



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:02 pm BST

PDB ID : 6AC6  
Title : Ab initio crystal structure of Selenomethionine labelled Mycobacterium smegmatis Mfd  
Authors : Putta, S.; Fox, G.C.; Walsh, M.A.; Rao, D.N.; Nagaraja, V.; Natesh, R.  
Deposited on : 2018-07-25  
Resolution : 2.99 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

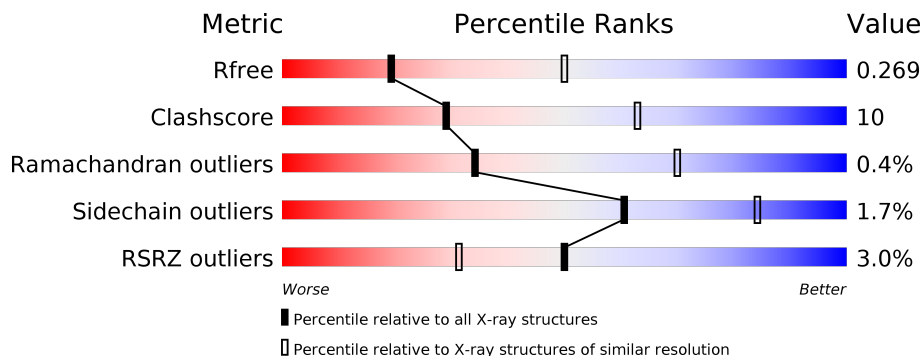
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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	1235	
1	B	1235	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 16853 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 Mycobacterium smegmatis Mfd.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	1154	8417	5293	1487	1606	6	25	0	0	0
1	B	1153	8337	5253	1473	1580	6	25	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	initiating methionine	UNP I7G7M2
A	-18	GLY	-	expression tag	UNP I7G7M2
A	-17	SER	-	expression tag	UNP I7G7M2
A	-16	SER	-	expression tag	UNP I7G7M2
A	-15	HIS	-	expression tag	UNP I7G7M2
A	-14	HIS	-	expression tag	UNP I7G7M2
A	-13	HIS	-	expression tag	UNP I7G7M2
A	-12	HIS	-	expression tag	UNP I7G7M2
A	-11	HIS	-	expression tag	UNP I7G7M2
A	-10	HIS	-	expression tag	UNP I7G7M2
A	-9	SER	-	expression tag	UNP I7G7M2
A	-8	SER	-	expression tag	UNP I7G7M2
A	-7	GLY	-	expression tag	UNP I7G7M2
A	-6	LEU	-	expression tag	UNP I7G7M2
A	-5	VAL	-	expression tag	UNP I7G7M2
A	-4	PRO	-	expression tag	UNP I7G7M2
A	-3	ARG	-	expression tag	UNP I7G7M2
A	-2	GLY	-	expression tag	UNP I7G7M2
A	-1	SER	-	expression tag	UNP I7G7M2
A	0	HIS	-	expression tag	UNP I7G7M2
B	-19	MSE	-	initiating methionine	UNP I7G7M2
B	-18	GLY	-	expression tag	UNP I7G7M2
B	-17	SER	-	expression tag	UNP I7G7M2
B	-16	SER	-	expression tag	UNP I7G7M2
B	-15	HIS	-	expression tag	UNP I7G7M2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP I7G7M2
B	-13	HIS	-	expression tag	UNP I7G7M2
B	-12	HIS	-	expression tag	UNP I7G7M2
B	-11	HIS	-	expression tag	UNP I7G7M2
B	-10	HIS	-	expression tag	UNP I7G7M2
B	-9	SER	-	expression tag	UNP I7G7M2
B	-8	SER	-	expression tag	UNP I7G7M2
B	-7	GLY	-	expression tag	UNP I7G7M2
B	-6	LEU	-	expression tag	UNP I7G7M2
B	-5	VAL	-	expression tag	UNP I7G7M2
B	-4	PRO	-	expression tag	UNP I7G7M2
B	-3	ARG	-	expression tag	UNP I7G7M2
B	-2	GLY	-	expression tag	UNP I7G7M2
B	-1	SER	-	expression tag	UNP I7G7M2
B	0	HIS	-	expression tag	UNP I7G7M2

