



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2016 – 10:54 AM EDT

PDB ID : 4ZEH
Title : High resolution structure of Gan1D, a putative 6-phospho-beta-galactosidase from *Geobacillus stearothermophilus*
Authors : Lansky, S.; Zehavi, A.; Dvir, H.; Shoham, Y.; Shoham, G.
Deposited on : 2015-04-20
Resolution : 1.33 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027790

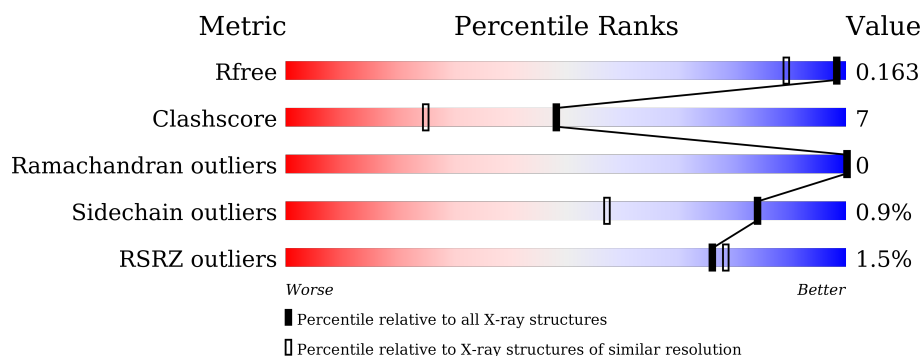
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.33 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}	91344	1723 (1.38-1.30)
Clashscore	102246	1806 (1.38-1.30)
Ramachandran outliers	100387	1749 (1.38-1.30)
Sidechain outliers	100360	1749 (1.38-1.30)
RSRZ outliers	91569	1721 (1.38-1.30)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	485	<div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	B	485	<div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	C	485	<div> <div>81%</div> <div>16%</div> <div>..</div> </div>
1	D	485	<div> <div>80%</div> <div>12%</div> <div>6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IMD	B	501	-	-	X	-
3	MPD	A	503	-	-	X	X
3	MPD	B	503	-	-	X	X
3	MPD	C	502	-	-	X	X
3	MPD	D	502	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18854 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 Putative 6-phospho-beta-galactobiosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	24	0
			4012	2584	680	732	16			
1	B	476	Total	C	N	O	S	0	23	0
			4027	2592	689	732	14			
1	C	474	Total	C	N	O	S	0	29	0
			4043	2607	685	735	16			
1	D	455	Total	C	N	O	S	0	19	0
			3854	2486	656	700	12			

There are 32 discrepancies between the modelled and reference sequences:

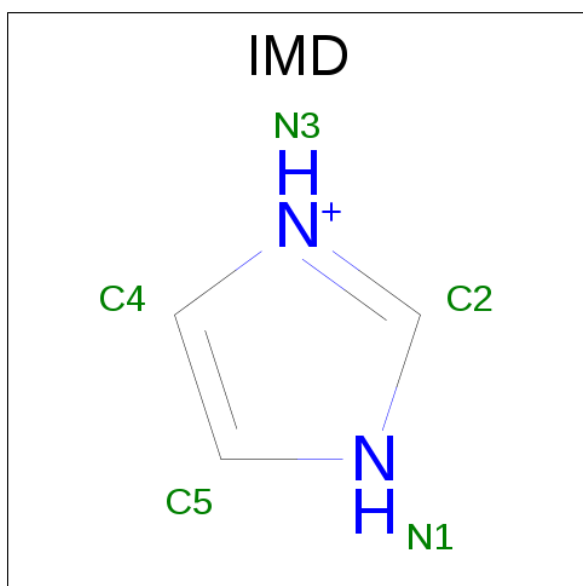
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP W8QF82
A	-5	ILE	-	expression tag	UNP W8QF82
A	-4	HIS	-	expression tag	UNP W8QF82
A	-3	HIS	-	expression tag	UNP W8QF82
A	-2	HIS	-	expression tag	UNP W8QF82
A	-1	HIS	-	expression tag	UNP W8QF82
A	0	HIS	-	expression tag	UNP W8QF82
A	1	HIS	-	expression tag	UNP W8QF82
B	-6	MET	-	initiating methionine	UNP W8QF82
B	-5	ILE	-	expression tag	UNP W8QF82
B	-4	HIS	-	expression tag	UNP W8QF82
B	-3	HIS	-	expression tag	UNP W8QF82
B	-2	HIS	-	expression tag	UNP W8QF82
B	-1	HIS	-	expression tag	UNP W8QF82
B	0	HIS	-	expression tag	UNP W8QF82
B	1	HIS	-	expression tag	UNP W8QF82
C	-6	MET	-	initiating methionine	UNP W8QF82
C	-5	ILE	-	expression tag	UNP W8QF82
C	-4	HIS	-	expression tag	UNP W8QF82
C	-3	HIS	-	expression tag	UNP W8QF82
C	-2	HIS	-	expression tag	UNP W8QF82

