.51
1:B:501:MSE:HE1	1:B:524:ILE:HG13	1.92	0.51
1:A:355:TRP:O	1:A:358:LYS:HG3	2.11	0.51
1:A:570:ARG:NH1	1:A:570:ARG:CG	2.66	0.51
1:A:909:GLU:HB3	1:A:911:LYS:NZ	2.25	0.51
1:A:389:TYR:HB3	1:A:400:ILE:HG22	1.93	0.51
1:B:239:LEU:O	1:B:239:LEU:HD12	2.10	0.51
1:B:658:ILE:HG22	1:B:662:MSE:CE	2.31	0.51
1:B:874:ILE:HA	1:B:878:GLN:OE1	2.11	0.51
1:B:149:GLU:HB3	1:B:152:LEU:HD13	1.92	0.51
1:A:393:SER:O	1:A:394:ARG:HB2	2.11	0.51
1:A:786:ARG:O	1:A:787:MSE:HG2	2.10	0.51
1:B:470:LEU:HD13	1:B:485:MSE:HE1	1.93	0.51
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.18	0.50
1:B:361:ASN:O	1:B:364:LYS:HB2	2.12	0.50
1:A:378:ASN:OD1	1:A:381:GLU:HG2	2.11	0.50
1:A:659:ALA:O	1:A:663:ILE:HG13	2.11	0.50
1:B:782:PHE:CE1	1:B:878:GLN:HB2	2.46	0.50
1:B:913:PRO:O	1:B:914:VAL:HG13	2.11	0.50
1:A:158:LEU:HD11	1:A:206:ILE:HD11	1.92	0.50
1:A:446:ALA:O	1:A:450:ILE:HB	2.11	0.50
1:B:259:PHE:CE1	1:B:289:ILE:HD13	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:GLN:O	1:A:280:GLN:HG3	2.11	0.50
1:A:298:TYR:CE2	1:A:761:ILE:HD11	2.47	0.50
1:A:888:ASP:O	1:A:908:ARG:NH1	2.45	0.50
1:B:151:LYS:CB	1:B:188:TYR:HE2	2.25	0.50
1:B:398:ARG:HG3	1:B:441:VAL:HB	1.93	0.50
1:A:293:LEU:HB2	1:A:294:PRO:HD3	1.92	0.50
1:B:481:ALA:C	1:B:485:MSE:HE3	2.31	0.50
1:B:221:ASP:OD1	1:B:221:ASP:C	2.50	0.50
1:A:911:LYS:H	1:A:911:LYS:CD	2.20	0.50
1:A:919:THR:HG21	1:A:921:ARG:NH2	2.27	0.50
1:B:63:LEU:C	1:B:67:LYS:HZ2	2.16	0.49
1:B:190:LEU:HD23	1:B:207:LEU:CD1	2.41	0.49
1:B:63:LEU:C	1:B:67:LYS:HZ1	2.16	0.49
1:B:375:HIS:CD2	1:B:385:VAL:HG11	2.47	0.49
1:B:874:ILE:HG23	1:B:878:GLN:HG2	1.94	0.49
1:B:234:ASP:OD2	1:B:237:LEU:HD13	2.13	0.49
1:B:293:LEU:N	1:B:294:PRO:CD	2.75	0.49
1:B:322:ASP:OD1	1:B:324:LYS:HB2	2.12	0.49
1:A:317:SER:HB3	1:A:332:VAL:HG22	1.95	0.49
1:B:345:ASP:OD1	1:B:345:ASP:C	2.51	0.49
1:A:697:PHE:CD1	1:A:697:PHE:C	2.86	0.49
1:A:707:ASN:OD1	1:A:711:ARG:NH1	2.45	0.49
1:B:151:LYS:HB2	1:B:188:TYR:CE2	2.48	0.49
1:B:162:ARG:CB	1:B:165:ILE:HG13	2.40	0.49
1:A:87:ASP:OD1	1:A:87:ASP:O	2.30	0.49
1:B:190:LEU:HD21	1:B:210:SER:CB	2.43	0.49
1:B:93:GLU:HG2	1:B:95:SER:H	1.78	0.48
1:B:459:ASN:OD1	1:B:459:ASN:C	2.52	0.48
1:B:884:PHE:HE2	1:B:905:LEU:HD21	1.78	0.48
1:A:297:ASP:OD2	1:A:921:ARG:NE	2.45	0.48