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

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

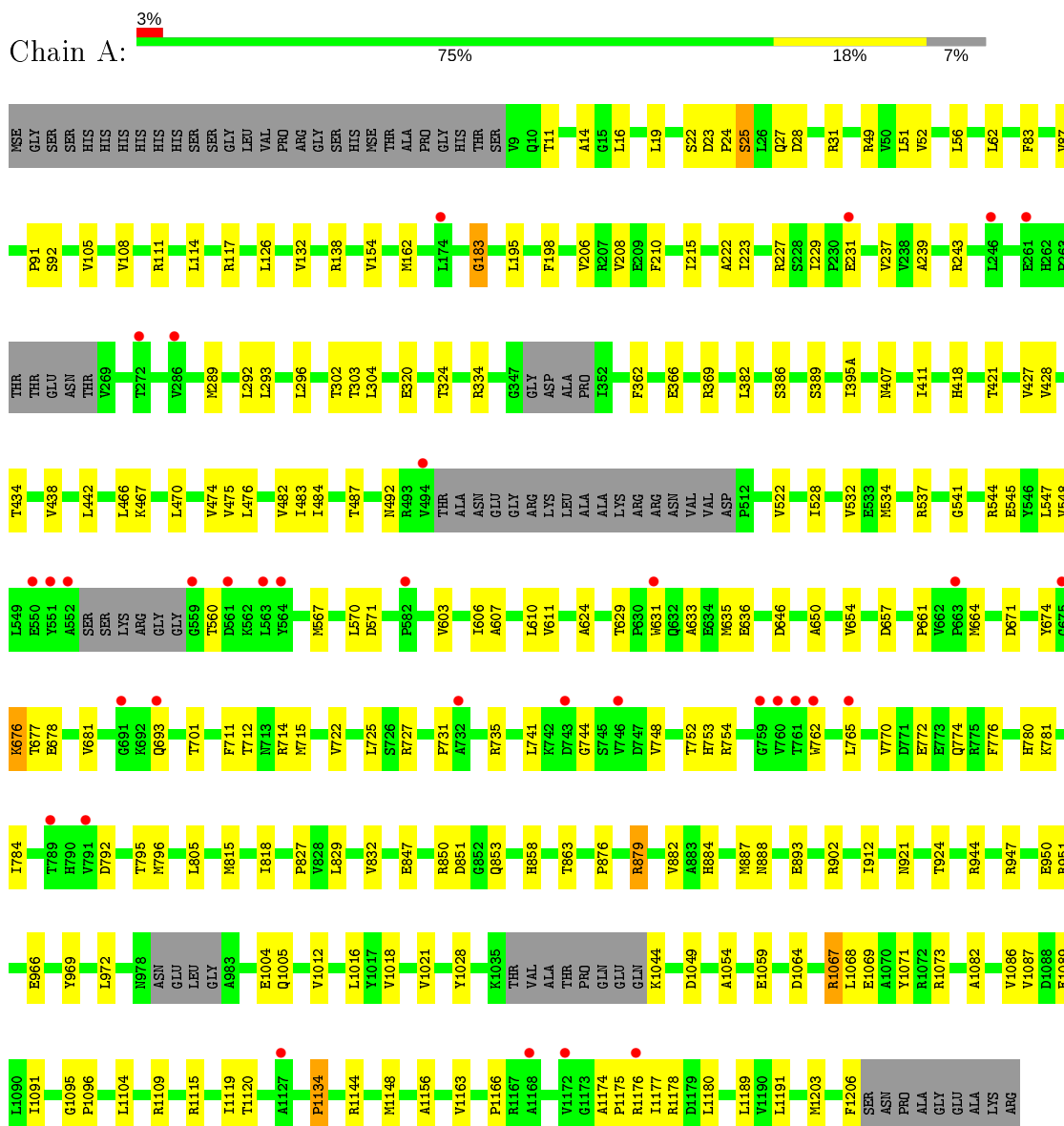
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	37	Total	O	0	0
			37	37		

### 3 Residue-property plots [i](#)

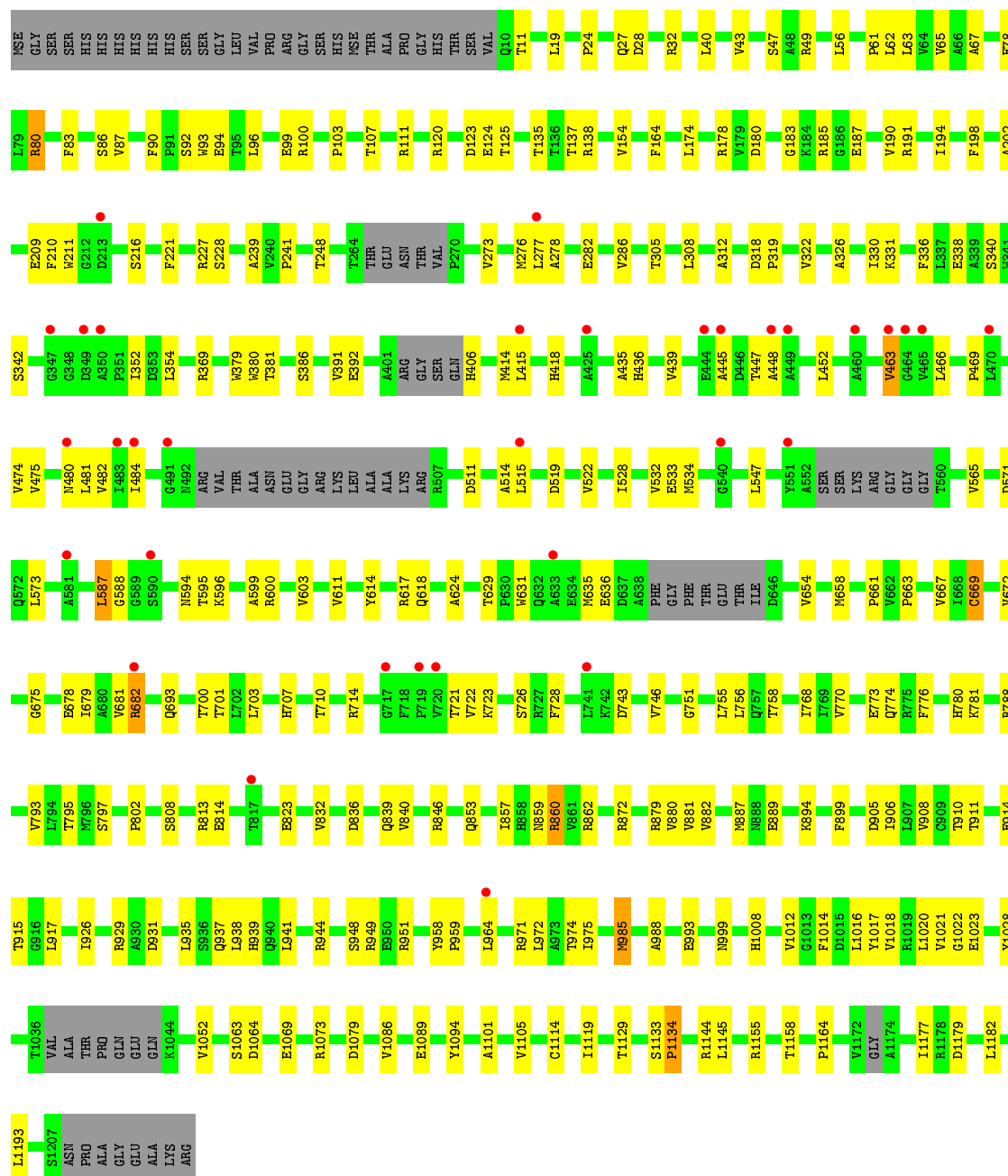
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



