



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:09 PM UTC

PDB ID : 3QG5 / pdb_00003qg5
Title : The Mre11:Rad50 complex forms an ATP dependent molecular clamp in DNA double-strand break repair
Authors : Lammens, K.
Deposited on : 2011-01-24
Resolution : 3.40 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

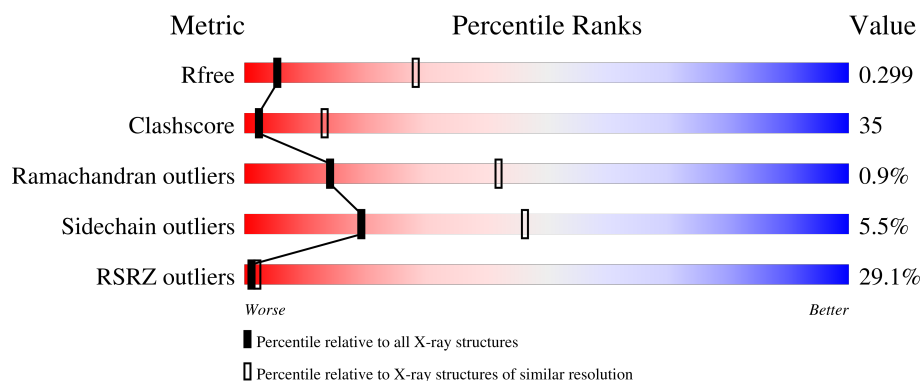
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	365	18% 47% 43% 5% .
1	B	365	60% 73% 22% . .
2	C	379	12% 51% 38% 6% .
2	D	379	18% 55% 37% . . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11601 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 rad50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	Se	95	0	0
			2799	1784	486	525	4			
1	B	349	Total	C	N	O	Se	371	0	0
			2799	1784	486	525	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	678	GLY	-	linker	UNP Q9X1X1
A	679	GLY	-	linker	UNP Q9X1X1
A	680	ALA	-	linker	UNP Q9X1X1
A	681	GLY	-	linker	UNP Q9X1X1
A	682	GLY	-	linker	UNP Q9X1X1
A	683	ALA	-	linker	UNP Q9X1X1
A	684	GLY	-	linker	UNP Q9X1X1
A	685	GLY	-	linker	UNP Q9X1X1
B	678	GLY	-	linker	UNP Q9X1X1
B	679	GLY	-	linker	UNP Q9X1X1
B	680	ALA	-	linker	UNP Q9X1X1
B	681	GLY	-	linker	UNP Q9X1X1
B	682	GLY	-	linker	UNP Q9X1X1
B	683	ALA	-	linker	UNP Q9X1X1
B	684	GLY	-	linker	UNP Q9X1X1
B	685	GLY	-	linker	UNP Q9X1X1

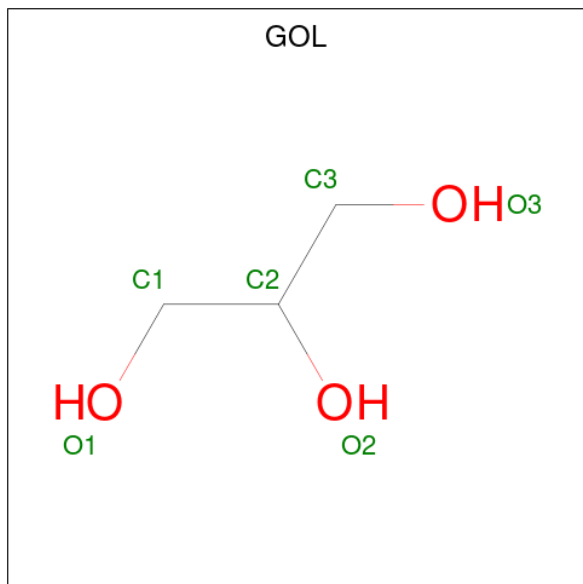
- Molecule 2 is a protein called Mre11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	362	Total	C	N	O	S	Se	127	0
			2985	1915	505	558	1	6		0
2	D	366	Total	C	N	O	S	Se	114	0
			3006	1928	512	559	1	6		0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	7	MSE	-	initiating methionine	UNP Q9X1X0
D	7	MSE	-	initiating methionine	UNP Q9X1X0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

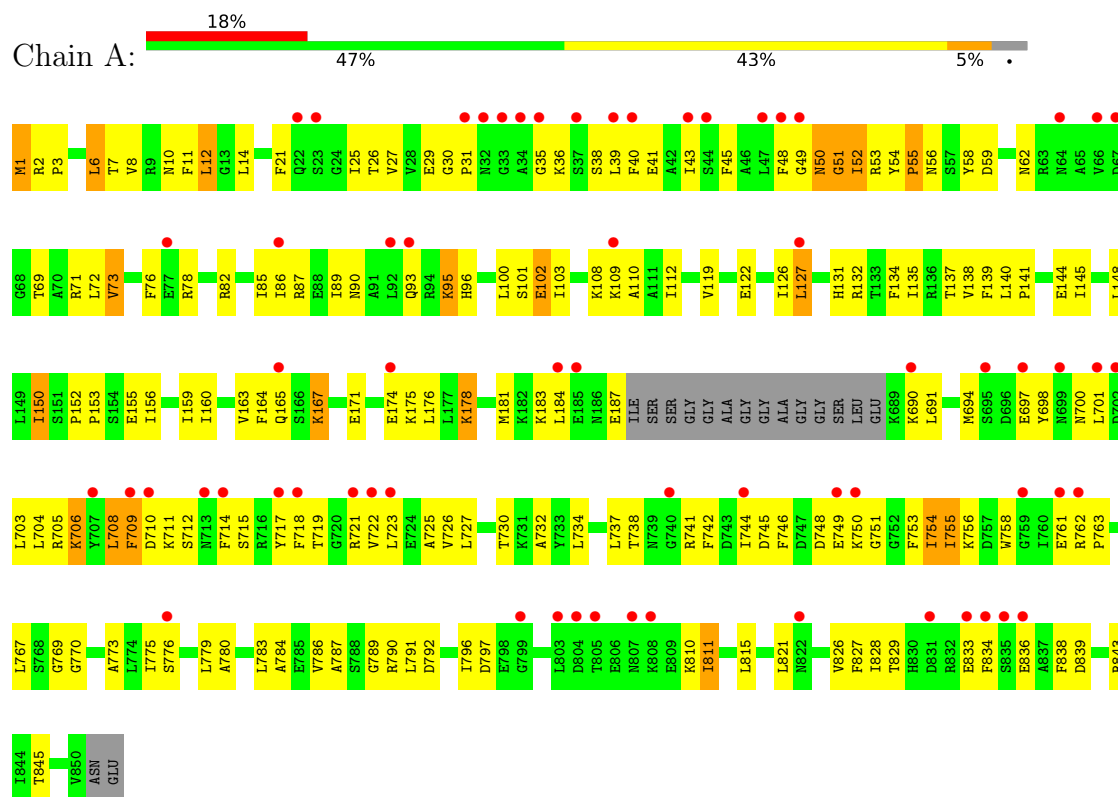


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

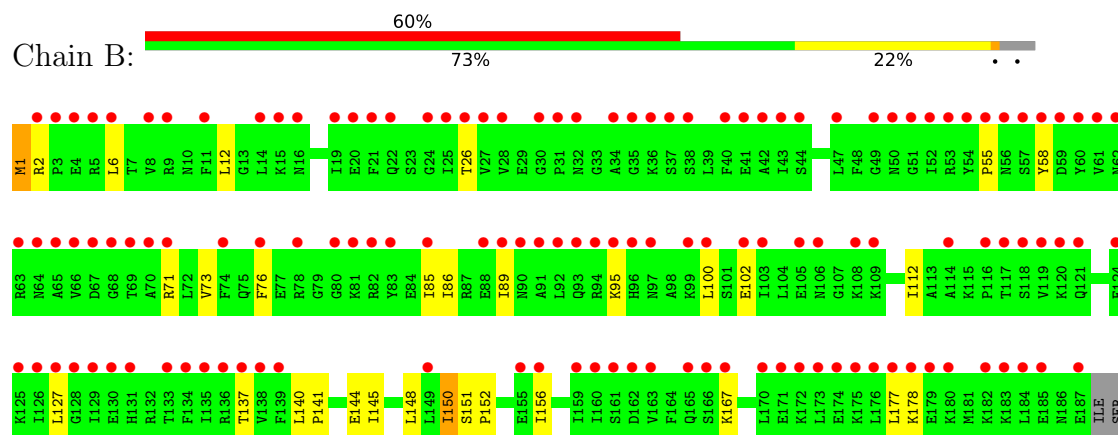
3 Residue-property plots

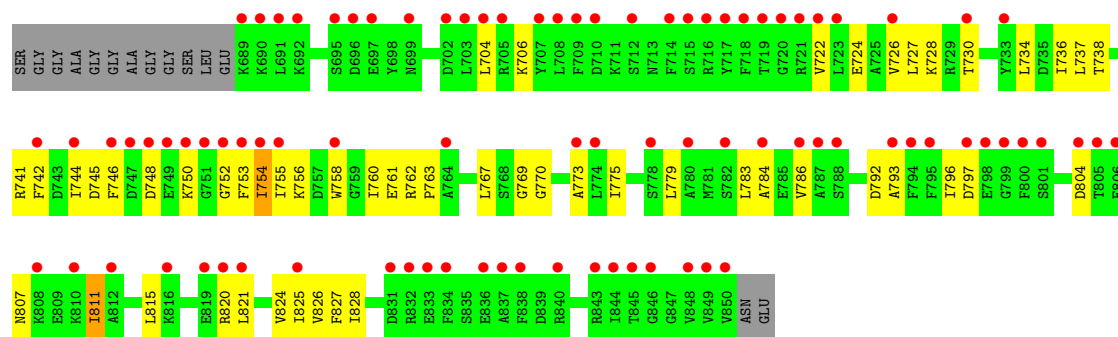
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: rad50