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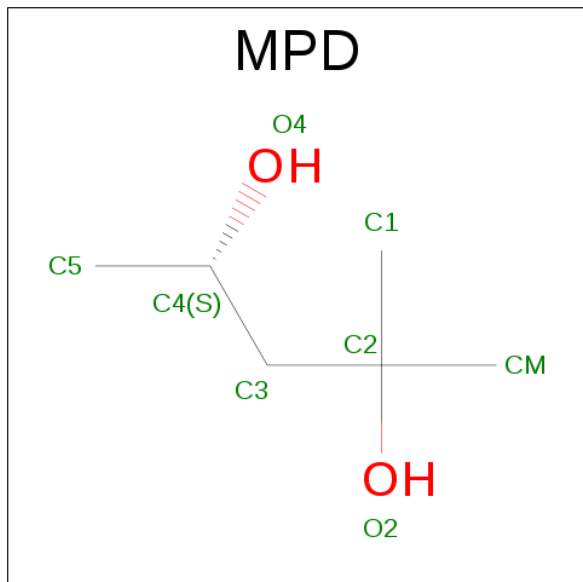
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	HIS	-	expression tag	UNP W8QF82
C	0	HIS	-	expression tag	UNP W8QF82
C	1	HIS	-	expression tag	UNP W8QF82
D	-6	MET	-	initiating methionine	UNP W8QF82
D	-5	ILE	-	expression tag	UNP W8QF82
D	-4	HIS	-	expression tag	UNP W8QF82
D	-3	HIS	-	expression tag	UNP W8QF82
D	-2	HIS	-	expression tag	UNP W8QF82
D	-1	HIS	-	expression tag	UNP W8QF82
D	0	HIS	-	expression tag	UNP W8QF82
D	1	HIS	-	expression tag	UNP W8QF82

- Molecule 2 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			5	3	2		
2	A	1	Total	C	N	0	0
			5	3	2		
2	B	1	Total	C	N	0	0
			5	3	2		
2	B	1	Total	C	N	0	0
			5	3	2		
2	C	1	Total	C	N	0	0
			5	3	2		
2	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 4 is water.

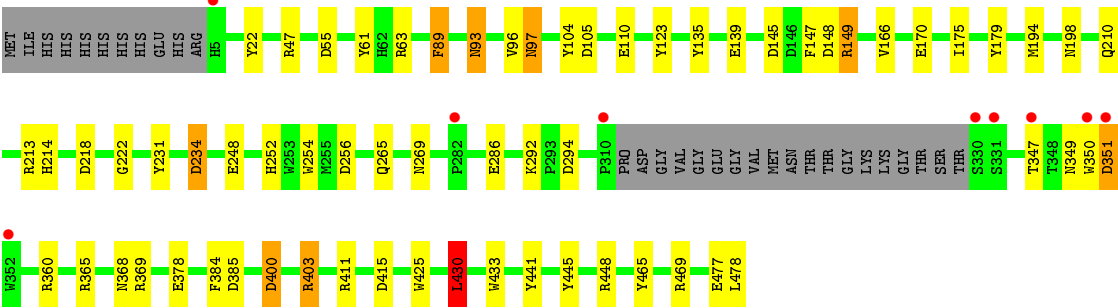
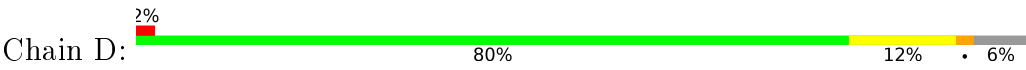
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	736	Total	O	0	0
			736	736		
4	B	677	Total	O	0	0
			677	677		
4	C	764	Total	O	0	0
			764	764		
4	D	679	Total	O	0	0
			679	679		