- Molecule 1: Mycobacterium smegmatis Mfd





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.71Å 158.87Å 207.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.19 – 2.99 47.19 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.19-2.99) 96.5 (47.19-2.99)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 3.01Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.218 , 0.270 0.219 , 0.269	Depositor DCC
$R_{free}$ test set	2788 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.7	Xtrriage
Anisotropy	0.389	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16853	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: 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	0.26	0/8542	0.44	0/11635
1	B	0.27	0/8461	0.45	2/11529 (0.0%)
All	All	0.26	0/17003	0.45	2/23164 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	80	ARG	NE-CZ-NH2	-5.16	117.72	120.30

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	8417	0	8131	145	0
1	B	8337	0	8022	174	0
2	A	15	0	0	2	0
2	B	10	0	0	0	0
3	A	37	0	0	2	0
3	B	37	0	0	2	0
All	All	16853	0	16153	316	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 10.

All (316) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:LEU:HD13	1:B:466:LEU:HG	1.43	0.95
1:B:330:ILE:HD12	1:B:331:LYS:N	1.91	0.86
1:A:674:TYR:HB3	1:A:818:ILE:HD11	1.62	0.81
1:B:636:GLU:HG2	1:B:682:ARG:HH11	1.48	0.79
1:B:532:VAL:HG23	1:B:533:GLU:HB3	1.64	0.77
1:B:1052:VAL:HG23	1:B:1179:ASP:HA	1.67	0.77
1:B:185:ARG:NH1	1:B:202:ALA:O	2.18	0.76
1:A:635:MSE:HG2	1:A:714:ARG:HH21	1.51	0.75
1:B:330:ILE:HD12	1:B:331:LYS:H	1.50	0.74
1:A:805:LEU:HD13	1:A:1018:VAL:HG23	1.71	0.73
1:A:195:LEU:HD23	1:A:208:VAL:HB	1.71	0.71
1:B:862:ARG:HD2	1:B:862:ARG:H	1.55	0.71
1:B:880:VAL:HG22	1:B:906:ILE:HB	1.71	0.71
1:B:617:ARG:NH1	1:B:663:PRO:O	2.25	0.70
1:B:185:ARG:NH2	1:B:823:GLU:O	2.25	0.70
1:B:587:LEU:H	1:B:587:LEU:HD23	1.58	0.69
1:A:92:SER:HB2	1:A:138:ARG:HD2	1.76	0.68
1:B:931:ASP:O	1:B:971:ARG:NH2	2.27	0.67
1:A:701:THR:HG21	1:A:727:ARG:HB3	1.76	0.67
1:A:52:VAL:HG21	1:A:382:LEU:HD22	1.76	0.66
1:B:92:SER:HB3	1:B:138:ARG:HD2	1.77	0.66
1:B:1145:LEU:HD13	1:B:1193:LEU:HD11	1.78	0.66
1:A:28:ASP:OD1	1:A:31:ARG:NH2	2.29	0.66
1:A:770:VAL:HB	1:A:795:THR:HG22	1.78	0.66
1:A:541:GLY:O	1:A:1178:ARG:NH1	2.28	0.66
1:A:243:ARG:HD3	1:A:289:MSE:HE1	1.76	0.66
1:B:599:ALA:O	1:B:603:VAL:HG23	1.96	0.66
1:B:209:GLU:O	1:B:216:SER:N	2.29	0.64
1:B:1144:ARG:NH2	3:B:1402:HOH:O	2.30	0.64
1:B:305:THR:HA	1:B:308:LEU:HD12	1.79	0.63
1:B:452:LEU:HB2	1:B:466:LEU:HD21	1.81	0.63
1:B:840:VAL:HG13	1:B:926:ILE:HD13	1.80	0.63
1:A:850:ARG:HH21	1:A:950:GLU:HG2	1.64	0.62
1:B:452:LEU:HB2	1:B:466:LEU:CG	2.30	0.62
1:B:860:ARG:CZ	1:B:862:ARG:HD3	2.29	0.62
1:B:154:VAL:HB	1:B:239:ALA:HB3	1.82	0.61
1:B:415:LEU:HD11	1:B:484:ILE:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:LEU:HB2	1:B:466:LEU:HG	1.82	0.61
1:B:701:THR:HG23	1:B:726:SER:HB3	1.82	0.61
1:B:452:LEU:HB2	1:B:466:LEU:CD2	2.30	0.61
1:A:138:ARG:NH2	2:A:1302:SO4:O1	2.33	0.61
1:B:164:PHE:HZ	1:B:190:VAL:HG23	1.65	0.61
