



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 03:42 pm BST

PDB ID : 1SR6  
Title : Structure of nucleotide-free scallop myosin S1  
Authors : Risal, D.; Gourinath, S.; Himmel, D.M.; Szent-Gyorgyi, A.G.; Cohen, C.  
Deposited on : 2004-03-22  
Resolution : 2.75 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

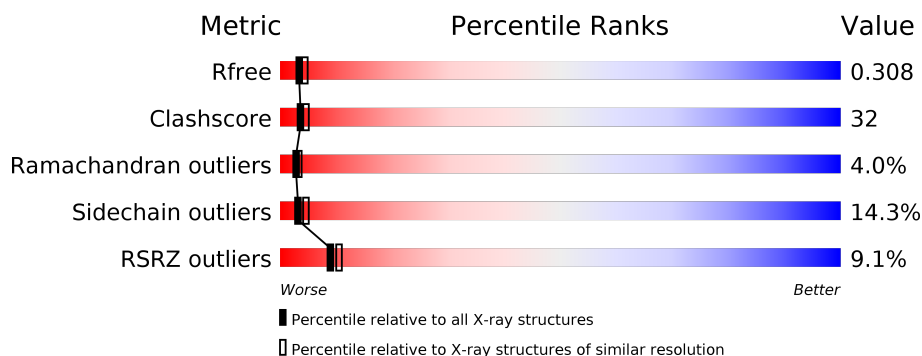
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	840	<div> <div>5%</div> <div> <div>51%</div> <div>35%</div> <div>9%</div> <div>5%</div> </div> </div>
2	B	156	<div> <div>33%</div> <div> <div>30%</div> <div>47%</div> <div>13%</div> <div>8%</div> </div> </div>
3	C	156	<div> <div>5%</div> <div> <div>58%</div> <div>36%</div> <div>5%</div> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8895 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 Myosin heavy chain, striated muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	S	0	0	0
			6419	4087	1104	1190	38			

- Molecule 2 is a protein called Myosin regulatory light chain, striated adductor muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	144	Total	C	N	O	S	0	0	0
			1145	720	182	234	9			

- Molecule 3 is a protein called Myosin essential light chain, striated adductor muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	155	Total	C	N	O	S	0	0	0
			1229	778	195	249	7			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Ca 1 1	0	0

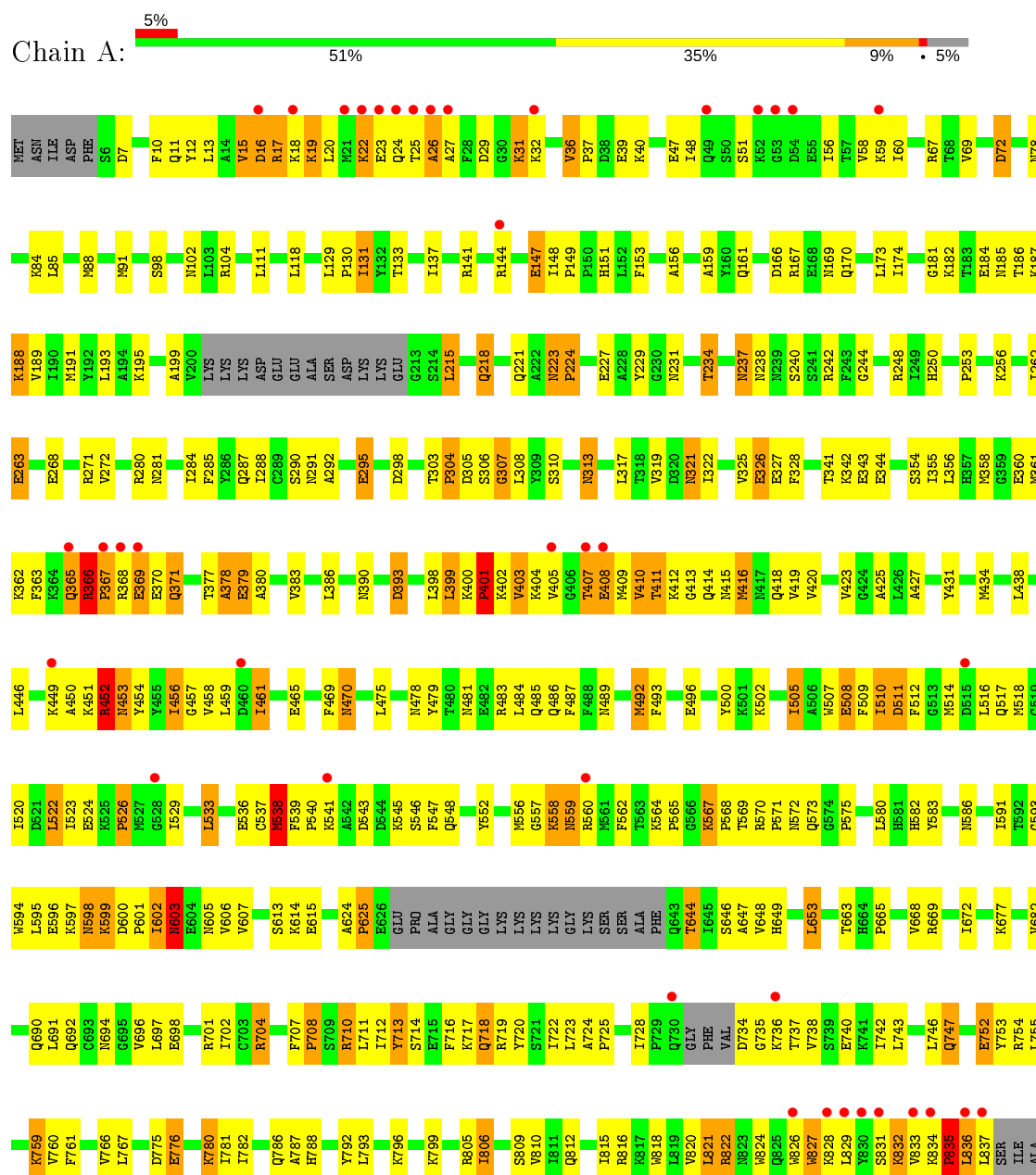
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	81	Total O 81 81	0	0
7	B	6	Total O 6 6	0	0
7	C	8	Total O 8 8	0	0

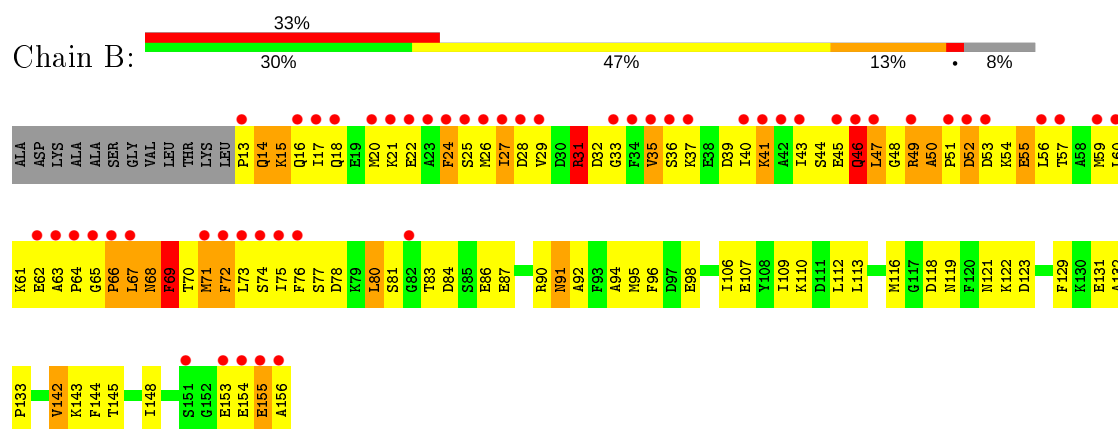
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

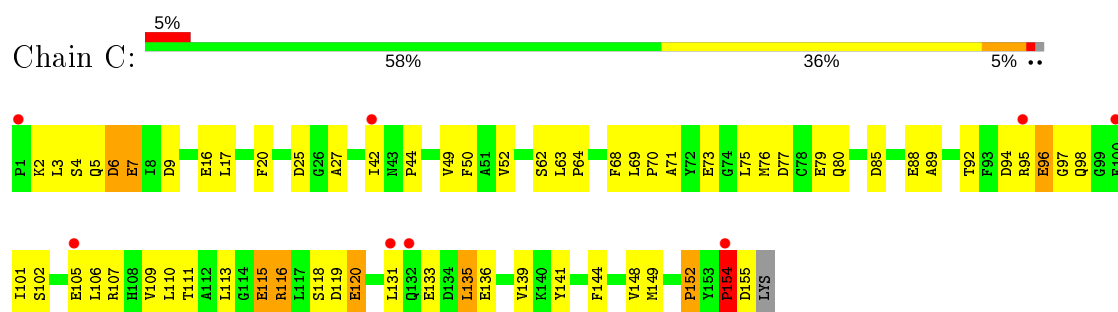
- Molecule 1: Myosin heavy chain, striated muscle



