Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2026 – 11:29 AM UTC

PDB ID	:	6JOW / pdb_00006jow
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

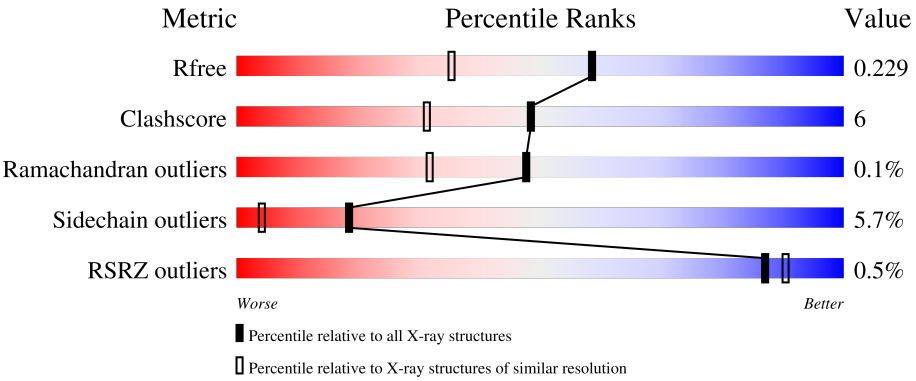
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	% 79% 19% .
1	B	762	83% 15% .
1	C	762	82% 16% .
1	D	762	83% 15% .

2 Entry composition (i)

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.

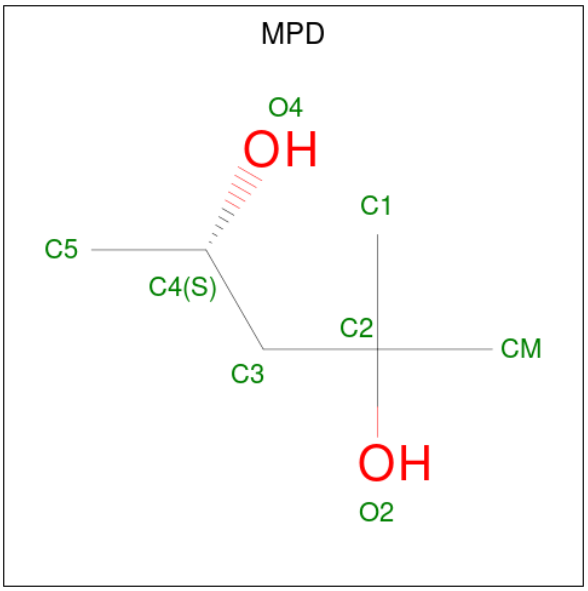
- Molecule 1 is a protein called Beta-galactosidase.

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 (CCD ID: 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 (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



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

- Molecule 4 is water.

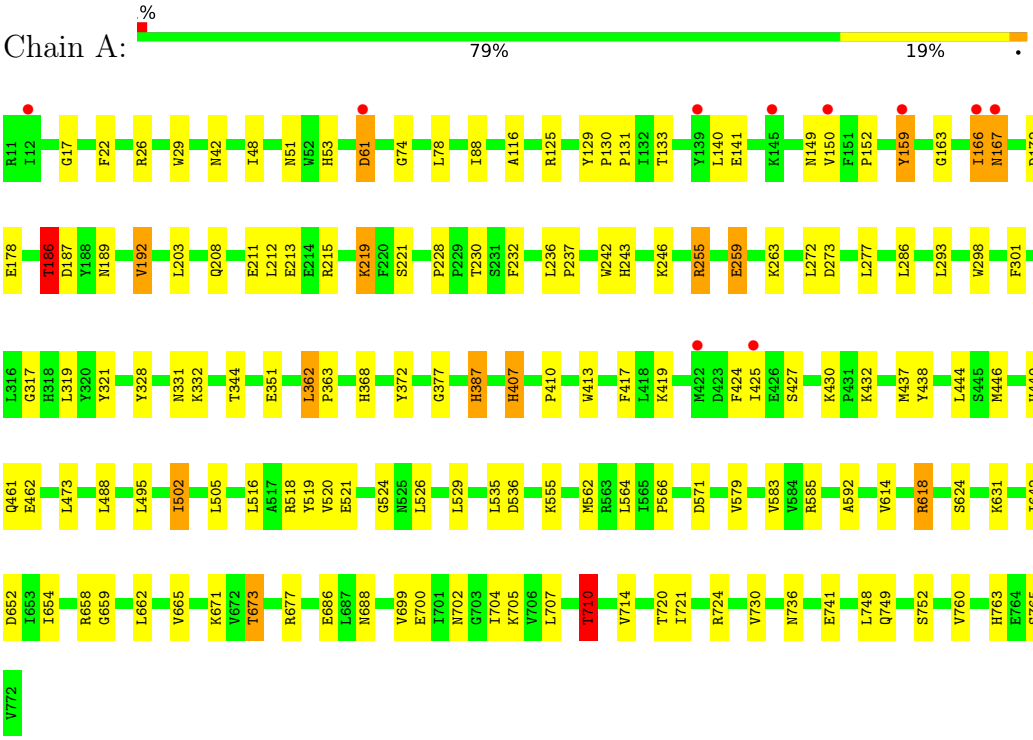
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	432	Total O 432 432	0	0
4	B	488	Total O 488 488	0	0
4	C	532	Total O 532 532	0	0
4	D	504	Total O 504 504	0	0