1:B:141:ILE:HG22	1:B:142:GLU:N	2.28	0.48
1:B:882:ILE:HG22	1:B:896:PHE:HE2	1.78	0.48
1:B:190:LEU:HD21	1:B:210:SER:HB2	1.94	0.48
1:B:211:PHE:CE1	1:B:225:LEU:HD13	2.48	0.48
1:B:242:PHE:CE2	1:B:273:LEU:HD21	2.48	0.48
1:A:405:LEU:HD22	1:A:423:LEU:HD21	1.95	0.48
1:B:117:TYR:HA	1:B:120:ASP:O	2.13	0.48
1:B:711:ARG:CZ	1:B:785:PRO:HG2	2.44	0.48
1:B:225:LEU:HD23	1:B:225:LEU:H	1.79	0.48
1:B:657:MSE:CE	1:B:681:ASN:HD21	2.25	0.48
1:B:912:GLU:N	1:B:913:PRO:HD3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:LEU:HB3	1:B:608:LEU:HD21	1.95	0.48
1:B:278:THR:HG22	1:B:287:LEU:CD2	2.44	0.48
1:B:758:VAL:HG23	1:B:874:ILE:HD13	1.95	0.48
1:A:343:THR:HG22	1:A:345:ASP:H	1.79	0.48
1:B:373:VAL:HG23	1:B:410:LEU:HD13	1.95	0.48
1:A:546:LEU:O	1:A:549:TYR:HB3	2.13	0.47
1:A:875:LEU:O	1:A:878:GLN:HB3	2.14	0.47
1:A:398:ARG:CG	1:A:398:ARG:NH1	2.56	0.47
1:B:716:GLN:O	1:B:716:GLN:CG	2.62	0.47
1:B:761:ILE:O	1:B:905:LEU:HB2	2.13	0.47
1:A:5:THR:HG23	1:A:8:PRO:HD2	1.97	0.47
1:A:175:ASP:OD2	1:A:178:SER:N	2.47	0.47
1:B:72:LEU:HD23	1:B:72:LEU:HA	1.72	0.47
1:B:189:LEU:HD23	1:B:189:LEU:O	2.14	0.47
1:B:214:LEU:HD12	1:B:217:MSE:CE	2.44	0.47
1:B:386:MSE:HE3	1:B:411:ILE:HD11	1.96	0.47
1:A:768:ILE:HG22	1:A:917:ILE:HG13	1.96	0.47
1:B:64:ILE:CA	1:B:67:LYS:HZ2	2.28	0.47
1:B:82:ALA:HB1	1:B:89:PHE:CE2	2.50	0.47
1:A:248:GLU:O	1:A:248:GLU:CD	2.52	0.47
1:A:430:ASN:HB3	1:A:439:VAL:CG2	2.45	0.47
1:B:181:GLU:O	1:B:185:ILE:HG23	2.14	0.47
1:B:478:GLY:HA3	1:B:513:ILE:CD1	2.45	0.47
1:B:353:LEU:HD23	1:B:353:LEU:HA	1.63	0.47
1:A:381:GLU:O	1:A:385:VAL:HG23	2.14	0.47
1:B:225:LEU:N	1:B:225:LEU:CD2	2.78	0.47
1:B:719:ASN:CB	1:B:722:THR:HG22	2.40	0.47
1:A:436:ASP:HB3	1:A:439:VAL:CG1	2.45	0.47
1:B:95:SER:O	1:B:99:GLU:HG2	2.15	0.47
1:B:202:PHE:CZ	1:B:206:ILE:HD11	2.49	0.47
1:B:743:PHE:N	1:B:744:PRO:CD	2.77	0.47
1:B:151:LYS:CD	1:B:152:LEU:HD12	2.45	0.46
1:B:185:ILE:CG1	1:B:186:ILE:N	2.78	0.46
1:B:539:MSE:HE2	1:B:550:GLY:C	2.35	0.46
1:A:602:VAL:HG12	1:A:625:LEU:CD2	2.45	0.46
1:B:181:GLU:OE1	1:B:181:GLU:CA	2.62	0.46
1:B:754:THR:HA	1:B:755:PRO:HD3	1.80	0.46
1:A:345:ASP:OD1	1:A:345:ASP:C	2.53	0.46
1:A:361:ASN:O	1:A:364:LYS:HB2	2.15	0.46
1:B:67:LYS:CD	1:B:67:LYS:N	2.77	0.46
1:B:222:TYR:CD2	1:B:241:LEU:HD11	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:GLY:HA3	1:B:407:GLY:O	2.16	0.46
