



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 04:09 AM BST

PDB ID : 6JOW  
Title : Exo-beta-D-glucosaminidase from *Pyrococcus furiosus*  
Authors : Mine, S.; Watanabe, M.  
Deposited on : 2019-03-24  
Resolution : 1.75 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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

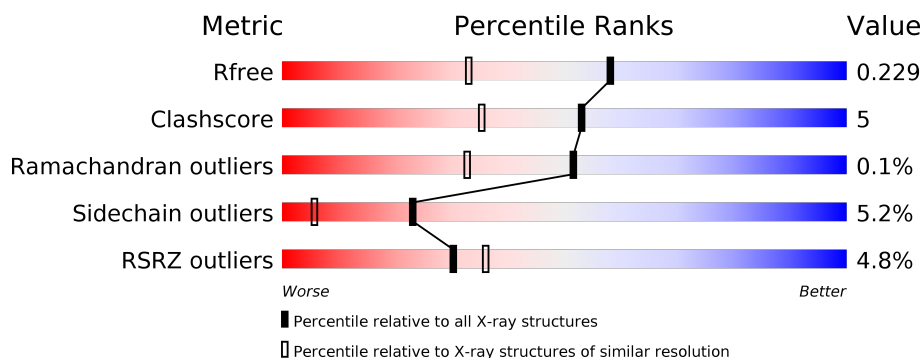
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	762	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>•</div> </div> </div>
1	B	762	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>•</div> </div> </div>
1	C	762	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>•</div> </div> </div>
1	D	762	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>•</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27343 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.

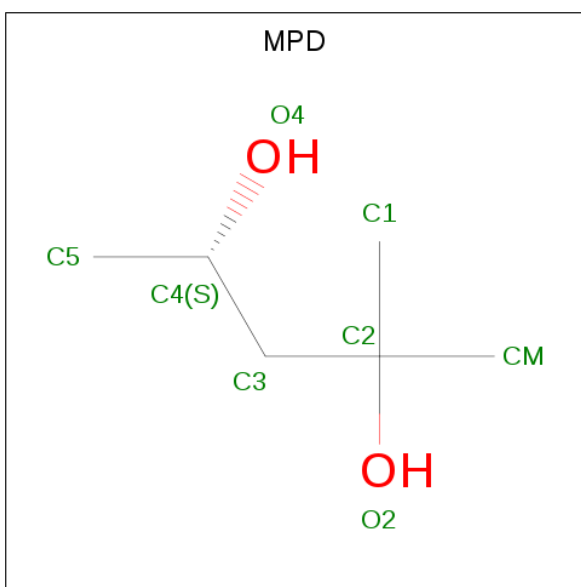
- Molecule 1 is a protein called Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	762	Total	C	N	O	S	0	2	0
			6326	4124	1040	1146	16			
1	B	762	Total	C	N	O	S	0	1	0
			6321	4121	1041	1144	15			
1	C	762	Total	C	N	O	S	0	3	0
			6344	4137	1042	1149	16			
1	D	762	Total	C	N	O	S	0	2	0
			6330	4130	1039	1146	15			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		

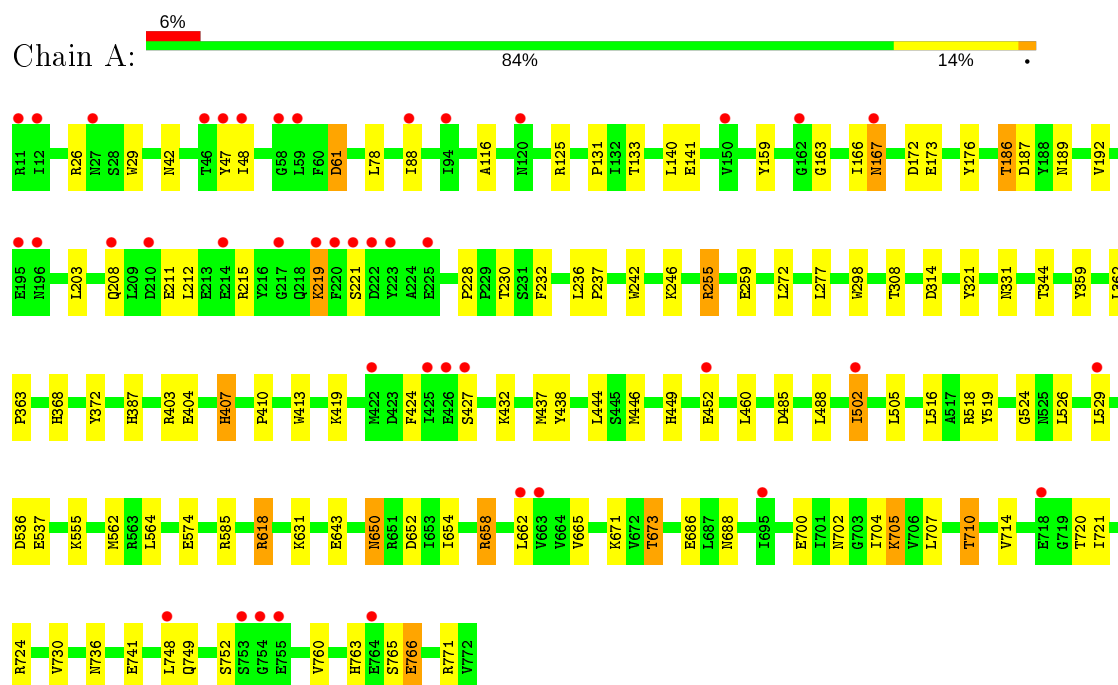
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	432	Total	O	0	0
			432	432		
4	B	488	Total	O	0	0
			488	488		
4	C	532	Total	O	0	0
			532	532		
4	D	504	Total	O	0	0
			504	504		