3 Residue-property plots (i)

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.

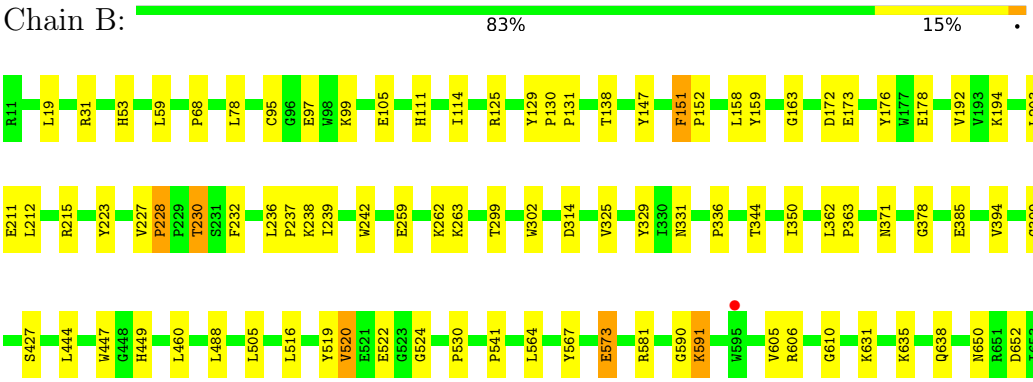
• Molecule 1: Beta-galactosidase

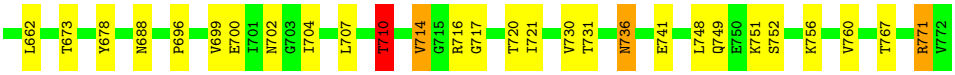
Chain A:



• Molecule 1: Beta-galactosidase

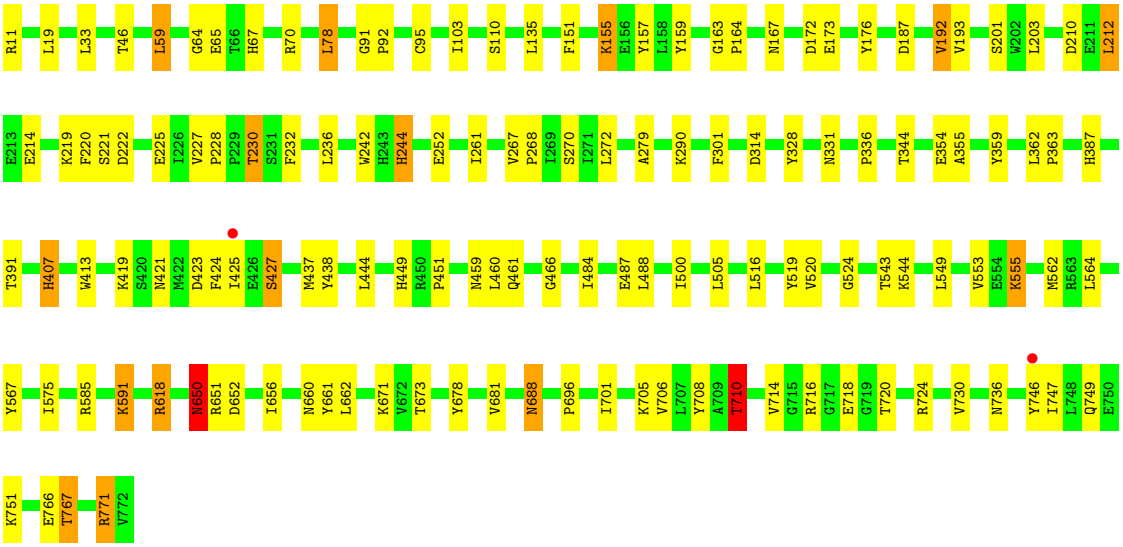
Chain B:





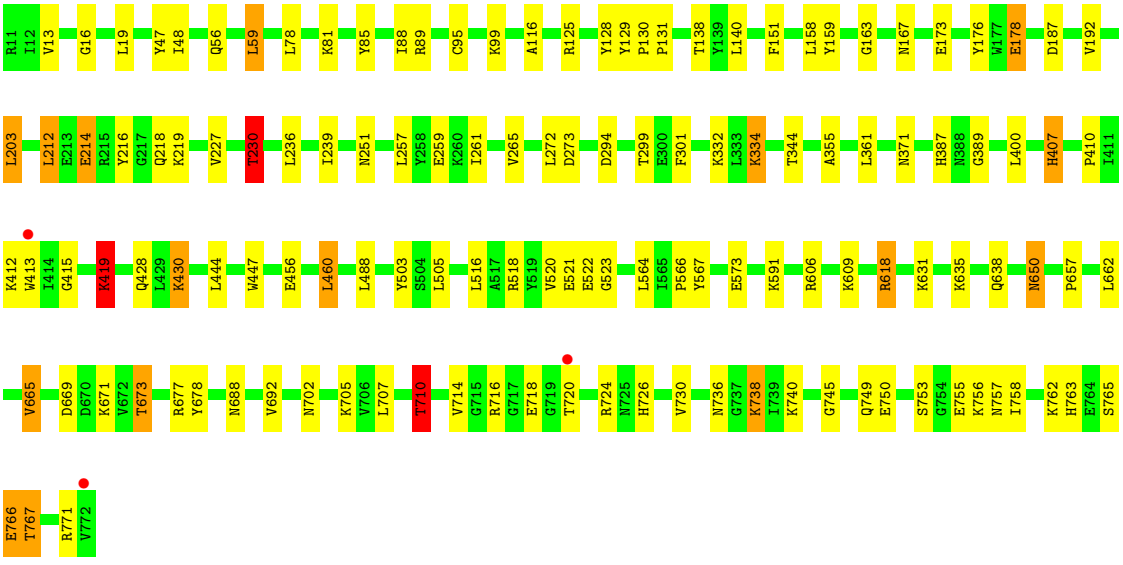
• Molecule 1: Beta-galactosidase

Chain C:



• Molecule 1: Beta-galactosidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.13Å 149.60Å 147.31Å 90.00° 102.07° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 30.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-1.75) 98.4 (30.00-1.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	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 (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	18.8	Xtriage
Anisotropy	0.788	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MPD, CA

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	1.29	37/6508 (0.6%)	1.44	23/8835 (0.3%)
1	B	1.19	14/6503 (0.2%)	1.39	19/8828 (0.2%)
1	C	1.24	20/6525 (0.3%)	1.35	20/8859 (0.2%)
1	D	1.20	14/6517 (0.2%)	1.38	21/8849 (0.2%)
All	All	1.23	85/26053 (0.3%)	1.39	83/35371 (0.2%)