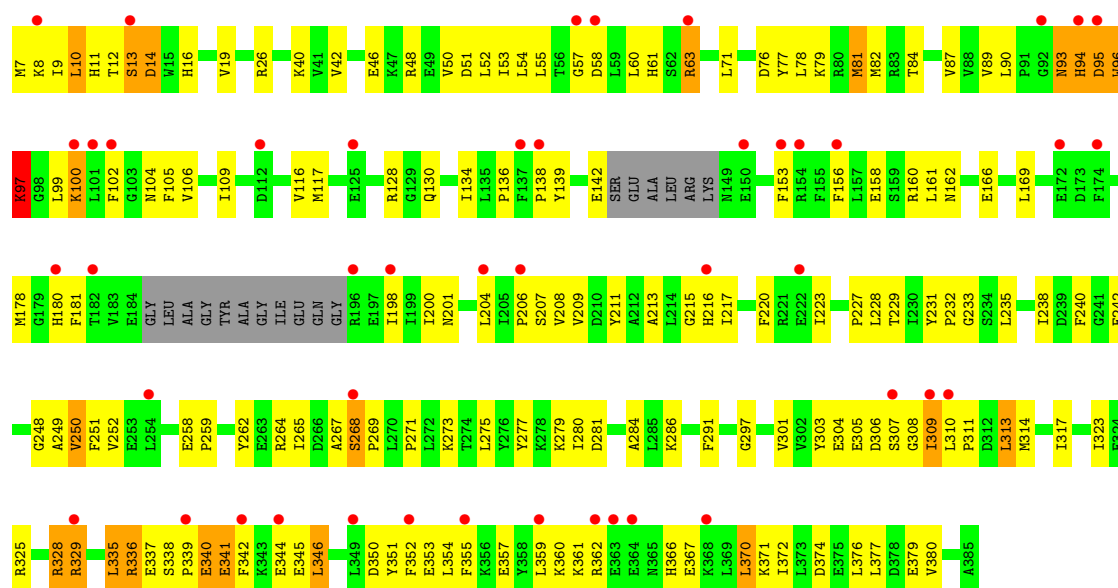


• Molecule 1: rad50

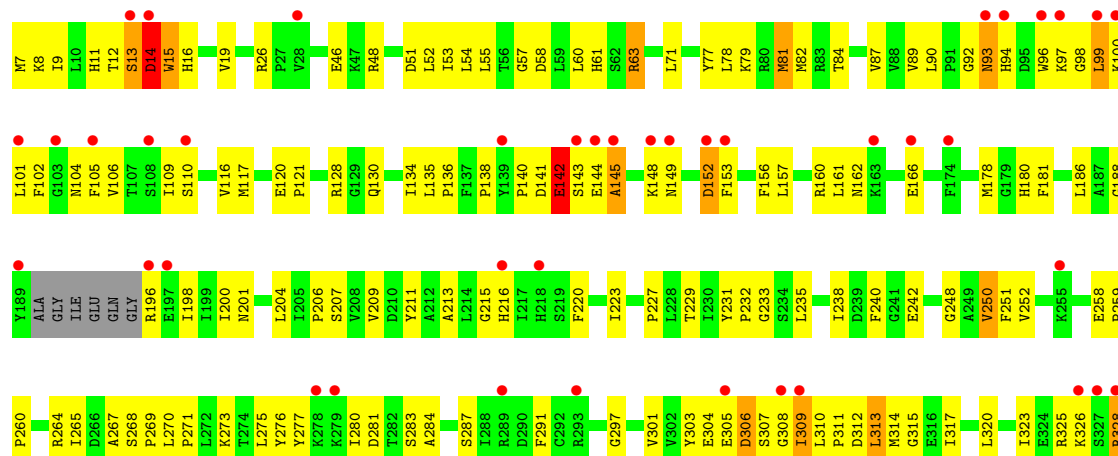


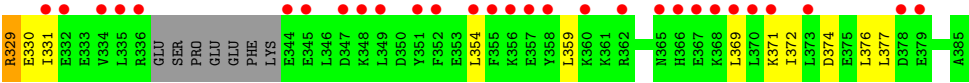


• Molecule 2: Mre11



• Molecule 2: Mre11





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	105.19Å 187.00Å 300.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 20.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-3.40) 98.2 (20.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.44Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.258 , 0.295 0.269 , 0.299	Depositor DCC
R_{free} test set	2020 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	93.7	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 79.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11601	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.33	0/2837	0.73	3/3797 (0.1%)
1	B	0.29	0/2837	0.71	2/3797 (0.1%)
2	C	0.35	0/3041	0.79	3/4086 (0.1%)
2	D	0.35	0/3061	0.84	10/4112 (0.2%)
All	All	0.33	0/11776	0.77	18/15792 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	15	TRP	N-CA-C	8.00	120.08	111.36
2	D	329	ARG	NE-CZ-NH2	7.95	126.35	119.20
2	C	97	LYS	N-CA-C	7.83	119.81	111.28
2	D	196	ARG	NE-CZ-NH2	7.46	125.92	119.20
2	D	329	ARG	NE-CZ-NH1	-7.37	114.13	121.50
2	D	196	ARG	NE-CZ-NH1	-7.00	114.50	121.50
1	A	753	PHE	N-CA-C	-6.82	99.33	109.15
1	A	709	PHE	N-CA-C	6.54	118.49	111.36
2	D	14	ASP	N-CA-C	6.33	119.79	110.30
2	D	93	ASN	N-CA-CB	6.22	121.76	112.30
2	C	329	ARG	NE-CZ-NH2	-5.54	114.22	119.20
2	D	329	ARG	CD-NE-CZ	5.49	132.08	124.40
2	C	329	ARG	CD-NE-CZ	5.41	131.98	124.40
1	B	748	ASP	N-CA-C	5.20	116.94	111.28
2	D	110	SER	N-CA-C	5.17	116.93	109.07
2	D	196	ARG	CD-NE-CZ	5.17	131.63	124.40
1	B	744	ILE	N-CA-C	5.09	115.24	108.11
1	A	754	ILE	N-CA-C	-5.01	101.20	108.36

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	2799	0	2870	254	0
1	B	2799	0	2870	82	0
2	C	2985	0	3006	257	0
2	D	3006	0	3038	247	0
3	A	6	0	8	0	0
3	D	6	0	8	0	0
All	All	11601	0	11800	767	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 35.