1:A:117:ARG:HG2	1:A:126:LEU:HB3	1.83	0.60
1:B:452:LEU:CD1	1:B:466:LEU:HG	2.24	0.60
1:B:678:GLU:HA	1:B:681:VAL:HG22	1.83	0.60
1:A:944:ARG:NH2	3:A:1401:HOH:O	2.32	0.59
1:A:611:VAL:HG21	1:A:1028:TYR:HB3	1.83	0.59
1:B:522:VAL:HG12	1:B:528:ILE:HG13	1.85	0.59
1:A:532:VAL:HB	1:A:548:VAL:HG23	1.83	0.58
1:B:802:PRO:HD3	1:B:993:GLU:HB3	1.83	0.58
1:B:722:VAL:HG23	1:B:723:LYS:H	1.67	0.58
1:B:929:ARG:HG3	1:B:959:PRO:HD3	1.84	0.58
1:A:1091:ILE:HG22	1:A:1096:PRO:HA	1.84	0.58
1:B:90:PHE:HB3	1:B:135:THR:HB	1.84	0.58
1:B:773:GLU:OE2	1:B:788:ARG:NH2	2.36	0.58
1:A:206:VAL:HG11	1:A:237:VAL:HG11	1.85	0.58
1:A:762:TRP:HB3	1:A:765:LEU:HB2	1.86	0.58
1:A:545:GLU:OE2	1:A:1067:ARG:NH1	2.36	0.58
1:B:935:LEU:HD11	1:B:985:MSE:SE	2.53	0.57
1:A:56:LEU:HB2	1:A:62:LEU:HD22	1.85	0.57
1:B:751:GLY:HA3	1:B:755:LEU:HD11	1.87	0.57
1:A:784:ILE:H	1:A:784:ILE:HD12	1.70	0.56
1:A:1119:ILE:HA	1:A:1134:PRO:HG2	1.85	0.56
1:A:772:GLU:OE1	1:A:774:GLN:NE2	2.36	0.56
1:B:78:GLU:HA	1:B:469:PRO:HG2	1.87	0.56
1:B:774:GLN:HB3	1:B:999:ASN:HD22	1.70	0.56
1:A:847:GLU:HG3	1:A:924:THR:HB	1.87	0.56
1:B:49:ARG:NH2	1:B:318:ASP:OD2	2.37	0.56
1:A:678:GLU:O	1:A:681:VAL:HG22	2.04	0.56
1:A:475:VAL:HG22	1:A:482:VAL:HG23	1.87	0.56
1:B:614:TYR:O	1:B:618:GLN:HG2	2.06	0.56
1:B:1101:ALA:O	1:B:1105:VAL:HG23	2.06	0.55
1:B:534:MSE:SE	1:B:547:LEU:HD13	2.56	0.55
1:A:780:HIS:O	1:A:784:ILE:HD12	2.05	0.55
1:A:882:VAL:HG23	1:A:887:MSE:HE1	1.88	0.55
1:A:83:PHE:HB2	1:A:87:VAL:HG23	1.88	0.55
1:A:847:GLU:O	1:A:850:ARG:HG2	2.06	0.55
1:A:606:ILE:O	1:A:610:LEU:HG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1119:ILE:HG23	1:A:1134:PRO:HD2	1.89	0.55
1:A:650:ALA:O	1:A:654:VAL:HG13	2.07	0.55
1:B:859:ASN:HA	1:B:910:THR:HG22	1.88	0.55
1:A:1012:VAL:HG22	1:A:1016:LEU:HD23	1.88	0.54
1:A:522:VAL:HG23	1:A:528:ILE:HD13	1.88	0.54
1:A:1109:ARG:HH21	1:A:1206:PHE:HA	1.71	0.54
1:B:414:MSE:HE1	1:B:482:VAL:HG11	1.88	0.54
1:B:629:THR:HG22	1:B:631:TRP:H	1.73	0.54
1:B:99:GLU:OE1	1:B:846:ARG:NH1	2.40	0.54
1:B:1073:ARG:NH2	1:B:1086:VAL:HG12	2.23	0.54
1:A:544:ARG:NH2	1:A:1049:ASP:OD1	2.41	0.54
1:B:178:ARG:NH2	1:B:190:VAL:HG11	2.23	0.54
1:B:164:PHE:CZ	1:B:190:VAL:HG23	2.43	0.54
1:B:938:LEU:HD11	1:B:975:ILE:HG21	1.88	0.54
1:B:603:VAL:HG13	1:B:1021:VAL:HG22	1.90	0.53
1:B:32:ARG:NH1	1:B:391:VAL:HG21	2.22	0.53
1:B:948:SER:OG	1:B:949:ARG:N	2.38	0.53
1:A:407:ASN:O	1:A:411:ILE:HG13	2.08	0.53
1:B:28:ASP:O	1:B:32:ARG:HG3	2.08	0.53
1:A:427:VAL:HG11	1:A:438:VAL:HG11	1.91	0.53
1:B:221:PHE:HA	1:B:228:SER:HA	1.90	0.53
1:B:19:LEU:HG	1:B:481:LEU:HD11	1.90	0.52
1:A:884:HIS:CD2	1:A:887:MSE:HE3	2.44	0.52
1:A:195:LEU:HD22	1:A:210:PHE:HE1	1.75	0.52
1:A:303:THR:OG1	1:A:304:LEU:N	2.43	0.52
1:B:700:THR:OG1	1:B:703:LEU:HD12	2.10	0.52
1:B:194:ILE:HG13	1:B:209:GLU:HG2	1.91	0.52
1:B:624:ALA:HB2	1:B:661:PRO:HB3	1.92	0.52
1:A:227:ARG:HD3	1:A:1089:GLU:HG3	1.90	0.52
1:B:100:ARG:HG3	1:B:340:SER:HB3	1.92	0.52
1:A:1109:ARG:NH2	1:A:1206:PHE:HA	2.26	0.51
1:B:565:VAL:HG11	1:B:573:LEU:HD11	1.92	0.51
1:B:547:LEU:HB3	1:B:565:VAL:HG13	1.92	0.51