- Molecule 2: Myosin regulatory light chain, striated adductor muscle



- Molecule 3: Myosin essential light chain, striated adductor muscle



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.59Å 51.11Å 162.33Å 90.00° 98.02° 90.00°	Depositor
Resolution (Å)	38.79 – 2.75 48.15 – 2.74	Depositor EDS
% Data completeness (in resolution range)	83.0 (38.79-2.75) 82.5 (48.15-2.74)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.74 (at 2.73Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.242 , 0.286 0.255 , 0.308	Depositor DCC
$R_{free}$ test set	1578 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.6	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 60.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8895	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CA, SO4

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	0.54	0/6548	0.65	3/8824 (0.0%)
2	B	0.55	0/1162	0.83	2/1551 (0.1%)
3	C	0.55	0/1254	0.64	0/1688
All	All	0.54	0/8964	0.67	5/12063 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	835	PRO	N-CA-C	6.66	129.42	112.10
1	A	366	ARG	N-CA-C	5.41	125.60	111.00
1	A	27	ALA	N-CA-C	-5.25	96.81	111.00
2	B	78	ASP	N-CA-C	5.23	125.13	111.00
2	B	24	PHE	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	6419	0	6423	374	10
2	B	1145	0	1115	151	0
3	C	1229	0	1158	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	1	0
5	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	81	0	0	17	0
7	B	6	0	0	0	0
7	C	8	0	0	0	0
All	All	8895	0	8696	552	10

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 32.