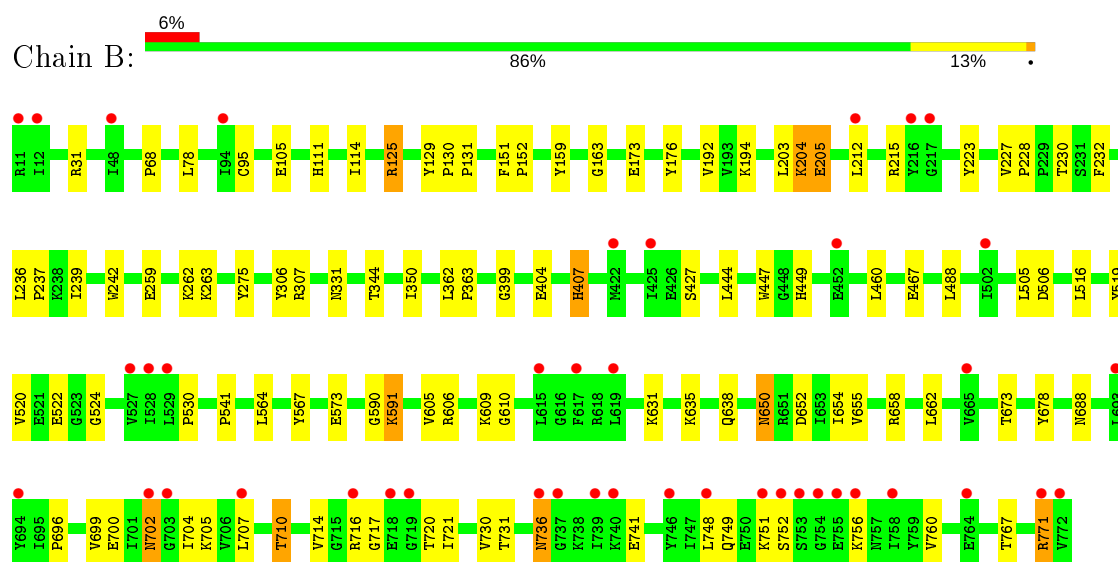
### 3 Residue-property plots

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.

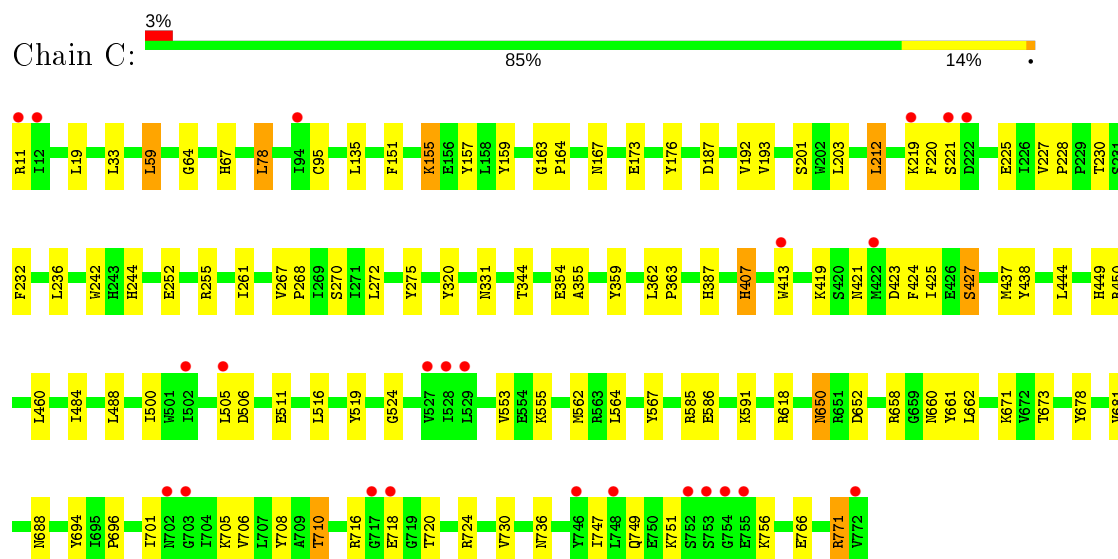
#### • Molecule 1: Beta-galactosidase



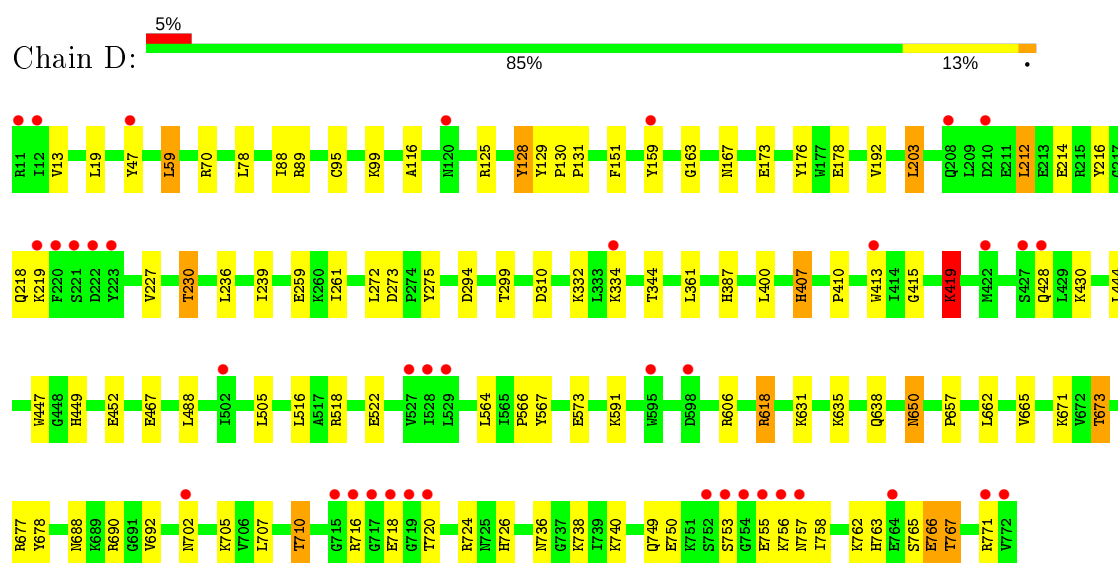
#### • Molecule 1: Beta-galactosidase



## ● Molecule 1: Beta-galactosidase



## ● Molecule 1: Beta-galactosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.13Å 149.60Å 147.31Å 90.00° 102.07° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 29.96 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-1.75) 98.1 (29.96-1.75)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.148 , 0.220 0.154 , 0.229	Depositor DCC
$R_{free}$ test set	17963 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.788	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	27343	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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

### 5.1 Standard geometry

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

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	0.92	10/6508 (0.2%)	1.04	9/8835 (0.1%)
1	B	0.85	4/6503 (0.1%)	0.99	4/8828 (0.0%)
1	C	0.90	4/6525 (0.1%)	0.99	5/8859 (0.1%)
1	D	0.85	6/6517 (0.1%)	0.97	8/8849 (0.1%)
All	All	0.88	24/26053 (0.1%)	1.00	26/35371 (0.1%)