1:B:889:ARG:NH2	1:B:914:VAL:CG1	2.79	0.46
1:B:867:LYS:HD2	1:B:867:LYS:N	2.31	0.46
1:A:278:THR:HA	1:A:287:LEU:HD11	1.97	0.46
1:A:608:LEU:HD12	1:A:608:LEU:HA	1.76	0.46
1:B:144:CYS:HA	1:B:147:ALA:HB3	1.98	0.46
1:A:504:TYR:O	1:A:508:THR:HG22	2.16	0.46
1:A:909:GLU:HB3	1:A:911:LYS:HZ2	1.80	0.46
1:A:501:MSE:HE1	1:A:524:ILE:HD11	1.97	0.46
1:A:919:THR:HG21	1:A:921:ARG:HH21	1.80	0.46
1:B:144:CYS:HB2	1:B:153:ALA:HB2	1.97	0.46
1:B:197:VAL:O	1:B:203:ARG:NH1	2.49	0.46
1:A:540:LEU:HD23	1:A:540:LEU:HA	1.72	0.46
1:B:162:ARG:O	1:B:166:ILE:HG13	2.16	0.46
1:B:259:PHE:CD2	1:B:902:VAL:HG11	2.50	0.46
1:A:919:THR:HG21	1:A:921:ARG:CZ	2.46	0.45
1:A:253:LEU:HD12	1:A:253:LEU:HA	1.71	0.45
1:A:289:ILE:HA	1:A:294:PRO:HG2	1.97	0.45
1:A:638:ILE:HD11	1:A:664:LEU:HD21	1.98	0.45
1:A:245:LEU:HD21	1:A:254:SER:HA	1.99	0.45
1:A:494:LYS:HA	1:A:495:PRO:HD3	1.73	0.45
1:B:158:LEU:HD12	1:B:158:LEU:HA	1.75	0.45
1:B:252:GLY:HA3	1:B:893:VAL:HG21	1.99	0.45
1:B:539:MSE:HE2	1:B:551:GLY:N	2.31	0.45
1:A:261:LEU:O	1:A:265:ALA:HB3	2.16	0.45
1:A:430:ASN:HB3	1:A:439:VAL:HG23	1.98	0.45
1:A:490:LEU:HD21	1:A:727:THR:CG2	2.46	0.45
1:B:203:ARG:O	1:B:207:LEU:HD22	2.16	0.45
1:B:242:PHE:HE2	1:B:273:LEU:HD21	1.81	0.45
1:B:688:ASN:C	1:B:688:ASN:OD1	2.54	0.45
1:B:913:PRO:O	1:B:914:VAL:CG1	2.64	0.45
1:B:136:ILE:CG2	1:B:137:PHE:N	2.79	0.45
1:B:226:ASN:O	1:B:230:VAL:CG2	2.65	0.45
1:A:89:PHE:CZ	1:A:101:ILE:HD11	2.51	0.45
1:B:67:LYS:HD2	1:B:67:LYS:N	2.30	0.45
1:B:546:LEU:O	1:B:549:TYR:HB3	2.17	0.45
1:B:596:LEU:CD2	1:B:725:LEU:HD11	2.45	0.45
1:B:882:ILE:HG22	1:B:882:ILE:O	2.16	0.45
1:A:353:LEU:N	1:A:354:PRO:CD	2.78	0.45
1:B:182:ASN:N	1:B:182:ASN:HD22	2.15	0.45
1:B:259:PHE:CE1	1:B:289:ILE:HG23	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:HIS:O	1:A:503:THR:OG1	2.35	0.45
1:B:209:LYS:NZ	1:B:209:LYS:HA	2.32	0.45
1:A:141:ILE:HG22	1:A:142:GLU:N	2.33	0.44
1:A:301:THR:HG22	1:A:871:MSE:HE1	1.98	0.44
1:B:433:THR:HG21	1:B:439:VAL:HG21	1.98	0.44
1:B:455:MSE:HE1	1:B:728:LYS:HA	1.99	0.44
1:B:581:ASP:HB3	1:B:616:HIS:CG	2.53	0.44
1:B:894:ARG:O	1:B:894:ARG:HG3	2.18	0.44
1:A:437:GLU:OE1	1:A:437:GLU:N	2.49	0.44
1:A:688:ASN:O	1:A:696:LYS:NZ	2.33	0.44
1:A:882:ILE:HD12	1:A:882:ILE:HA	1.75	0.44