All (552) 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)
2:B:49:ARG:CZ	2:B:50:ALA:HA	1.68	1.21
2:B:21:LYS:HB2	2:B:69:PHE:CZ	1.82	1.15
1:A:215:LEU:H	1:A:215:LEU:HD22	1.11	1.08
2:B:49:ARG:NH2	2:B:50:ALA:HA	1.68	1.07
2:B:49:ARG:HH21	2:B:51:PRO:HD2	1.21	1.06
1:A:792:TYR:CD2	3:C:152:PRO:HD3	1.95	1.01
2:B:48:GLY:O	2:B:49:ARG:HG3	1.61	1.00
1:A:48:ILE:HA	1:A:58:VAL:HG12	1.45	0.98
2:B:69:PHE:O	2:B:69:PHE:CD1	2.18	0.96
1:A:321:ASN:H	1:A:321:ASN:HD22	1.11	0.96
1:A:341:THR:HB	1:A:344:GLU:HG3	1.47	0.96
2:B:24:PHE:CG	2:B:69:PHE:HB2	2.02	0.95
2:B:52:ASP:O	2:B:55:GLU:OE2	1.84	0.95
1:A:17:ARG:H	1:A:17:ARG:HD3	1.33	0.94
2:B:51:PRO:HB2	2:B:55:GLU:CG	1.98	0.93
3:C:52:VAL:HG21	3:C:75:LEU:HD21	1.48	0.93
2:B:49:ARG:C	2:B:49:ARG:NE	2.23	0.91
2:B:44:SER:HB3	2:B:49:ARG:NH2	1.85	0.91
2:B:49:ARG:CZ	2:B:50:ALA:CA	2.50	0.90
1:A:470:ASN:N	1:A:470:ASN:HD22	1.71	0.88
2:B:21:LYS:HB2	2:B:69:PHE:CE2	2.09	0.88
1:A:407:THR:O	1:A:408:GLU:HG2	1.73	0.87
1:A:407:THR:O	1:A:407:THR:HG22	1.73	0.86
2:B:67:LEU:O	2:B:68:ASN:HB3	1.75	0.86
1:A:792:TYR:CE2	3:C:152:PRO:HD3	2.10	0.85
2:B:44:SER:HB3	2:B:49:ARG:CZ	2.07	0.85
1:A:822:ARG:HB3	1:A:822:ARG:HH11	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:LEU:HD21	1:A:461:ILE:HD11	1.59	0.84
1:A:569:THR:HG22	1:A:570:ARG:HG2	1.58	0.84
2:B:51:PRO:CB	2:B:55:GLU:HG3	2.07	0.83
2:B:49:ARG:NH2	2:B:51:PRO:HD2	1.91	0.83
1:A:215:LEU:H	1:A:215:LEU:CD2	1.89	0.83
1:A:837:LEU:O	1:A:837:LEU:HD23	1.79	0.82
1:A:365:GLN:O	1:A:367:PRO:HD3	1.80	0.81
1:A:836:LEU:H	1:A:836:LEU:HD23	1.45	0.81
1:A:321:ASN:H	1:A:321:ASN:ND2	1.78	0.81
2:B:51:PRO:HB2	2:B:55:GLU:OE1	1.79	0.80
1:A:564:LYS:HG3	1:A:565:PRO:HD2	1.63	0.80
1:A:708:PRO:O	1:A:710:ARG:HD3	1.81	0.80
2:B:51:PRO:HB2	2:B:55:GLU:HG3	1.65	0.79
1:A:321:ASN:HD22	1:A:321:ASN:N	1.75	0.79
1:A:17:ARG:HD3	1:A:17:ARG:N	1.97	0.78
1:A:410:VAL:HG12	1:A:411:THR:H	1.48	0.77
1:A:694:ASN:HD22	1:A:696:VAL:HG13	1.49	0.77
1:A:400:LYS:HG3	1:A:412:LYS:O	1.85	0.77
1:A:723:LEU:HD13	1:A:746:LEU:HD11	1.66	0.76
2:B:49:ARG:O	2:B:49:ARG:NE	2.17	0.76
1:A:380:ALA:N	7:A:1000:HOH:O	2.18	0.75
1:A:390:ASN:HB3	1:A:393:ASP:HB2	1.67	0.75
1:A:728:ILE:HD12	1:A:738:VAL:HG13	1.67	0.75
1:A:818:TRP:HB2	2:B:148:ILE:HG23	1.69	0.75
2:B:48:GLY:O	2:B:49:ARG:CG	2.35	0.75
1:A:319:VAL:HB	1:A:322:ILE:HB	1.69	0.74
2:B:44:SER:CB	2:B:49:ARG:CZ	2.63	0.74
1:A:415:ASN:H	1:A:418:GLN:HB2	1.51	0.74
1:A:831:SER:HA	1:A:834:LYS:HG2	1.70	0.74
2:B:20:MET:HG3	2:B:73:LEU:HD21	1.69	0.74
2:B:28:ASP:CG	2:B:31:ARG:HA	2.09	0.73
2:B:44:SER:CB	2:B:49:ARG:NH2	2.51	0.73
3:C:95:ARG:HD2	3:C:95:ARG:H	1.52	0.73
1:A:812:GLN:HE22	2:B:118:ASP:H	1.33	0.73
1:A:833:VAL:O	1:A:833:VAL:HG12	1.87	0.73
1:A:22:LYS:HA	1:A:22:LYS:NZ	2.02	0.73
1:A:215:LEU:N	1:A:215:LEU:HD22	1.96	0.73
1:A:822:ARG:NH1	2:B:156:ALA:HB2	2.04	0.72
1:A:736:LYS:NZ	1:A:755:LEU:HB3	2.04	0.72
2:B:51:PRO:HB2	2:B:55:GLU:CD	2.09	0.72
1:A:736:LYS:HZ3	1:A:755:LEU:HB3	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:LYS:HG2	1:A:740:GLU:OE2	1.90	0.71
1:A:826:TRP:CZ2	2:B:59:MET:HB3	2.26	0.71
1:A:452:ARG:H	1:A:452:ARG:HD3	1.56	0.71
1:A:368:ARG:HA	1:A:368:ARG:HE	1.56	0.70
1:A:690:GLN:O	1:A:694:ASN:HB2	1.91	0.70
1:A:360:GLU:O	1:A:379:GLU:HG2	1.92	0.70
1:A:250:HIS:HB3	1:A:452:ARG:HG3	1.74	0.70
1:A:407:THR:CG2	1:A:407:THR:O	2.39	0.70
1:A:399:LEU:O	1:A:401:PRO:CD	2.40	0.69
1:A:691:LEU:HD22	1:A:696:VAL:HG21	1.74	0.69
1:A:736:LYS:NZ	1:A:755:LEU:HD13	2.07	0.69
2:B:20:MET:HE1	2:B:72:PHE:HD2	1.55	0.69
1:A:11:GLN:HE21	1:A:12:TYR:HE1	1.41	0.69
1:A:291:ASN:HB2	1:A:304:PRO:HB3	1.74	0.69
1:A:310:SER:HA	1:A:313:ASN:ND2	2.09	0.69
1:A:221:GLN:O	1:A:224:PRO:HD2	1.93	0.68
1:A:25:THR:HG22	1:A:25:THR:O	1.93	0.68
1:A:399:LEU:O	1:A:401:PRO:HD2	1.93	0.68
1:A:489:ASN:HB3	1:A:512:PHE:CB	2.24	0.68
2:B:35:VAL:O	2:B:36:SER:HB2	1.92	0.68
1:A:500:TYR:HD2	1:A:509:PHE:CE1	2.11	0.68
1:A:828:LYS:O	1:A:832:LYS:HB3	1.93	0.68
2:B:76:PHE:O	2:B:80:LEU:HB2	1.94	0.68
1:A:403:VAL:HG13	1:A:404:LYS:N	2.08	0.68
1:A:746:LEU:O	1:A:747:GLN:HG2	1.93	0.68
1:A:13:LEU:HD21	1:A:131:ILE:CG2	2.25	0.67
1:A:310:SER:HA	1:A:313:ASN:HD21	1.58	0.67
1:A:496:GLU:HG3	1:A:500:TYR:CE2	2.29	0.67
2:B:155:GLU:HG3	2:B:156:ALA:N	2.08	0.67
1:A:792:TYR:CE1	3:C:152:PRO:HG3	2.28	0.67
1:A:543:ASP:O	1:A:546:SER:HB3	1.95	0.67
3:C:44:PRO:HB3	3:C:75:LEU:HD12	1.75	0.67
1:A:72:ASP:HB2	7:A:1002:HOH:O	1.94	0.67
1:A:836:LEU:HD23	1:A:836:LEU:N	2.10	0.67
1:A:558:LYS:HA	1:A:558:LYS:HE3	1.75	0.67
1:A:253:PRO:HG3	1:A:453:ASN:ND2	2.11	0.66
1:A:719:ARG:HA	7:A:993:HOH:O	1.93	0.66
1:A:537:CYS:HB3	1:A:599:LYS:HE2	1.76	0.66
1:A:185:ASN:O	1:A:189:VAL:HG23	1.96	0.66
1:A:184:GLU:O	1:A:188:LYS:HD2	1.95	0.66
2:B:45:GLU:HB3	2:B:49:ARG:NH1	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:VAL:CG2	1:A:111:LEU:HD11	2.27	0.65
1:A:470:ASN:N	1:A:470:ASN:ND2	2.45	0.65
1:A:692:GLN:HA	1:A:697:LEU:HD12	1.78	0.65
2:B:35:VAL:HG12	2:B:36:SER:H	1.61	0.65
1:A:174:ILE:HG12	1:A:668:VAL:HB	1.79	0.65
2:B:24:PHE:CD2	2:B:24:PHE:O	2.51	0.64
2:B:45:GLU:C	2:B:47:LEU:H	2.01	0.64
1:A:15:VAL:HG12	1:A:16:ASP:H	1.62	0.64
1:A:36:VAL:HG11	1:A:69:VAL:HG11	1.79	0.64
2:B:131:GLU:HG3	2:B:131:GLU:O	1.97	0.64
3:C:131:LEU:HD13	3:C:144:PHE:HB2	1.77	0.64
2:B:33:GLY:O	2:B:68:ASN:HB2	1.98	0.64
1:A:822:ARG:HB3	1:A:822:ARG:NH1	2.12	0.64
2:B:49:ARG:C	2:B:49:ARG:HE	2.01	0.64
2:B:41:LYS:O	2:B:45:GLU:HG2	1.97	0.64
1:A:31:LYS:C	1:A:32:LYS:HE2	2.18	0.64
1:A:148:ILE:HG12	1:A:149:PRO:HD2	1.80	0.63
1:A:736:LYS:HZ1	1:A:755:LEU:HD13	1.64	0.63
3:C:42:ILE:HG22	3:C:44:PRO:HD3	1.81	0.63
1:A:792:TYR:CG	3:C:152:PRO:HD3	2.32	0.63
1:A:25:THR:O	1:A:26:ALA:HB2	1.98	0.62
1:A:365:GLN:HG3	1:A:366:ARG:H	1.64	0.62
3:C:94:ASP:OD2	3:C:97:GLY:HA2	1.99	0.62
1:A:244:GLY:HA3	1:A:461:ILE:HG23	1.82	0.62
1:A:712:ILE:HG22	1:A:759:LYS:HB3	1.80	0.62
1:A:500:TYR:HD2	1:A:509:PHE:HE1	1.45	0.62
1:A:818:TRP:CB	2:B:148:ILE:HG23	2.30	0.62
1:A:88:MET:HG2	1:A:102:ASN:HD22	1.65	0.61
1:A:341:THR:HG22	1:A:343:GLU:N	2.16	0.61
3:C:42:ILE:HD11	3:C:76:MET:HG2	1.81	0.61
1:A:717:LYS:HG3	1:A:718:GLN:N	2.15	0.61