- Molecule 1: Putative 6-phospho-beta-galactobiosidase





● Molecule 1: Putative 6-phospho-beta-galactobiosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.97Å 78.10Å 92.09Å 102.36° 93.54° 91.74°	Depositor
Resolution (Å)	30.85 – 1.33 30.83 – 1.33	Depositor EDS
% Data completeness (in resolution range)	88.2 (30.85-1.33) 85.0 (30.83-1.33)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 1.33Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.136 , 0.161 0.139 , 0.163	Depositor DCC
R_{free} test set	19050 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	18854	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.70 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4822e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: MPD, IMD

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	1.36	20/4208 (0.5%)	1.39	54/5716 (0.9%)
1	B	1.35	8/4220 (0.2%)	1.35	38/5733 (0.7%)
1	C	1.34	16/4256 (0.4%)	1.35	38/5779 (0.7%)
1	D	1.38	14/4034 (0.3%)	1.36	46/5485 (0.8%)
All	All	1.36	58/16718 (0.3%)	1.36	176/22713 (0.8%)

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	B	0	1

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	ASP	C-N	-15.65	0.98	1.34
1	D	248	GLU	CD-OE2	-9.50	1.15	1.25
1	D	351[A]	ASP	N-CA	9.33	1.65	1.46
1	D	351[B]	ASP	N-CA	9.33	1.65	1.46
1	A	110	GLU	CD-OE2	-8.27	1.16	1.25
1	C	110	GLU	CD-OE1	-8.24	1.16	1.25
1	D	22	TYR	CE2-CZ	-6.99	1.29	1.38
1	C	248	GLU	CD-OE2	-6.67	1.18	1.25
1	C	227	TYR	CE2-CZ	-6.66	1.29	1.38
1	A	387	LEU	C-N	-6.26	1.19	1.34
1	D	110	GLU	CD-OE2	-6.20	1.18	1.25
1	D	22	TYR	CD1-CE1	5.96	1.48	1.39
1	A	47	ARG	CZ-NH2	-5.85	1.25	1.33
1	A	391	ASP	C-N	-5.83	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	123	TYR	CE1-CZ	-5.81	1.30	1.38
1	C	160	ASP	CG-OD1	5.81	1.38	1.25
1	A	161	ARG	C-N	-5.78	1.20	1.34
1	C	164	TYR	CG-CD1	-5.78	1.31	1.39
1	D	104	TYR	CE2-CZ	5.75	1.46	1.38
1	D	400[A]	ASP	CA-C	5.74	1.67	1.52
1	D	400[B]	ASP	CA-C	5.74	1.67	1.52
1	A	196	GLU	CD-OE2	5.64	1.31	1.25
1	C	352	TRP	CB-CG	-5.60	1.40	1.50
1	A	397	TYR	C-N	-5.58	1.21	1.34
1	A	61	TYR	CZ-OH	5.56	1.47	1.37
1	A	164	TYR	CG-CD1	-5.56	1.31	1.39
1	C	350	TRP	CE3-CZ3	5.55	1.47	1.38
1	A	323	GLY	N-CA	-5.55	1.37	1.46
1	A	47	ARG	CD-NE	-5.54	1.37	1.46
1	C	397	TYR	CB-CG	-5.50	1.43	1.51
1	B	123	TYR	CE1-CZ	-5.49	1.31	1.38
1	A	477	GLU	CD-OE1	5.48	1.31	1.25
1	C	384[A]	PHE	C-N	-5.47	1.21	1.34
1	C	384[B]	PHE	C-N	-5.47	1.21	1.34
1	C	452	SER	CB-OG	-5.42	1.35	1.42
1	C	170	GLU	CD-OE1	5.41	1.31	1.25
1	A	416	GLY	N-CA	-5.39	1.38	1.46
1	C	352	TRP	CE3-CZ3	-5.38	1.29	1.38
1	B	227	TYR	CE2-CZ	-5.37	1.31	1.38
1	B	292[A]	LYS	CA-C	5.34	1.66	1.52
1	B	292[B]	LYS	CA-C	5.34	1.66	1.52
1	A	61	TYR	CE2-CZ	-5.33	1.31	1.38
1	D	445	TYR	CE1-CZ	-5.30	1.31	1.38
1	A	195	TYR	CE1-CZ	-5.29	1.31	1.38
1	B	196	GLU	CD-OE2	5.26	1.31	1.25
1	A	47	ARG	CA-C	5.25	1.66	1.52
1	B	177	PHE	CG-CD2	-5.25	1.30	1.38
1	B	215	TYR	CE1-CZ	-5.22	1.31	1.38
1	D	97[A]	ASN	CG-OD1	-5.22	1.12	1.24
1	D	97[B]	ASN	CG-OD1	-5.22	1.12	1.24
1	D	170	GLU	CD-OE1	5.19	1.31	1.25
1	A	79	TYR	CE2-CZ	-5.19	1.31	1.38
1	C	235	SER	CB-OG	5.18	1.49	1.42
1	A	94	GLY	N-CA	5.18	1.53	1.46
1	C	109	GLU	C-N	5.15	1.45	1.34
1	A	110	GLU	CD-OE1	-5.11	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	247	GLU	CD-OE1	-5.08	1.20	1.25
1	B	98	GLU	CD-OE2	5.07	1.31	1.25