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

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	404	GLU	CD-OE2	-13.07	1.11	1.25
1	C	749	GLN	CD-NE2	12.75	1.64	1.32
1	A	61	ASP	CG-OD1	9.09	1.46	1.25
1	B	399	GLY	C-O	7.89	1.36	1.23
1	D	419	LYS	C-O	7.80	1.38	1.23
1	A	574	GLU	CD-OE2	7.67	1.34	1.25
1	D	467	GLU	CD-OE2	-7.62	1.17	1.25
1	A	167	ASN	CG-ND2	7.33	1.51	1.32
1	A	133	THR	C-O	7.22	1.37	1.23
1	B	467	GLU	CD-OE2	-6.61	1.18	1.25
1	D	452	GLU	CD-OE1	6.55	1.32	1.25
1	C	354	GLU	CD-OE2	6.47	1.32	1.25
1	D	452	GLU	CD-OE2	6.43	1.32	1.25
1	D	566	PRO	C-O	6.18	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	586	GLU	CD-OE2	-6.07	1.19	1.25
1	A	61	ASP	CG-OD2	5.94	1.39	1.25
1	D	99	LYS	C-O	5.89	1.34	1.23
1	A	404	GLU	CD-OE2	-5.84	1.19	1.25
1	C	511	GLU	CD-OE1	5.76	1.31	1.25
1	A	537	GLU	CD-OE2	-5.73	1.19	1.25
1	B	350	ILE	C-O	5.70	1.34	1.23
1	A	502	ILE	C-O	5.64	1.34	1.23
1	A	141	GLU	C-O	5.17	1.33	1.23
1	A	42	ASN	C-O	5.01	1.32	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ASP	CB-CG-OD1	-9.44	109.80	118.30
1	A	61	ASP	CB-CG-OD2	-8.15	110.97	118.30
1	A	618	ARG	CG-CD-NE	-7.73	95.56	111.80
1	D	720	THR	CA-CB-OG1	7.46	124.67	109.00
1	D	70	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	D	125	ARG	CG-CD-NE	-6.70	97.72	111.80
1	C	255	ARG	NE-CZ-NH1	-6.35	117.13	120.30
1	C	450	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	D	128	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	A	658	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	306	TYR	CB-CG-CD1	-5.74	117.56	121.00
1	B	125[A]	ARG	CG-CD-NE	-5.66	99.92	111.80
1	B	125[B]	ARG	CG-CD-NE	-5.66	99.92	111.80
1	C	694	TYR	CB-CG-CD1	5.54	124.33	121.00
1	C	658	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	308	THR	CA-CB-OG1	-5.36	97.75	109.00
1	D	618	ARG	CG-CD-NE	-5.35	100.56	111.80
1	D	310	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	47	TYR	CB-CG-CD2	5.29	124.18	121.00
1	A	125	ARG	CG-CD-NE	-5.25	100.77	111.80
1	A	403	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	D	690	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	359	TYR	CB-CG-CD1	5.13	124.08	121.00
1	D	128	TYR	CB-CG-CD1	5.09	124.05	121.00
1	C	320	TYR	CB-CG-CD1	5.08	124.05	121.00
1	B	307	ARG	NE-CZ-NH1	-5.03	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	ILE	Mainchain
1	A	61	ASP	Sidechain

## 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	6326	0	6257	73	0
1	B	6321	0	6256	65	0
1	C	6344	0	6265	62	0
1	D	6330	0	6259	66	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	16	0	28	4	0
3	B	16	0	28	7	0
3	C	16	0	28	8	0
3	D	16	0	28	4	0
4	A	432	0	0	21	0
4	B	488	0	0	18	0
4	C	532	0	0	13	0
4	D	504	0	0	15	0
All	All	27343	0	25149	273	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 5.