1:B:728:LYS:HB2	1:B:728:LYS:NZ	2.32	0.44
1:A:373:VAL:HG23	1:A:410:LEU:HD13	2.00	0.44
1:A:497:ALA:HB1	1:A:501:MSE:HE1	1.98	0.44
1:A:617:VAL:O	1:A:621:THR:HG23	2.17	0.44
1:B:909:GLU:N	1:B:910:PRO:CD	2.80	0.44
1:A:427:ILE:CD1	1:A:446:ALA:HB1	2.46	0.44
1:A:641:LEU:HA	1:A:641:LEU:HD23	1.84	0.44
1:B:185:ILE:HG13	1:B:186:ILE:N	2.33	0.44
1:A:348:PHE:O	1:A:352:ASN:ND2	2.49	0.44
1:A:761:ILE:HG13	1:A:902:VAL:HG13	2.00	0.44
1:B:149:GLU:HB3	1:B:152:LEU:CD1	2.48	0.44
1:B:717:LEU:HD11	1:B:733:LEU:CD1	2.45	0.44
1:A:919:THR:HG23	1:A:921:ARG:N	2.31	0.44
1:B:162:ARG:NH1	1:B:164:ASP:OD1	2.51	0.44
1:A:85:ALA:O	1:A:86:LYS:HB2	2.17	0.44
1:B:245:LEU:HD13	1:B:254:SER:HA	2.00	0.44
1:B:291:SER:HB2	1:B:293:LEU:CD1	2.48	0.44
1:A:321:LEU:HB3	1:A:328:PHE:CG	2.53	0.43
1:B:239:LEU:HD12	1:B:239:LEU:C	2.39	0.43
1:B:780:ASP:OD1	1:B:780:ASP:N	2.39	0.43
1:A:393:SER:O	1:A:394:ARG:CB	2.66	0.43
1:A:596:LEU:HD12	1:A:596:LEU:C	2.39	0.43
1:A:879:SER:HB3	1:A:898:GLY:O	2.18	0.43
1:B:163:LEU:HD13	1:B:206:ILE:HD13	2.01	0.43
1:B:472:ASN:OD1	1:B:472:ASN:O	2.36	0.43
1:B:887:ASP:OD1	1:B:887:ASP:N	2.43	0.43
1:B:151:LYS:CB	1:B:188:TYR:CE2	3.01	0.43
1:B:650:ASP:OD1	1:B:651:PHE:N	2.52	0.43
1:A:158:LEU:HD12	1:A:158:LEU:HA	1.79	0.43
1:B:773:MSE:HE3	1:B:773:MSE:HB2	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:ILE:HG23	1:B:521:LEU:HD22	2.01	0.43
1:B:889:ARG:HH22	1:B:914:VAL:CG1	2.31	0.43
1:B:89:PHE:HD1	1:B:90:ASP:N	2.15	0.43
1:B:761:ILE:CG1	1:B:762:ARG:N	2.81	0.43
1:A:169:ALA:O	1:A:173:LYS:HG2	2.18	0.43
1:B:160:GLY:O	1:B:161:TYR:HB2	2.19	0.43
1:B:189:LEU:C	1:B:189:LEU:CD2	2.87	0.43
1:B:311:ILE:HD13	1:B:311:ILE:HA	1.85	0.43
1:B:719:ASN:HB3	1:B:722:THR:CG2	2.44	0.43
1:B:719:ASN:ND2	1:B:722:THR:HG22	2.34	0.43
1:A:122:GLN:HA	1:A:122:GLN:OE1	2.19	0.43
1:A:145:LEU:CD2	1:A:150:LEU:HD12	2.48	0.43
1:B:188:TYR:CE1	1:B:192:LEU:HD13	2.53	0.43
1:B:214:LEU:HD12	1:B:217:MSE:HE2	2.01	0.43
1:B:497:ALA:O	1:B:501:MSE:HG3	2.18	0.43
1:A:921:ARG:HE	1:A:921:ARG:HB3	1.48	0.43
1:B:241:LEU:HD12	1:B:241:LEU:C	2.34	0.43
1:B:515:ARG:HB2	1:B:546:LEU:HD22	2.00	0.43
1:A:265:ALA:HB1	1:A:269:LEU:HD22	2.00	0.43
1:A:919:THR:CG2	1:A:921:ARG:HB3	2.49	0.43
1:A:138:GLU:O	1:A:142:GLU:HG2	2.19	0.42