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 (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	749	GLN	CD-NE2	14.99	1.64	1.33
1	A	61	ASP	CG-OD1	11.00	1.46	1.25
1	D	419	LYS	C-O	10.71	1.38	1.24
1	A	133	THR	C-O	10.39	1.37	1.24
1	D	566	PRO	C-O	10.05	1.35	1.23
1	A	502	ILE	C-O	9.63	1.34	1.24
1	B	399	GLY	C-O	8.67	1.36	1.23
1	A	167	ASN	CG-ND2	8.54	1.51	1.33
1	B	350	ILE	C-O	8.42	1.34	1.24
1	D	99	LYS	C-O	8.38	1.34	1.24
1	C	459	ASN	C-O	8.10	1.32	1.23
1	A	141	GLU	C-O	7.69	1.33	1.24
1	A	642	ILE	C-O	7.56	1.32	1.24
1	B	404	GLU	CD-OE2	-7.41	1.11	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	290	LYS	C-O	7.31	1.32	1.24
1	A	61	ASP	CG-OD2	7.20	1.39	1.25
1	A	152	PRO	C-O	7.07	1.32	1.24
1	A	462	GLU	N-CA	6.92	1.54	1.46
1	A	319	LEU	C-O	6.84	1.32	1.24
1	B	238	LYS	C-O	6.78	1.32	1.24
1	C	746	TYR	C-O	6.76	1.32	1.23
1	A	42	ASN	C-O	6.58	1.32	1.24
1	A	317	GLY	C-O	6.55	1.31	1.23
1	C	244	HIS	ND1-CE1	6.50	1.39	1.32
1	B	299	THR	C-O	6.47	1.31	1.24
1	C	651	ARG	C-O	6.41	1.32	1.24
1	A	293	LEU	C-O	6.37	1.31	1.24
1	B	378	GLY	C-O	6.35	1.28	1.24
1	A	521	GLU	C-O	6.32	1.31	1.24
1	B	581	ARG	C-O	6.29	1.31	1.23
1	A	535	LEU	N-CA	6.27	1.53	1.45
1	A	315	ARG	C-O	6.26	1.32	1.24
1	A	566	PRO	C-O	6.22	1.31	1.23
1	D	412	LYS	N-CA	6.17	1.53	1.46
1	D	503	TYR	C-O	-6.17	1.16	1.24
1	A	286	LEU	C-O	6.17	1.31	1.24
1	D	158	LEU	C-O	6.16	1.31	1.23
1	B	211	GLU	C-O	6.15	1.31	1.24
1	C	70	ARG	C-O	6.10	1.32	1.24
1	D	745	GLY	C-O	6.07	1.31	1.24
1	A	166	ILE	C-N	6.05	1.41	1.33
1	C	549	LEU	C-O	5.95	1.31	1.24
1	C	46	THR	C-O	5.93	1.31	1.23
1	A	592	ALA	C-O	5.92	1.31	1.23
1	C	487	GLU	C-O	5.84	1.31	1.24
1	A	473	LEU	N-CA	5.84	1.53	1.46
1	C	575	ILE	C-O	5.81	1.30	1.24
1	A	387	HIS	CE1-NE2	5.78	1.38	1.32
1	D	412	LYS	C-O	5.77	1.30	1.24
1	A	571	ASP	C-O	5.75	1.30	1.23
1	C	656	ILE	N-CA	5.69	1.50	1.46
1	A	583	VAL	C-O	5.66	1.30	1.24
1	A	332	LYS	C-O	5.65	1.30	1.24
1	A	495	LEU	C-O	-5.58	1.17	1.24
1	A	579	VAL	CA-C	5.55	1.59	1.52
1	B	302	TRP	C-O	-5.46	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	624	SER	N-CA	5.45	1.53	1.46
1	A	150	VAL	C-O	5.42	1.30	1.24
1	A	351	GLU	C-O	5.37	1.30	1.23
1	A	53	HIS	C-O	5.36	1.31	1.24
1	A	362	LEU	N-CA	5.35	1.51	1.46
1	A	17	GLY	C-O	5.34	1.29	1.23
1	C	543	THR	C-O	5.33	1.29	1.24
1	B	53	HIS	CE1-NE2	5.31	1.37	1.32
1	D	355	ALA	C-O	5.25	1.30	1.24
1	C	103	ILE	N-CA	5.23	1.52	1.46
1	D	460	LEU	C-O	5.22	1.30	1.24
1	D	521	GLU	C-O	5.22	1.30	1.24
1	C	591	LYS	N-CA	5.21	1.52	1.46
1	B	172	ASP	C-O	-5.20	1.17	1.23
1	C	328	TYR	C-O	5.20	1.30	1.24
1	A	301	PHE	N-CA	5.20	1.52	1.46
1	C	688	ASN	C-O	-5.18	1.17	1.24
1	A	263	LYS	C-O	-5.17	1.17	1.24
1	C	314	ASP	C-O	5.16	1.30	1.24
1	D	371	ASN	C-O	5.15	1.30	1.24
1	B	99	LYS	C-O	5.12	1.30	1.24
1	D	48	ILE	C-O	5.10	1.29	1.24
1	D	669	ASP	C-O	5.09	1.29	1.23
1	A	273	ASP	CG-OD2	5.08	1.35	1.25
1	A	74	GLY	C-O	5.08	1.29	1.23
1	C	749	GLN	CD-OE1	5.05	1.33	1.23
1	B	371	ASN	C-O	5.04	1.30	1.24
1	B	178	GLU	C-O	5.04	1.30	1.23
1	C	110	SER	C-O	5.03	1.30	1.24