All (273) 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:C:424:PHE:O	1:C:427:SER:HB2	1.48	1.12
1:D:294:ASP:HB2	4:D:1371:HOH:O	1.62	0.98
3:D:902:MPD:HM3	4:D:1003:HOH:O	1.63	0.97
1:D:95:CYS:SG	3:D:902:MPD:H13	2.10	0.91
1:D:766:GLU:HG2	4:D:1391:HOH:O	1.74	0.88
1:D:767:THR:HB	4:D:1073:HOH:O	1.72	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:803:MPD:HM3	4:C:908:HOH:O	1.75	0.87
1:B:771:ARG:HB3	4:B:1053:HOH:O	1.76	0.86
1:C:95:CYS:SG	3:C:803:MPD:H13	2.19	0.83
1:A:671:LYS:HE2	1:A:688[A]:ASN:OD1	1.77	0.82
3:B:901:MPD:HM3	4:B:1400:HOH:O	1.78	0.81
1:C:591:LYS:HE3	3:C:801:MPD:HM1	1.62	0.80
1:A:673:THR:HG22	4:A:1027:HOH:O	1.80	0.80
1:B:31:ARG:NH1	4:B:1001:HOH:O	2.15	0.78
1:D:178:GLU:OE1	4:D:1001:HOH:O	2.02	0.76
1:D:573:GLU:H	1:D:635:LYS:HZ2	1.33	0.76
3:C:803:MPD:H4	4:C:1288:HOH:O	1.87	0.75
1:D:95:CYS:SG	3:D:902:MPD:C1	2.75	0.74
1:B:771:ARG:CB	4:B:1053:HOH:O	2.34	0.72
1:D:702:ASN:HD22	1:D:716:ARG:HG2	1.56	0.70
1:C:449:HIS:ND1	4:C:905:HOH:O	2.25	0.70
1:A:536:ASP:OD2	4:A:901:HOH:O	2.08	0.70
1:B:259:GLU:HG2	4:B:1434:HOH:O	1.92	0.69
1:A:688[A]:ASN:ND2	4:A:904:HOH:O	2.25	0.69
1:C:331:ASN:HB2	4:C:1122:HOH:O	1.93	0.69
1:A:331:ASN:HB2	4:A:1257:HOH:O	1.93	0.68
1:C:671:LYS:HE2	1:C:688:ASN:OD1	1.95	0.66
1:B:331:ASN:HB2	4:B:1088:HOH:O	1.95	0.66
1:A:766:GLU:HG2	4:A:1278:HOH:O	1.95	0.66
1:A:449:HIS:ND1	4:A:908:HOH:O	2.29	0.65
1:A:585:ARG:NH1	4:A:907:HOH:O	2.29	0.65
1:B:654:ILE:CD1	4:B:1076:HOH:O	2.45	0.65
1:B:173:GLU:OE2	3:B:902:MPD:H31	1.97	0.65
1:C:344:THR:O	1:C:407:HIS:HE1	1.78	0.65
1:A:555:LYS:HG3	4:A:1169:HOH:O	1.96	0.65
1:A:167:ASN:ND2	1:A:298:TRP:CZ2	2.67	0.63
1:C:192:VAL:HG22	1:C:193:VAL:HG13	1.79	0.63
1:A:368:HIS:HD2	4:A:1279:HOH:O	1.81	0.62
1:B:631:LYS:HE2	4:B:1098:HOH:O	1.99	0.62
1:D:449:HIS:ND1	4:D:1004:HOH:O	2.30	0.62
1:A:763:HIS:HD2	1:A:765:SER:O	1.81	0.62
1:C:413[B]:TRP:CE3	1:C:724:ARG:HD2	2.34	0.62
1:D:259[A]:GLU:OE1	4:D:1002:HOH:O	2.16	0.61
1:D:671:LYS:HG3	1:D:688:ASN:OD1	2.01	0.60
1:A:654:ILE:HD11	4:A:1005:HOH:O	2.00	0.60
1:D:606:ARG:HD3	4:D:1209:HOH:O	2.01	0.60
1:A:344:THR:O	1:A:407:HIS:HE1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:ASP:CB	4:D:1371:HOH:O	2.35	0.60
1:B:407:HIS:H	1:B:407:HIS:CD2	2.19	0.60
1:A:159:TYR:HA	1:A:163:GLY:O	2.01	0.60
1:A:410:PRO:HA	1:A:413:TRP:CD1	2.38	0.59
1:B:654:ILE:HD11	4:B:1076:HOH:O	2.02	0.59
1:D:407:HIS:CD2	1:D:407:HIS:H	2.19	0.59
1:D:413[A]:TRP:CE3	1:D:724:ARG:HD2	2.37	0.59
1:B:591:LYS:HB2	1:B:591:LYS:NZ	2.18	0.59
1:C:236:LEU:HD11	1:C:444:LEU:HD21	1.84	0.59
1:C:650:ASN:HD22	1:C:650:ASN:C	2.06	0.58
1:C:173:GLU:OE2	3:C:803:MPD:H32	2.03	0.58
1:D:216:TYR:HB3	1:D:218:GLN:OE1	2.03	0.58
1:D:236:LEU:HD11	1:D:444:LEU:HD21	1.85	0.58
1:D:413[A]:TRP:CD2	1:D:724:ARG:HD2	2.39	0.58
1:D:19:LEU:HD23	1:D:19:LEU:C	2.24	0.57
1:A:720:THR:HG22	1:A:771:ARG:HG2	1.87	0.56
1:D:410:PRO:HA	1:D:413[B]:TRP:CD1	2.40	0.56
1:B:204:LYS:HG3	1:B:223:TYR:CE2	2.40	0.56
1:D:705:LYS:HB3	1:D:736:ASN:HB2	1.88	0.56
1:A:407:HIS:H	1:A:407:HIS:CD2	2.24	0.56
1:A:654:ILE:CD1	4:A:1005:HOH:O	2.53	0.56
3:A:802:MPD:H4	4:A:914:HOH:O	2.04	0.56
1:B:702:ASN:ND2	1:B:716:ARG:HB3	2.21	0.55
1:C:720:THR:HG22	1:C:771:ARG:HG2	1.88	0.55
1:C:232:PHE:HB3	1:C:449:HIS:CE1	2.42	0.55
1:C:421:ASN:ND2	1:C:661:TYR:OH	2.33	0.55
1:D:59:LEU:HD12	1:D:59:LEU:C	2.27	0.55
1:A:654:ILE:HB	1:A:665:VAL:HB	1.89	0.55
1:A:255:ARG:O	1:A:259:GLU:HG2	2.06	0.55
1:B:650:ASN:HD22	1:B:652:ASP:H	1.53	0.55
1:A:766:GLU:CG	4:A:1278:HOH:O	2.54	0.54
1:C:591:LYS:HE3	3:C:801:MPD:CM	2.35	0.54
1:C:252:GLU:OE1	4:C:901:HOH:O	2.18	0.54
1:A:362:LEU:HB2	1:A:363:PRO:HD3	1.90	0.54
1:D:332:LYS:O	1:D:334:LYS:NZ	2.41	0.54
1:A:189:ASN:OD1	4:A:902:HOH:O	2.18	0.54
1:C:650:ASN:HD22	1:C:652:ASP:H	1.54	0.54
1:C:710:THR:CG2	4:C:1000:HOH:O	2.55	0.54
1:B:263:LYS:HE2	4:B:1378:HOH:O	2.08	0.54
1:C:33:LEU:HD12	1:C:78:LEU:HD13	1.90	0.53
1:C:407:HIS:CD2	1:C:407:HIS:H	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:518:ARG:O	1:D:522:GLU:HG2	2.07	0.53
1:A:236:LEU:HD11	1:A:444:LEU:HD21	1.90	0.53
1:B:232:PHE:HB3	1:B:449:HIS:CE1	2.43	0.53
1:B:650:ASN:ND2	1:B:652:ASP:H	2.06	0.53