All (767) 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:174:GLU:HG2	1:A:709:PHE:CE1	1.61	1.34
2:D:306:ASP:HB2	2:D:325:ARG:NH1	1.40	1.30
1:A:3:PRO:HB2	1:A:21:PHE:CE1	1.67	1.29
2:D:14:ASP:OD2	2:D:57:GLY:HA3	1.29	1.27
2:D:306:ASP:CB	2:D:325:ARG:NH1	1.96	1.27
2:D:306:ASP:CB	2:D:325:ARG:HH11	1.50	1.24
2:D:148:LYS:HB3	2:D:152:ASP:CB	1.66	1.23
2:C:340:GLU:O	2:C:341:GLU:HG2	1.39	1.22
2:C:346:LEU:HD12	2:C:346:LEU:O	1.39	1.20
1:A:25:ILE:HD11	1:A:827:PHE:CE1	1.76	1.19
2:D:148:LYS:HD2	2:D:152:ASP:CG	1.68	1.19
1:A:3:PRO:HB2	1:A:21:PHE:CD1	1.81	1.15
2:C:40:LYS:NZ	2:C:268:SER:OG	1.79	1.15
2:C:308:GLY:HA2	2:C:309:ILE:HB	1.27	1.15
1:B:738:THR:HG21	1:B:742:PHE:HD2	1.04	1.14
2:D:142:GLU:HG2	2:D:143:SER:N	1.66	1.10
2:D:149:ASN:O	2:D:153:PHE:HB3	1.50	1.10
2:C:308:GLY:CA	2:C:309:ILE:HB	1.83	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:93:ASN:HB2	2:C:139:TYR:HB3	1.14	1.08
1:A:25:ILE:HD11	1:A:827:PHE:HE1	1.07	1.06
1:A:174:GLU:HA	1:A:709:PHE:HZ	1.15	1.06
2:D:149:ASN:HA	2:D:153:PHE:HB2	1.09	1.06
1:B:26:THR:O	1:B:826:VAL:HA	1.54	1.06
1:A:90:ASN:ND2	1:A:93:GLN:OE1	1.89	1.05
2:C:338:SER:N	2:C:339:PRO:HD3	1.67	1.05
1:B:741:ARG:CZ	1:B:742:PHE:CZ	2.40	1.05
2:D:149:ASN:HD22	2:D:153:PHE:CB	1.68	1.05
1:A:722:VAL:HG23	1:A:726:VAL:CG2	1.86	1.05
2:D:149:ASN:HD22	2:D:153:PHE:HB3	1.22	1.05
1:A:708:LEU:HD23	1:A:708:LEU:C	1.81	1.03
2:D:79:LYS:HA	2:D:82:MSE:HE2	1.39	1.03
1:B:762:ARG:HH12	2:D:283:SER:HA	1.21	1.02
1:A:722:VAL:O	1:A:726:VAL:HB	1.58	1.02
1:A:722:VAL:HG23	1:A:726:VAL:HG21	1.06	1.02
2:C:79:LYS:HA	2:C:82:MSE:HE2	1.41	1.01
1:A:714:PHE:CE1	2:C:355:PHE:HA	1.96	1.01
2:D:14:ASP:HB3	2:D:58:ASP:N	1.77	0.99
1:B:738:THR:HG21	1:B:742:PHE:CD2	1.96	0.99
2:D:148:LYS:HB3	2:D:152:ASP:HB3	1.44	0.98
1:A:714:PHE:CZ	2:C:355:PHE:HB2	1.97	0.98
1:A:723:LEU:CD2	1:A:746:PHE:CD2	2.46	0.98
1:A:721:ARG:HG3	2:C:354:LEU:HD11	1.46	0.98
2:D:13:SER:HB2	2:D:232:PRO:HB2	1.46	0.98
2:D:149:ASN:CA	2:D:153:PHE:HB2	1.94	0.97
2:D:306:ASP:OD1	2:D:306:ASP:C	2.07	0.97
1:A:174:GLU:HG2	1:A:709:PHE:HE1	0.85	0.96
1:A:174:GLU:HA	1:A:709:PHE:CZ	1.99	0.96
2:D:148:LYS:CA	2:D:152:ASP:HB2	1.96	0.96
2:D:144:GLU:OE2	2:D:152:ASP:HB3	1.65	0.95
1:A:174:GLU:CG	1:A:709:PHE:HE1	1.80	0.94
1:A:722:VAL:CG2	1:A:726:VAL:HG21	1.97	0.94
1:A:3:PRO:HB2	1:A:21:PHE:HE1	1.26	0.93
2:D:92:GLY:O	2:D:94:HIS:CD2	2.21	0.93
2:C:11:HIS:CE1	2:C:232:PRO:HG2	2.04	0.93
2:C:161:LEU:HD13	2:C:204:LEU:HB3	1.50	0.93
2:D:148:LYS:O	2:D:152:ASP:CB	2.16	0.93
2:C:96:TRP:HE1	2:C:99:LEU:HB2	1.33	0.92
2:D:148:LYS:HB3	2:D:152:ASP:HB2	1.49	0.92
2:D:161:LEU:HD13	2:D:204:LEU:HB3	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:HB	1:A:96:HIS:HD2	1.34	0.92
2:C:308:GLY:HA2	2:C:309:ILE:CB	2.00	0.92
2:D:306:ASP:HB3	2:D:325:ARG:NH1	1.84	0.91
2:D:142:GLU:HG2	2:D:143:SER:H	1.36	0.91
2:D:149:ASN:ND2	2:D:153:PHE:CB	2.33	0.91
2:C:11:HIS:CE1	2:C:232:PRO:CG	2.53	0.91
1:B:758:TRP:HD1	2:D:287:SER:HG	1.16	0.91
2:C:96:TRP:NE1	2:C:99:LEU:HB2	1.85	0.90
1:A:719:THR:O	1:A:722:VAL:HG12	1.70	0.90
2:D:149:ASN:HA	2:D:153:PHE:CB	1.99	0.90
1:B:741:ARG:CZ	1:B:742:PHE:HZ	1.83	0.89
2:C:13:SER:HB2	2:C:232:PRO:HB2	1.53	0.89
2:D:149:ASN:ND2	2:D:153:PHE:CG	2.41	0.89
1:A:723:LEU:HD23	1:A:746:PHE:CD2	2.06	0.88
2:C:306:ASP:HA	2:C:325:ARG:HH11	1.38	0.88
1:A:3:PRO:CB	1:A:21:PHE:CE1	2.56	0.87
2:D:148:LYS:CB	2:D:152:ASP:HB2	2.02	0.87
1:A:708:LEU:HB2	2:C:355:PHE:CZ	2.10	0.87
2:D:148:LYS:CB	2:D:152:ASP:CB	2.51	0.87
2:D:153:PHE:HZ	2:D:198:ILE:HD12	1.37	0.87
1:A:25:ILE:CD1	1:A:827:PHE:HE1	1.85	0.87
2:C:335:LEU:O	2:C:336:ARG:HG2	1.74	0.87
2:D:12:THR:HG22	2:D:55:LEU:HD23	1.56	0.86
1:A:50:ASN:O	1:A:131:HIS:NE2	2.08	0.86
1:A:714:PHE:CG	2:C:355:PHE:HD1	1.92	0.86
1:A:78:ARG:HD3	1:A:127:LEU:HD22	1.55	0.86
1:A:714:PHE:CE1	2:C:355:PHE:CA	2.59	0.85
2:D:280:ILE:O	2:D:307:SER:HB3	1.76	0.85
2:D:280:ILE:N	2:D:307:SER:OG	2.09	0.85
1:A:706:LYS:HE3	1:A:706:LYS:HA	1.59	0.85
2:C:93:ASN:HB2	2:C:139:TYR:CB	2.03	0.85
1:A:714:PHE:CD2	2:C:355:PHE:HD1	1.94	0.84
2:C:11:HIS:ND1	2:C:232:PRO:HG3	1.92	0.84
2:D:148:LYS:O	2:D:152:ASP:HB2	1.77	0.84
1:B:758:TRP:CD1	2:D:287:SER:HG	1.95	0.84
2:D:11:HIS:CE1	2:D:213:ALA:HB1	2.13	0.84
2:D:12:THR:CG2	2:D:55:LEU:CD2	2.57	0.83
1:B:755:ILE:HD13	1:B:767:LEU:HD11	1.58	0.83
1:A:174:GLU:CG	1:A:709:PHE:CE1	2.56	0.83
2:D:14:ASP:OD2	2:D:57:GLY:CA	2.23	0.83
1:A:723:LEU:HD21	1:A:746:PHE:CD2	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:310:LEU:HD23	2:D:310:LEU:H	1.45	0.82
2:D:60:LEU:HD12	2:D:96:TRP:CZ2	2.14	0.82
1:A:708:LEU:HD23	1:A:708:LEU:O	1.80	0.81
1:A:708:LEU:HA	2:C:355:PHE:CE1	2.16	0.81
1:A:706:LYS:HE2	1:A:710:ASP:CG	2.06	0.81
2:D:96:TRP:CZ2	2:D:99:LEU:HD22	2.16	0.81
1:A:3:PRO:CB	1:A:21:PHE:CD1	2.63	0.81
2:C:13:SER:OG	2:C:232:PRO:HD2	1.81	0.80
1:B:151:SER:O	1:B:752:GLY:HA2	1.80	0.80
1:A:738:THR:HG22	1:A:741:ARG:HB3	1.62	0.80
1:B:758:TRP:HZ2	2:D:276:TYR:O	1.65	0.80
2:C:40:LYS:HZ2	2:C:268:SER:HG	1.30	0.80
2:D:148:LYS:O	2:D:152:ASP:CA	2.29	0.80
1:B:738:THR:HG22	1:B:741:ARG:HB3	1.62	0.79
2:C:11:HIS:ND1	2:C:232:PRO:CG	2.46	0.79
2:D:94:HIS:HB3	2:D:96:TRP:CZ3	2.18	0.79
2:D:141:ASP:O	2:D:142:GLU:HB3	1.83	0.79
1:A:3:PRO:O	1:A:21:PHE:HD1	1.66	0.78
1:B:758:TRP:CZ2	2:D:276:TYR:O	2.36	0.78
2:D:149:ASN:O	2:D:153:PHE:CB	2.30	0.78
1:A:708:LEU:C	1:A:708:LEU:CD2	2.54	0.78
1:A:719:THR:O	1:A:722:VAL:CG1	2.31	0.78
2:C:96:TRP:HZ3	2:D:97:LYS:HD3	1.47	0.78
2:C:340:GLU:O	2:C:341:GLU:CG	2.27	0.78
1:A:714:PHE:CG	2:C:355:PHE:CD1	2.71	0.78
2:C:63:ARG:HB2	2:C:94:HIS:O	1.83	0.78
2:D:148:LYS:O	2:D:153:PHE:N	2.17	0.78
2:D:148:LYS:C	2:D:152:ASP:HB2	2.09	0.78
1:A:722:VAL:O	1:A:726:VAL:CB	2.30	0.77
2:D:94:HIS:ND1	2:D:96:TRP:HZ3	1.83	0.77
1:A:49:GLY:HA2	1:A:87:ARG:NH2	2.00	0.77
1:B:26:THR:O	1:B:826:VAL:CA	2.31	0.77
1:A:704:LEU:HD22	2:C:372:ILE:CD1	2.13	0.77
2:C:337:GLU:C	2:C:339:PRO:HD3	2.09	0.77
1:B:758:TRP:HD1	2:D:287:SER:OG	1.66	0.76
2:C:338:SER:N	2:C:339:PRO:CD	2.47	0.76
2:D:54:LEU:HG	2:D:178:MSE:HE2	1.68	0.76
2:C:268:SER:N	2:C:269:PRO:CD	2.49	0.75
2:D:11:HIS:HB3	2:D:250:VAL:HG13	1.67	0.75
2:D:14:ASP:HB3	2:D:58:ASP:CA	2.17	0.75
1:A:29:GLU:O	1:A:843:ARG:HA	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:PHE:CZ	2:D:198:ILE:HD12	2.21	0.75
1:A:3:PRO:CB	1:A:21:PHE:HE1	1.98	0.74
1:A:714:PHE:HE1	2:C:355:PHE:HA	1.51	0.74
2:C:346:LEU:HD12	2:C:346:LEU:C	2.13	0.74
1:A:52:ILE:HD11	1:A:135:ILE:HD12	1.69	0.74
2:C:54:LEU:HG	2:C:178:MSE:HE2	1.67	0.74
2:C:311:PRO:O	2:C:313:LEU:HD12	1.88	0.73
2:D:12:THR:CG2	2:D:55:LEU:HD23	2.17	0.73
2:D:16:HIS:O	2:D:19:VAL:HG12	1.87	0.73
2:C:311:PRO:O	2:C:313:LEU:CD1	2.36	0.73
1:A:40:PHE:CZ	1:A:139:PHE:HB2	2.23	0.73
2:D:148:LYS:CD	2:D:152:ASP:CG	2.55	0.73
1:A:714:PHE:CD2	2:C:355:PHE:CD1	2.76	0.73
2:D:148:LYS:O	2:D:152:ASP:N	2.22	0.73
2:D:306:ASP:CA	2:D:325:ARG:HH11	2.02	0.73
1:B:704:LEU:HD22	2:D:372:ILE:HD11	1.71	0.72
1:B:762:ARG:NH1	2:D:283:SER:HA	2.01	0.72
2:C:14:ASP:OD1	2:C:57:GLY:HA3	1.90	0.72
2:D:14:ASP:CG	2:D:58:ASP:H	1.97	0.72
1:A:174:GLU:HG2	1:A:709:PHE:CZ	2.25	0.72
1:A:703:LEU:HD12	1:A:704:LEU:N	2.04	0.72
1:A:25:ILE:HD11	1:A:827:PHE:CD1	2.25	0.72
2:D:26:ARG:NH2	2:D:314:MSE:O	2.22	0.72
2:C:346:LEU:O	2:C:346:LEU:CD1	2.30	0.72
1:A:26:THR:HB	1:A:826:VAL:HG12	1.72	0.72
1:A:738:THR:HG21	1:A:742:PHE:HD2	1.55	0.72
2:C:116:VAL:HG11	2:C:136:PRO:HB3	1.71	0.72
2:D:16:HIS:CD2	2:D:238:ILE:HD11	2.24	0.71
2:D:92:GLY:O	2:D:94:HIS:HD2	1.70	0.71
2:D:134:ILE:HD12	2:D:178:MSE:HE3	1.72	0.71
2:D:306:ASP:CB	2:D:325:ARG:HH12	1.99	0.71
1:A:714:PHE:CZ	2:C:355:PHE:CB	2.71	0.71
2:C:93:ASN:CB	2:C:139:TYR:HB3	2.08	0.71
1:A:714:PHE:CD1	2:C:355:PHE:HD1	2.09	0.71
2:C:328:ARG:HH21	2:C:328:ARG:HG3	1.54	0.71
2:C:328:ARG:HH21	2:C:328:ARG:CG	2.04	0.70
2:C:8:LYS:HB3	2:C:251:PHE:HE1	1.57	0.70
1:B:140:LEU:HB3	1:B:145:ILE:HD11	1.71	0.70
2:D:14:ASP:CB	2:D:58:ASP:N	2.53	0.70
2:D:144:GLU:O	2:D:145:ALA:HB3	1.91	0.70
2:D:116:VAL:HG11	2:D:136:PRO:HB3	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:148:LYS:HD2	2:D:152:ASP:OD1	1.91	0.70
1:A:140:LEU:HB3	1:A:145:ILE:HD11	1.72	0.70
1:A:174:GLU:CA	1:A:709:PHE:HZ	2.00	0.70
1:A:789:GLY:HA2	2:C:346:LEU:HD11	1.73	0.70
1:A:3:PRO:O	1:A:21:PHE:CD1	2.45	0.70
1:B:26:THR:N	1:B:825:ILE:O	2.20	0.70
2:C:96:TRP:CD1	2:C:99:LEU:HB2	2.27	0.69
2:C:309:ILE:HG22	2:C:309:ILE:O	1.90	0.69
1:B:738:THR:CG2	1:B:742:PHE:HD2	1.95	0.69
2:D:148:LYS:HD2	2:D:152:ASP:OD2	1.91	0.69