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	ASP	CB-CG-OD1	14.28	131.15	118.30
1	A	448	ARG	NE-CZ-NH2	-13.93	113.34	120.30
1	A	448	ARG	NE-CZ-NH1	13.01	126.81	120.30
1	A	160	ASP	CB-CG-OD1	12.92	129.93	118.30
1	A	398	ARG	NE-CZ-NH2	12.81	126.70	120.30
1	B	213	ARG	NE-CZ-NH2	-12.04	114.28	120.30
1	C	449	ASP	CB-CG-OD1	11.62	128.75	118.30
1	B	141	ARG	NE-CZ-NH2	-11.59	114.51	120.30
1	A	365	ARG	NE-CZ-NH2	-11.13	114.73	120.30
1	B	231	TYR	CB-CG-CD1	10.80	127.48	121.00
1	D	63[A]	ARG	NE-CZ-NH1	-10.34	115.13	120.30
1	D	63[B]	ARG	NE-CZ-NH1	-10.34	115.13	120.30
1	B	231	TYR	CB-CG-CD2	-10.22	114.87	121.00
1	D	231	TYR	CB-CG-CD1	9.55	126.73	121.00
1	A	47	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	C	365	ARG	NE-CZ-NH2	-9.47	115.57	120.30
1	B	63[A]	ARG	NE-CZ-NH1	-9.45	115.58	120.30
1	B	63[B]	ARG	NE-CZ-NH1	-9.45	115.58	120.30
1	D	365	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	A	403	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	C	234	ASP	CB-CG-OD1	9.13	126.52	118.30
1	C	448	ARG	NE-CZ-NH2	-9.11	115.74	120.30
1	D	149	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	C	448	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	B	213	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	A	63[A]	ARG	NE-CZ-NH1	-8.70	115.95	120.30
1	A	63[B]	ARG	NE-CZ-NH1	-8.70	115.95	120.30
1	B	79	TYR	CB-CG-CD1	8.65	126.19	121.00
1	A	403	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	B	365	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	C	249	PHE	CB-CG-CD2	-8.31	114.98	120.80
1	D	430	LEU	CB-CG-CD1	-7.80	97.73	111.00
1	C	190	ASP	CB-CG-OD1	7.76	125.29	118.30
1	C	160	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	D	294	ASP	CB-CG-OD2	7.50	125.05	118.30
1	A	79	TYR	CB-CG-CD2	-7.46	116.52	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	123	TYR	CB-CG-CD2	7.30	125.38	121.00
1	C	145	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	A	161	ARG	O-C-N	-7.19	111.19	122.70
1	D	123	TYR	CB-CG-CD1	-7.12	116.73	121.00
1	B	448	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	C	385	ASP	CB-CG-OD1	7.03	124.63	118.30
1	B	400	ASP	CB-CG-OD1	-6.98	112.02	118.30
1	D	234	ASP	CB-CG-OD1	6.97	124.57	118.30
1	C	249	PHE	CB-CG-CD1	6.95	125.67	120.80
1	C	63[A]	ARG	NE-CZ-NH1	-6.93	116.84	120.30
1	C	63[B]	ARG	NE-CZ-NH1	-6.93	116.84	120.30
1	B	190[A]	ASP	CB-CG-OD1	6.89	124.50	118.30
1	B	190[B]	ASP	CB-CG-OD1	6.89	124.50	118.30
1	D	385	ASP	CB-CG-OD1	6.88	124.49	118.30
1	A	384	PHE	N-CA-C	-6.87	92.46	111.00
1	A	365	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	C	396	ASP	CB-CG-OD1	6.78	124.40	118.30
1	D	55	ASP	CB-CG-OD1	6.77	124.39	118.30
1	A	160	ASP	C-N-CA	6.73	138.52	121.70
1	A	160	ASP	O-C-N	-6.72	111.95	122.70
1	D	256	ASP	CB-CG-OD1	6.66	124.30	118.30
1	C	400[A]	ASP	CB-CG-OD1	6.64	124.28	118.30
1	C	400[B]	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	161	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	D	63[A]	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	D	63[B]	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	C	355	ASP	CB-CG-OD2	-6.56	112.40	118.30
1	A	384	PHE	CB-CA-C	6.55	123.50	110.40
1	D	148	ASP	CB-CG-OD1	6.54	124.18	118.30
1	D	256	ASP	CB-CG-OD2	-6.50	112.44	118.30
1	D	179	TYR	CB-CG-CD1	6.49	124.89	121.00
1	B	294	ASP	CB-CG-OD2	6.46	124.11	118.30
1	A	160	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	B	141	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	C	236	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	398	ARG	NH1-CZ-NH2	-6.36	112.41	119.40
1	A	391	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	D	89	PHE	CB-CG-CD2	6.30	125.21	120.80
1	B	448	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	D	411	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	C	55	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	C	430	LEU	CB-CG-CD1	-6.24	100.40	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	TYR	CB-CG-CD2	6.22	124.73	121.00
1	C	47	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	C	400[A]	ASP	CB-CG-OD2	-6.18	112.73	118.30
1	C	400[B]	ASP	CB-CG-OD2	-6.18	112.73	118.30
1	B	411	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	B	360	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	C	415	ASP	CB-CG-OD1	6.14	123.83	118.30
1	D	411	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	C	148	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	145	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	D	145	ASP	CB-CG-OD1	6.02	123.72	118.30