1:A:173:GLU:HA	1:A:272:LEU:O	2.08	0.53
1:A:344:THR:HG21	1:A:372:TYR:HB3	1.91	0.53
1:A:432:LYS:HE2	1:A:643:GLU:O	2.09	0.53
1:B:736:ASN:ND2	1:B:736:ASN:O	2.37	0.53
1:A:173:GLU:OE2	3:A:802:MPD:H53	2.08	0.53
1:A:741:GLU:OE2	1:A:771:ARG:HD2	2.09	0.53
1:C:555:LYS:HG3	4:C:951:HOH:O	2.08	0.52
1:C:650:ASN:ND2	1:C:652:ASP:H	2.07	0.52
1:D:407:HIS:HD2	1:D:407:HIS:H	1.57	0.52
1:A:387:HIS:HA	1:B:567:TYR:CD2	2.45	0.52
1:C:437[B]:MET:HE3	1:C:437[B]:MET:HA	1.92	0.52
1:B:194:LYS:HE2	4:B:1141:HOH:O	2.09	0.51
1:A:232:PHE:HB3	1:A:449:HIS:CE1	2.45	0.51
1:A:671:LYS:CE	1:A:688[A]:ASN:OD1	2.54	0.51
1:D:740:LYS:HE3	1:D:771:ARG:HG2	1.93	0.50
1:A:730:VAL:CG2	1:A:760:VAL:CG1	2.89	0.50
1:B:720:THR:HG22	1:B:771:ARG:HG3	1.92	0.50
1:C:167:ASN:ND2	1:C:270:SER:OG	2.45	0.50
1:D:763:HIS:HD2	1:D:765:SER:O	1.95	0.50
1:B:227:VAL:HG23	4:B:1187:HOH:O	2.12	0.50
1:A:236:LEU:HB3	1:A:237:PRO:HD3	1.93	0.50
1:D:673:THR:HG22	4:D:1049:HOH:O	2.11	0.50
1:B:228:PRO:HB3	1:B:242:TRP:CZ3	2.47	0.50
1:C:484:ILE:HD11	1:C:500:ILE:HD13	1.93	0.50
1:B:650:ASN:C	1:B:650:ASN:HD22	2.16	0.49
1:B:771:ARG:CG	4:B:1053:HOH:O	2.58	0.49
1:D:273:ASP:OD1	1:D:299:THR:HA	2.11	0.49
1:B:606:ARG:NH2	4:B:1015:HOH:O	2.44	0.49
1:B:68:PRO:CD	3:B:901:MPD:HM1	2.42	0.49
1:C:720:THR:HG22	1:C:771:ARG:CG	2.42	0.49
1:A:246:LYS:HE3	4:A:1133:HOH:O	2.12	0.49
1:D:738:LYS:HA	1:D:757:ASN:HD22	1.77	0.49
1:B:236:LEU:HD11	1:B:444:LEU:HD21	1.94	0.49
1:D:400:LEU:CD1	4:D:1155:HOH:O	2.61	0.49
1:B:427:SER:HB2	1:B:658:ARG:O	2.13	0.49
3:D:902:MPD:H4	4:D:1290:HOH:O	2.11	0.49
1:C:413[B]:TRP:CE3	1:C:724:ARG:CD	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:PHE:O	1:A:427:SER:OG	2.19	0.48
1:A:48:ILE:HD11	1:A:88:ILE:HD11	1.94	0.48
1:B:741:GLU:HB3	1:B:771:ARG:HD2	1.93	0.48
1:D:428:GLN:HB2	1:D:430:LYS:HE3	1.95	0.48
1:B:696:PRO:HB2	1:B:699:VAL:CG1	2.44	0.48
3:C:803:MPD:H11	4:C:908:HOH:O	2.12	0.48
1:C:362:LEU:HB2	1:C:363:PRO:HD3	1.96	0.47
1:C:678:TYR:O	1:C:681:VAL:HG22	2.14	0.47
1:B:173:GLU:OE2	3:B:902:MPD:H53	2.15	0.47
1:B:205:GLU:HA	1:B:205:GLU:OE1	2.09	0.47
1:D:573:GLU:H	1:D:635:LYS:NZ	2.09	0.47
1:B:68:PRO:HD3	3:B:901:MPD:HM1	1.96	0.47
1:A:686:GLU:HG2	1:A:688[A]:ASN:ND2	2.30	0.47
1:A:688[A]:ASN:CG	4:A:904:HOH:O	2.54	0.47
1:A:710:THR:O	1:A:710:THR:CG2	2.63	0.47
1:B:591:LYS:HD2	4:B:1477:HOH:O	2.14	0.47
1:D:710:THR:O	1:D:710:THR:CG2	2.63	0.47
1:A:173:GLU:OE2	3:A:802:MPD:H31	2.15	0.47
1:B:159:TYR:HA	1:B:163:GLY:O	2.15	0.46
1:B:520:VAL:O	1:B:610:GLY:HA3	2.14	0.46
1:D:665:VAL:HB	1:D:692:VAL:HG22	1.98	0.46
1:B:215:ARG:NH2	1:B:237:PRO:HB3	2.31	0.46
1:C:407:HIS:HD2	1:C:407:HIS:H	1.61	0.46
1:C:413[A]:TRP:CH2	4:C:1048:HOH:O	2.56	0.46
1:D:650:ASN:C	1:D:650:ASN:HD22	2.17	0.46
1:D:710:THR:HG23	4:D:1395:HOH:O	2.15	0.46
1:B:662:LEU:HD13	1:B:678:TYR:CE2	2.49	0.46
1:C:201:SER:HB2	4:C:1201:HOH:O	2.15	0.46
1:D:415:GLY:O	1:D:419:LYS:HD3	2.14	0.46
1:C:151:PHE:CZ	1:C:261:ILE:HG12	2.51	0.46
1:B:631:LYS:NZ	4:B:1019:HOH:O	2.47	0.46
1:C:19:LEU:HD23	1:C:19:LEU:C	2.36	0.46
1:A:529:LEU:HD23	1:A:529:LEU:N	2.31	0.46
1:C:220:PHE:HA	1:C:225:GLU:OE1	2.16	0.46
1:B:239:ILE:HG22	1:B:447:TRP:CH2	2.51	0.46
1:B:704:ILE:HD12	1:B:721:ILE:HG13	1.97	0.46
1:B:707:LEU:HD23	1:B:756:LYS:HE3	1.98	0.46
1:C:228:PRO:HB3	1:C:242:TRP:CZ3	2.51	0.46
1:C:78:LEU:HA	1:C:78:LEU:HD23	1.73	0.46
1:B:95:CYS:SG	3:B:902:MPD:H32	2.56	0.45
1:B:407:HIS:H	1:B:407:HIS:HD2	1.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:TYR:HA	1:D:163:GLY:O	2.16	0.45
3:B:902:MPD:H4	4:B:1048:HOH:O	2.15	0.45
1:C:437[B]:MET:HG3	1:C:438:TYR:N	2.32	0.45
1:A:407:HIS:HD2	1:A:407:HIS:H	1.64	0.45
1:D:19:LEU:C	1:D:19:LEU:CD2	2.85	0.45
1:A:26:ARG:HA	1:A:29:TRP:CE2	2.52	0.45
1:C:387:HIS:HA	1:D:567:TYR:CD2	2.52	0.45
1:D:47:TYR:HA	1:D:89:ARG:O	2.16	0.45
1:A:650:ASN:C	1:A:650:ASN:HD22	2.20	0.45
1:D:239:ILE:HG22	1:D:447:TRP:CH2	2.52	0.45
1:A:519:TYR:CZ	1:A:524:GLY:HA3	2.51	0.44
1:B:702:ASN:CG	1:B:717:GLY:O	2.55	0.44
1:D:216:TYR:CD1	1:D:216:TYR:N	2.86	0.44
1:A:650:ASN:ND2	1:A:652:ASP:H	2.16	0.44
1:A:650:ASN:HD22	1:A:652:ASP:H	1.64	0.44
1:A:705:LYS:HB3	1:A:736:ASN:HB2	2.00	0.44
1:B:519:TYR:CZ	1:B:524:GLY:HA3	2.53	0.44