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	710	THR	CB-CA-C	10.38	123.99	111.22
1	D	720	THR	CA-CB-OG1	10.05	124.67	109.60
1	A	710	THR	CB-CA-C	9.17	122.50	111.22
1	C	710	THR	CB-CA-C	8.89	122.96	111.50
1	B	151	PHE	CA-CB-CG	-8.15	105.65	113.80
1	D	710	THR	CB-CA-C	8.04	121.11	111.22
1	A	308	THR	CA-CB-OG1	-7.90	97.75	109.60
1	A	618	ARG	CG-CD-NE	-7.47	95.56	112.00
1	C	230	THR	CB-CA-C	6.91	119.72	109.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	391	THR	CA-CB-OG1	-6.87	99.30	109.60
1	A	51	ASN	CA-CB-CG	6.80	119.40	112.60
1	D	125	ARG	CG-CD-NE	-6.49	97.72	112.00
1	C	336	PRO	O-C-N	-6.43	118.13	121.15
1	D	138	THR	CA-CB-OG1	-6.40	100.01	109.60
1	B	228	PRO	N-CA-CB	6.39	106.77	103.19
1	D	618	ARG	CB-CA-C	-6.23	100.71	111.30
1	A	213	GLU	CA-C-O	-6.22	112.81	119.97
1	A	618	ARG	CB-CA-C	-6.21	100.74	111.30
1	C	544	LYS	CA-C-O	-6.15	114.55	121.00
1	C	618	ARG	CB-CA-C	-6.03	101.05	111.30
1	A	259	GLU	N-CA-C	-5.96	104.86	111.36
1	A	614	VAL	CA-C-O	-5.95	114.20	120.39
1	D	214	GLU	CA-C-N	5.93	128.23	120.28
1	D	214	GLU	C-N-CA	5.93	128.23	120.28
1	D	389	GLY	CA-C-O	-5.86	114.40	121.67
1	D	251	ASN	CA-C-N	5.81	128.07	120.28
1	D	251	ASN	C-N-CA	5.81	128.07	120.28
1	C	461	GLN	N-CA-C	-5.79	104.87	111.07
1	A	314	ASP	O-C-N	5.75	128.94	122.22
1	C	354	GLU	CA-C-O	-5.68	114.40	120.42
1	A	178	GLU	N-CA-C	-5.65	105.68	112.58
1	C	650	ASN	CA-C-O	-5.63	114.25	120.33
1	A	417	PHE	CA-C-O	-5.63	114.91	120.82
1	C	451	PRO	CA-C-N	5.63	128.09	120.38
1	C	451	PRO	C-N-CA	5.63	128.09	120.38
1	C	301	PHE	CA-CB-CG	-5.61	108.19	113.80
1	B	138	THR	CA-CB-OG1	-5.61	101.19	109.60
1	A	149	ASN	CA-C-O	-5.60	113.17	120.00
1	D	16	GLY	CA-C-N	5.57	125.90	121.61
1	D	16	GLY	C-N-CA	5.57	125.90	121.61
1	B	158	LEU	CA-C-N	5.53	127.96	120.38
1	B	158	LEU	C-N-CA	5.53	127.96	120.38
1	A	677	ARG	CB-CA-C	5.53	118.98	110.14
1	B	325	VAL	N-CA-C	-5.52	105.15	110.72
1	D	257	LEU	CA-C-O	-5.51	115.04	120.82
1	B	210	ASP	CA-CB-CG	5.49	118.09	112.60
1	C	555	LYS	CB-CA-C	5.48	119.27	110.29
1	A	377	GLY	CA-C-O	-5.47	116.60	121.41
1	D	140	LEU	CA-C-O	-5.42	114.81	120.55
1	A	22	PHE	CA-CB-CG	5.39	119.19	113.80
1	B	329	TYR	CA-C-O	-5.39	114.26	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	222	ASP	CA-C-O	-5.35	115.55	121.33
1	D	334	LYS	CB-CA-C	5.28	118.94	111.86
1	D	301	PHE	CA-CB-CG	-5.28	108.52	113.80
1	D	187	ASP	CA-CB-CG	5.25	117.85	112.60
1	B	147	TYR	CA-C-O	-5.22	114.20	120.10
1	D	85	TYR	CA-C-O	-5.21	115.48	121.47
1	D	618	ARG	CG-CD-NE	-5.20	100.56	112.00
1	B	230	THR	CB-CA-C	5.18	117.12	109.29
1	A	461	GLN	N-CA-C	-5.18	105.76	111.71
1	B	211	GLU	CA-C-N	5.17	127.21	120.28
1	B	211	GLU	C-N-CA	5.17	127.21	120.28
1	A	192	VAL	CA-C-O	-5.16	114.67	120.25
1	A	328	TYR	N-CA-C	-5.16	104.92	111.11
1	C	466	GLY	CA-C-N	5.16	127.19	120.28
1	C	466	GLY	C-N-CA	5.16	127.19	120.28
1	A	659	GLY	CA-C-N	5.13	129.29	120.72
1	A	659	GLY	C-N-CA	5.13	129.29	120.72
1	B	97	GLU	CB-CG-CD	5.13	121.32	112.60
1	A	125	ARG	CG-CD-NE	-5.11	100.77	112.00
1	B	714	VAL	CB-CA-C	5.10	115.75	110.70
1	B	336	PRO	N-CA-CB	5.10	105.87	103.22
1	A	159	TYR	CA-C-O	-5.09	114.34	120.10
1	C	279	ALA	N-CA-C	-5.08	105.92	111.82
1	C	65	GLU	CB-CA-C	-5.07	102.38	110.79
1	D	178	GLU	N-CA-C	-5.06	105.76	112.24
1	C	767	THR	CB-CA-C	5.04	119.00	109.37
1	B	394	VAL	CA-C-N	5.02	129.27	122.19
1	B	394	VAL	C-N-CA	5.02	129.27	122.19
1	B	385	GLU	CB-CG-CD	5.02	121.13	112.60
1	D	230	THR	CB-CA-C	5.01	116.86	109.29
1	C	210	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	186	THR	N-CA-CB	-5.00	103.31	111.66