1:B:533:GLU:HG3	1:B:534:MSE:N	2.25	0.51
1:A:727:ARG:NH2	1:A:893:GLU:OE2	2.43	0.51
1:B:768:ILE:HB	1:B:793:VAL:HG22	1.91	0.51
1:A:1044:LYS:O	1:A:1115:ARG:NH1	2.44	0.51
1:B:935:LEU:HD23	1:B:971:ARG:HG3	1.92	0.51
1:B:326:ALA:O	1:B:330:ILE:HG13	2.11	0.51
1:B:93:TRP:CE2	1:B:103:PRO:HG3	2.46	0.51
1:B:120:ARG:NH1	1:B:123:ASP:OD2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:THR:HB	1:B:322:VAL:HG13	1.91	0.51
1:B:594:ASN:ND2	3:B:1403:HOH:O	2.32	0.51
1:A:624:ALA:HB2	1:A:661:PRO:HA	1.92	0.50
1:A:715:MSE:CE	1:A:748:VAL:HG11	2.42	0.50
1:A:91:PRO:HD2	1:A:111:ARG:HG3	1.93	0.50
1:A:607:ALA:O	1:A:611:VAL:HG22	2.12	0.50
1:A:693:GLN:HE22	1:A:744:GLY:HA2	1.76	0.50
1:A:847:GLU:OE2	1:A:850:ARG:NH1	2.44	0.50
1:B:11:THR:OG1	1:B:11:THR:O	2.24	0.50
1:A:701:THR:HG22	1:A:752:THR:HG21	1.94	0.50
1:B:124:GLU:H	1:B:124:GLU:CD	2.15	0.50
1:A:162:MSE:HE1	1:A:215:ILE:HD11	1.94	0.50
1:B:435:ALA:O	1:B:439:VAL:HG13	2.12	0.49
1:B:917:LEU:C	1:B:944:ARG:HH21	2.16	0.49
1:B:1008:HIS:O	1:B:1012:VAL:HG12	2.11	0.49
1:B:635:MSE:O	1:B:714:ARG:NH2	2.34	0.49
1:B:83:PHE:HB2	1:B:87:VAL:HG23	1.95	0.49
1:B:180:ASP:HB2	1:B:1063:SER:HB2	1.95	0.49
1:B:823:GLU:OE2	1:B:823:GLU:N	2.45	0.49
1:A:366:GLU:OE1	1:A:369:ARG:NH1	2.46	0.48
1:A:829:LEU:HG	1:A:951:ARG:HD3	1.93	0.48
1:A:547:LEU:HD22	1:A:1068:LEU:HD11	1.94	0.48
1:B:43:VAL:HG21	1:B:386:SER:HA	1.94	0.48
1:B:882:VAL:HA	1:B:908:VAL:O	2.12	0.48
1:A:741:LEU:HD12	1:A:762:TRP:HA	1.96	0.48
1:A:1120:THR:HG23	1:A:1134:PRO:HG3	1.95	0.48
1:A:853:GLN:OE1	1:A:921:ASN:ND2	2.47	0.48
1:B:971:ARG:O	1:B:974:THR:OG1	2.30	0.48
1:B:635:MSE:HE1	1:B:682:ARG:HD3	1.96	0.48
1:A:780:HIS:O	1:A:784:ILE:CD1	2.61	0.48
1:A:1166:PRO:HG2	1:A:1177:ILE:HD13	1.95	0.48
1:B:937:GLN:OE1	1:B:937:GLN:N	2.47	0.48
1:A:154:VAL:HB	1:A:239:ALA:HB3	1.95	0.48
1:A:195:LEU:HD22	1:A:210:PHE:CE1	2.49	0.47
1:B:63:LEU:HD22	1:B:308:LEU:HD11	1.96	0.47
1:B:857:ILE:HD11	1:B:914:GLU:HG3	1.96	0.47
1:A:19:LEU:O	1:A:22:SER:HB3	2.14	0.47
1:A:87:VAL:HG22	1:A:132:VAL:HB	1.95	0.47
1:A:635:MSE:HE2	1:A:635:MSE:HB3	1.85	0.47
1:B:1114:CYS:HB3	1:B:1119:ILE:HB	1.95	0.47
1:B:174:LEU:HD22	1:B:241:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1163:VAL:HG21	1:A:1189:LEU:HD11	1.97	0.47
1:A:11:THR:HB	1:A:14:ALA:HB2	1.96	0.47
1:A:947:ARG:HD3	3:A:1401:HOH:O	2.14	0.47
1:B:1155:ARG:HB2	1:B:1158:THR:OG1	2.15	0.47
1:A:1071:TYR:HE1	1:A:1104:LEU:HD11	1.80	0.47
1:B:164:PHE:HD1	1:B:210:PHE:CE2	2.33	0.47
1:B:1129:THR:HG22	1:B:1164:PRO:HA	1.97	0.47
1:B:853:GLN:NE2	1:B:899:PHE:O	2.48	0.47
1:A:395(A):ILE:HG12	1:A:476:LEU:HD23	1.97	0.46
1:B:1133:SER:HB3	1:B:1134:PRO:HD3	1.96	0.46
1:B:43:VAL:HG13	1:B:392:GLU:HA	1.97	0.46
1:B:278:ALA:O	1:B:282:GLU:HG3	2.15	0.46
1:B:1017:TYR:O	1:B:1021:VAL:HG23	2.14	0.46
1:B:65:VAL:HG22	1:B:135:THR:HG23	1.97	0.46
1:A:183:GLY:HA2	1:A:223:ILE:HD12	1.96	0.46
1:B:832:VAL:HG21	1:B:972:LEU:HB3	1.97	0.46
1:B:958:TYR:CG	1:B:964:LEU:HD11	2.50	0.46
1:B:1177:ILE:HG13	1:B:1182:LEU:HB2	1.98	0.46
1:B:183:GLY:N	1:B:187:GLU:OE2	2.36	0.46
1:B:40:LEU:HB3	1:B:380:TRP:CD1	2.51	0.46