1:C:159:TYR:HA	1:C:163:GLY:O	2.18	0.44
1:C:424:PHE:O	1:C:427:SER:CB	2.41	0.44
1:C:59:LEU:HD12	1:C:59:LEU:C	2.37	0.44
1:C:701:ILE:HG23	1:C:716:ARG:NH1	2.33	0.44
1:A:172:ASP:O	1:A:173:GLU:C	2.56	0.44
1:B:720:THR:HG22	1:B:771:ARG:CG	2.48	0.44
1:B:344:THR:O	1:B:407:HIS:HE1	2.00	0.44
1:B:204:LYS:HG3	1:B:223:TYR:CD2	2.53	0.44
1:A:116:ALA:HB3	1:A:131:PRO:HB2	2.00	0.43
1:C:747:ILE:HD12	1:C:747:ILE:N	2.33	0.43
1:A:167:ASN:ND2	1:A:298:TRP:HZ2	2.15	0.43
1:A:427:SER:HB2	1:A:658:ARG:O	2.18	0.43
1:C:227:VAL:HG22	4:C:1369:HOH:O	2.17	0.43
1:D:173:GLU:HA	1:D:272:LEU:O	2.18	0.43
1:B:591:LYS:HB2	1:B:591:LYS:HZ2	1.82	0.43
1:B:662:LEU:HD13	1:B:678:TYR:CD2	2.53	0.43
1:A:208:GLN:O	1:A:211:GLU:HB2	2.19	0.43
1:A:437[A]:MET:HG3	1:A:438:TYR:N	2.33	0.43
1:A:631:LYS:CE	4:A:1293:HOH:O	2.66	0.43
1:C:662:LEU:HA	1:C:662:LEU:HD12	1.86	0.43
1:A:631:LYS:HE2	4:A:927:HOH:O	2.18	0.43
1:D:662:LEU:HD12	1:D:662:LEU:HA	1.86	0.43
1:A:321:TYR:OH	1:A:437[A]:MET:HG2	2.19	0.42
1:D:344:THR:O	1:D:407:HIS:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:657:PRO:HA	1:D:662:LEU:HD12	2.01	0.42
1:C:244:HIS:ND1	4:C:915:HOH:O	2.36	0.42
1:B:655:VAL:HG13	1:B:662:LEU:HG	2.02	0.42
4:B:1175:HOH:O	3:C:801:MPD:HM3	2.20	0.42
1:D:662:LEU:HD13	1:D:678:TYR:CE2	2.54	0.42
1:A:255:ARG:HH21	1:A:255:ARG:HB3	1.84	0.42
1:D:203:LEU:HG	1:D:212:LEU:HD21	2.01	0.42
1:C:173:GLU:HA	1:C:272:LEU:O	2.19	0.42
1:D:230:THR:HG21	4:D:1355:HOH:O	2.20	0.42
1:A:662:LEU:HD12	1:A:662:LEU:HA	1.88	0.42
1:C:355:ALA:HB1	1:C:359:TYR:CE2	2.54	0.42
1:D:203:LEU:HD12	1:D:203:LEU:HA	1.92	0.42
1:D:631:LYS:HE2	4:D:1226:HOH:O	2.20	0.42
1:D:88:ILE:HD12	1:D:88:ILE:HA	1.94	0.42
1:D:413[A]:TRP:CD2	1:D:724:ARG:CD	3.02	0.41
1:D:151:PHE:CZ	1:D:261:ILE:HG12	2.55	0.41
1:A:368:HIS:CE1	4:A:1242:HOH:O	2.72	0.41
1:A:704:ILE:HD12	1:A:721:ILE:HG13	2.01	0.41
1:C:553:VAL:HG12	1:C:585:ARG:HD3	2.01	0.41
1:D:707:LEU:HD23	1:D:756:LYS:HE3	2.02	0.41
1:A:186:THR:HG23	1:A:187:ASP:HB2	2.02	0.41
1:A:368:HIS:HE1	4:A:1242:HOH:O	2.02	0.41
1:B:151:PHE:N	1:B:152:PRO:CD	2.84	0.41
1:D:766:GLU:HG3	1:D:766:GLU:H	1.50	0.41
1:B:130:PRO:HA	1:B:131:PRO:HD3	1.92	0.41
1:C:157:TYR:O	1:C:164:PRO:HD2	2.20	0.41
1:C:519:TYR:CZ	1:C:524:GLY:HA3	2.55	0.41
1:C:696:PRO:O	1:C:708:TYR:HA	2.20	0.41
1:D:128:TYR:O	1:D:129:TYR:C	2.59	0.41
1:A:502:ILE:HD12	1:A:526:LEU:HD22	2.03	0.41
1:B:362:LEU:HB2	1:B:363:PRO:HD3	2.01	0.41
1:B:573:GLU:HB2	1:B:635:LYS:NZ	2.36	0.41
1:D:212:LEU:HD12	1:D:212:LEU:HA	1.96	0.41
1:D:726:HIS:HA	1:D:766:GLU:HB3	2.03	0.41
1:A:432:LYS:CE	1:A:643:GLU:O	2.68	0.41
1:B:105:GLU:OE2	1:B:125[B]:ARG:NH2	2.53	0.41
1:C:64:GLY:HA2	1:C:67:HIS:O	2.21	0.41
1:B:129:TYR:O	1:B:130:PRO:C	2.59	0.41
1:C:567:TYR:CD1	1:D:387:HIS:HA	2.56	0.41
1:A:228:PRO:HB3	1:A:242:TRP:CZ3	2.56	0.41
1:A:730:VAL:HG23	1:A:760:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:705:LYS:HG2	1:C:736:ASN:HD22	1.86	0.41
1:B:590:GLY:HA3	1:B:605:VAL:HG22	2.02	0.40
1:C:212:LEU:HA	1:C:212:LEU:HD12	1.94	0.40
1:A:219:LYS:HD2	1:A:219:LYS:N	2.35	0.40
1:A:437[B]:MET:HE3	1:A:485:ASP:HB2	2.03	0.40
3:A:802:MPD:C4	4:A:914:HOH:O	2.67	0.40
1:B:710:THR:HG22	1:B:731:THR:HA	2.03	0.40
1:C:155:LYS:CD	4:C:1291:HOH:O	2.69	0.40
1:D:116:ALA:HB3	1:D:131:PRO:HB2	2.03	0.40
1:A:215:ARG:HB3	1:A:215:ARG:CZ	2.51	0.40
1:C:187:ASP:O	1:C:192:VAL:HG21	2.21	0.40
1:C:267:VAL:HB	1:C:268:PRO:HD2	2.04	0.40
1:D:130:PRO:HA	1:D:131:PRO:HD3	1.93	0.40
1:D:361:LEU:HD21	1:D:665:VAL:HG11	2.04	0.40
1:B:111:HIS:O	1:B:114:ILE:HG12	2.20	0.40
1:B:749:GLN:HB3	1:B:760:VAL:HB	2.03	0.40
1:A:277:LEU:HD21	1:A:446:MET:SD	2.62	0.40
1:B:407:HIS:CD2	1:B:407:HIS:N	2.88	0.40
1:B:702:ASN:HD21	1:B:716:ARG:HB3	1.86	0.40
1:D:606:ARG:HG3	1:D:606:ARG:HH11	1.87	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	762/762 (100%)	727 (95%)	34 (4%)	1 (0%)	51	33
1	B	761/762 (100%)	726 (95%)	35 (5%)	0	100	100
1	C	763/762 (100%)	733 (96%)	29 (4%)	1 (0%)	51	33
1	D	762/762 (100%)	726 (95%)	35 (5%)	1 (0%)	51	33
All	All	3048/3048 (100%)	2912 (96%)	133 (4%)	3 (0%)	51	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	758	ILE
1	C	718	GLU
1	A	702	ASN