1:A:469:PHE:C	1:A:470:ASN:HD22	2.04	0.61
1:A:280:ARG:HB2	7:A:1049:HOH:O	2.01	0.61
1:A:377:THR:O	1:A:380:ALA:N	2.31	0.61
1:A:826:TRP:HZ2	2:B:59:MET:HB3	1.66	0.61
2:B:24:PHE:CD1	2:B:69:PHE:HB2	2.35	0.61
3:C:111:THR:O	3:C:116:ARG:HG2	2.01	0.61
1:A:694:ASN:ND2	1:A:696:VAL:HG13	2.15	0.60
1:A:793:LEU:O	1:A:796:LYS:HB3	2.01	0.60
2:B:27:ILE:HA	2:B:43:ILE:HD13	1.83	0.60
1:A:404:LYS:HG3	1:A:409:MET:HE3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LYS:HG3	1:A:565:PRO:CD	2.28	0.60
1:A:780:LYS:N	1:A:780:LYS:HE3	2.16	0.60
1:A:18:LYS:NZ	1:A:22:LYS:HD2	2.16	0.60
1:A:341:THR:HG22	1:A:343:GLU:H	1.66	0.60
2:B:63:ALA:C	2:B:65:GLY:H	2.03	0.60
1:A:796:LYS:HD3	3:C:152:PRO:HB3	1.83	0.60
1:A:776:GLU:O	1:A:780:LYS:HD2	2.01	0.60
1:A:508:GLU:O	1:A:509:PHE:HB2	2.00	0.60
2:B:51:PRO:CB	2:B:55:GLU:CG	2.70	0.60
3:C:105:GLU:O	3:C:109:VAL:HG23	2.01	0.60
1:A:36:VAL:CG1	1:A:69:VAL:HG11	2.32	0.59
1:A:500:TYR:CD2	1:A:509:PHE:CE1	2.90	0.59
1:A:182:LYS:HG2	4:A:992:SO4:O3	2.03	0.59
1:A:29:ASP:OD2	1:A:32:LYS:HD2	2.02	0.59
1:A:415:ASN:HB2	1:A:418:GLN:OE1	2.03	0.59
1:A:489:ASN:HB3	1:A:512:PHE:HB3	1.83	0.59
2:B:28:ASP:OD2	2:B:31:ARG:HA	2.03	0.59
1:A:313:ASN:HA	1:A:317:LEU:HD21	1.85	0.59
1:A:31:LYS:O	1:A:32:LYS:HE2	2.01	0.59
1:A:416:MET:O	1:A:420:VAL:HG13	2.03	0.59
1:A:399:LEU:O	1:A:414:GLN:HG3	2.03	0.59
3:C:49:VAL:HG23	3:C:50:PHE:CD2	2.38	0.59
1:A:186:THR:HG23	1:A:458:VAL:HG11	1.84	0.58
1:A:272:VAL:HA	1:A:281:ASN:HD21	1.67	0.58
1:A:522:LEU:HD13	1:A:580:LEU:HD11	1.84	0.58
1:A:707:PHE:CE2	1:A:754:ARG:HG3	2.38	0.58
2:B:55:GLU:CG	2:B:55:GLU:O	2.51	0.58
2:B:24:PHE:CD2	2:B:69:PHE:HB2	2.39	0.58
1:A:361:MET:CE	1:A:380:ALA:HA	2.34	0.58
1:A:404:LYS:HA	1:A:409:MET:HB2	1.86	0.58
1:A:690:GLN:O	1:A:694:ASN:N	2.36	0.58
2:B:21:LYS:CB	2:B:69:PHE:CZ	2.74	0.58
1:A:23:GLU:CG	1:A:23:GLU:O	2.52	0.57
1:A:552:TYR:HD2	1:A:556:MET:HG2	1.68	0.57
2:B:49:ARG:NE	2:B:50:ALA:N	2.51	0.57
2:B:67:LEU:HG	2:B:68:ASN:N	2.19	0.57
1:A:692:GLN:HG2	7:A:1015:HOH:O	2.04	0.57
1:A:11:GLN:HG2	1:A:12:TYR:CD1	2.40	0.57
1:A:493:PHE:CD2	1:A:511:ASP:HA	2.40	0.57
1:A:603:ASN:HB3	1:A:606:VAL:H	1.69	0.56
1:A:173:LEU:N	1:A:173:LEU:HD12	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ALA:HB2	1:A:325:VAL:HG13	1.87	0.56
3:C:71:ALA:O	3:C:75:LEU:HD23	2.05	0.56
1:A:223:ASN:HB3	1:A:224:PRO:HD3	1.87	0.56
1:A:736:LYS:O	1:A:740:GLU:HG3	2.06	0.56
2:B:49:ARG:CD	2:B:49:ARG:C	2.74	0.56
2:B:24:PHE:CD2	2:B:69:PHE:CB	2.89	0.56
1:A:407:THR:O	1:A:408:GLU:CG	2.51	0.56
1:A:23:GLU:O	1:A:23:GLU:HG2	2.06	0.56
1:A:287:GLN:HB3	1:A:328:PHE:HB2	1.88	0.56
1:A:522:LEU:HD11	1:A:562:PHE:HB2	1.87	0.56
3:C:49:VAL:HG23	3:C:50:PHE:HD2	1.70	0.56
1:A:832:LYS:HE2	2:B:47:LEU:HB3	1.87	0.55
2:B:54:LYS:C	2:B:56:LEU:H	2.09	0.55
1:A:215:LEU:HG	7:A:1069:HOH:O	2.06	0.55
1:A:22:LYS:HZ3	1:A:22:LYS:HA	1.71	0.55
2:B:112:LEU:HD23	2:B:116:MET:SD	2.46	0.55
2:B:45:GLU:HB3	2:B:49:ARG:HH11	1.71	0.55
3:C:3:LEU:HD22	3:C:7:GLU:HB3	1.88	0.55
1:A:377:THR:O	1:A:378:ALA:C	2.44	0.55
3:C:52:VAL:HG21	3:C:75:LEU:CD2	2.29	0.55
2:B:55:GLU:O	2:B:55:GLU:CD	2.44	0.55
1:A:377:THR:O	1:A:379:GLU:N	2.39	0.55
1:A:399:LEU:O	1:A:401:PRO:HD3	2.07	0.55
1:A:537:CYS:HB3	1:A:599:LYS:CE	2.37	0.55
1:A:567:LYS:HB3	1:A:567:LYS:NZ	2.21	0.55
2:B:21:LYS:CB	2:B:69:PHE:CE2	2.87	0.55
3:C:107:ARG:O	3:C:111:THR:HG23	2.07	0.54
2:B:20:MET:HG3	2:B:73:LEU:CD2	2.37	0.54
3:C:42:ILE:C	3:C:44:PRO:HD3	2.28	0.54
1:A:833:VAL:O	1:A:833:VAL:CG1	2.53	0.54
2:B:49:ARG:O	2:B:50:ALA:HB2	2.08	0.54
1:A:371:GLN:OE1	1:A:413:GLY:HA2	2.08	0.54
1:A:489:ASN:HB3	1:A:512:PHE:HB2	1.88	0.54
2:B:35:VAL:HB	2:B:67:LEU:HD21	1.90	0.54
2:B:51:PRO:CA	2:B:55:GLU:HG3	2.38	0.54
1:A:368:ARG:HA	1:A:368:ARG:NE	2.21	0.54
1:A:571:PRO:O	1:A:572:ASN:HB3	2.07	0.54
1:A:583:TYR:HD1	1:A:698:GLU:HG3	1.73	0.54
1:A:834:LYS:NZ	1:A:834:LYS:HB3	2.23	0.53
2:B:49:ARG:HD2	2:B:51:PRO:CD	2.39	0.53
1:A:326:GLU:OE1	1:A:326:GLU:HA	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:VAL:O	2:B:29:VAL:CG1	2.55	0.53
1:A:173:LEU:HD12	1:A:173:LEU:H	1.74	0.53
2:B:20:MET:O	2:B:24:PHE:N	2.41	0.53
1:A:580:LEU:HD23	1:A:582:HIS:CE1	2.42	0.53
1:A:724:ALA:O	1:A:728:ILE:HG12	2.09	0.53
1:A:170:GLN:O	1:A:456:ILE:HA	2.09	0.53
1:A:250:HIS:HB3	1:A:452:ARG:CG	2.37	0.53
1:A:812:GLN:O	1:A:816:ARG:HG3	2.07	0.53
2:B:55:GLU:OE2	2:B:55:GLU:C	2.47	0.53
1:A:786:GLN:NE2	3:C:115:GLU:O	2.42	0.53
1:A:313:ASN:HD22	1:A:313:ASN:C	2.12	0.53
1:A:805:ARG:HG3	3:C:20:PHE:CE2	2.44	0.53
1:A:510:ILE:O	1:A:511:ASP:HB2	2.09	0.53
1:A:560:ARG:HD2	1:A:560:ARG:O	2.09	0.53
2:B:45:GLU:N	2:B:49:ARG:NH1	2.57	0.53
1:A:227:GLU:HA	1:A:231:ASN:OD1	2.09	0.53
1:A:288:ILE:HD11	1:A:356:LEU:HD11	1.90	0.53
1:A:379:GLU:O	1:A:383:VAL:HG23	2.09	0.53
1:A:792:TYR:CE2	3:C:152:PRO:CD	2.90	0.53
2:B:49:ARG:CD	2:B:50:ALA:N	2.71	0.53
2:B:106:ILE:HG23	2:B:107:GLU:N	2.24	0.52
2:B:26:MET:O	2:B:29:VAL:HG23	2.08	0.52
2:B:17:ILE:HG23	2:B:73:LEU:HD13	1.91	0.52
2:B:36:SER:HB3	2:B:39:ASP:HB2	1.91	0.52
1:A:18:LYS:HZ1	1:A:22:LYS:HD2	1.73	0.52
1:A:361:MET:HE3	1:A:383:VAL:HG21	1.92	0.52
1:A:734:ASP:HB3	1:A:737:THR:OG1	2.09	0.52
1:A:786:GLN:HE22	3:C:115:GLU:C	2.12	0.52
1:A:824:TRP:CZ2	1:A:826:TRP:HD1	2.28	0.52
2:B:69:PHE:CD1	2:B:69:PHE:C	2.83	0.52
1:A:231:ASN:HA	1:A:240:SER:O	2.10	0.52
1:A:696:VAL:HG23	1:A:697:LEU:N	2.24	0.52
1:A:796:LYS:HB2	3:C:152:PRO:CG	2.39	0.52
1:A:487:PHE:CZ	1:A:665:PRO:HG3	2.44	0.52
3:C:144:PHE:O	3:C:148:VAL:HG23	2.10	0.52
1:A:479:TYR:OH	1:A:524:GLU:HB3	2.09	0.52
3:C:131:LEU:HD11	3:C:139:VAL:HB	1.92	0.52
1:A:712:ILE:O	1:A:714:SER:N	2.43	0.51
1:A:712:ILE:CG2	1:A:759:LYS:HB3	2.40	0.51
1:A:16:ASP:HB2	1:A:19:LYS:HB3	1.91	0.51
1:A:360:GLU:C	1:A:379:GLU:HG2	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:ARG:HD2	2:B:50:ALA:N	2.24	0.51
2:B:37:LYS:HD3	2:B:60:LEU:HD13	1.93	0.51
1:A:537:CYS:C	1:A:539:PHE:H	2.14	0.51
1:A:796:LYS:HB2	3:C:152:PRO:HG2	1.93	0.51
2:B:92:ALA:O	2:B:95:MET:HB2	2.11	0.51
1:A:15:VAL:HB	7:A:995:HOH:O	2.09	0.51
1:A:36:VAL:HG12	1:A:37:PRO:HD2	1.93	0.51
1:A:60:ILE:HD11	1:A:67:ARG:HD2	1.92	0.51