1:B:176:GLN:O	1:B:177:ASP:HB2	2.18	0.42
1:B:894:ARG:HG3	1:B:894:ARG:HH11	1.84	0.42
1:A:4:THR:HB	1:A:5:THR:H	1.54	0.42
1:A:619:CYS:HB2	1:A:652:VAL:HG22	2.01	0.42
1:B:372:GLY:HA2	1:B:411:ILE:HG12	2.00	0.42
1:B:782:PHE:CE2	1:B:878:GLN:HB2	2.54	0.42
1:B:895:LYS:CD	1:B:896:PHE:H	2.17	0.42
1:B:918:GLU:CB	1:B:923:MSE:CE	2.97	0.42
1:A:106:ILE:HD11	1:A:140:MSE:HG2	2.01	0.42
1:A:518:ALA:HB1	1:A:550:GLY:CA	2.47	0.42
1:B:202:PHE:O	1:B:206:ILE:HG12	2.18	0.42
1:B:214:LEU:HG	1:B:225:LEU:HD21	2.01	0.42
1:B:257:ILE:C	1:B:257:ILE:HD12	2.39	0.42
1:B:889:ARG:NH2	1:B:914:VAL:HG12	2.34	0.42
1:B:68:VAL:HG22	1:B:69:TYR:N	2.34	0.42
1:B:770:LYS:HE2	1:B:917:ILE:HG12	2.01	0.42
1:A:28:ILE:HG23	1:A:39:ILE:HD13	2.02	0.42
1:B:231:ASN:HD22	1:B:231:ASN:H	1.65	0.42
1:B:352:ASN:ND2	1:B:352:ASN:N	2.66	0.42
1:B:387:ALA:N	1:B:388:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:LEU:O	1:B:393:SER:HB3	2.19	0.42
1:A:174:LEU:C	1:A:174:LEU:HD12	2.40	0.42
1:B:767:ALA:O	1:B:769:PRO:CD	2.67	0.42
1:A:257:ILE:HD13	1:A:257:ILE:HA	1.89	0.42
1:A:282:TYR:HE2	1:A:286:LEU:HD12	1.85	0.42
1:A:602:VAL:O	1:A:606:VAL:HG22	2.19	0.42
1:B:638:ILE:CD1	1:B:664:LEU:HD21	2.48	0.42
1:A:776:TYR:CE2	1:A:865:PRO:HD3	2.55	0.42
1:B:82:ALA:HB1	1:B:89:PHE:CD2	2.55	0.42
1:A:68:VAL:O	1:A:72:LEU:HG	2.20	0.42
1:B:243:LYS:HB3	1:B:243:LYS:HE3	1.81	0.42
1:B:670:LYS:HE2	1:B:670:LYS:HB3	1.94	0.42
1:A:278:THR:HG22	1:A:279:ALA:N	2.35	0.42
1:A:444:HIS:ND1	1:A:480:ALA:HB2	2.35	0.42
1:A:450:ILE:HD12	1:A:462:VAL:HG23	2.02	0.42
1:A:454:ALA:O	1:A:457:SER:HB3	2.19	0.42
1:B:170:LEU:HD23	1:B:170:LEU:HA	1.76	0.42
1:B:259:PHE:CD1	1:B:289:ILE:HG23	2.55	0.42
1:B:283:ASP:OD1	1:B:284:PRO:HD2	2.19	0.42
1:B:307:LYS:HE2	1:B:345:ASP:OD2	2.20	0.42
1:A:76:GLU:OE1	1:A:76:GLU:N	2.51	0.41
1:B:245:LEU:HD23	1:B:245:LEU:HA	1.73	0.41
1:B:353:LEU:N	1:B:354:PRO:HD3	2.34	0.41
1:A:110:VAL:HG11	1:A:159:GLU:HG3	2.02	0.41
1:A:117:TYR:CE1	1:A:121:GLU:HB3	2.56	0.41
1:A:214:LEU:HD11	1:A:224:THR:HG22	2.01	0.41
1:A:361:ASN:HA	1:A:399:PHE:CE2	2.54	0.41
1:A:389:TYR:HE2	2:A:2010:HOH:O	2.02	0.41
1:A:549:TYR:CE1	1:A:586:ALA:HB2	2.56	0.41
1:A:891:VAL:HA	1:A:892:PRO:HD3	1.90	0.41
1:B:692:GLU:N	1:B:692:GLU:OE1	2.53	0.41
1:B:768:ILE:HA	1:B:769:PRO:HD2	1.90	0.41
1:A:175:ASP:O	1:A:176:GLN:CB	2.68	0.41