### 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	684/682 (100%)	649 (95%)	35 (5%)	24	6
1	B	683/682 (100%)	645 (94%)	38 (6%)	21	5
1	C	685/682 (100%)	650 (95%)	35 (5%)	24	6
1	D	684/682 (100%)	650 (95%)	34 (5%)	24	6
All	All	2736/2728 (100%)	2594 (95%)	142 (5%)	23	6

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	140	LEU
1	A	176	TYR
1	A	186	THR
1	A	192	VAL
1	A	203	LEU
1	A	212	LEU
1	A	219	LYS
1	A	221	SER
1	A	230	THR
1	A	255	ARG
1	A	314	ASP
1	A	407	HIS
1	A	419	LYS
1	A	452	GLU
1	A	460	LEU
1	A	488	LEU

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Mol	Chain	Res	Type
1	A	505	LEU
1	A	516	LEU
1	A	518	ARG
1	A	562	MET
1	A	564	LEU
1	A	618	ARG
1	A	650	ASN
1	A	673	THR
1	A	700	GLU
1	A	705	LYS
1	A	707	LEU
1	A	710	THR
1	A	714	VAL
1	A	724	ARG
1	A	748	LEU
1	A	749	GLN
1	A	752	SER
1	A	766	GLU
1	B	78	LEU
1	B	176	TYR
1	B	192	VAL
1	B	203	LEU
1	B	204	LYS
1	B	205	GLU
1	B	212	LEU
1	B	230	THR
1	B	262	LYS
1	B	275	TYR
1	B	407	HIS
1	B	460	LEU
1	B	488	LEU
1	B	505	LEU
1	B	506	ASP
1	B	516	LEU
1	B	522	GLU
1	B	530	PRO
1	B	541	PRO
1	B	564	LEU
1	B	591	LYS
1	B	609	LYS
1	B	638	GLN
1	B	650	ASN

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Mol	Chain	Res	Type
1	B	673	THR
1	B	688	ASN
1	B	700	GLU
1	B	702	ASN
1	B	705	LYS
1	B	710	THR
1	B	714	VAL
1	B	730	VAL
1	B	736	ASN
1	B	748	LEU
1	B	751	LYS
1	B	752	SER
1	B	767	THR
1	B	771	ARG
1	C	11	ARG
1	C	59	LEU
1	C	78	LEU
1	C	135	LEU
1	C	155	LYS
1	C	176	TYR
1	C	203	LEU
1	C	212	LEU
1	C	219	LYS
1	C	221	SER
1	C	230	THR
1	C	275	TYR
1	C	407	HIS
1	C	419	LYS
1	C	423	ASP
1	C	425	ILE
1	C	427	SER
1	C	460	LEU
1	C	488	LEU
1	C	505	LEU
1	C	506	ASP
1	C	516	LEU
1	C	562	MET
1	C	564	LEU
1	C	618	ARG
1	C	650	ASN
1	C	660	ASN
1	C	673	THR

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Mol	Chain	Res	Type
1	C	706	VAL
1	C	710	THR
1	C	730	VAL
1	C	751	LYS
1	C	756	LYS
1	C	766	GLU
1	C	771	ARG
1	D	13	VAL
1	D	59	LEU
1	D	78	LEU
1	D	167	ASN
1	D	176	TYR
1	D	192	VAL
1	D	203	LEU
1	D	212	LEU
1	D	214	GLU
1	D	219	LYS
1	D	227	VAL
1	D	230	THR
1	D	275	TYR
1	D	407	HIS
1	D	419	LYS
1	D	488	LEU
1	D	505	LEU
1	D	516	LEU
1	D	564	LEU
1	D	591	LYS
1	D	618	ARG
1	D	638	GLN
1	D	650	ASN
1	D	673	THR
1	D	677	ARG
1	D	710	THR
1	D	718	GLU
1	D	749	GLN
1	D	750	GLU
1	D	753	SER
1	D	755	GLU
1	D	762	LYS
1	D	766	GLU
1	D	767	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	251	ASN
1	A	407	HIS
1	A	638	GLN
1	A	650	ASN
1	A	660	ASN
1	A	763	HIS
1	B	69	GLN
1	B	407	HIS
1	B	449	HIS
1	B	496	GLN
1	B	650	ASN
1	B	688	ASN
1	B	702	ASN
1	C	167	ASN
1	C	196	ASN
1	C	407	HIS
1	C	421	ASN
1	C	428	GLN
1	C	525	ASN
1	C	650	ASN
1	C	763	HIS
1	D	167	ASN
1	D	407	HIS
1	D	650	ASN
1	D	702	ASN
1	D	763	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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
3	MPD	C	801	-	7,7,7	0.83	0	9,10,10	1.21	1 (11%)
3	MPD	B	901	-	7,7,7	0.34	0	9,10,10	0.77	0
3	MPD	B	902	-	7,7,7	0.63	0	9,10,10	1.00	1 (11%)
3	MPD	D	901	-	7,7,7	0.41	0	9,10,10	0.37	0
3	MPD	C	803	-	7,7,7	0.98	0	9,10,10	0.73	0
3	MPD	A	803	-	7,7,7	0.36	0	9,10,10	0.41	0
3	MPD	A	802	-	7,7,7	1.03	1 (14%)	9,10,10	0.86	0
3	MPD	D	902	-	7,7,7	1.43	2 (28%)	9,10,10	1.41	1 (11%)

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	MPD	C	801	-	-	0/5/5/5	-
3	MPD	B	901	-	-	4/5/5/5	-
3	MPD	B	902	-	-	2/5/5/5	-
3	MPD	D	901	-	-	3/5/5/5	-
3	MPD	C	803	-	-	3/5/5/5	-
3	MPD	A	803	-	-	0/5/5/5	-
3	MPD	A	802	-	-	2/5/5/5	-
3	MPD	D	902	-	-	2/5/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	902	MPD	O4-C4	2.55	1.54	1.43
3	D	902	MPD	O2-C2	2.20	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	MPD	O2-C2	2.02	1.49	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	902	MPD	O4-C4-C3	3.21	124.33	111.36
3	C	801	MPD	C5-C4-C3	2.17	121.92	111.69
3	B	902	MPD	O2-C2-CM	2.11	114.86	108.08

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	901	MPD	O2-C2-C3-C4
3	B	901	MPD	CM-C2-C3-C4
3	A	802	MPD	C2-C3-C4-C5
3	C	803	MPD	O2-C2-C3-C4
3	B	902	MPD	C2-C3-C4-C5
3	D	902	MPD	C2-C3-C4-O4
3	B	901	MPD	C1-C2-C3-C4
3	D	901	MPD	C1-C2-C3-C4
3	C	803	MPD	C1-C2-C3-C4
3	C	803	MPD	CM-C2-C3-C4
3	D	901	MPD	O2-C2-C3-C4
3	D	902	MPD	C2-C3-C4-C5
3	B	901	MPD	C2-C3-C4-O4
3	B	902	MPD	C2-C3-C4-O4
3	D	901	MPD	C2-C3-C4-O4
3	A	802	MPD	C2-C3-C4-O4