1:B:872:ARG:NH2	1:B:880:VAL:O	2.47	0.46
1:B:1079:ASP:OD1	1:B:1079:ASP:N	2.48	0.46
1:B:369:ARG:HG3	1:B:379:TRP:CG	2.50	0.46
1:B:47:SER:OG	1:B:474:VAL:HG12	2.15	0.46
1:B:693:GLN:NE2	1:B:743:ASP:O	2.47	0.46
1:B:728:PHE:HE1	1:B:894:LYS:HD3	1.81	0.46
1:A:487:THR:HG22	1:A:492:ASN:O	2.15	0.46
1:A:567:MSE:SE	1:A:570:LEU:HD11	2.65	0.46
1:B:1014:PHE:O	1:B:1018:VAL:HG22	2.16	0.46
1:B:352:ILE:O	1:B:354:LEU:HD12	2.16	0.46
1:A:1120:THR:H	1:A:1134:PRO:CG	2.28	0.46
1:A:23:ASP:OD2	1:A:25:SER:HB3	2.16	0.46
1:A:753:HIS:HB2	1:A:780:HIS:CE1	2.51	0.46
1:B:338:GLU:O	1:B:342:SER:HB3	2.16	0.46
1:B:61:PRO:HB2	1:B:312:ALA:HB2	1.98	0.46
1:A:676:LYS:HD2	1:A:796:MSE:HE3	1.98	0.45
1:B:475:VAL:HG13	1:B:482:VAL:HG22	1.97	0.45
1:B:667:VAL:HG12	1:B:795:THR:HB	1.98	0.45
1:A:49:ARG:HA	1:A:52:VAL:HG22	1.98	0.45
1:B:1012:VAL:CG2	1:B:1016:LEU:HD23	2.47	0.45
1:A:1071:TYR:CE1	1:A:1104:LEU:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1156:ALA:N	2:A:1301:SO4:O1	2.46	0.45
1:A:776:PHE:O	1:A:781:LYS:NZ	2.50	0.45
1:B:191:ARG:HD2	1:B:1094:TYR:HD1	1.82	0.45
1:A:1087:VAL:O	1:A:1091:ILE:HG13	2.16	0.45
1:A:657:ASP:N	1:A:657:ASP:OD1	2.49	0.45
1:A:1120:THR:H	1:A:1134:PRO:HG3	1.81	0.45
1:A:1148:MSE:HE2	1:A:1148:MSE:HB2	1.84	0.45
1:A:712:THR:HG22	1:A:722:VAL:HG13	1.99	0.45
1:A:851:ASP:O	1:A:902:ARG:NH2	2.49	0.45
1:B:770:VAL:HG22	1:B:795:THR:HA	1.98	0.45
1:B:882:VAL:O	1:B:887:MSE:HE1	2.16	0.45
1:A:320:GLU:O	1:A:324:THR:HG23	2.17	0.44
1:A:571:ASP:OD1	1:A:571:ASP:N	2.50	0.44
1:A:966:GLU:HA	1:A:969:TYR:CE2	2.51	0.44
1:B:276:MSE:HG3	1:B:286:VAL:HG11	1.98	0.44
1:B:83:PHE:HB3	1:B:86:SER:HB2	1.98	0.44
1:A:418:HIS:O	1:A:421:THR:HB	2.17	0.44
1:A:832:VAL:HG21	1:A:972:LEU:HB3	2.00	0.44
1:B:938:LEU:HA	1:B:941:LEU:HD12	1.99	0.44
1:A:629:THR:HG22	1:A:631:TRP:H	1.83	0.44
1:A:681:VAL:HG12	1:A:711:PHE:CE1	2.52	0.44
1:A:162:MSE:HE3	1:A:162:MSE:HB2	1.63	0.44
1:B:707:HIS:HA	1:B:710:THR:HG22	1.99	0.44
1:A:292:LEU:O	1:A:296:LEU:N	2.44	0.44
1:A:195:LEU:CD2	1:A:208:VAL:HB	2.44	0.44
1:B:452:LEU:O	1:B:466:LEU:HD21	2.18	0.44
1:A:1069:GLU:OE2	1:A:1073:ARG:NH2	2.51	0.44
1:A:428:VAL:HA	1:A:466:LEU:O	2.18	0.44
1:B:56:LEU:HB2	1:B:62:LEU:HD22	2.00	0.44
1:B:80:ARG:HG3	1:B:80:ARG:HH11	1.83	0.44
1:A:1004:GLU:HG2	1:A:1005:GLN:N	2.33	0.44
1:A:105:VAL:HA	1:A:108:VAL:HG22	1.99	0.44
1:A:302:THR:OG1	1:A:303:THR:N	2.50	0.44
1:A:676:LYS:HG2	1:A:796:MSE:SE	2.68	0.43
1:B:96:LEU:HD12	1:B:336:PHE:CG	2.53	0.43
1:B:935:LEU:HD12	1:B:988:ALA:HB2	1.99	0.43
1:A:428:VAL:HG21	1:A:470:LEU:HD12	1.99	0.43
1:A:633:ALA:HA	1:A:636:GLU:HG3	2.00	0.43
1:A:1059:GLU:OE1	1:A:1059:GLU:N	2.46	0.43
1:A:386:SER:HG	1:B:406:HIS:N	2.16	0.43
1:B:448:ALA:O	1:B:463:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:HD21	1:A:483:ILE:HD13	2.00	0.43
1:A:784:ILE:N	1:A:784:ILE:HD12	2.34	0.43
1:A:664:MSE:N	1:A:792:ASP:OD1	2.45	0.43
1:B:319:PRO:HG3	1:B:381:THR:HG23	2.01	0.43
1:A:534:MSE:HE2	1:A:1064:ASP:HB3	2.00	0.43
1:A:1191:LEU:HD23	1:A:1191:LEU:HA	1.87	0.43
1:B:24:PRO:HA	1:B:27:GLN:HB2	2.00	0.43
1:A:427:VAL:HA	1:A:484:ILE:O	2.19	0.43
1:A:731:PRO:O	1:A:735:ARG:HB3	2.19	0.43