1:A:721:ASP:CG	1:A:899:ASN:HD21	2.23	0.41
1:B:236:GLY:O	1:B:240:GLN:HG3	2.20	0.41
1:B:380:LEU:HG	1:B:381:GLU:N	2.35	0.41
1:A:481:ALA:O	1:A:485:MSE:HE3	2.21	0.41
1:A:642:ASP:HB3	1:A:643:PRO:CD	2.46	0.41
1:B:63:LEU:O	1:B:66:SER:HB2	2.20	0.41
1:B:561:GLY:O	1:B:597:ARG:HG3	2.20	0.41
1:B:683:LEU:HD23	1:B:683:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:LEU:HA	1:A:683:LEU:HD23	1.74	0.41
1:B:124:TYR:CG	1:B:162:ARG:NH1	2.89	0.41
1:B:398:ARG:HG3	1:B:441:VAL:CB	2.50	0.41
1:B:418:ASP:OD1	1:B:419:THR:N	2.53	0.41
1:A:306:ASN:ND2	1:A:306:ASN:N	2.68	0.41
1:B:593:PHE:O	1:B:596:LEU:HD13	2.21	0.41
1:B:923:MSE:HE2	1:B:923:MSE:HB3	1.84	0.41
1:A:158:LEU:HD11	1:A:206:ILE:HD13	2.00	0.41
1:A:184:LYS:NZ	1:A:184:LYS:HB2	2.35	0.41
1:A:222:TYR:HA	1:A:225:LEU:HB2	2.03	0.41
1:A:314:LEU:HA	1:A:314:LEU:HD23	1.74	0.41
1:B:217:MSE:HE3	1:B:219:ASN:O	2.20	0.41
1:B:482:ALA:CA	1:B:485:MSE:HE3	2.48	0.41
1:A:192:LEU:HD12	1:A:192:LEU:HA	1.95	0.41
1:B:231:ASN:N	1:B:231:ASN:ND2	2.64	0.41
1:B:489:MSE:HE3	1:B:494:LYS:HD3	2.02	0.41
1:A:230:VAL:HG13	1:A:265:ALA:HA	2.03	0.41
1:A:743:PHE:N	1:A:744:PRO:CD	2.84	0.41
1:B:114:SER:HG	1:B:161:TYR:HE2	1.67	0.41
1:B:291:SER:HB2	1:B:293:LEU:HD12	2.03	0.41
1:B:291:SER:CB	1:B:293:LEU:HD12	2.50	0.41
1:B:686:ILE:HD11	1:B:700:CYS:HA	2.01	0.41
1:B:787:MSE:O	1:B:788:TYR:CB	2.69	0.41
1:A:298:TYR:CZ	1:A:761:ILE:HD11	2.56	0.41
1:A:526:TYR:HA	1:A:557:LEU:HB3	2.02	0.41
1:A:754:THR:HG23	2:A:2024:HOH:O	2.21	0.41
1:B:74:GLU:CD	1:B:74:GLU:N	2.73	0.41
1:B:548:ARG:NH1	1:B:578:ASP:OD1	2.54	0.41
1:B:913:PRO:C	1:B:914:VAL:HG13	2.41	0.41
1:A:572:LEU:O	1:A:576:VAL:HG23	2.21	0.40
1:A:881:TYR:HE1	1:B:72:LEU:HD11	1.85	0.40
1:B:101:ILE:HA	1:B:101:ILE:HD12	1.85	0.40
1:B:268:GLN:O	1:B:272:ILE:HG13	2.20	0.40
1:B:470:LEU:HB2	1:B:485:MSE:CE	2.44	0.40
1:A:7:ALA:N	1:A:8:PRO:CD	2.82	0.40
1:A:572:LEU:HA	1:A:572:LEU:HD23	1.86	0.40
1:B:122:GLN:O	1:B:125:THR:HB	2.21	0.40
1:A:436:ASP:OD1	1:A:438:ASP:N	2.54	0.40
1:A:650:ASP:OD1	1:A:651:PHE:N	2.53	0.40
1:B:645:THR:O	1:B:653:ARG:HG2	2.21	0.40
1:B:711:ARG:HA	2:B:2028:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:GLN:OE1	1:A:128:ILE:HG21	2.21	0.40
1:B:60:MSE:O	1:B:63:LEU:HB3	2.21	0.40
1:B:424:LYS:O	1:B:428:VAL:HG22	2.22	0.40