3:C:42:ILE:HG22	3:C:44:PRO:CD	2.40	0.51
2:B:20:MET:HE3	2:B:69:PHE:CD1	2.46	0.51
1:A:370:GLU:HG3	1:A:370:GLU:O	2.11	0.51
1:A:380:ALA:HB2	7:A:1000:HOH:O	2.11	0.51
1:A:486:GLN:NE2	1:A:517:GLN:HG2	2.25	0.51
1:A:13:LEU:HD21	1:A:131:ILE:HG21	1.92	0.50
1:A:133:THR:O	1:A:137:ILE:HG13	2.11	0.50
1:A:354:SER:O	1:A:358:MET:HG3	2.11	0.50
1:A:361:MET:HE1	1:A:380:ALA:HA	1.93	0.50
1:A:401:PRO:HG3	1:A:603:ASN:HD21	1.77	0.50
1:A:747:GLN:O	1:A:747:GLN:CG	2.59	0.50
2:B:60:LEU:HD23	2:B:60:LEU:O	2.11	0.50
2:B:24:PHE:CZ	2:B:68:ASN:HA	2.45	0.50
1:A:591:ILE:HA	1:A:594:TRP:NE1	2.27	0.50
2:B:69:PHE:O	2:B:69:PHE:HD1	1.84	0.50
1:A:169:ASN:HB2	1:A:663:THR:HG22	1.93	0.50
1:A:711:LEU:HD11	1:A:767:LEU:HD21	1.94	0.50
2:B:68:ASN:CG	2:B:68:ASN:O	2.49	0.50
1:A:713:TYR:CE2	1:A:736:LYS:HD2	2.47	0.50
1:A:242:ARG:HD2	1:A:268:GLU:OE2	2.12	0.50
1:A:415:ASN:O	1:A:419:VAL:HG23	2.12	0.50
1:A:753:TYR:O	1:A:754:ARG:HG2	2.12	0.50
1:A:523:ILE:HD11	1:A:580:LEU:HD21	1.93	0.50
3:C:152:PRO:O	3:C:154:PRO:HD2	2.12	0.50
1:A:104:ARG:HG3	1:A:682:VAL:HG11	1.94	0.49
1:A:366:ARG:HG2	1:A:369:GLU:O	2.12	0.49
1:A:59:LYS:HB2	1:A:59:LYS:NZ	2.26	0.49
1:A:59:LYS:HB2	1:A:59:LYS:HZ2	1.77	0.49
1:A:821:LEU:HD22	1:A:827:TRP:CD1	2.46	0.49
1:A:88:MET:HA	1:A:91:MET:HG3	1.94	0.49
1:A:15:VAL:HG21	1:A:84:LYS:HD3	1.94	0.49
2:B:91:ASN:HA	2:B:94:ALA:HB3	1.93	0.49
1:A:816:ARG:O	1:A:820:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:ILE:HD11	3:C:76:MET:CG	2.42	0.49
1:A:736:LYS:HZ2	1:A:740:GLU:CD	2.15	0.49
2:B:21:LYS:HD3	2:B:69:PHE:CE2	2.47	0.49
1:A:218:GLN:HB3	1:A:446:LEU:CD2	2.42	0.49
1:A:284:ILE:HG23	1:A:285:PHE:N	2.28	0.49
1:A:736:LYS:HE3	7:A:1044:HOH:O	2.12	0.49
2:B:62:GLU:O	2:B:75:ILE:HG12	2.12	0.49
1:A:306:SER:C	1:A:308:LEU:H	2.16	0.49
1:A:465:GLU:H	1:A:478:ASN:HD21	1.60	0.49
1:A:505:ILE:HD13	1:A:505:ILE:O	2.12	0.49
1:A:599:LYS:O	1:A:601:PRO:HD3	2.13	0.49
3:C:118:SER:OG	3:C:120:GLU:HG3	2.13	0.49
3:C:88:GLU:O	3:C:92:THR:HG23	2.12	0.49
1:A:603:ASN:O	1:A:607:VAL:HG23	2.12	0.49
1:A:557:GLY:CA	7:A:1040:HOH:O	2.61	0.48
2:B:35:VAL:HG12	2:B:36:SER:N	2.28	0.48
2:B:60:LEU:C	2:B:62:GLU:H	2.15	0.48
2:B:24:PHE:HZ	2:B:68:ASN:HA	1.78	0.48
1:A:559:ASN:HB3	1:A:562:PHE:HB3	1.95	0.48
1:A:704:ARG:HB3	7:A:1014:HOH:O	2.12	0.48
1:A:713:TYR:CZ	1:A:736:LYS:HD2	2.48	0.48
2:B:17:ILE:HG23	2:B:73:LEU:CD1	2.43	0.48
2:B:26:MET:C	2:B:28:ASP:H	2.15	0.48
1:A:290:SER:O	1:A:291:ASN:HB3	2.13	0.48
1:A:723:LEU:HB3	1:A:746:LEU:HD21	1.94	0.48
2:B:45:GLU:CA	2:B:49:ARG:HH11	2.26	0.48
1:A:649:HIS:O	1:A:653:LEU:HB2	2.13	0.48
2:B:49:ARG:CZ	2:B:49:ARG:O	2.62	0.48
2:B:56:LEU:O	2:B:60:LEU:HB2	2.13	0.48
1:A:256:LYS:HB2	7:A:1041:HOH:O	2.13	0.48
1:A:290:SER:HB2	1:A:325:VAL:HG22	1.96	0.48
1:A:591:ILE:HA	1:A:594:TRP:CE2	2.49	0.48
1:A:724:ALA:N	1:A:725:PRO:HD3	2.28	0.48
1:A:262:ILE:HG22	1:A:263:GLU:N	2.29	0.48
1:A:644:THR:O	1:A:648:VAL:HG23	2.13	0.48
2:B:21:LYS:HD3	2:B:69:PHE:HE2	1.79	0.48
3:C:95:ARG:N	3:C:95:ARG:HD2	2.27	0.48
1:A:15:VAL:HG22	1:A:111:LEU:HD11	1.96	0.48
1:A:148:ILE:CG1	1:A:149:PRO:HD2	2.43	0.48
1:A:568:PRO:HA	1:A:573:GLN:OE1	2.13	0.48
1:A:677:LYS:HG3	7:A:1064:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:ALA:HB1	1:A:625:PRO:HD2	1.95	0.48
2:B:63:ALA:O	2:B:65:GLY:N	2.41	0.48
3:C:69:LEU:CB	3:C:70:PRO:HD3	2.43	0.48
1:A:361:MET:CE	1:A:383:VAL:HG21	2.43	0.47
1:A:453:ASN:HB3	1:A:454:TYR:CD2	2.49	0.47
1:A:25:THR:O	1:A:26:ALA:CB	2.62	0.47
1:A:144:ARG:O	1:A:147:GLU:HG3	2.14	0.47
2:B:131:GLU:OE2	2:B:155:GLU:HB3	2.15	0.47
1:A:826:TRP:HZ2	2:B:59:MET:O	1.97	0.47
2:B:49:ARG:HD2	2:B:51:PRO:HD2	1.95	0.47
1:A:572:ASN:O	1:A:572:ASN:CG	2.52	0.47
1:A:533:LEU:HD22	1:A:598:ASN:OD1	2.14	0.47
1:A:415:ASN:OD1	1:A:416:MET:N	2.48	0.47
1:A:167:ARG:HD2	1:A:454:TYR:OH	2.15	0.47
2:B:129:PHE:HA	2:B:132:ALA:HB2	1.96	0.47
3:C:106:LEU:O	3:C:110:LEU:HG	2.15	0.47
1:A:129:LEU:CD1	1:A:131:ILE:HD11	2.45	0.47
1:A:250:HIS:CG	1:A:452:ARG:HG3	2.50	0.47
1:A:307:GLY:HA2	1:A:313:ASN:HB3	1.97	0.47
1:A:533:LEU:HG	1:A:547:PHE:CZ	2.50	0.47
1:A:514:MET:C	1:A:516:LEU:H	2.17	0.46
1:A:303:THR:O	1:A:305:ASP:N	2.41	0.46
1:A:234:THR:HG23	1:A:237:ASN:O	2.16	0.46
1:A:722:ILE:HD11	3:C:89:ALA:HA	1.98	0.46
1:A:500:TYR:CE2	1:A:509:PHE:CZ	3.04	0.46
1:A:514:MET:C	1:A:516:LEU:N	2.68	0.46
1:A:595:LEU:N	1:A:595:LEU:HD12	2.30	0.46
1:A:692:GLN:CA	1:A:697:LEU:HD12	2.45	0.46
1:A:403:VAL:O	1:A:409:MET:HB2	2.16	0.46
1:A:483:ARG:HD2	1:A:520:ILE:HD13	1.97	0.46
2:B:29:VAL:O	2:B:29:VAL:HG12	2.14	0.46
1:A:826:TRP:CZ3	2:B:40:ILE:HD13	2.50	0.46
3:C:109:VAL:HG13	3:C:113:LEU:HD12	1.98	0.46
1:A:415:ASN:HB3	1:A:418:GLN:H	1.80	0.46
2:B:49:ARG:NE	2:B:50:ALA:HA	2.26	0.46
1:A:405:VAL:H	1:A:409:MET:HA	1.80	0.46
2:B:70:THR:O	2:B:70:THR:HG22	2.15	0.46
1:A:431:TYR:HA	1:A:434:MET:HE3	1.98	0.46
1:A:7:ASP:HB3	1:A:10:PHE:HD1	1.81	0.45
2:B:24:PHE:CD2	2:B:69:PHE:HB3	2.51	0.45
1:A:400:LYS:HD3	1:A:411:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:HIS:CB	1:A:452:ARG:HG3	2.42	0.45
1:A:486:GLN:HE22	1:A:517:GLN:HG2	1.81	0.45
1:A:752:GLU:HG3	1:A:766:VAL:CG2	2.46	0.45
1:A:137:ILE:HG12	1:A:153:PHE:CE2	2.51	0.45
1:A:644:THR:HG23	1:A:647:ALA:HB3	1.98	0.45
2:B:16:GLN:O	2:B:20:MET:N	2.49	0.45
2:B:45:GLU:C	2:B:47:LEU:N	2.68	0.45
3:C:95:ARG:CD	3:C:95:ARG:H	2.24	0.45
1:A:788:HIS:CE1	3:C:149:MET:HG2	2.52	0.45
2:B:109:ILE:O	2:B:113:LEU:HG	2.17	0.45
2:B:144:PHE:CE1	2:B:148:ILE:HD11	2.52	0.45
2:B:67:LEU:O	2:B:68:ASN:CB	2.52	0.45
1:A:11:GLN:HG2	1:A:12:TYR:CE1	2.51	0.45
2:B:39:ASP:O	2:B:43:ILE:HG13	2.16	0.45
2:B:45:GLU:CB	2:B:49:ARG:NH1	2.78	0.45
1:A:405:VAL:CG2	1:A:410:VAL:HG23	2.46	0.45
1:A:502:LYS:O	1:A:502:LYS:HG2	2.17	0.45
1:A:593:GLY:O	1:A:596:GLU:HG2	2.17	0.45
2:B:15:LYS:HB3	2:B:15:LYS:HE3	1.78	0.45
2:B:21:LYS:O	2:B:21:LYS:HD2	2.17	0.45
2:B:26:MET:C	2:B:28:ASP:N	2.70	0.45
2:B:53:ASP:O	2:B:53:ASP:CG	2.55	0.45
1:A:829:LEU:O	1:A:833:VAL:HG23	2.17	0.45
1:A:781:ILE:HG21	3:C:85:ASP:O	2.17	0.45
1:A:156:ALA:O	1:A:159:ALA:HB3	2.17	0.45
1:A:591:ILE:H	1:A:591:ILE:HG13	1.67	0.45
1:A:720:TYR:O	1:A:742:ILE:HD13	2.17	0.45
2:B:69:PHE:HA	2:B:72:PHE:CB	2.47	0.45