2:D:8:LYS:HB3	2:D:251:PHE:HE1	1.58	0.69
2:D:14:ASP:HB3	2:D:58:ASP:H	1.56	0.69
2:D:153:PHE:HZ	2:D:198:ILE:CD1	2.05	0.69
2:D:311:PRO:O	2:D:313:LEU:HD13	1.93	0.69
2:C:134:ILE:HD12	2:C:178:MSE:HE3	1.73	0.69
1:A:708:LEU:HA	2:C:355:PHE:HE1	1.57	0.69
2:D:328:ARG:HH21	2:D:328:ARG:HG3	1.56	0.69
2:D:313:LEU:HD13	2:D:313:LEU:N	2.08	0.69
1:A:51:GLY:C	1:A:52:ILE:HG13	2.16	0.69
1:A:770:GLY:N	1:A:811:ILE:HD12	2.08	0.69
1:A:52:ILE:CD1	1:A:135:ILE:HD12	2.23	0.68
2:C:280:ILE:HB	2:C:310:LEU:HD21	1.75	0.68
2:D:14:ASP:CB	2:D:58:ASP:H	2.06	0.68
1:A:6:LEU:HG	1:A:43:ILE:HG12	1.74	0.68
2:C:360:LYS:HA	2:C:366:HIS:CB	2.23	0.68
2:D:328:ARG:HH21	2:D:328:ARG:CG	2.06	0.68
2:D:149:ASN:ND2	2:D:153:PHE:HB3	1.99	0.68
1:B:770:GLY:N	1:B:811:ILE:HD12	2.08	0.68
1:A:48:PHE:CG	1:A:131:HIS:HB2	2.28	0.68
2:D:14:ASP:HB3	2:D:58:ASP:C	2.18	0.68
2:D:63:ARG:HB3	2:D:94:HIS:ND1	2.09	0.67
2:D:235:LEU:O	2:D:269:PRO:HG3	1.95	0.67
2:D:313:LEU:O	2:D:317:ILE:N	2.27	0.67
2:C:63:ARG:HB3	2:C:95:ASP:HA	1.76	0.67
1:A:69:THR:HG22	1:A:90:ASN:HB2	1.77	0.67
1:A:714:PHE:CD1	2:C:355:PHE:CD1	2.82	0.67
1:A:100:LEU:HD22	1:A:112:ILE:HD12	1.75	0.67
1:A:184:LEU:HG	1:A:698:TYR:HB2	1.77	0.67
2:D:13:SER:OG	2:D:232:PRO:HD2	1.95	0.67
2:D:312:ASP:OD2	2:D:315:GLY:HA3	1.94	0.67
1:A:3:PRO:HB2	1:A:21:PHE:HD1	1.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:16:HIS:O	2:C:19:VAL:HG12	1.95	0.66
1:A:721:ARG:O	1:A:725:ALA:HB3	1.95	0.66
2:D:306:ASP:HB2	2:D:325:ARG:HH12	1.51	0.66
2:C:313:LEU:HD12	2:C:313:LEU:N	2.10	0.66
1:B:758:TRP:NE1	2:D:277:TYR:CZ	2.63	0.66
1:A:165:GLN:CD	2:C:352:PHE:HE2	2.03	0.66
1:A:721:ARG:HG3	2:C:354:LEU:CD1	2.23	0.66
2:C:63:ARG:HD2	2:C:94:HIS:HB3	1.78	0.66
1:A:714:PHE:CE2	2:C:355:PHE:HD1	2.14	0.66
2:D:78:LEU:O	2:D:82:MSE:HG3	1.96	0.66
2:D:306:ASP:OD1	2:D:306:ASP:O	2.13	0.65
1:A:176:LEU:HD21	2:C:379:GLU:HG2	1.78	0.65
1:B:100:LEU:HD22	1:B:112:ILE:HD12	1.78	0.65
2:C:12:THR:HG22	2:C:249:ALA:HB2	1.78	0.65
2:D:153:PHE:O	2:D:157:LEU:HG	1.97	0.65
2:D:148:LYS:HB3	2:D:152:ASP:CG	2.21	0.65
1:A:52:ILE:CG1	1:A:135:ILE:HD12	2.27	0.65
1:A:82:ARG:HG3	1:A:103:ILE:HB	1.79	0.65
2:C:104:ASN:HB2	2:C:117:MSE:HE1	1.78	0.65
2:C:340:GLU:OE1	2:C:341:GLU:N	2.30	0.65
2:D:148:LYS:CD	2:D:152:ASP:OD1	2.44	0.65
1:A:722:VAL:HA	1:A:726:VAL:HG23	1.80	0.64
2:C:10:LEU:HB2	2:C:50:VAL:HG11	1.79	0.64
2:C:340:GLU:C	2:C:341:GLU:HG2	2.21	0.64
2:C:10:LEU:HD13	2:C:10:LEU:C	2.22	0.64
2:C:360:LYS:HA	2:C:366:HIS:HB3	1.79	0.64
2:C:267:ALA:CB	2:C:269:PRO:HD3	2.27	0.64
2:C:306:ASP:CA	2:C:325:ARG:HH11	2.10	0.64
2:C:335:LEU:O	2:C:336:ARG:CG	2.46	0.64
2:D:12:THR:CG2	2:D:55:LEU:HD22	2.27	0.64
2:D:12:THR:HG21	2:D:55:LEU:CD2	2.26	0.64
2:C:336:ARG:HG3	2:C:337:GLU:N	2.13	0.64
1:A:723:LEU:HD21	1:A:746:PHE:CE2	2.33	0.63
2:C:355:PHE:CE2	2:C:359:LEU:HD21	2.33	0.63
2:D:92:GLY:O	2:D:93:ASN:OD1	2.16	0.63
1:A:30:GLY:H	1:A:36:LYS:HD3	1.63	0.63
1:B:762:ARG:NH2	2:D:283:SER:OG	2.31	0.63
2:C:63:ARG:CB	2:C:94:HIS:O	2.46	0.63
2:C:78:LEU:O	2:C:82:MSE:HG3	1.98	0.63
2:C:308:GLY:HA3	2:C:309:ILE:HB	1.76	0.63
1:A:744:ILE:HG22	1:A:755:ILE:HG13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:104:ASN:HB2	2:D:117:MSE:HE1	1.79	0.63
2:C:267:ALA:HB3	2:C:269:PRO:HD3	1.81	0.62
2:D:13:SER:HB2	2:D:232:PRO:CB	2.27	0.62
2:C:96:TRP:CZ3	2:D:97:LYS:HD3	2.31	0.62
2:D:144:GLU:HG3	2:D:148:LYS:HB2	1.80	0.62
1:A:89:ILE:HB	1:A:96:HIS:CD2	2.26	0.62
2:D:313:LEU:N	2:D:313:LEU:CD1	2.62	0.62
1:A:101:SER:HB2	1:A:109:LYS:HB3	1.82	0.62
2:C:105:PHE:HE2	2:D:106:VAL:HG11	1.65	0.62
2:D:149:ASN:HD22	2:D:149:ASN:C	2.06	0.61
1:A:137:THR:HG23	1:A:784:ALA:HB1	1.81	0.61
1:A:12:LEU:O	1:A:38:SER:HB3	2.00	0.61
2:D:152:ASP:O	2:D:156:PHE:CB	2.49	0.61
1:B:137:THR:HG23	1:B:784:ALA:HB1	1.81	0.61
2:C:307:SER:O	2:C:310:LEU:CD2	2.49	0.61
2:D:9:ILE:HB	2:D:252:VAL:HG13	1.81	0.61
2:C:26:ARG:NH2	2:C:314:MSE:O	2.33	0.61
1:A:738:THR:HG21	1:A:742:PHE:CD2	2.36	0.61
1:A:52:ILE:HG12	1:A:135:ILE:HD12	1.83	0.60
2:C:350:ASP:OD1	2:C:353:GLU:HB3	2.01	0.60
1:B:755:ILE:CD1	1:B:767:LEU:HD11	2.30	0.60
2:D:144:GLU:OE2	2:D:148:LYS:HB3	2.00	0.60
2:C:81:MSE:HB3	2:C:87:VAL:HG11	1.82	0.60
1:A:1:MSE:HG3	1:A:76:PHE:HB2	1.84	0.60
1:A:171:GLU:O	1:A:174:GLU:HB3	2.02	0.60
2:C:342:PHE:O	2:C:344:GLU:HG2	2.02	0.60
2:D:313:LEU:HD13	2:D:313:LEU:H	1.65	0.60
2:D:326:LYS:HG3	2:D:330:GLU:HB2	1.84	0.60
1:B:741:ARG:HG3	1:B:758:TRP:CE2	2.37	0.60
1:A:36:LYS:HD2	1:A:829:THR:O	2.01	0.60
1:A:727:LEU:HD13	1:A:745:ASP:HA	1.82	0.60
1:A:134:PHE:CZ	1:A:138:VAL:HG11	2.37	0.59
2:C:11:HIS:HB3	2:C:250:VAL:HG13	1.83	0.59
1:A:2:ARG:HG3	1:A:792:ASP:CB	2.33	0.59
1:B:758:TRP:CD1	2:D:277:TYR:HH	2.21	0.59
1:A:711:LYS:O	1:A:715:SER:HB3	2.01	0.59
1:A:48:PHE:CZ	1:A:131:HIS:HA	2.37	0.59
1:A:183:LYS:O	1:A:187:GLU:HG2	2.03	0.59
1:B:811:ILE:N	1:B:811:ILE:HD13	2.17	0.59
1:A:164:PHE:CG	1:A:718:PHE:HZ	2.21	0.58
1:A:811:ILE:HD13	1:A:811:ILE:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ARG:HG3	1:B:792:ASP:CB	2.33	0.58
2:C:40:LYS:NZ	2:C:268:SER:HG	1.90	0.58
2:D:144:GLU:O	2:D:145:ALA:CB	2.51	0.58
1:A:721:ARG:CG	2:C:354:LEU:HD11	2.29	0.58
1:B:760:ILE:HD11	2:D:291:PHE:HA	1.84	0.58
1:A:3:PRO:CB	1:A:21:PHE:HD1	2.12	0.58
1:A:45:PHE:CE1	1:A:49:GLY:O	2.56	0.58
1:A:704:LEU:HD22	2:C:372:ILE:HD12	1.85	0.58
2:D:81:MSE:HB3	2:D:87:VAL:HG11	1.84	0.58
2:C:181:PHE:CG	2:C:200:ILE:HD12	2.38	0.58
2:C:366:HIS:O	2:C:370:LEU:HD23	2.03	0.58
2:D:16:HIS:O	2:D:19:VAL:CG1	2.51	0.58
1:A:714:PHE:CE1	2:C:355:PHE:CB	2.87	0.58
2:C:313:LEU:CD1	2:C:313:LEU:H	2.16	0.58
2:C:211:TYR:HE2	2:C:213:ALA:HB2	1.68	0.58
1:A:145:ILE:HG22	1:A:776:SER:OG	2.04	0.57
1:A:722:VAL:CG2	1:A:726:VAL:CG2	2.70	0.57
1:A:741:ARG:HG3	1:A:758:TRP:CE2	2.38	0.57
1:B:2:ARG:HG3	1:B:792:ASP:HB3	1.86	0.57
2:D:12:THR:HG21	2:D:55:LEU:HD22	1.84	0.57
1:B:741:ARG:HD3	1:B:742:PHE:CD2	2.40	0.57
1:B:750:LYS:HD2	1:B:754:ILE:HD11	1.87	0.57
2:C:11:HIS:HE1	2:C:232:PRO:CG	2.13	0.57
2:D:280:ILE:HB	2:D:307:SER:HB2	1.87	0.57
1:A:714:PHE:CE2	2:C:355:PHE:CD1	2.92	0.57
2:C:102:PHE:CE2	2:C:106:VAL:HG21	2.40	0.57
2:D:369:LEU:O	2:D:372:ILE:HG13	2.03	0.57
1:A:773:ALA:HB1	1:A:815:LEU:HD21	1.86	0.57
1:B:756:LYS:HA	1:B:761:GLU:HA	1.86	0.57
1:B:773:ALA:HB1	1:B:815:LEU:HD21	1.87	0.57
2:C:346:LEU:C	2:C:346:LEU:CD1	2.76	0.57
1:B:1:MSE:HG3	1:B:76:PHE:HB2	1.85	0.57
1:A:723:LEU:O	1:A:727:LEU:HB2	2.04	0.56
2:D:304:GLU:HG3	2:D:305:GLU:H	1.70	0.56
1:A:755:ILE:HD13	1:A:767:LEU:HD11	1.87	0.56
2:C:313:LEU:O	2:C:317:ILE:N	2.34	0.56
2:D:310:LEU:HD23	2:D:310:LEU:N	2.17	0.56
1:A:2:ARG:HG3	1:A:792:ASP:HB3	1.88	0.56
2:D:54:LEU:HG	2:D:178:MSE:CE	2.36	0.56
2:D:211:TYR:HE2	2:D:213:ALA:HB2	1.71	0.56
2:D:306:ASP:HB3	2:D:325:ARG:HH11	1.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:PRO:HD3	1:A:845:THR:HG22	1.87	0.56
1:B:152:PRO:O	1:B:156:ILE:HG13	2.06	0.56
2:C:96:TRP:HZ3	2:D:97:LYS:CD	2.16	0.56
2:C:96:TRP:CZ3	2:D:97:LYS:CD	2.88	0.56
1:A:152:PRO:O	1:A:156:ILE:HG13	2.05	0.56
2:C:13:SER:HB2	2:C:233:GLY:N	2.21	0.56
2:C:181:PHE:CD2	2:C:200:ILE:HD12	2.40	0.56
2:D:372:ILE:O	2:D:376:LEU:HG	2.06	0.56
1:B:26:THR:O	1:B:827:PHE:N	2.38	0.56
1:A:756:LYS:HA	1:A:761:GLU:HA	1.87	0.56
2:C:11:HIS:NE2	2:C:213:ALA:HB1	2.21	0.55
2:C:335:LEU:O	2:C:336:ARG:CB	2.55	0.55
1:A:155:GLU:O	1:A:159:ILE:HG12	2.05	0.55
1:A:721:ARG:O	1:A:725:ALA:CB	2.54	0.55
1:A:7:THR:HB	1:A:73:VAL:HG22	1.89	0.55
2:C:55:LEU:HD12	2:C:89:VAL:HG22	1.88	0.55
2:C:313:LEU:HD12	2:C:313:LEU:H	1.69	0.55
1:A:163:VAL:HG13	1:A:164:PHE:CD1	2.41	0.55
1:A:722:VAL:O	1:A:726:VAL:N	2.39	0.55
1:B:736:ILE:HD13	1:B:821:LEU:HD23	1.89	0.55
1:A:148:LEU:O	1:A:148:LEU:HD23	2.07	0.55
2:C:54:LEU:HG	2:C:178:MSE:CE	2.36	0.55
2:C:215:GLY:O	2:C:216:HIS:HB3	2.07	0.55
2:D:207:SER:HA	2:D:227:PRO:HG3	1.89	0.55
1:A:711:LYS:HA	1:A:715:SER:HB3	1.87	0.55
2:D:55:LEU:HD12	2:D:89:VAL:HG22	1.89	0.55
1:A:49:GLY:HA2	1:A:87:ARG:HH22	1.71	0.54
2:C:16:HIS:CD2	2:C:238:ILE:HD11	2.42	0.54
2:C:357:GLU:HA	2:C:360:LYS:HG2	1.88	0.54
1:A:711:LYS:HA	1:A:715:SER:CB	2.37	0.54
2:C:158:GLU:HA	2:C:161:LEU:HD12	1.89	0.54
2:C:207:SER:HA	2:C:227:PRO:HG3	1.89	0.54
1:B:156:ILE:HD12	1:B:746:PHE:CE1	2.41	0.54
2:C:109:ILE:CD1	2:D:106:VAL:HG13	2.36	0.54
1:A:14:LEU:HD21	1:A:39:LEU:HD23	1.90	0.54
2:C:9:ILE:HB	2:C:252:VAL:HG13	1.89	0.54
2:D:181:PHE:CD2	2:D:200:ILE:HD12	2.43	0.54
1:B:734:LEU:HB3	1:B:742:PHE:O	2.08	0.54
2:D:328:ARG:CG	2:D:328:ARG:NH2	2.69	0.54