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	801	MPD	3	0
3	B	901	MPD	3	0
3	B	902	MPD	4	0
3	C	803	MPD	5	0
3	A	802	MPD	4	0
3	D	902	MPD	4	0



## 5.7 Other polymers

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	762/762 (100%)	0.02	42 (5%)	25 31	20, 36, 68, 109	0
1	B	762/762 (100%)	-0.06	42 (5%)	25 31	19, 32, 67, 117	0
1	C	762/762 (100%)	-0.23	24 (3%)	49 55	19, 29, 66, 95	0
1	D	762/762 (100%)	-0.08	39 (5%)	28 34	21, 33, 68, 107	0
All	All	3048/3048 (100%)	-0.09	147 (4%)	30 36	19, 32, 67, 117	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	ARG	7.1
1	B	11	ARG	5.2
1	B	718	GLU	5.2
1	D	221	SER	4.9
1	B	425	ILE	4.8
1	A	217	GLY	4.8
1	B	755	GLU	4.8
1	A	150	VAL	4.7
1	A	422	MET	4.6
1	B	702	ASN	4.4
1	C	11	ARG	4.2
1	C	12	ILE	4.2
1	A	220	PHE	4.0
1	B	772	VAL	4.0
1	A	718	GLU	4.0
1	D	220	PHE	3.9
1	D	413[A]	TRP	3.9
1	B	754	GLY	3.9
1	C	718	GLU	3.9
1	A	210	ASP	3.8
1	B	529	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	94	ILE	3.6
1	D	754	GLY	3.6
1	D	12	ILE	3.6
1	A	425	ILE	3.5
1	A	47	TYR	3.5
1	A	221	SER	3.5
1	A	219	LYS	3.4
1	D	428	GLN	3.4
1	B	751	LYS	3.4
1	D	502	ILE	3.3
1	C	772	VAL	3.2
1	C	422	MET	3.2
1	B	12	ILE	3.2
1	C	748	LEU	3.2
1	C	702	ASN	3.2
1	A	222	ASP	3.1
1	D	718	GLU	3.1
1	A	48	ILE	3.1
1	B	528	ILE	3.1
1	C	94	ILE	3.1
1	C	502	ILE	3.0
1	B	746	TYR	3.0
1	B	719	GLY	3.0
1	A	748	LEU	3.0
1	C	755	GLU	3.0
1	A	764	GLU	2.9
1	D	716	ARG	2.9
1	B	527	VAL	2.9
1	D	219	LYS	2.9
1	B	217	GLY	2.9
1	A	502	ILE	2.9
1	D	222	ASP	2.9
1	C	746	TYR	2.9
1	D	159	TYR	2.9
1	A	214	GLU	2.8
1	C	754	GLY	2.8
1	A	529	LEU	2.8
1	C	529	LEU	2.8
1	D	210	ASP	2.8
1	B	736	ASN	2.8
1	C	752	SER	2.8
1	D	427	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	753	SER	2.8
1	D	755	GLU	2.8
1	B	422	MET	2.8
1	D	756	LYS	2.8
1	A	167	ASN	2.7
1	B	615	LEU	2.7
1	A	208	GLN	2.7
1	B	716	ARG	2.7
1	A	755	GLU	2.6
1	B	502	ILE	2.6
1	A	225	GLU	2.6
1	B	617	PHE	2.6
1	A	452	GLU	2.6
1	C	528	ILE	2.6
1	A	46	THR	2.6
1	D	529	LEU	2.6
1	B	752	SER	2.6
1	A	120	ASN	2.6
1	C	717	GLY	2.6
1	D	528	ILE	2.6
1	D	772	VAL	2.6
1	D	422	MET	2.6
1	D	752	SER	2.5
1	A	427	SER	2.5
1	B	703	GLY	2.5
1	A	195	GLU	2.5
1	D	720	THR	2.5
1	D	527	VAL	2.5
1	B	771	ARG	2.5
1	A	162	GLY	2.5
1	D	598	ASP	2.4
1	D	702	ASN	2.4
1	A	88	ILE	2.4
1	C	219	LYS	2.4
1	A	12	ILE	2.4
1	B	764	GLU	2.4
1	A	754	GLY	2.4
1	C	505	LEU	2.3
1	C	221	SER	2.3
1	B	748	LEU	2.3
1	C	413[A]	TRP	2.3
1	B	753	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	756	LYS	2.3
1	D	764	GLU	2.3
1	B	94	ILE	2.3
1	D	334	LYS	2.3
1	D	47	TYR	2.3
1	A	196	ASN	2.3
1	D	223	TYR	2.2
1	B	737	GLY	2.2
1	D	719	GLY	2.2
1	D	757	ASN	2.2
1	B	758	ILE	2.2
1	A	753	SER	2.2
1	A	223	TYR	2.2
1	C	527	VAL	2.2
1	B	48	ILE	2.2
1	D	717	GLY	2.2
1	B	452	GLU	2.2
1	D	771	ARG	2.2
1	A	59	LEU	2.2
1	A	662	LEU	2.2
1	C	222	ASP	2.2
1	D	595	TRP	2.2
1	A	58	GLY	2.1
1	D	208	GLN	2.1
1	A	426	GLU	2.1
1	D	120	ASN	2.1
1	B	216	TYR	2.1
1	B	212	LEU	2.1
1	B	619	LEU	2.1
1	B	740	LYS	2.1
1	C	753	SER	2.1
1	B	739	ILE	2.1
1	C	703	GLY	2.1
1	A	27	ASN	2.1
1	B	693	LEU	2.1
1	B	707	LEU	2.1
1	B	694	TYR	2.0
1	D	715	GLY	2.0
1	A	663	VAL	2.0
1	A	695	ILE	2.0
1	D	11	ARG	2.0
1	B	665	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
3	MPD	B	902	8/8	0.62	0.26	32,47,54,63	0
3	MPD	C	801	8/8	0.75	0.25	46,53,65,99	0
3	MPD	A	802	8/8	0.77	0.20	45,50,55,60	0
3	MPD	C	803	8/8	0.79	0.23	43,52,68,70	0
3	MPD	A	803	8/8	0.86	0.18	32,38,60,62	0
3	MPD	D	902	8/8	0.86	0.16	36,42,58,69	0
3	MPD	B	901	8/8	0.96	0.07	31,34,36,38	0
3	MPD	D	901	8/8	0.96	0.09	24,32,35,39	0
2	CA	C	802	1/1	0.99	0.03	47,47,47,47	0
2	CA	A	801	1/1	0.99	0.07	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.