1:B:534:MSE:HB3	1:B:534:MSE:HE3	1.99	0.43
1:B:675:GLY:O	1:B:679:ILE:HD12	2.19	0.43
1:B:669:CYS:HA	1:B:797:SER:O	2.19	0.43
1:B:776:PHE:HB2	1:B:781:LYS:HG3	2.00	0.42
1:B:436:HIS:O	1:B:439:VAL:HG22	2.19	0.42
1:B:445:ALA:O	1:B:447:THR:N	2.52	0.42
1:B:511:ASP:O	1:B:1069:GLU:HG3	2.20	0.42
1:A:1082:ALA:O	1:A:1086:VAL:HG23	2.19	0.42
1:A:863:THR:OG1	1:A:863:THR:O	2.37	0.42
1:B:1016:LEU:O	1:B:1020:LEU:HG	2.20	0.42
1:B:721:THR:OG1	1:B:746:VAL:HA	2.20	0.42
1:A:603:VAL:CG1	1:A:1021:VAL:HA	2.50	0.42
1:A:827:PRO:O	1:A:951:ARG:NH1	2.52	0.42
1:B:83:PHE:HB2	1:B:87:VAL:CG2	2.49	0.42
1:B:571:ASP:N	1:B:571:ASP:OD1	2.53	0.42
1:B:596:LYS:O	1:B:600:ARG:HB2	2.19	0.42
1:B:894:LYS:HB2	1:B:894:LYS:HE2	1.82	0.42
1:A:51:LEU:HD11	1:A:474:VAL:HG11	2.01	0.42
1:B:958:TYR:HB2	1:B:959:PRO:HD2	2.02	0.42
1:A:24:PRO:HA	1:A:27:GLN:HB2	2.02	0.42
1:A:603:VAL:HG11	1:A:1021:VAL:HA	2.01	0.42
1:B:514:ALA:O	1:B:515:LEU:HD12	2.20	0.42
1:B:654:VAL:O	1:B:658:MSE:HB2	2.20	0.42
1:B:123:ASP:CG	1:B:125:THR:HG22	2.40	0.42
1:B:600:ARG:NH2	1:B:1023:GLU:OE1	2.52	0.41
1:B:611:VAL:HG21	1:B:1028:TYR:HB3	2.02	0.41
1:B:273:VAL:O	1:B:277:LEU:HD12	2.20	0.41
1:A:676:LYS:HD3	1:A:796:MSE:HB3	2.01	0.41
1:B:1012:VAL:HG21	1:B:1016:LEU:HD23	2.02	0.41
1:B:879:ARG:HG2	1:B:905:ASP:OD2	2.20	0.41
1:B:939:HIS:HB2	1:B:975:ILE:HD11	2.02	0.41
1:A:1178:ARG:HB2	1:A:1178:ARG:HE	1.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:VAL:O	1:A:442:LEU:HG	2.21	0.41
1:A:428:VAL:HG11	1:A:470:LEU:HB2	2.02	0.41
1:B:67:ALA:O	1:B:137:THR:HG22	2.19	0.41
1:B:227:ARG:HD3	1:B:1089:GLU:HG3	2.00	0.41
1:B:418:HIS:NE2	1:B:480:ASN:OD1	2.38	0.41
1:A:222:ALA:HB2	1:A:229:ILE:HD11	2.01	0.41
1:A:879:ARG:HD3	1:B:879:ARG:HD3	2.02	0.41
1:B:814:GLU:N	1:B:814:GLU:OE2	2.53	0.41
1:A:293:LEU:HD22	1:A:293:LEU:H	1.84	0.41
1:B:107:THR:O	1:B:111:ARG:HG3	2.21	0.41
1:B:836:ASP:HB3	1:B:839:GLN:HB2	2.03	0.41
1:A:677:THR:O	1:A:681:VAL:HG13	2.20	0.41
1:A:725:LEU:HD21	1:A:754:ARG:HE	1.85	0.41
1:A:876:PRO:HB2	1:B:881:VAL:HG12	2.02	0.41
1:B:911:THR:O	1:B:915:THR:HG23	2.21	0.41
1:B:879:ARG:HG2	1:B:879:ARG:H	1.69	0.41
1:A:1054:ALA:HB1	1:A:1104:LEU:HA	2.03	0.41
1:A:1064:ASP:OD1	1:A:1067:ARG:NH2	2.54	0.41
1:A:1091:ILE:HA	1:A:1095:GLY:O	2.21	0.41
1:A:858:HIS:NE2	1:A:863:THR:HG23	2.35	0.41
1:B:889:GLU:H	1:B:889:GLU:CD	2.23	0.41
1:B:94:GLU:HG2	1:B:951:ARG:HD2	2.03	0.41
1:A:671:ASP:N	1:A:671:ASP:OD1	2.47	0.40
1:A:138:ARG:HG3	1:A:362:PHE:CE1	2.56	0.40
1:A:434:THR:OG1	1:A:434:THR:O	2.36	0.40
1:A:912:ILE:HD12	1:A:912:ILE:H	1.86	0.40
1:A:1174:ALA:HB3	1:A:1175:PRO:HD3	2.02	0.40
1:A:544:ARG:HH22	1:A:1049:ASP:HA	1.87	0.40
1:B:808:SER:HB3	1:B:1022:GLY:HA2	2.03	0.40
1:B:191:ARG:HD2	1:B:1094:TYR:CD1	2.56	0.40
1:B:594:ASN:OD1	1:B:595:THR:N	2.54	0.40
1:B:756:LEU:HD11	1:B:780:HIS:HA	2.03	0.40
1:B:788:ARG:NH1	1:B:813:ARG:HH12	2.19	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	1140/1235 (92%)	1081 (95%)	56 (5%)	3 (0%)	41	74
1	B	1137/1235 (92%)	1070 (94%)	61 (5%)	6 (0%)	29	66
All	All	2277/2470 (92%)	2151 (94%)	117 (5%)	9 (0%)	34	70