1:B:722:VAL:O	1:B:726:VAL:HB	2.08	0.54
2:D:181:PHE:CG	2:D:200:ILE:HD12	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:16:HIS:O	2:C:19:VAL:CG1	2.55	0.54
1:A:178:LYS:HA	1:A:181:MSE:HE2	1.89	0.54
1:A:708:LEU:CB	2:C:355:PHE:CZ	2.88	0.54
2:D:7:MSE:HE1	2:D:52:LEU:HB2	1.90	0.54
1:A:717:TYR:CD2	2:C:354:LEU:HD21	2.43	0.54
1:A:762:ARG:NH1	2:C:286:LYS:HD3	2.23	0.54
2:C:13:SER:CB	2:C:233:GLY:N	2.70	0.54
2:D:215:GLY:O	2:D:216:HIS:HB3	2.07	0.53
1:B:741:ARG:HG3	1:B:758:TRP:CZ2	2.43	0.53
2:D:94:HIS:ND1	2:D:96:TRP:CZ3	2.70	0.53
2:D:149:ASN:ND2	2:D:149:ASN:C	2.64	0.53
1:B:727:LEU:HD13	1:B:745:ASP:HA	1.90	0.53
1:B:762:ARG:HH22	2:D:283:SER:C	2.15	0.53
1:A:833:GLU:O	1:A:836:GLU:HG3	2.08	0.53
2:C:280:ILE:CB	2:C:310:LEU:HD21	2.37	0.53
2:C:307:SER:O	2:C:310:LEU:HD21	2.09	0.53
2:C:96:TRP:CD1	2:C:96:TRP:O	2.61	0.53
1:B:148:LEU:HD23	1:B:148:LEU:O	2.09	0.53
2:C:273:LYS:HG2	2:C:291:PHE:CZ	2.43	0.53
2:D:54:LEU:CG	2:D:178:MSE:HE2	2.39	0.53
2:C:102:PHE:CE2	2:C:106:VAL:CG2	2.92	0.53
2:C:128:ARG:HB2	2:C:130:GLN:HE22	1.73	0.53
2:D:313:LEU:HB2	2:D:320:LEU:HD23	1.90	0.53
1:A:31:PRO:HD2	1:A:845:THR:HA	1.91	0.53
1:A:49:GLY:CA	1:A:87:ARG:HH22	2.22	0.53
2:C:308:GLY:HA2	2:C:309:ILE:CG1	2.38	0.53
2:D:268:SER:N	2:D:269:PRO:CD	2.71	0.53
2:C:93:ASN:CB	2:C:139:TYR:CD2	2.91	0.52
1:A:102:GLU:O	1:A:102:GLU:HG3	2.09	0.52
1:B:1:MSE:CG	1:B:76:PHE:HB2	2.39	0.52
2:C:280:ILE:H	2:C:307:SER:CB	2.22	0.52
1:A:27:VAL:HG11	1:A:838:PHE:HB2	1.90	0.52
1:A:175:LYS:HA	1:A:178:LYS:NZ	2.25	0.52
2:C:12:THR:HG22	2:C:249:ALA:CB	2.40	0.52
2:D:11:HIS:CE1	2:D:213:ALA:CB	2.88	0.52
2:C:201:ASN:HB3	2:C:204:LEU:HG	1.91	0.52
1:A:714:PHE:CE1	2:C:355:PHE:HD1	2.27	0.52
1:A:714:PHE:HE2	2:C:351:TYR:CE1	2.28	0.52
1:B:156:ILE:HD13	1:B:753:PHE:CE2	2.45	0.52
2:D:156:PHE:O	2:D:160:ARG:HD3	2.09	0.52
1:A:717:TYR:CE2	2:C:354:LEU:HD21	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:LEU:HD21	2:C:265:ILE:HD12	1.92	0.52
1:A:714:PHE:CE1	2:C:355:PHE:CD1	2.98	0.52
2:C:11:HIS:O	2:C:249:ALA:HB1	2.10	0.52
2:C:46:GLU:HG2	2:C:84:THR:OG1	2.08	0.52
2:D:273:LYS:HG2	2:D:291:PHE:CZ	2.45	0.52
2:C:7:MSE:HE1	2:C:52:LEU:HB2	1.91	0.52
2:C:267:ALA:C	2:C:269:PRO:HD3	2.35	0.52
2:C:268:SER:N	2:C:269:PRO:HD3	2.23	0.52
1:A:12:LEU:HD11	1:A:53:ARG:NE	2.25	0.51
1:A:164:PHE:CB	1:A:718:PHE:HZ	2.23	0.51
2:D:98:GLY:O	2:D:101:LEU:HB2	2.10	0.51
1:A:131:HIS:O	1:A:135:ILE:HG12	2.10	0.51
2:C:13:SER:CB	2:C:232:PRO:HB2	2.33	0.51
2:D:301:VAL:CG2	2:D:323:ILE:HG12	2.40	0.51
2:D:46:GLU:HG2	2:D:84:THR:OG1	2.09	0.51
1:A:48:PHE:CD1	1:A:131:HIS:HB2	2.46	0.51
2:C:79:LYS:HG3	2:D:105:PHE:HE1	1.75	0.51
1:A:164:PHE:HB2	1:A:718:PHE:HZ	1.75	0.51
2:D:128:ARG:HB2	2:D:130:GLN:HE22	1.75	0.51
1:A:1:MSE:CG	1:A:76:PHE:HB2	2.40	0.51
1:A:3:PRO:O	1:A:21:PHE:HB2	2.10	0.51
1:A:108:LYS:HD2	1:A:109:LYS:O	2.10	0.51
2:D:16:HIS:CD2	2:D:238:ILE:CD1	2.94	0.51
1:A:184:LEU:CD1	1:A:698:TYR:HB2	2.41	0.51
2:D:201:ASN:HB3	2:D:204:LEU:HG	1.92	0.51
2:C:372:ILE:O	2:C:376:LEU:HG	2.11	0.51
2:D:223:ILE:HB	2:D:229:THR:HB	1.93	0.51
1:A:178:LYS:NZ	1:A:178:LYS:HB3	2.25	0.50
2:C:97:LYS:O	2:C:100:LYS:HG3	2.10	0.50
2:C:313:LEU:CD1	2:C:313:LEU:N	2.72	0.50
1:A:790:ARG:HG2	2:C:345:GLU:OE1	2.11	0.50
2:C:223:ILE:HB	2:C:229:THR:HB	1.92	0.50
1:B:738:THR:CG2	1:B:741:ARG:HB3	2.37	0.50
2:C:93:ASN:HB3	2:C:139:TYR:CD2	2.46	0.50
2:D:9:ILE:HB	2:D:252:VAL:CG1	2.40	0.50
2:D:152:ASP:O	2:D:156:PHE:HB3	2.12	0.50
2:D:280:ILE:O	2:D:307:SER:CB	2.54	0.50
1:A:730:THR:HG21	1:A:744:ILE:HD11	1.93	0.50
1:A:714:PHE:CZ	2:C:355:PHE:HD1	2.30	0.50
2:C:11:HIS:ND1	2:C:232:PRO:HG2	2.16	0.50
2:C:304:GLU:HG3	2:C:305:GLU:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:301:VAL:HG22	2:D:323:ILE:HG12	1.92	0.50
2:C:340:GLU:C	2:C:341:GLU:CG	2.82	0.50
1:B:758:TRP:CH2	2:D:276:TYR:N	2.78	0.50
2:C:153:PHE:CZ	2:C:198:ILE:HD12	2.47	0.50
2:C:268:SER:N	2:C:269:PRO:HD2	2.25	0.50
2:C:281:ASP:H	2:C:284:ALA:HB3	1.77	0.50
2:D:102:PHE:CE2	2:D:106:VAL:HG21	2.47	0.50
1:B:724:GLU:O	1:B:728:LYS:HB2	2.11	0.50
2:C:301:VAL:HG22	2:C:323:ILE:HG12	1.94	0.50
2:D:152:ASP:O	2:D:156:PHE:HB2	2.11	0.50
1:A:810:LYS:HE3	2:C:279:LYS:NZ	2.27	0.49
2:C:11:HIS:CE1	2:C:232:PRO:HG3	2.32	0.49
2:D:99:LEU:O	2:D:102:PHE:HB3	2.12	0.49
1:A:95:LYS:HB2	1:A:95:LYS:NZ	2.26	0.49
1:A:741:ARG:HG3	1:A:758:TRP:CZ2	2.47	0.49
1:B:156:ILE:CD1	1:B:746:PHE:CE1	2.95	0.49
2:C:19:VAL:HG23	2:C:61:HIS:CE1	2.46	0.49
2:D:281:ASP:H	2:D:284:ALA:HB3	1.75	0.49
1:A:25:ILE:HG23	1:A:25:ILE:O	2.12	0.49
2:C:54:LEU:CG	2:C:178:MSE:HE2	2.39	0.49
2:C:328:ARG:CG	2:C:328:ARG:NH2	2.68	0.49
2:D:148:LYS:HA	2:D:152:ASP:HB2	1.87	0.49
2:C:10:LEU:HD13	2:C:11:HIS:N	2.27	0.49
2:C:116:VAL:CG1	2:C:136:PRO:HB3	2.41	0.49
2:C:309:ILE:O	2:C:309:ILE:CG2	2.60	0.49
2:C:306:ASP:HA	2:C:325:ARG:NH1	2.18	0.49
2:D:148:LYS:C	2:D:152:ASP:CB	2.79	0.49
1:A:184:LEU:HB3	1:A:698:TYR:HD1	1.78	0.49
1:A:3:PRO:C	1:A:21:PHE:HD1	2.21	0.49
1:A:723:LEU:HD23	1:A:746:PHE:CG	2.48	0.49
1:B:1:MSE:HG2	1:B:2:ARG:N	2.27	0.49
1:A:167:LYS:NZ	1:A:167:LYS:HB3	2.27	0.49
2:C:13:SER:HB2	2:C:232:PRO:CB	2.36	0.49
1:A:1:MSE:HG2	1:A:2:ARG:N	2.28	0.48
1:A:723:LEU:HD23	1:A:746:PHE:HD2	1.74	0.48
1:A:35:GLY:O	1:A:39:LEU:HB2	2.13	0.48
2:C:301:VAL:CG2	2:C:323:ILE:HG12	2.42	0.48
2:C:307:SER:O	2:C:310:LEU:HG	2.13	0.48
1:A:100:LEU:HB2	1:A:119:VAL:HG13	1.94	0.48
1:A:738:THR:CG2	1:A:741:ARG:HB3	2.36	0.48
2:C:48:ARG:HD3	2:C:251:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:PHE:O	1:A:839:ASP:C	2.54	0.48
1:B:783:LEU:O	1:B:786:VAL:HG12	2.13	0.48
1:A:691:LEU:HA	1:A:694:MSE:HE2	1.95	0.48
2:C:235:LEU:O	2:C:269:PRO:HG3	2.13	0.48
1:B:745:ASP:O	1:B:754:ILE:HB	2.12	0.48
2:C:109:ILE:HD11	2:D:109:ILE:HD11	1.95	0.48
2:D:63:ARG:HD3	2:D:94:HIS:CE1	2.49	0.48
2:D:308:GLY:HA2	2:D:309:ILE:C	2.38	0.48
1:B:734:LEU:HD11	1:B:775:ILE:HA	1.96	0.48
2:C:7:MSE:CE	2:C:52:LEU:HB2	2.44	0.48
1:B:1:MSE:HG3	1:B:76:PHE:CD2	2.49	0.48
2:C:10:LEU:CD1	2:C:12:THR:HG23	2.44	0.48
2:D:144:GLU:OE2	2:D:152:ASP:CB	2.52	0.48
2:C:42:VAL:HG22	2:C:81:MSE:SE	2.64	0.47
2:D:15:TRP:O	2:D:16:HIS:HB2	2.13	0.47
2:D:258:GLU:HB3	2:D:259:PRO:HD2	1.96	0.47
1:A:137:THR:CG2	1:A:791:LEU:HD11	2.43	0.47
2:C:280:ILE:N	2:C:307:SER:OG	2.47	0.47
2:D:14:ASP:HB3	2:D:58:ASP:O	2.14	0.47
1:B:58:TYR:HA	1:B:89:ILE:HD11	1.95	0.47
2:C:10:LEU:C	2:C:10:LEU:CD1	2.87	0.47
2:D:7:MSE:CE	2:D:52:LEU:HB2	2.44	0.47
1:A:1:MSE:HG3	1:A:76:PHE:CD2	2.47	0.47
1:A:101:SER:HA	1:A:110:ALA:O	2.14	0.47
2:C:277:TYR:O	2:C:303:TYR:HA	2.13	0.47
2:D:102:PHE:CE2	2:D:106:VAL:CG2	2.98	0.47
2:D:277:TYR:O	2:D:303:TYR:HA	2.14	0.47
1:A:690:LYS:O	1:A:694:MSE:HG3	2.14	0.47
1:A:783:LEU:O	1:A:786:VAL:HG12	2.14	0.47
2:C:258:GLU:HB3	2:C:259:PRO:HD2	1.96	0.47
1:A:78:ARG:HD3	1:A:127:LEU:CD2	2.36	0.47
1:A:708:LEU:CA	2:C:355:PHE:CZ	2.98	0.47
1:B:71:ARG:CZ	1:B:86:ILE:HG21	2.45	0.47
2:D:19:VAL:HG23	2:D:61:HIS:CE1	2.50	0.47
1:A:734:LEU:HD11	1:A:775:ILE:HA	1.97	0.47
2:C:366:HIS:C	2:C:370:LEU:HD23	2.40	0.47
2:D:116:VAL:CG1	2:D:136:PRO:HB3	2.42	0.47
2:D:271:PRO:O	2:D:297:GLY:HA3	2.15	0.47
1:A:58:TYR:HA	1:A:89:ILE:HD11	1.95	0.47
1:A:102:GLU:HB3	1:A:112:ILE:HD11	1.97	0.47
2:D:313:LEU:HB3	2:D:317:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ILE:HD13	1:A:135:ILE:HG23	1.97	0.47
1:A:11:PHE:CE1	1:A:12:LEU:HD23	2.50	0.46
1:A:706:LYS:HE2	1:A:710:ASP:OD1	2.14	0.46
2:D:48:ARG:HD3	2:D:251:PHE:CE2	2.50	0.46
2:C:95:ASP:OD1	2:C:95:ASP:N	2.45	0.46
2:D:141:ASP:O	2:D:142:GLU:CB	2.58	0.46
2:D:148:LYS:HD3	2:D:152:ASP:OD1	2.14	0.46
1:A:714:PHE:CZ	2:C:355:PHE:CD1	3.03	0.46
1:B:736:ILE:O	1:B:820:ARG:NH2	2.49	0.46
2:C:102:PHE:C	2:C:102:PHE:CD2	2.92	0.46
2:D:206:PRO:HB2	2:D:209:VAL:HG13	1.97	0.46
1:A:174:GLU:CG	1:A:709:PHE:CZ	2.95	0.46
2:C:53:ILE:HG21	2:C:81:MSE:HG3	1.97	0.46
2:D:149:ASN:ND2	2:D:153:PHE:CD2	2.84	0.46
2:D:149:ASN:C	2:D:153:PHE:CB	2.87	0.46
1:A:122:GLU:O	1:A:126:ILE:HG13	2.15	0.46
1:A:184:LEU:CG	1:A:698:TYR:HB2	2.44	0.46
1:A:697:GLU:O	1:A:701:LEU:HG	2.16	0.46
2:C:206:PRO:HB2	2:C:209:VAL:HG13	1.97	0.46
2:C:248:GLY:HA3	2:C:265:ILE:O	2.16	0.46
2:C:355:PHE:O	2:C:359:LEU:HD13	2.15	0.46
1:B:762:ARG:HH22	2:D:283:SER:CA	2.28	0.46
1:B:141:PRO:HG2	1:B:144:GLU:HB2	1.98	0.46
2:C:240:PHE:C	2:C:242:GLU:H	2.24	0.46
2:C:337:GLU:C	2:C:339:PRO:CD	2.86	0.46
1:A:141:PRO:HG2	1:A:144:GLU:HB2	1.98	0.46
2:D:377:LEU:HD13	2:D:377:LEU:O	2.16	0.46
1:A:156:ILE:O	1:A:160:ILE:HG12	2.15	0.46