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 (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	6326	0	6257	75	0
1	B	6321	0	6256	66	0
1	C	6344	0	6265	65	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	22	0
4	B	488	0	0	18	0
4	C	532	0	0	12	0
4	D	504	0	0	15	0
All	All	27343	0	25149	279	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 6.

All (279) 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:573:GLU:H	1:D:635:LYS:HZ2	1.20	0.88
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:173:GLU:OE2	3:B:902:MPD:H31	1.97	0.65
1:B:654:ILE:CD1	4:B:1076:HOH:O	2.45	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:650:ASN:C	1:C:650:ASN:HD22	2.06	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:A:763:HIS:HD2	1:A:765:SER:O	1.81	0.62
1:D:19:LEU:HD23	1:D:19:LEU:C	2.24	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
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:D:59:LEU:C	1:D:59:LEU:HD12	2.27	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:H	1:D:407:HIS:CD2	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:B:650:ASN:HD22	1:B:650:ASN:C	2.16	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
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:O	1:B:736:ASN:ND2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:D:407:HIS:HD2	1.57	0.52
1:A:387:HIS:HA	1:B:567:TYR:CD2	2.45	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:A:688[A]:ASN:CG	4:A:904:HOH:O	2.54	0.51
1:D:650:ASN:C	1:D:650:ASN:HD22	2.17	0.51
1:C:437[B]:MET:HE3	1:C:437[B]:MET:HA	1.93	0.50
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:19:LEU:C	1:C:19:LEU:HD23	2.36	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:771:ARG:CG	4:B:1053:HOH:O	2.58	0.49
1:C:59:LEU:HD12	1:C:59:LEU:C	2.37	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:D:19:LEU:C	1:D:19:LEU:CD2	2.85	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:A:650:ASN:C	1:A:650:ASN:HD22	2.20	0.49
1:B:702:ASN:CG	1:B:717:GLY:O	2.55	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:A:172:ASP:O	1:A:173:GLU:C	2.56	0.48
1:C:413[B]:TRP:CE3	1:C:724:ARG:CD	2.96	0.48
1:A:48:ILE:HD11	1:A:88:ILE:HD11	1.94	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:437[B]:MET:HE3	4:A:915:HOH:O	2.12	0.48
1:B:741:GLU:HB3	1:B:771:ARG:HD2	1.93	0.48
1:B:573:GLU:H	1:B:635:LYS:HZ2	1.61	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:OE1	1:B:205:GLU:HA	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: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:H	1:C:407:HIS:HD2	1.61	0.46
1:C:413[A]:TRP:CH2	4:C:1048:HOH:O	2.56	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:A:529:LEU:N	1:A:529:LEU:HD23	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:78:LEU:HD23	1:C:78:LEU:HA	1.73	0.46
1:C:228:PRO:HB3	1:C:242:TRP:CZ3	2.51	0.46
1:B:95:CYS:SG	3:B:902:MPD:H32	2.56	0.45
1:B:129:TYR:O	1:B:130:PRO:C	2.59	0.45
1:B:407:HIS:H	1:B:407:HIS:HD2	1.60	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437[B]:MET:HG3	1:C:438:TYR:N	2.32	0.45
1:D:128:TYR:O	1:D:129:TYR:C	2.59	0.45
1:A:407:HIS:H	1:A:407:HIS:HD2	1.64	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:D:239:ILE:HG22	1:D:447:TRP:CH2	2.52	0.45
1:A:129:TYR:O	1:A:130:PRO:C	2.60	0.44
1:A:519:TYR:CZ	1:A:524:GLY:HA3	2.51	0.44
1:D:216:TYR:N	1:D:216:TYR:CD1	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:701:ILE:HG23	1:C:716:ARG:NH1	2.33	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:HD12	1:C:662:LEU:HA	1.86	0.43
1:A:631:LYS:HE2	4:A:927:HOH:O	2.18	0.43
1:D:81:LYS:NZ	4:D:1036:HOH:O	2.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:523:GLY:HA2	1:D:609:LYS:C	2.44	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:C:172:ASP:O	1:C:173:GLU:C	2.63	0.41
1:D:413[A]:TRP:CD2	1:D:724:ARG:CD	3.02	0.41
1:C:91:GLY:HA3	1:C:92:PRO:C	2.45	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:H	1:D:766:GLU:HG3	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: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: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
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:HD12	1:C:212:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:HD2	1:A:219:LYS:N	2.35	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:19:LEU:C	1:C:19:LEU:CD2	2.94	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:CZ	1:A:215:ARG:HB3	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:A:243:HIS:CE1	1:A:446:MET:HE1	2.56	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:HH11	1:D:606:ARG:HG3	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%)	48	32
1	B	761/762 (100%)	726 (95%)	35 (5%)	0	100	100
1	C	763/762 (100%)	733 (96%)	29 (4%)	1 (0%)	48	32
1	D	762/762 (100%)	726 (95%)	35 (5%)	1 (0%)	48	32
All	All	3048/3048 (100%)	2912 (96%)	133 (4%)	3 (0%)	48	32