1	C	455	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	227	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	D	351[A]	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	D	351[B]	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	145	ASP	CB-CG-OD1	5.98	123.68	118.30
1	B	458	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	277	GLU	CG-CD-OE2	5.86	130.03	118.30
1	B	145	ASP	CB-CG-OD2	-5.86	113.02	118.30
1	D	360	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	A	360	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	B	160	ASP	CB-CG-OD1	5.84	123.55	118.30
1	D	47	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	D	403[A]	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	D	403[B]	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	294	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	145	ASP	CB-CG-OD1	5.76	123.48	118.30
1	B	437	TYR	CB-CG-CD1	-5.76	117.55	121.00
1	C	141	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	D	213	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	D	22	TYR	CG-CD1-CE1	-5.72	116.72	121.30
1	B	55	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	139	GLU	OE1-CD-OE2	5.67	130.10	123.30
1	C	411	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	B	194[A]	MET	CG-SD-CE	5.62	109.19	100.20
1	B	194[B]	MET	CG-SD-CE	5.62	109.19	100.20
1	C	145	ASP	CB-CG-OD1	5.61	123.35	118.30
1	D	148	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	D	147	PHE	CB-CG-CD1	-5.57	116.90	120.80
1	B	157	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	164	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	D	441	TYR	CB-CG-CD2	-5.54	117.67	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63[A]	ARG	CA-C-O	5.51	131.67	120.10
1	B	63[B]	ARG	CA-C-O	5.51	131.67	120.10
1	A	79	TYR	CB-CG-CD1	5.50	124.30	121.00
1	A	341	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	C	457	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	227	TYR	CB-CG-CD1	5.47	124.28	121.00
1	C	76	LEU	CB-CA-C	-5.47	99.81	110.20
1	A	385	ASP	N-CA-C	-5.45	96.29	111.00
1	D	415	ASP	CB-CG-OD1	5.44	123.20	118.30
1	D	403[A]	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	403[B]	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	365	ARG	O-C-N	-5.40	114.05	122.70
1	A	66	GLU	OE1-CD-OE2	5.39	129.77	123.30
1	A	449	ASP	CB-CG-OD1	5.36	123.12	118.30
1	C	109	GLU	O-C-N	-5.36	114.13	122.70
1	A	93	ASN	C-N-CA	-5.35	111.07	122.30
1	A	295	PHE	CB-CG-CD2	5.35	124.54	120.80
1	C	106	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	249	PHE	CB-CG-CD1	-5.33	117.07	120.80
1	B	234	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	411	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	256	ASP	CB-CG-OD2	-5.33	113.51	118.30
1	D	448	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	141	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	91	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	295	PHE	CB-CG-CD1	-5.29	117.10	120.80
1	A	164	TYR	CD1-CE1-CZ	-5.27	115.05	119.80
1	B	106	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	403	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	B	351	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	D	105	ASP	CB-CG-OD2	-5.22	113.61	118.30
1	B	458	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	469	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	150	TYR	CB-CG-CD1	5.20	124.12	121.00
1	C	135	TYR	CG-CD2-CE2	5.17	125.44	121.30
1	D	135	TYR	CD1-CE1-CZ	5.16	124.45	119.80
1	A	403	ARG	O-C-N	5.16	130.96	122.70
1	A	453[A]	GLU	CA-C-O	5.15	130.92	120.10
1	A	453[B]	GLU	CA-C-O	5.15	130.92	120.10
1	B	284	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	D	210	GLN	O-C-N	-5.14	114.47	122.70
1	C	133	ASP	CB-CG-OD2	-5.14	113.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157[A]	ARG	CA-C-O	5.14	130.89	120.10
1	A	157[B]	ARG	CA-C-O	5.14	130.89	120.10
1	D	105	ASP	CB-CG-OD1	5.14	122.93	118.30
1	D	147	PHE	CB-CG-CD2	5.14	124.40	120.80
1	C	148	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	D	218	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	D	465	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	A	396	ASP	CB-CG-OD1	5.08	122.87	118.30
1	B	39	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	400[A]	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	A	400[B]	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	D	22	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	A	238[A]	GLU	CG-CD-OE1	5.04	128.38	118.30
1	A	238[B]	GLU	CG-CD-OE1	5.04	128.38	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	290	ALA	Mainchain