1:A:164:PHE:CZ	1:A:787:ALA:HB2	2.51	0.46
1:B:726:VAL:CG2	1:B:786:VAL:HG11	2.46	0.46
2:D:14:ASP:CG	2:D:58:ASP:N	2.68	0.46
2:D:77:TYR:O	2:D:81:MSE:HB2	2.16	0.46
1:A:779:LEU:HD23	1:A:779:LEU:O	2.16	0.45
1:B:779:LEU:HD23	1:B:779:LEU:O	2.16	0.45
2:C:215:GLY:O	2:C:216:HIS:CB	2.64	0.45
2:C:377:LEU:O	2:C:380:VAL:HG12	2.16	0.45
2:D:248:GLY:HA3	2:D:265:ILE:O	2.16	0.45
1:A:71:ARG:CZ	1:A:86:ILE:HG21	2.46	0.45
1:B:738:THR:CG2	1:B:742:PHE:CD2	2.83	0.45
2:C:77:TYR:O	2:C:81:MSE:HB2	2.17	0.45
2:D:240:PHE:C	2:D:242:GLU:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ARG:C	1:A:132:ARG:HD3	2.41	0.45
1:A:148:LEU:HD23	1:A:148:LEU:C	2.42	0.45
2:C:105:PHE:CE2	2:D:106:VAL:HG11	2.49	0.45
2:D:148:LYS:O	2:D:152:ASP:C	2.58	0.45
2:D:304:GLU:OE1	2:D:328:ARG:HD3	2.16	0.45
2:D:93:ASN:OD1	2:D:93:ASN:C	2.60	0.45
2:D:117:MSE:HE3	2:D:117:MSE:HB2	1.93	0.45
1:A:810:LYS:HE3	2:C:279:LYS:HZ1	1.82	0.45
2:D:149:ASN:CA	2:D:153:PHE:CB	2.74	0.45
1:A:730:THR:O	1:A:734:LEU:HD23	2.16	0.45
2:C:153:PHE:HZ	2:C:198:ILE:HD12	1.82	0.45
2:D:53:ILE:HB	2:D:87:VAL:HG12	1.99	0.45
1:A:3:PRO:CG	1:A:21:PHE:CD1	2.99	0.44
1:A:745:ASP:HB2	1:A:754:ILE:HD11	1.99	0.44
1:A:160:ILE:HG13	1:A:722:VAL:HG11	1.99	0.44
2:C:271:PRO:O	2:C:297:GLY:HA3	2.16	0.44
2:D:96:TRP:CE2	2:D:99:LEU:HD22	2.52	0.44
2:C:96:TRP:CD1	2:C:99:LEU:CB	2.99	0.44
2:D:102:PHE:C	2:D:102:PHE:CD2	2.93	0.44
1:A:748:ASP:O	1:A:749:GLU:C	2.60	0.44
1:B:730:THR:O	1:B:734:LEU:HD23	2.18	0.44
2:C:8:LYS:HB3	2:C:251:PHE:CE1	2.45	0.44
2:C:162:ASN:O	2:C:166:GLU:HG2	2.18	0.44
2:C:220:PHE:CG	2:C:264:ARG:NH1	2.86	0.44
1:A:78:ARG:HG3	1:A:127:LEU:HD13	2.00	0.44
2:C:109:ILE:HD12	2:D:106:VAL:HG13	1.99	0.44
2:D:12:THR:HG22	2:D:55:LEU:CD2	2.27	0.44
1:A:3:PRO:HG2	1:A:21:PHE:CD1	2.53	0.44
1:A:41:GLU:CD	1:A:53:ARG:HG3	2.43	0.44
1:A:55:PRO:HG2	1:A:56:ASN:H	1.83	0.44
1:A:714:PHE:HE1	2:C:355:PHE:CA	2.15	0.44
1:A:732:ALA:HB1	2:C:342:PHE:CD1	2.53	0.44
2:D:63:ARG:H	2:D:63:ARG:HG2	1.46	0.44
1:A:755:ILE:HG23	1:A:762:ARG:O	2.18	0.44
2:C:211:TYR:CE2	2:C:213:ALA:HB2	2.52	0.44
2:D:305:GLU:HA	2:D:305:GLU:OE1	2.17	0.43
1:A:769:GLY:HA3	1:A:811:ILE:HD11	2.00	0.43
2:D:60:LEU:HD11	2:D:71:LEU:HD23	2.00	0.43
2:D:267:ALA:O	2:D:268:SER:OG	2.30	0.43
2:D:303:TYR:O	2:D:325:ARG:HA	2.17	0.43
1:A:27:VAL:HG13	1:A:27:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:PHE:CD1	1:A:49:GLY:O	2.72	0.43
1:A:165:GLN:CD	2:C:352:PHE:CE2	2.90	0.43
1:A:184:LEU:HD21	1:A:694:MSE:HB3	2.00	0.43
1:A:708:LEU:CA	2:C:355:PHE:CE1	2.96	0.43
1:A:783:LEU:O	1:A:783:LEU:HD23	2.18	0.43
1:B:758:TRP:CH2	2:D:276:TYR:O	2.71	0.43
2:C:303:TYR:O	2:C:325:ARG:HA	2.19	0.43
2:D:280:ILE:H	2:D:307:SER:HG	1.64	0.43
1:A:90:ASN:HB3	1:A:93:GLN:HB2	2.00	0.43
1:B:755:ILE:HD11	1:B:775:ILE:HD13	2.01	0.43
2:C:267:ALA:O	2:C:268:SER:CB	2.66	0.43
2:C:96:TRP:CD1	2:C:96:TRP:C	2.97	0.43
2:C:345:GLU:OE1	2:C:345:GLU:HA	2.19	0.43
1:A:10:ASN:O	1:A:62:ASN:HB2	2.19	0.43
1:A:174:GLU:CA	1:A:709:PHE:CZ	2.86	0.43
1:A:783:LEU:HD23	1:A:783:LEU:C	2.43	0.43
1:A:828:ILE:HG22	1:A:828:ILE:O	2.18	0.43
2:C:10:LEU:CD2	2:C:265:ILE:HD12	2.48	0.43
2:C:371:LYS:HA	2:C:374:ASP:OD2	2.19	0.43
2:D:19:VAL:HB	2:D:61:HIS:CG	2.54	0.43
1:A:52:ILE:O	1:A:52:ILE:HG22	2.19	0.43
1:B:769:GLY:HA3	1:B:811:ILE:HD11	1.99	0.43
2:D:162:ASN:O	2:D:166:GLU:HG2	2.19	0.43
2:D:215:GLY:O	2:D:216:HIS:CB	2.64	0.43
2:D:275:LEU:HD11	2:D:291:PHE:CE2	2.53	0.43
1:A:108:LYS:HD2	1:A:109:LYS:N	2.34	0.43
1:A:797:ASP:HB3	1:A:828:ILE:HB	2.01	0.43
1:B:797:ASP:HB3	1:B:828:ILE:HB	2.00	0.43
2:C:128:ARG:HB2	2:C:130:GLN:NE2	2.32	0.43
2:D:275:LEU:HB2	2:D:301:VAL:HG12	2.01	0.43
2:D:328:ARG:HA	2:D:331:ILE:HG22	2.01	0.43
2:C:53:ILE:HB	2:C:87:VAL:HG12	2.00	0.43
2:C:76:ASP:C	2:C:76:ASP:OD1	2.62	0.42
2:D:207:SER:HA	2:D:227:PRO:CG	2.48	0.42
2:D:313:LEU:CB	2:D:320:LEU:HD23	2.48	0.42
1:B:148:LEU:HD23	1:B:148:LEU:C	2.43	0.42
2:C:51:ASP:OD1	2:C:128:ARG:HD3	2.18	0.42
1:A:153:PRO:HD3	1:A:751:GLY:O	2.18	0.42
1:A:754:ILE:HD12	1:A:754:ILE:O	2.19	0.42
2:D:94:HIS:CB	2:D:96:TRP:CZ3	2.97	0.42
2:D:220:PHE:CG	2:D:264:ARG:NH1	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:PRO:O	2:D:270:LEU:C	2.61	0.42
1:A:71:ARG:NH1	1:A:86:ILE:HD13	2.34	0.42
1:B:762:ARG:NH2	2:D:283:SER:O	2.50	0.42
2:D:51:ASP:OD1	2:D:128:ARG:HD3	2.19	0.42
2:D:312:ASP:CG	2:D:315:GLY:H	2.28	0.42
1:A:85:ILE:HG12	1:A:100:LEU:HA	2.02	0.42
2:C:63:ARG:HD2	2:C:94:HIS:CB	2.46	0.42
2:C:275:LEU:HB2	2:C:301:VAL:HG12	2.02	0.42
2:C:360:LYS:HA	2:C:366:HIS:HB2	1.98	0.42
2:D:53:ILE:HG21	2:D:81:MSE:HG3	2.02	0.42
2:D:371:LYS:HA	2:D:374:ASP:OD2	2.19	0.42
1:A:51:GLY:O	1:A:52:ILE:HG13	2.19	0.42
1:A:56:ASN:HB3	1:A:59:ASP:OD2	2.20	0.42
1:A:164:PHE:HB2	1:A:718:PHE:CZ	2.52	0.42
2:C:14:ASP:HB3	2:C:58:ASP:N	2.35	0.42
2:C:134:ILE:O	2:C:136:PRO:HD3	2.20	0.42
1:A:39:LEU:HD13	1:A:39:LEU:C	2.44	0.42
1:A:145:ILE:HG23	1:A:780:ALA:HB2	2.02	0.42
1:B:71:ARG:NH1	1:B:86:ILE:HD13	2.34	0.42
1:B:140:LEU:O	1:B:796:ILE:HA	2.19	0.42
1:B:156:ILE:CD1	1:B:753:PHE:CE2	3.02	0.42
2:D:8:LYS:HB3	2:D:251:PHE:CE1	2.46	0.42
1:A:721:ARG:O	1:A:725:ALA:N	2.51	0.42
1:B:793:ALA:HA	1:B:824:VAL:O	2.19	0.42
2:D:120:GLU:HA	2:D:121:PRO:HD3	1.82	0.42
2:D:149:ASN:ND2	2:D:153:PHE:HB2	2.29	0.42
1:A:12:LEU:HD13	1:A:54:TYR:HE2	1.84	0.42
2:D:63:ARG:O	2:D:96:TRP:HE3	2.03	0.42
1:A:7:THR:O	1:A:72:LEU:HA	2.20	0.41
1:A:78:ARG:CG	1:A:127:LEU:HD13	2.49	0.41
1:A:762:ARG:HG3	1:A:763:PRO:HD2	2.02	0.41
2:C:11:HIS:HD2	2:C:54:LEU:HB3	1.85	0.41
2:C:207:SER:HA	2:C:227:PRO:CG	2.49	0.41
1:A:6:LEU:HD13	1:A:6:LEU:O	2.20	0.41
1:A:8:VAL:HG11	1:A:14:LEU:HD22	2.02	0.41
1:A:176:LEU:HD21	2:C:379:GLU:CG	2.47	0.41
1:A:705:ARG:HG2	1:A:706:LYS:N	2.35	0.41
1:A:708:LEU:HD23	1:A:709:PHE:N	2.32	0.41
1:A:178:LYS:HB3	1:A:178:LYS:HZ3	1.84	0.41
1:B:758:TRP:NE1	2:D:277:TYR:HH	2.18	0.41
2:C:217:ILE:O	2:C:233:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:273:LYS:HG3	2:C:275:LEU:CD1	2.51	0.41
2:D:13:SER:CB	2:D:233:GLY:N	2.84	0.41
2:D:128:ARG:HB2	2:D:130:GLN:NE2	2.34	0.41
2:D:144:GLU:OE2	2:D:148:LYS:CB	2.69	0.41
2:D:259:PRO:HA	2:D:260:PRO:HD3	1.87	0.41
2:D:273:LYS:HG3	2:D:275:LEU:CD1	2.51	0.41
2:C:97:LYS:HA	2:C:100:LYS:HG3	2.03	0.41
1:A:78:ARG:CD	1:A:127:LEU:HD13	2.50	0.41
1:A:140:LEU:O	1:A:796:ILE:HA	2.20	0.41
2:C:11:HIS:HD2	2:C:54:LEU:CB	2.34	0.41
2:C:275:LEU:HD11	2:C:291:PHE:CE2	2.55	0.41
1:B:85:ILE:HD11	1:B:100:LEU:HG	2.02	0.41
1:B:804:ASP:OD1	1:B:807:ASN:HB2	2.21	0.41
2:C:280:ILE:CB	2:C:310:LEU:CD2	2.99	0.41
2:D:149:ASN:O	2:D:149:ASN:ND2	2.43	0.41
2:D:180:HIS:CE1	2:D:216:HIS:HB2	2.56	0.41
2:D:206:PRO:O	2:D:227:PRO:HG2	2.20	0.41
1:B:737:LEU:HD21	1:B:821:LEU:HG	2.03	0.41
2:C:60:LEU:HD11	2:C:71:LEU:HD23	2.03	0.41
2:C:366:HIS:O	2:C:367:GLU:C	2.64	0.41
2:C:13:SER:H	2:C:232:PRO:HB2	1.86	0.41
2:C:117:MSE:HE3	2:C:117:MSE:HB2	1.91	0.41
2:C:169:LEU:HD21	2:C:208:VAL:HG11	2.03	0.41
2:C:366:HIS:HB2	2:C:370:LEU:HD21	2.02	0.41
2:D:90:LEU:HD11	2:D:138:PRO:HB3	2.02	0.41
1:A:700:ASN:O	1:A:703:LEU:HG	2.20	0.41
1:A:706:LYS:HE3	1:A:706:LYS:CA	2.41	0.41
1:A:706:LYS:HE2	1:A:710:ASP:OD2	2.19	0.41
2:C:9:ILE:HB	2:C:252:VAL:CG1	2.50	0.41
2:C:220:PHE:HD1	2:C:231:TYR:O	2.04	0.41
2:C:228:LEU:HD21	2:C:262:TYR:CD2	2.56	0.41
2:D:19:VAL:HG23	2:D:61:HIS:NE2	2.36	0.41
2:C:90:LEU:HD11	2:C:138:PRO:HB3	2.02	0.41
2:C:206:PRO:O	2:C:227:PRO:HG2	2.21	0.41
1:A:41:GLU:OE2	1:A:52:ILE:N	2.43	0.40
1:A:95:LYS:NZ	1:A:95:LYS:CB	2.84	0.40
1:B:762:ARG:HG3	1:B:763:PRO:HD2	2.02	0.40
2:C:14:ASP:HB3	2:C:58:ASP:H	1.86	0.40
2:C:156:PHE:O	2:C:160:ARG:HD3	2.21	0.40
2:C:180:HIS:CE1	2:C:216:HIS:HB2	2.56	0.40
2:D:135:LEU:HD22	2:D:135:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:LEU:HD21	1:A:821:LEU:HG	2.04	0.40
2:C:11:HIS:HE1	2:C:232:PRO:HG2	1.71	0.40
2:D:186:LEU:C	2:D:188:GLY:H	2.29	0.40
1:A:714:PHE:HE2	2:C:351:TYR:CZ	2.39	0.40
2:C:14:ASP:OD1	2:C:14:ASP:N	2.55	0.40
2:C:105:PHE:HE2	2:D:106:VAL:CG1	2.32	0.40
1:A:85:ILE:HD11	1:A:100:LEU:HG	2.04	0.40
1:A:834:PHE:O	1:A:838:PHE:CE2	2.75	0.40
2:D:220:PHE:HD1	2:D:231:TYR:O	2.04	0.40
2:C:307:SER:O	2:C:310:LEU:CG	2.70	0.40
2:D:134:ILE:O	2:D:136:PRO:HD3	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	345/365 (94%)	314 (91%)	27 (8%)	4 (1%)	10	35
1	B	345/365 (94%)	315 (91%)	28 (8%)	2 (1%)	21	50
2	C	356/379 (94%)	330 (93%)	23 (6%)	3 (1%)	16	44
2	D	360/379 (95%)	330 (92%)	27 (8%)	3 (1%)	16	44
All	All	1406/1488 (94%)	1289 (92%)	105 (8%)	12 (1%)	14	42