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 (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	684/682 (100%)	645 (94%)	39 (6%)	18	4
1	B	683/682 (100%)	646 (95%)	37 (5%)	20	5
1	C	685/682 (100%)	648 (95%)	37 (5%)	20	5
1	D	684/682 (100%)	641 (94%)	43 (6%)	16	3
All	All	2736/2728 (100%)	2580 (94%)	156 (6%)	18	4

All (156) 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	425	ILE
1	A	430	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	520	VAL
1	A	562	MET
1	A	564	LEU
1	A	618	ARG
1	A	650	ASN
1	A	673	THR
1	A	699	VAL
1	A	700	GLU
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	A	767	THR
1	B	19	LEU
1	B	59	LEU
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	314	ASP
1	B	407	HIS
1	B	460	LEU
1	B	488	LEU
1	B	505	LEU
1	B	516	LEU
1	B	520	VAL
1	B	522	GLU
1	B	530	PRO
1	B	541	PRO
1	B	564	LEU

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Mol	Chain	Res	Type
1	B	573	GLU
1	B	591	LYS
1	B	638	GLN
1	B	673	THR
1	B	688	ASN
1	B	700	GLU
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	192	VAL
1	C	203	LEU
1	C	212	LEU
1	C	214	GLU
1	C	219	LYS
1	C	221	SER
1	C	230	THR
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	516	LEU
1	C	520	VAL
1	C	562	MET
1	C	564	LEU
1	C	618	ARG
1	C	650	ASN

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Mol	Chain	Res	Type
1	C	660	ASN
1	C	673	THR
1	C	706	VAL
1	C	710	THR
1	C	714	VAL
1	C	730	VAL
1	C	751	LYS
1	C	766	GLU
1	C	767	THR
1	C	771	ARG
1	D	13	VAL
1	D	56	GLN
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	265	VAL
1	D	407	HIS
1	D	419	LYS
1	D	430	LYS
1	D	456	GLU
1	D	460	LEU
1	D	488	LEU
1	D	505	LEU
1	D	516	LEU
1	D	520	VAL
1	D	564	LEU
1	D	591	LYS
1	D	618	ARG
1	D	638	GLN
1	D	650	ASN
1	D	665	VAL
1	D	673	THR
1	D	677	ARG
1	D	710	THR

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Mol	Chain	Res	Type
1	D	714	VAL
1	D	718	GLU
1	D	730	VAL
1	D	738	LYS
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	69	GLN
1	A	196	ASN
1	A	206	ASN
1	A	251	ASN
1	A	407	HIS
1	A	496	GLN
1	A	525	ASN
1	A	620	GLN
1	A	638	GLN
1	A	650	ASN
1	A	660	ASN
1	A	763	HIS
1	B	69	GLN
1	B	80	GLN
1	B	368	HIS
1	B	407	HIS
1	B	449	HIS
1	B	650	ASN
1	B	688	ASN
1	B	702	ASN
1	C	167	ASN
1	C	196	ASN
1	C	368	HIS
1	C	388	ASN
1	C	407	HIS
1	C	421	ASN