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1134	PRO
1	B	588	GLY
1	A	560	THR
1	A	1134	PRO
1	B	248	THR
1	B	758	THR
1	B	463	VAL
1	B	672	VAL
1	A	183	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	827/961 (86%)	809 (98%)	18 (2%)	52	80
1	B	807/961 (84%)	798 (99%)	9 (1%)	73	90
All	All	1634/1922 (85%)	1607 (98%)	27 (2%)	60	84

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	114	LEU
1	A	198	PHE
1	A	231	GLU
1	A	334	ARG
1	A	389	SER
1	A	467	LYS
1	A	537	ARG
1	A	646	ASP
1	A	676	LYS
1	A	815	MSE
1	A	879	ARG
1	A	888	ASN
1	A	1067	ARG
1	A	1144	ARG
1	A	1176	ARG
1	A	1180	LEU
1	A	1203	MSE
1	B	198	PHE
1	B	211	TRP
1	B	519	ASP
1	B	587	LEU
1	B	669	CYS
1	B	682	ARG
1	B	860	ARG
1	B	985	MSE
1	B	1064	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	594	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](#)

5 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
2	SO4	A	1301	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	B	1301	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	A	1303	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	B	1302	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	A	1302	-	4,4,4	0.14	0	6,6,6	0.11	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	SO4	1	0
2	A	1302	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	1129/1235 (91%)	0.11	34 (3%)	50 31	43, 76, 115, 138	0
1	B	1128/1235 (91%)	0.10	33 (2%)	51 32	46, 82, 116, 153	0
All	All	2257/2470 (91%)	0.11	67 (2%)	50 31	43, 78, 115, 153	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	717	GLY	4.6
1	B	463	VAL	4.5
1	A	552	ALA	4.3
1	B	540	GLY	4.2
1	B	349	ASP	4.1
1	A	551	TYR	3.8
1	B	682	ARG	3.5
1	A	746	VAL	3.5
1	A	1172	VAL	3.3
1	B	213	ASP	3.2
1	B	633	ALA	3.2
1	B	491	GLY	3.2
1	B	964	LEU	3.2
1	A	762	TRP	3.1
1	B	445	ALA	3.0
1	A	550	GLU	3.0
1	A	563	LEU	2.9
1	B	581	ALA	2.9
1	A	743	ASP	2.9
1	B	444	GLU	2.9
1	B	515	LEU	2.8
1	A	1127	ALA	2.8
1	A	559	GLY	2.8
1	A	691	GLY	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	765	LEU	2.7
1	B	720	VAL	2.7
1	B	551	TYR	2.7
1	B	480	ASN	2.7
1	A	561	ASP	2.7
1	A	261	GLU	2.7
1	A	789	THR	2.7
1	B	464	GLY	2.6
1	A	791	VAL	2.6
1	B	425	ALA	2.5
1	A	582	PRO	2.5
1	A	246	LEU	2.5
1	A	286	VAL	2.4
1	A	631	TRP	2.4
1	A	663	PRO	2.4
1	B	817	THR	2.4
1	A	174	LEU	2.4
1	B	347	GLY	2.3
1	A	693	GLN	2.3
1	B	350	ALA	2.3
1	B	460	ALA	2.3
1	A	760	VAL	2.3
1	B	719	PRO	2.3
1	A	761	THR	2.3
1	A	494	VAL	2.2
1	B	277	LEU	2.2
1	A	732	ALA	2.2
1	A	675	GLY	2.2
1	A	1176	ARG	2.2
1	B	483	ILE	2.1
1	B	465	VAL	2.1
1	B	415	LEU	2.1
1	B	484	ILE	2.1
1	B	449	ALA	2.1
1	A	564	TYR	2.1
1	A	1168	ALA	2.0
1	B	448	ALA	2.0
1	A	231	GLU	2.0
1	B	470	LEU	2.0
1	A	759	GLY	2.0
1	B	741	LEU	2.0
1	B	590	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	272	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	SO4	B	1302	5/5	0.81	0.16	121,128,130,135	0
2	SO4	A	1303	5/5	0.97	0.17	78,81,90,90	0
2	SO4	A	1302	5/5	0.97	0.18	63,63,64,64	0
2	SO4	B	1301	5/5	0.98	0.15	61,66,69,76	0
2	SO4	A	1301	5/5	0.98	0.13	63,69,78,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.