1:A:834:LYS:H	1:A:835:PRO:HD2	1.82	0.45
3:C:17:LEU:O	3:C:20:PHE:HB3	2.17	0.45
2:B:45:GLU:CA	2:B:49:ARG:NH1	2.80	0.44
1:A:287:GLN:NE2	1:A:327:GLU:HG3	2.32	0.44
1:A:361:MET:HE2	1:A:380:ALA:HA	1.99	0.44
1:A:386:LEU:HD23	7:A:1018:HOH:O	2.16	0.44
1:A:806:ILE:O	1:A:810:VAL:HG23	2.17	0.44
1:A:365:GLN:CG	1:A:366:ARG:H	2.24	0.44
1:A:452:ARG:H	1:A:452:ARG:CD	2.15	0.44
1:A:580:LEU:O	1:A:586:ASN:HA	2.18	0.44
1:A:722:ILE:HD11	3:C:88:GLU:C	2.37	0.44
2:B:96:PHE:CD2	2:B:112:LEU:HD11	2.53	0.44
2:B:121:ASN:OD1	2:B:123:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:THR:CG2	1:A:25:THR:O	2.64	0.44
1:A:405:VAL:HG23	1:A:410:VAL:HG23	1.99	0.44
2:B:121:ASN:O	2:B:123:ASP:N	2.51	0.44
3:C:101:ILE:HD11	3:C:105:GLU:CG	2.47	0.44
1:A:291:ASN:ND2	1:A:304:PRO:HG2	2.33	0.43
1:A:669:ARG:HB3	1:A:694:ASN:HD21	1.83	0.43
1:A:713:TYR:CE1	1:A:760:VAL:HB	2.53	0.43
1:A:836:LEU:HG	1:A:837:LEU:H	1.83	0.43
1:A:88:MET:HG2	1:A:102:ASN:ND2	2.29	0.43
1:A:548:GLN:HE21	1:A:552:TYR:HE1	1.66	0.43
1:A:602:ILE:CG2	1:A:602:ILE:O	2.65	0.43
1:A:787:ALA:HB1	3:C:44:PRO:O	2.19	0.43
3:C:4:SER:C	3:C:6:ASP:N	2.72	0.43
1:A:129:LEU:HA	1:A:130:PRO:HD3	1.87	0.43
1:A:181:GLY:O	1:A:185:ASN:ND2	2.49	0.43
1:A:15:VAL:HG23	1:A:111:LEU:HD11	1.99	0.43
1:A:567:LYS:HD2	1:A:567:LYS:C	2.39	0.43
1:A:567:LYS:HZ2	1:A:567:LYS:HB3	1.83	0.43
3:C:101:ILE:HG22	3:C:141:TYR:HD1	1.84	0.43
1:A:193:LEU:HD11	1:A:456:ILE:HD13	2.01	0.43
1:A:215:LEU:N	1:A:215:LEU:CD2	2.68	0.43
1:A:321:ASN:ND2	1:A:321:ASN:N	2.45	0.43
3:C:63:LEU:HA	3:C:64:PRO:HD3	1.86	0.43
1:A:15:VAL:HG12	1:A:16:ASP:N	2.32	0.43
2:B:14:GLN:OE1	2:B:15:LYS:HB3	2.19	0.43
2:B:24:PHE:CG	2:B:69:PHE:CB	2.88	0.43
2:B:46:GLN:O	2:B:47:LEU:HG	2.18	0.43
2:B:56:LEU:HA	2:B:59:MET:HB2	2.00	0.43
1:A:361:MET:HG2	1:A:379:GLU:HB3	2.00	0.43
2:B:106:ILE:HG23	2:B:107:GLU:H	1.83	0.43
2:B:83:THR:OG1	2:B:84:ASP:N	2.52	0.43
3:C:133:GLU:HA	3:C:139:VAL:HG12	2.01	0.43
1:A:22:LYS:HZ2	1:A:22:LYS:HA	1.80	0.42
1:A:295:GLU:HG2	1:A:295:GLU:H	1.56	0.42
1:A:307:GLY:HA2	1:A:313:ASN:CB	2.49	0.42
2:B:73:LEU:O	2:B:77:SER:HB2	2.19	0.42
1:A:24:GLN:C	1:A:26:ALA:H	2.22	0.42
1:A:734:ASP:HB3	1:A:737:THR:CB	2.50	0.42
3:C:96:GLU:H	3:C:96:GLU:HG2	1.36	0.42
1:A:166:ASP:O	1:A:167:ARG:HB2	2.20	0.42
1:A:398:LEU:HD21	1:A:423:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:ILE:HG12	2:B:148:ILE:HD11	2.01	0.42
2:B:55:GLU:CD	2:B:55:GLU:C	2.77	0.42
1:A:379:GLU:HB3	7:A:1000:HOH:O	2.20	0.42
1:A:613:SER:OG	1:A:614:LYS:N	2.53	0.42
1:A:403:VAL:HG21	1:A:412:LYS:NZ	2.34	0.42
1:A:248:ARG:HA	1:A:457:GLY:HA2	2.02	0.42
1:A:500:TYR:CD2	1:A:509:PHE:CZ	3.08	0.42
1:A:716:PHE:CZ	1:A:743:LEU:HD21	2.55	0.42
2:B:18:GLN:O	2:B:22:GLU:HG2	2.19	0.42
1:A:512:PHE:CG	1:A:702:ILE:HD12	2.55	0.42
1:A:821:LEU:HD23	1:A:821:LEU:HA	1.72	0.42
1:A:223:ASN:CB	1:A:224:PRO:HD3	2.48	0.42
1:A:701:ARG:NH1	7:A:1008:HOH:O	2.52	0.42
1:A:131:ILE:HG22	1:A:151:HIS:HE2	1.85	0.42
1:A:362:LYS:HD2	1:A:363:PHE:H	1.84	0.42
1:A:736:LYS:HD3	7:A:1044:HOH:O	2.19	0.42
1:A:78:ASN:ND2	1:A:98:SER:HB2	2.34	0.42
1:A:229:TYR:CZ	1:A:284:ILE:HG12	2.54	0.41
1:A:450:ALA:O	1:A:452:ARG:N	2.52	0.41
1:A:583:TYR:CD1	1:A:698:GLU:HG3	2.55	0.41
2:B:86:GLU:HG2	2:B:145:THR:HG22	2.01	0.41
2:B:87:GLU:O	2:B:91:ASN:HB2	2.20	0.41
1:A:313:ASN:ND2	1:A:313:ASN:C	2.73	0.41
1:A:402:LYS:HB3	1:A:605:ASN:ND2	2.34	0.41
1:A:580:LEU:HD23	1:A:582:HIS:NE2	2.36	0.41
2:B:69:PHE:HA	2:B:72:PHE:HB2	2.01	0.41
1:A:541:LYS:O	1:A:541:LYS:HG2	2.21	0.41
1:A:696:VAL:HG23	1:A:697:LEU:H	1.85	0.41
1:A:822:ARG:CB	1:A:822:ARG:NH1	2.83	0.41
3:C:101:ILE:HG12	3:C:102:SER:N	2.35	0.41
1:A:481:ASN:HA	1:A:484:LEU:HB2	2.03	0.41
1:A:598:ASN:HD21	1:A:646:SER:H	1.67	0.41
1:A:712:ILE:HA	1:A:759:LYS:HA	2.03	0.41
1:A:782:ILE:O	1:A:786:GLN:HG3	2.20	0.41
1:A:834:LYS:HB2	1:A:835:PRO:HD3	2.03	0.41
2:B:21:LYS:O	2:B:25:SER:HB2	2.21	0.41
1:A:169:ASN:CB	1:A:663:THR:HG22	2.50	0.41
1:A:672:ILE:HG23	1:A:672:ILE:O	2.20	0.41
1:A:712:ILE:O	1:A:713:TYR:C	2.58	0.41
3:C:98:GLN:HG3	3:C:98:GLN:O	2.21	0.41
1:A:51:SER:HB3	1:A:56:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:GLU:HG3	1:A:766:VAL:HG22	2.02	0.41
2:B:15:LYS:HG2	2:B:15:LYS:O	2.20	0.41
2:B:45:GLU:N	2:B:49:ARG:CZ	2.84	0.41
1:A:425:ALA:HB1	1:A:601:PRO:O	2.21	0.41
1:A:818:TRP:CD1	2:B:148:ILE:HA	2.56	0.41
2:B:142:VAL:HG12	2:B:143:LYS:N	2.34	0.41
2:B:45:GLU:CB	2:B:49:ARG:HH11	2.32	0.41
1:A:792:TYR:CZ	3:C:152:PRO:HD3	2.55	0.41
1:A:118:LEU:HG	1:A:492:MET:HE3	2.02	0.41
1:A:291:ASN:HD22	1:A:304:PRO:HG2	1.86	0.41
1:A:355:ILE:HG23	1:A:427:ALA:HB1	2.03	0.41
2:B:54:LYS:C	2:B:56:LEU:N	2.74	0.41
2:B:66:PRO:O	2:B:71:MET:CG	2.69	0.41
1:A:707:PHE:HB3	1:A:761:PHE:HB3	2.02	0.41
2:B:13:PRO:HG2	2:B:16:GLN:NE2	2.36	0.41
2:B:106:ILE:HG13	2:B:110:LYS:HD2	2.03	0.40
2:B:49:ARG:HD2	2:B:51:PRO:HD3	2.02	0.40
1:A:129:LEU:HD12	1:A:131:ILE:HD11	2.03	0.40
1:A:485:GLN:HG2	1:A:583:TYR:CE1	2.56	0.40
2:B:132:ALA:HA	2:B:133:PRO:HD3	1.88	0.40
2:B:32:ASP:OD1	2:B:32:ASP:N	2.53	0.40
1:A:174:ILE:HG22	1:A:182:LYS:HB2	2.04	0.40
1:A:538:MET:H	1:A:538:MET:HG2	1.52	0.40
1:A:85:LEU:HB3	1:A:102:ASN:HD21	1.85	0.40
3:C:27:ALA:HB1	3:C:62:SER:HB2	2.03	0.40
1:A:552:TYR:O	1:A:556:MET:HB3	2.22	0.40
1:A:567:LYS:HD2	1:A:568:PRO:O	2.21	0.40
1:A:571:PRO:O	1:A:572:ASN:CB	2.69	0.40
1:A:593:GLY:O	1:A:597:LYS:HG3	2.22	0.40
2:B:13:PRO:CB	2:B:16:GLN:HE21	2.34	0.40
1:A:18:LYS:HD3	1:A:22:LYS:HG3	2.03	0.40
1:A:780:LYS:CA	1:A:780:LYS:HE3	2.52	0.40
2:B:24:PHE:CE2	2:B:69:PHE:HB3	2.56	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:CG	1:A:368:ARG:NH1[1_655]	0.56	1.64
1:A:144:ARG:NE	1:A:368:ARG:NH2[1_655]	1.09	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:CD	1:A:368:ARG:CZ[1_655]	1.35	0.85
1:A:144:ARG:CD	1:A:368:ARG:NH1[1_655]	1.52	0.68
1:A:144:ARG:CB	1:A:368:ARG:NH1[1_655]	1.53	0.67
1:A:144:ARG:CG	1:A:368:ARG:CZ[1_655]	1.62	0.58
1:A:144:ARG:NE	1:A:368:ARG:CZ[1_655]	1.69	0.51
1:A:144:ARG:CD	1:A:368:ARG:NH2[1_655]	1.95	0.25
1:A:144:ARG:NE	1:A:368:ARG:NH1[1_655]	2.15	0.05
1:A:144:ARG:CD	1:A:368:ARG:NE[1_655]	2.16	0.04