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Mol	Chain	Res	Type
1	C	428	GLN
1	C	449	HIS
1	C	496	GLN
1	C	620	GLN
1	C	650	ASN
1	C	763	HIS
1	D	56	GLN
1	D	80	GLN
1	D	167	ASN
1	D	407	HIS
1	D	496	GLN
1	D	620	GLN
1	D	638	GLN
1	D	650	ASN
1	D	702	ASN
1	D	757	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 oligosaccharides 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	B	902	-	7,7,7	0.66	0	9,10,10	1.00	1 (11%)
3	MPD	D	901	-	7,7,7	0.43	0	9,10,10	0.40	0
3	MPD	D	902	-	7,7,7	1.47	2 (28%)	9,10,10	1.42	1 (11%)
3	MPD	A	803	-	7,7,7	0.38	0	9,10,10	0.38	0
3	MPD	C	803	-	7,7,7	1.01	1 (14%)	9,10,10	0.74	0
3	MPD	C	801	-	7,7,7	0.86	0	9,10,10	1.23	1 (11%)
3	MPD	B	901	-	7,7,7	0.35	0	9,10,10	0.75	0
3	MPD	A	802	-	7,7,7	1.08	1 (14%)	9,10,10	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	B	902	-	-	2/5/5/5	-
3	MPD	D	901	-	-	4/5/5/5	-
3	MPD	D	902	-	-	1/5/5/5	-
3	MPD	A	803	-	-	0/5/5/5	-
3	MPD	C	803	-	-	3/5/5/5	-
3	MPD	C	801	-	-	1/5/5/5	-
3	MPD	B	901	-	-	4/5/5/5	-
3	MPD	A	802	-	-	2/5/5/5	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	902	MPD	O4-C4	2.70	1.54	1.43
3	D	902	MPD	O2-C2	2.26	1.50	1.44
3	A	802	MPD	O2-C2	2.07	1.49	1.44
3	C	803	MPD	O4-C4	2.06	1.51	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	902	MPD	O4-C4-C3	3.26	124.33	111.35
3	C	801	MPD	C5-C4-C3	2.21	121.92	111.67
3	B	902	MPD	O2-C2-CM	2.21	114.86	107.99

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	MPD	C2-C3-C4-C5
3	B	901	MPD	O2-C2-C3-C4
3	B	901	MPD	CM-C2-C3-C4
3	D	902	MPD	C2-C3-C4-O4
3	B	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	C1-C2-C3-C4
3	B	902	MPD	C2-C3-C4-C5
3	C	803	MPD	O2-C2-C3-C4
3	D	901	MPD	O2-C2-C3-C4
3	A	802	MPD	C2-C3-C4-O4
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	C	801	MPD	CM-C2-C3-C4
3	D	901	MPD	CM-C2-C3-C4

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	MPD	4	0
3	D	902	MPD	4	0
3	C	803	MPD	5	0
3	C	801	MPD	3	0
3	B	901	MPD	3	0
3	A	802	MPD	4	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	762/762 (100%)	-0.29	10 (1%)	75	81	14, 36, 68, 109	2 (0%)
1	B	762/762 (100%)	-0.42	1 (0%)	92	93	19, 32, 67, 117	1 (0%)
1	C	762/762 (100%)	-0.45	2 (0%)	90	92	13, 28, 66, 95	3 (0%)
1	D	762/762 (100%)	-0.36	3 (0%)	88	91	17, 33, 68, 107	2 (0%)
All	All	3048/3048 (100%)	-0.38	16 (0%)	87	90	13, 32, 67, 117	8 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	VAL	4.9
1	A	167	ASN	4.3
1	A	159	TYR	3.2
1	C	746	TYR	2.9
1	A	166	ILE	2.9
1	D	720	THR	2.6
1	D	413[A]	TRP	2.6
1	C	425	ILE	2.4
1	D	772	VAL	2.3
1	A	425	ILE	2.3
1	A	61	ASP	2.2
1	A	139	TYR	2.2
1	A	12	ILE	2.2
1	A	145	LYS	2.1
1	A	422	MET	2.0
1	B	595	TRP	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 oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MPD	B	902	8/8	0.64	0.24	32,47,54,63	0
3	MPD	C	801	8/8	0.79	0.18	46,53,65,99	0
3	MPD	A	802	8/8	0.80	0.16	45,50,55,60	0
3	MPD	C	803	8/8	0.83	0.17	43,52,68,70	0
3	MPD	D	902	8/8	0.84	0.14	36,42,58,69	0
3	MPD	A	803	8/8	0.93	0.10	32,38,60,62	0
3	MPD	B	901	8/8	0.95	0.09	31,34,36,38	0
3	MPD	D	901	8/8	0.97	0.07	24,32,35,39	0
2	CA	C	802	1/1	0.98	0.05	47,47,47,47	0
2	CA	A	801	1/1	0.99	0.08	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.