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	268	SER
2	C	309	ILE
1	A	51	GLY
2	C	336	ARG

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Mol	Chain	Res	Type
2	D	145	ALA
1	A	52	ILE
1	B	55	PRO
2	D	140	PRO
2	D	142	GLU
1	A	55	PRO
1	A	150	ILE
1	B	150	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/307 (99%)	286 (94%)	17 (6%)	19	46
1	B	303/307 (99%)	289 (95%)	14 (5%)	24	50
2	C	331/335 (99%)	308 (93%)	23 (7%)	14	40
2	D	331/335 (99%)	315 (95%)	16 (5%)	23	50
All	All	1268/1284 (99%)	1198 (94%)	70 (6%)	19	46

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	6	LEU
1	A	12	LEU
1	A	50	ASN
1	A	73	VAL
1	A	95	LYS
1	A	102	GLU
1	A	127	LEU
1	A	150	ILE
1	A	167	LYS
1	A	178	LYS
1	A	706	LYS
1	A	708	LEU

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Mol	Chain	Res	Type
1	A	712	SER
1	A	750	LYS
1	A	755	ILE
1	A	811	ILE
1	B	1	MSE
1	B	6	LEU
1	B	12	LEU
1	B	73	VAL
1	B	95	LYS
1	B	102	GLU
1	B	127	LEU
1	B	150	ILE
1	B	167	LYS
1	B	177	LEU
1	B	178	LYS
1	B	706	LYS
1	B	754	ILE
1	B	811	ILE
2	C	10	LEU
2	C	13	SER
2	C	14	ASP
2	C	63	ARG
2	C	81	MSE
2	C	93	ASN
2	C	94	HIS
2	C	95	ASP
2	C	96	TRP
2	C	97	LYS
2	C	100	LYS
2	C	142	GLU
2	C	250	VAL
2	C	313	LEU
2	C	328	ARG
2	C	329	ARG
2	C	335	LEU
2	C	340	GLU
2	C	341	GLU
2	C	346	LEU
2	C	361	LYS
2	C	362	ARG
2	C	370	LEU
2	D	13	SER

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Mol	Chain	Res	Type
2	D	14	ASP
2	D	63	ARG
2	D	81	MSE
2	D	99	LEU
2	D	100	LYS
2	D	142	GLU
2	D	152	ASP
2	D	250	VAL
2	D	306	ASP
2	D	309	ILE
2	D	313	LEU
2	D	328	ARG
2	D	329	ARG
2	D	354	LEU
2	D	359	LEU

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	64	ASN
1	A	75	GLN
1	A	96	HIS
1	A	121	GLN
1	A	700	ASN
1	B	64	ASN
1	B	93	GLN
1	B	96	HIS
1	B	121	GLN
2	C	93	ASN
2	C	180	HIS
2	C	216	HIS
2	D	72	HIS
2	D	149	ASN
2	D	216	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	D	3968	-	5,5,5	0.41	0	5,5,5	0.24	0
3	GOL	A	3968	-	5,5,5	0.40	0	5,5,5	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	3968	-	-	2/4/4/4	-
3	GOL	A	3968	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3968	GOL	O1-C1-C2-C3
3	D	3968	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	3968	GOL	O1-C1-C2-O2
3	D	3968	GOL	O1-C1-C2-O2

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	345/365 (94%)	0.85	64 (18%) 3 4	28, 79, 185, 328	75 (21%)
1	B	318/365 (87%)	3.75	219 (68%) 0 0	3, 54, 187, 391	277 (87%)
2	C	354/379 (93%)	0.78	46 (12%) 7 8	27, 80, 164, 279	85 (24%)
2	D	355/379 (93%)	1.04	70 (19%) 3 4	21, 78, 186, 363	81 (22%)
All	All	1372/1488 (92%)	1.55	399 (29%) 1 2	3, 76, 184, 391	518 (37%)

All (399) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	55	PRO	14.7
1	B	129	ILE	14.6
1	B	83	TYR	13.8
1	B	704	LEU	13.4
1	B	699	ASN	12.9
1	B	719	THR	12.7
1	B	43	ILE	12.2
1	B	106	ASN	11.6
1	B	74	PHE	11.5
1	B	19	ILE	10.6
1	B	162	ASP	10.5
2	D	335	LEU	10.4
1	B	845	THR	10.3
1	B	804	ASP	10.3
2	D	351	TYR	10.1
1	B	102	GLU	10.1
1	B	49	GLY	9.9
1	B	127	LEU	9.9
1	B	848	VAL	9.7
1	B	702	ASP	9.5
1	B	753	PHE	9.4