1:A:129:ILE:HG22	1:A:130:ASP:N	2.35	0.40
1:B:314:LEU:HA	1:B:314:LEU:HD23	1.84	0.40
1:B:561:GLY:O	1:B:597:ARG:NH1	2.53	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	843/963 (88%)	829 (98%)	14 (2%)	0	100	100
1	B	798/963 (83%)	783 (98%)	14 (2%)	1 (0%)	51	78
All	All	1641/1926 (85%)	1612 (98%)	28 (2%)	1 (0%)	51	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	910	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	694/792 (88%)	612 (88%)	82 (12%)	5	12
1	B	623/792 (79%)	546 (88%)	77 (12%)	4	11
All	All	1317/1584 (83%)	1158 (88%)	159 (12%)	5	11

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	26	GLU
1	A	49	LEU
1	A	57	ASP
1	A	87	ASP
1	A	101	ILE
1	A	107	GLU
1	A	118	THR
1	A	174	LEU
1	A	179	THR
1	A	183	VAL
1	A	187	ASN
1	A	209	LYS
1	A	215	MSE
1	A	220	CYS
1	A	223	LEU
1	A	262	VAL
1	A	266	SER
1	A	269	LEU
1	A	278	THR
1	A	280	GLN
1	A	297	ASP
1	A	304	LEU
1	A	307	LYS
1	A	321	LEU
1	A	343	THR
1	A	344	THR
1	A	345	ASP
1	A	347	SER
1	A	352	ASN
1	A	353	LEU
1	A	356	LEU
1	A	360	GLN
1	A	380	LEU
1	A	389	TYR

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Mol	Chain	Res	Type
1	A	390	LEU
1	A	398	ARG
1	A	427	ILE
1	A	433	THR
1	A	450	ILE
1	A	461	GLU
1	A	462	VAL
1	A	503	THR
1	A	508	THR
1	A	530	GLU
1	A	547	LEU
1	A	570	ARG
1	A	585	ARG
1	A	604	ARG
1	A	607	GLN
1	A	608	LEU
1	A	619	CYS
1	A	680	LYS
1	A	683	LEU
1	A	686	ILE
1	A	692	GLU
1	A	711	ARG
1	A	718	GLU
1	A	722	THR
1	A	724	THR
1	A	734	VAL
1	A	758	VAL
1	A	773	MSE
1	A	779	GLU
1	A	860	LYS
1	A	871	MSE
1	A	874	ILE
1	A	877	GLN
1	A	880	ARG
1	A	882	ILE
1	A	885	ILE
1	A	894	ARG
1	A	903	VAL
1	A	908	ARG
1	A	909	GLU
1	A	911	LYS
1	A	914	VAL

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Mol	Chain	Res	Type
1	A	917	ILE
1	A	919	THR
1	A	920	VAL
1	A	921	ARG
1	A	923	MSE
1	B	63	LEU
1	B	68	VAL
1	B	74	GLU
1	B	89	PHE
1	B	91	ILE
1	B	92	ASP
1	B	95	SER
1	B	97	PHE
1	B	99	GLU
1	B	101	ILE
1	B	125	THR
1	B	134	THR
1	B	136	ILE
1	B	140	MSE
1	B	141	ILE
1	B	143	LYS
1	B	159	GLU
1	B	179	THR
1	B	181	GLU
1	B	183	VAL
1	B	204	SER
1	B	205	SER
1	B	207	LEU
1	B	209	LYS
1	B	214	LEU
1	B	219	ASN
1	B	221	ASP
1	B	223	LEU
1	B	225	LEU
1	B	227	LYS
1	B	230	VAL
1	B	231	ASN
1	B	248	GLU
1	B	257	ILE
1	B	259	PHE
1	B	274	VAL
1	B	280	GLN