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	793/840 (94%)	685 (86%)	78 (10%)	30 (4%)	<b>3</b>	<b>4</b>
2	B	142/156 (91%)	108 (76%)	24 (17%)	10 (7%)	<b>1</b>	<b>1</b>
3	C	153/156 (98%)	139 (91%)	10 (6%)	4 (3%)	<b>5</b>	<b>8</b>
All	All	1088/1152 (94%)	932 (86%)	112 (10%)	44 (4%)	<b>3</b>	<b>3</b>

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	ALA
1	A	366	ARG
1	A	378	ALA
1	A	401	PRO
1	A	407	THR
1	A	449	LYS
1	A	451	LYS
1	A	452	ARG
1	A	508	GLU
1	A	510	ILE
1	A	625	PRO

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Mol	Chain	Res	Type
1	A	708	PRO
1	A	713	TYR
1	A	835	PRO
2	B	68	ASN
1	A	26	ALA
1	A	526	PRO
1	A	529	ILE
1	A	603	ASN
2	B	47	LEU
2	B	52	ASP
2	B	69	PHE
2	B	122	LYS
3	C	25	ASP
3	C	116	ARG
3	C	154	PRO
1	A	304	PRO
1	A	511	ASP
2	B	31	ARG
1	A	15	VAL
1	A	399	LEU
1	A	408	GLU
3	C	135	LEU
1	A	365	GLN
1	A	538	MET
2	B	35	VAL
2	B	50	ALA
2	B	46	GLN
1	A	735	GLY
1	A	307	GLY
1	A	367	PRO
1	A	575	PRO
1	A	540	PRO
2	B	64	PRO