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Mol	Chain	Res	Type	RSRZ
1	B	175	LYS	9.3
1	B	714	PHE	8.8
1	B	722	VAL	8.8
2	D	347	ASP	8.8
1	B	120	LYS	8.7
1	B	136	ARG	8.6
1	B	58	TYR	8.5
2	C	307	SER	8.3
1	B	138	VAL	8.3
1	B	22	GLN	8.1
1	B	103	ILE	8.1
1	B	746	PHE	8.0
1	B	139	PHE	7.9
2	C	342	PHE	7.7
1	B	748	ASP	7.6
1	B	707	TYR	7.5
1	B	108	LYS	7.5
1	B	834	PHE	7.4
1	B	69	THR	7.4
1	B	57	SER	7.3
1	B	21	PHE	7.3
1	B	128	GLY	7.2
1	B	97	ASN	7.1
2	C	153	PHE	7.0
1	B	54	TYR	6.9
1	B	92	LEU	6.8
1	B	820	ARG	6.8
1	A	723	LEU	6.7
1	B	806	GLU	6.7
1	B	16	ASN	6.7
1	B	799	GLY	6.6
1	B	78	ARG	6.6
1	B	165	GLN	6.6
1	B	173	LEU	6.5
1	B	723	LEU	6.5
2	C	101	LEU	6.4
1	B	844	ILE	6.4
1	B	800	PHE	6.4
1	B	752	GLY	6.3
1	B	718	PHE	6.3
1	B	708	LEU	6.2
1	B	836	GLU	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	788	SER	6.1
1	B	38	SER	6.1
1	B	99	LYS	6.1
1	B	787	ALA	6.1
1	B	715	SER	6.1
1	B	135	ILE	6.1
1	B	749	GLU	6.0
1	B	60	TYR	5.9
1	B	47	LEU	5.9
1	B	695	SER	5.8
1	B	798	GLU	5.7
1	B	9	ARG	5.7
1	B	703	LEU	5.7
1	B	160	ILE	5.7
2	D	345	GLU	5.6
1	A	699	ASN	5.6
1	B	124	GLU	5.6
1	B	130	GLU	5.5
1	B	59	ASP	5.5
1	B	6	LEU	5.4
2	D	373	LEU	5.4
1	B	691	LEU	5.4
1	B	161	SER	5.4
2	D	355	PHE	5.4
1	B	53	ARG	5.3
1	B	716	ARG	5.3
2	C	154	ARG	5.3
1	B	114	ALA	5.3
1	A	722	VAL	5.2
2	D	344	GLU	5.2
1	B	20	GLU	5.1
2	D	370	LEU	5.1
2	C	94	HIS	5.1
1	B	25	ILE	5.1
1	B	163	VAL	5.1
1	B	750	LYS	5.1
1	B	42	ALA	5.1
1	B	179	GLU	5.0
1	B	24	GLY	5.0
1	B	837	ALA	5.0
1	B	14	LEU	5.0
1	A	804	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
2	C	344	GLU	4.9
2	D	362	ARG	4.9
2	D	152	ASP	4.9
1	B	187	GLU	4.8
1	B	50	ASN	4.8
2	D	308	GLY	4.8
2	C	216	HIS	4.8
1	B	833	GLU	4.8
1	A	709	PHE	4.7
1	B	91	ALA	4.7
1	B	64	ASN	4.7
1	B	174	GLU	4.7
1	A	803	LEU	4.7
1	B	26	THR	4.6
1	B	773	ALA	4.6
2	D	348	LYS	4.6
2	D	357	GLU	4.6
1	B	747	ASP	4.6
1	B	44	SER	4.6
2	D	371	LYS	4.5
1	B	801	SER	4.5
1	B	182	LYS	4.5
1	B	5	ARG	4.5
1	B	88	GLU	4.4
1	B	51	GLY	4.4
1	A	759	GLY	4.3
2	D	97	LYS	4.3
1	B	177	LEU	4.3
1	B	100	LEU	4.3
1	B	744	ILE	4.3
1	B	185	GLU	4.3
1	B	61	VAL	4.3
1	B	11	PHE	4.2
2	D	369	LEU	4.2
1	B	95	LYS	4.2
1	A	23	SER	4.2
1	B	15	LYS	4.2
1	B	40	PHE	4.2
1	A	707	TYR	4.2
2	D	349	LEU	4.2
2	D	153	PHE	4.2
1	B	149	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	90	ASN	4.1
1	B	170	LEU	4.1
2	D	331	ILE	4.1
1	B	76	PHE	4.1
2	D	148	LYS	4.1
1	B	184	LEU	4.1
2	D	326	LYS	4.1
2	D	149	ASN	4.1
2	D	367	GLU	4.1
2	D	378	ASP	4.0
1	A	805	THR	4.0
1	A	67	ASP	4.0
1	B	133	THR	4.0
1	B	125	LYS	4.0
1	B	838	PHE	4.0
1	B	65	ALA	4.0
1	B	70	ALA	4.0
1	B	117	THR	4.0
2	D	327	SER	4.0
1	B	726	VAL	3.9
2	D	352	PHE	3.8
1	B	94	ARG	3.8
1	B	721	ARG	3.8
1	B	697	GLU	3.8
1	A	64	ASN	3.8
1	B	849	VAL	3.8
1	B	52	ILE	3.8
1	B	808	LYS	3.7
1	B	56	ASN	3.7
1	B	778	SER	3.7
1	B	67	ASP	3.7
1	A	713	ASN	3.7
1	B	832	ARG	3.7
2	D	96	TRP	3.7
1	A	714	PHE	3.7
2	C	352	PHE	3.6
1	B	66	VAL	3.6
1	B	846	GLY	3.6
2	D	13	SER	3.6
1	B	831	ASP	3.6
2	D	101	LEU	3.6
1	B	755	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	131	HIS	3.5
1	A	833	GLU	3.5
1	B	689	LYS	3.5
2	D	278	LYS	3.5
1	B	31	PRO	3.5
1	A	92	LEU	3.4
2	C	58	ASP	3.4
1	A	690	LYS	3.4
1	B	36	LYS	3.4
1	B	720	GLY	3.4
1	A	749	GLU	3.4
2	C	359	LEU	3.4
2	C	198	ILE	3.4
2	C	95	ASP	3.4
2	D	189	TYR	3.4
1	B	176	LEU	3.3
1	B	30	GLY	3.3
1	B	119	VAL	3.3
1	A	835	SER	3.3
1	B	121	GLN	3.3
1	A	43	ILE	3.3
1	B	793	ALA	3.3
1	A	35	GLY	3.3
1	B	93	GLN	3.2
1	B	32	ASN	3.2
1	B	178	LYS	3.2
2	D	99	LEU	3.2
1	B	805	THR	3.2
1	A	808	LYS	3.2
1	B	717	TYR	3.2
1	A	44	SER	3.1
1	A	86	ILE	3.1
1	B	2	ARG	3.1
2	D	332	GLU	3.1
1	B	156	ILE	3.1
2	C	92	GLY	3.1
2	C	222	GLU	3.1
2	D	305	GLU	3.1
1	A	127	LEU	3.0
2	C	63	ARG	3.0
1	B	733	TYR	3.0
2	C	180	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	365	ASN	3.0
1	B	37	SER	3.0
2	C	138	PRO	3.0
2	D	218	HIS	3.0
1	A	48	PHE	3.0
1	B	840	ARG	3.0
1	B	710	ASP	3.0
1	B	751	GLY	3.0
1	B	116	PRO	3.0
1	B	27	VAL	3.0
2	D	334	VAL	3.0
1	B	705	ARG	2.9
2	C	329	ARG	2.9
2	D	144	GLU	2.9
1	A	34	ALA	2.9
2	D	14	ASP	2.9
2	D	328	ARG	2.9
1	A	717	TYR	2.9
2	D	108	SER	2.9
1	B	105	GLU	2.9
2	C	206	PRO	2.9
1	A	174	GLU	2.8
2	C	174	PHE	2.8
1	B	782	SER	2.8
1	B	780	ALA	2.8
1	A	831	ASP	2.8
1	B	786	VAL	2.8
1	B	690	LYS	2.8
1	A	37	SER	2.8
1	B	85	ILE	2.8
2	D	110	SER	2.8
1	B	41	GLU	2.8
1	A	77	GLU	2.8
1	B	825	ILE	2.8
2	C	156	PHE	2.7
1	B	118	SER	2.7
2	C	150	GLU	2.7
2	D	105	PHE	2.7
2	D	279	LYS	2.7
2	D	139	TYR	2.7
2	D	358	TYR	2.7
1	A	32	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	204	LEU	2.7
1	B	62	ASN	2.7
1	B	709	PHE	2.7
2	C	100	LYS	2.7
2	D	143	SER	2.7
1	B	821	LEU	2.7
1	A	701	LEU	2.6
1	B	71	ARG	2.6
1	A	39	LEU	2.6
1	B	774	LEU	2.6
2	C	13	SER	2.6
2	C	112	ASP	2.6
2	C	349	LEU	2.6
1	B	843	ARG	2.6
1	B	35	GLY	2.6
2	D	197	GLU	2.6
1	B	784	ALA	2.6
2	D	356	LYS	2.6
1	B	183	LYS	2.5
2	C	309	ILE	2.5
2	D	145	ALA	2.5
2	C	355	PHE	2.5
1	A	185	GLU	2.5
1	B	692	LYS	2.5
1	A	47	LEU	2.5
1	B	81	LYS	2.4
2	D	293	ARG	2.4
1	B	80	GLY	2.4
1	B	126	ILE	2.4
1	A	836	GLU	2.4
2	D	94	HIS	2.4
2	D	366	HIS	2.4
1	A	750	LYS	2.4
2	C	362	ARG	2.4
2	D	100	LYS	2.4
1	A	702	ASP	2.4
1	A	740	GLY	2.3
2	D	255	LYS	2.3
2	C	137	PHE	2.3
1	A	66	VAL	2.3
1	B	28	VAL	2.3
1	A	744	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	336	ARG	2.3
1	A	822	ASN	2.3
1	A	710	ASP	2.3
1	A	697	GLU	2.3
1	B	4	GLU	2.3
2	D	166	GLU	2.3
1	A	109	LYS	2.3
1	B	172	LYS	2.3
2	C	196	ARG	2.3
1	B	758	TRP	2.3
2	C	57	GLY	2.3
1	B	137	THR	2.3
1	B	819	GLU	2.3
1	B	712	SER	2.3
2	D	93	ASN	2.3
1	A	22	GLN	2.3
1	B	3	PRO	2.3
1	A	799	GLY	2.3
1	B	167	LYS	2.3
1	B	159	ILE	2.2
1	A	695	SER	2.2
2	C	268	SER	2.2
1	A	40	PHE	2.2
1	B	730	THR	2.2
1	A	807	ASN	2.2
1	B	754	ILE	2.2
1	B	8	VAL	2.2
1	B	742	PHE	2.2
1	B	96	HIS	2.2
2	D	216	HIS	2.2
1	A	93	GLN	2.2
1	A	776	SER	2.2
1	B	155	GLU	2.2
1	B	171	GLU	2.2
2	C	172	GLU	2.2
2	C	363	GLU	2.2
1	B	810	LYS	2.2
2	C	368	LYS	2.2
2	D	163	LYS	2.2
2	D	360	LYS	2.2
2	D	368	LYS	2.2
1	A	721	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	795	PHE	2.2
2	C	102	PHE	2.2
2	D	28	VAL	2.1
1	B	34	ALA	2.1
1	B	812	ALA	2.1
2	C	339	PRO	2.1
1	A	718	PHE	2.1
1	B	89	ILE	2.1
1	A	184	LEU	2.1
1	B	180	LYS	2.1
2	D	354	LEU	2.1
1	A	762	ARG	2.1
1	A	49	GLY	2.1
2	C	364	GLU	2.1
2	C	8	LYS	2.1
2	C	182	THR	2.1
2	C	254	LEU	2.1
1	B	764	ALA	2.1
1	B	696	ASP	2.1
1	A	165	GLN	2.1
1	B	68	GLY	2.1
2	D	174	PHE	2.1
1	B	109	LYS	2.1
1	B	816	LYS	2.1
1	B	63	ARG	2.1
2	D	196	ARG	2.1
1	A	761	GLU	2.1
1	B	134	PHE	2.1
1	B	794	PHE	2.1
2	D	379	GLU	2.1
1	B	166	SER	2.0
1	B	82	ARG	2.0
2	D	289	ARG	2.0
1	B	850	VAL	2.0
2	C	310	LEU	2.0
2	D	309	ILE	2.0
1	B	797	ASP	2.0
1	A	33	GLY	2.0
1	A	834	PHE	2.0
2	D	103	GLY	2.0
1	A	31	PRO	2.0
2	C	125	GLU	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	3968	6/6	0.90	0.21	56,83,86,86	0
3	GOL	A	3968	6/6	0.96	0.10	53,55,58,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.