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Mol	Chain	Res	Type
1	B	289	ILE
1	B	295	THR
1	B	324	LYS
1	B	347	SER
1	B	350	LYS
1	B	352	ASN
1	B	360	GLN
1	B	380	LEU
1	B	381	GLU
1	B	389	TYR
1	B	393	SER
1	B	398	ARG
1	B	428	VAL
1	B	431	SER
1	B	437	GLU
1	B	462	VAL
1	B	464	GLU
1	B	503	THR
1	B	508	THR
1	B	524	ILE
1	B	543	ASP
1	B	565	ASN
1	B	570	ARG
1	B	596	LEU
1	B	600	THR
1	B	607	GLN
1	B	610	SER
1	B	623	PHE
1	B	654	GLN
1	B	683	LEU
1	B	725	LEU
1	B	728	LYS
1	B	765	ASP
1	B	766	GLN
1	B	868	VAL
1	B	879	SER
1	B	885	ILE
1	B	887	ASP
1	B	889	ARG
1	B	895	LYS

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

Mol	Chain	Res	Type
1	A	305	ASN
1	A	340	HIS
1	A	425	ASN
1	A	667	GLN
1	A	681	ASN
1	A	899	ASN
1	B	182	ASN
1	B	300	ASN
1	B	329	HIS
1	B	360	GLN
1	B	506	GLN
1	B	510	HIS
1	B	635	GLN
1	B	681	ASN
1	B	899	ASN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	829/963 (86%)	0.42	25 (3%)	50 51	40, 73, 114, 144	0
1	B	782/963 (81%)	0.43	35 (4%)	33 31	35, 80, 136, 173	0
All	All	1611/1926 (83%)	0.42	60 (3%)	41 41	35, 75, 129, 173	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	884	PHE	6.5
1	B	83	LEU	5.3
1	A	920	VAL	4.2
1	B	396	SER	3.8
1	A	860	LYS	3.6
1	A	401	LYS	3.5
1	A	443	LEU	3.5
1	A	440	ASP	3.4
1	B	130	ASP	3.3
1	B	175	ASP	3.2
1	B	299	TYR	3.0
1	B	442	LEU	3.0
1	B	395	ALA	3.0
1	B	915	ALA	2.9
1	A	427	ILE	2.9
1	B	303	LEU	2.9
1	A	891	VAL	2.9
1	B	912	GLU	2.9
1	B	79	VAL	2.8
1	B	226	ASN	2.6
1	B	890	PHE	2.6
1	B	761	ILE	2.6
1	A	721	ASP	2.6
1	B	89	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	921	ARG	2.6
1	A	442	LEU	2.5
1	B	905	LEU	2.5
1	A	408	LEU	2.5
1	A	317	SER	2.5
1	A	396	SER	2.5
1	A	760	GLY	2.4
1	B	179	THR	2.4
1	B	222	TYR	2.4
1	B	286	LEU	2.4
1	A	758	VAL	2.4
1	A	686	ILE	2.4
1	B	262	VAL	2.4
1	A	781	ALA	2.3
1	B	150	LEU	2.3
1	B	101	ILE	2.3
1	B	273	LEU	2.3
1	A	355	TRP	2.3
1	B	920	VAL	2.3
1	B	253	LEU	2.3
1	A	513	ILE	2.2
1	B	91	ILE	2.2
1	A	356	LEU	2.2
1	B	62	ALA	2.2
1	A	759	ILE	2.1
1	B	61	ALA	2.1
1	A	359	ALA	2.1
1	A	905	LEU	2.1
1	B	66	SER	2.1
1	A	861	TYR	2.1
1	B	213	PHE	2.1
1	B	771	PHE	2.1
1	B	675	VAL	2.1
1	A	470	LEU	2.0
1	A	921	ARG	2.0
1	B	304	LEU	2.0

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

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.