### 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	698/732 (95%)	608 (87%)	90 (13%)	4	6
2	B	125/133 (94%)	99 (79%)	26 (21%)	1	1
3	C	131/132 (99%)	111 (85%)	20 (15%)	2	4
All	All	954/997 (96%)	818 (86%)	136 (14%)	3	4

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	17	ARG
1	A	19	LYS
1	A	20	LEU
1	A	22	LYS
1	A	31	LYS
1	A	36	VAL
1	A	39	GLU
1	A	40	LYS
1	A	47	GLU
1	A	72	ASP
1	A	131	ILE
1	A	141	ARG
1	A	147	GLU
1	A	161	GLN
1	A	187	LYS
1	A	188	LYS
1	A	191	MET
1	A	195	LYS
1	A	215	LEU
1	A	218	GLN
1	A	223	ASN
1	A	224	PRO
1	A	234	THR
1	A	237	ASN
1	A	238	ASN
1	A	263	GLU
1	A	271	ARG
1	A	295	GLU
1	A	298	ASP
1	A	313	ASN
1	A	321	ASN
1	A	326	GLU
1	A	342	LYS

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Mol	Chain	Res	Type
1	A	366	ARG
1	A	369	GLU
1	A	371	GLN
1	A	379	GLU
1	A	393	ASP
1	A	401	PRO
1	A	403	VAL
1	A	410	VAL
1	A	411	THR
1	A	416	MET
1	A	438	LEU
1	A	452	ARG
1	A	453	ASN
1	A	456	ILE
1	A	461	ILE
1	A	470	ASN
1	A	475	LEU
1	A	492	MET
1	A	505	ILE
1	A	507	TRP
1	A	518	MET
1	A	522	LEU
1	A	526	PRO
1	A	533	LEU
1	A	536	GLU
1	A	538	MET
1	A	545	LYS
1	A	558	LYS
1	A	559	ASN
1	A	567	LYS
1	A	598	ASN
1	A	599	LYS
1	A	600	ASP
1	A	602	ILE
1	A	603	ASN
1	A	615	GLU
1	A	644	THR
1	A	653	LEU
1	A	704	ARG
1	A	710	ARG
1	A	718	GLN
1	A	747	GLN

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Mol	Chain	Res	Type
1	A	752	GLU
1	A	759	LYS
1	A	775	ASP
1	A	776	GLU
1	A	780	LYS
1	A	799	LYS
1	A	806	ILE
1	A	809	SER
1	A	821	LEU
1	A	822	ARG
1	A	827	TRP
1	A	832	LYS
1	A	835	PRO
1	A	836	LEU
2	B	14	GLN
2	B	15	LYS
2	B	27	ILE
2	B	31	ARG
2	B	41	LYS
2	B	46	GLN
2	B	49	ARG
2	B	55	GLU
2	B	57	THR
2	B	61	LYS
2	B	66	PRO
2	B	67	LEU
2	B	69	PHE
2	B	71	MET
2	B	72	PHE
2	B	74	SER
2	B	80	LEU
2	B	81	SER
2	B	90	ARG
2	B	91	ASN
2	B	98	GLU
2	B	119	ASN
2	B	142	VAL
2	B	153	GLU
2	B	154	GLU
2	B	155	GLU
3	C	2	LYS
3	C	5	GLN

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Mol	Chain	Res	Type
3	C	6	ASP
3	C	7	GLU
3	C	9	ASP
3	C	16	GLU
3	C	68	PHE
3	C	73	GLU
3	C	77	ASP
3	C	79	GLU
3	C	80	GLN
3	C	96	GLU
3	C	115	GLU
3	C	119	ASP
3	C	120	GLU
3	C	135	LEU
3	C	136	GLU
3	C	152	PRO
3	C	154	PRO
3	C	155	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	33	ASN
1	A	90	ASN
1	A	162	ASN
1	A	237	ASN
1	A	238	ASN
1	A	287	GLN
1	A	291	ASN
1	A	297	ASN
1	A	313	ASN
1	A	321	ASN
1	A	346	GLN
1	A	453	ASN
1	A	470	ASN
1	A	478	ASN
1	A	481	ASN
1	A	485	GLN
1	A	486	GLN
1	A	489	ASN
1	A	517	GLN

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Mol	Chain	Res	Type
1	A	555	HIS
1	A	572	ASN
1	A	577	HIS
1	A	603	ASN
1	A	654	ASN
1	A	694	ASN
1	A	769	ASN
1	A	786	GLN
1	A	812	GLN
2	B	16	GLN
2	B	91	ASN
3	C	138	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SO4	A	992	-	4,4,4	0.18	0	6,6,6	0.09	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	992	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	801/840 (95%)	0.30	40 (4%) 28 35	22, 47, 93, 166	0
2	B	144/156 (92%)	1.62	52 (36%) 0 0	27, 93, 136, 189	0
3	C	155/156 (99%)	0.32	8 (5%) 27 33	33, 55, 83, 117	0
All	All	1100/1152 (95%)	0.48	100 (9%) 9 10	22, 50, 118, 189	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	156	ALA	13.5
1	A	836	LEU	8.6
2	B	64	PRO	7.1
1	A	837	LEU	6.9
2	B	36	SER	6.8
2	B	40	ILE	6.5
2	B	29	VAL	6.5
2	B	60	LEU	6.5
1	A	25	THR	6.2
2	B	34	PHE	5.9
2	B	63	ALA	5.6
1	A	367	PRO	5.5
2	B	155	GLU	5.1
2	B	75	ILE	5.0
2	B	18	GLN	4.8
2	B	72	PHE	4.5
2	B	17	ILE	4.5
2	B	35	VAL	4.5
2	B	74	SER	4.4
2	B	25	SER	4.3
1	A	407	THR	4.2
1	A	368	ARG	4.2
1	A	24	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	24	PHE	4.1
2	B	67	LEU	4.1
2	B	154	GLU	4.0
2	B	73	LEU	4.0
2	B	13	PRO	4.0
1	A	53	GLY	3.9
2	B	76	PHE	3.9
1	A	49	GLN	3.8
2	B	41	LYS	3.8
2	B	53	ASP	3.7
2	B	42	ALA	3.7
1	A	59	LYS	3.6
2	B	16	GLN	3.6
2	B	46	GLN	3.5
2	B	49	ARG	3.5
1	A	829	LEU	3.4
2	B	22	GLU	3.4
2	B	82	GLY	3.3
2	B	20	MET	3.2
2	B	33	GLY	3.1
2	B	59	MET	3.1
1	A	833	VAL	3.0
1	A	21	MET	3.0
3	C	1	PRO	3.0
1	A	144	ARG	3.0
2	B	151	SER	3.0
1	A	736	LYS	2.9
1	A	23	GLU	2.9
3	C	95	ARG	2.9
3	C	154	PRO	2.9
1	A	826	TRP	2.8
1	A	834	LYS	2.8
1	A	830	TYR	2.8
1	A	26	ALA	2.8
2	B	57	THR	2.8
2	B	47	LEU	2.8
2	B	45	GLU	2.8
2	B	37	LYS	2.8
2	B	27	ILE	2.8
2	B	52	ASP	2.7
2	B	66	PRO	2.6
1	A	16	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	43	ILE	2.5
3	C	42	ILE	2.5
2	B	28	ASP	2.5
2	B	71	MET	2.4
1	A	828	LYS	2.4
1	A	54	ASP	2.4
1	A	52	LYS	2.4
2	B	56	LEU	2.4
1	A	18	LYS	2.3
1	A	449	LYS	2.3
2	B	153	GLU	2.3
3	C	105	GLU	2.3
3	C	100	PHE	2.3
3	C	131	LEU	2.3
2	B	23	ALA	2.3
1	A	541	LYS	2.3
1	A	515	ASP	2.3
1	A	408	GLU	2.2
1	A	831	SER	2.2
1	A	528	GLY	2.2
2	B	65	GLY	2.2
2	B	26	MET	2.2
3	C	132	GLN	2.2
1	A	22	LYS	2.2
1	A	32	LYS	2.2
1	A	27	ALA	2.2
1	A	560	ARG	2.1
1	A	405	VAL	2.1
1	A	460	ASP	2.1
2	B	62	GLU	2.1
2	B	21	LYS	2.1
2	B	51	PRO	2.1
1	A	730	GLN	2.1
1	A	369	GLU	2.0
1	A	365	GLN	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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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
5	MG	B	990	1/1	0.14	0.13	124,124,124,124	0
6	CA	C	991	1/1	0.69	0.23	98,98,98,98	0
4	SO4	A	992	5/5	0.96	0.30	83,87,89,93	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.