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	4012	0	3874	44	0
1	B	4027	0	3879	71	0
1	C	4043	0	3915	63	0
1	D	3854	0	3698	45	0
2	A	10	0	10	0	0
2	B	10	0	10	5	0
2	C	5	0	5	0	0
2	D	5	0	5	1	0
3	A	8	0	14	16	0
3	B	8	0	14	19	0
3	C	8	0	13	10	0
3	D	8	0	14	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	736	0	0	20	0
4	B	677	0	0	32	1
4	C	764	0	0	40	0
4	D	679	0	0	22	1
All	All	18854	0	15451	228	1

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 7.

All (228) 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:452:SER:HB3	4:C:677:HOH:O	1.45	1.14
3:C:502:MPD:HM3	4:C:1021:HOH:O	1.49	1.13
1:A:433:TRP:HD1	3:A:503:MPD:H52	1.10	1.10
1:C:114:HIS:HE1	4:C:1095:HOH:O	1.37	1.08
1:B:112[B]:ARG:HD2	4:B:794:HOH:O	1.56	1.06
1:A:433:TRP:CD1	3:A:503:MPD:H52	1.93	1.03
1:C:132[A]:MET:HE1	4:C:1174:HOH:O	1.60	1.00
2:B:501:IMD:H5	4:B:1081:HOH:O	1.61	0.99
1:A:99[A]:LYS:HE3	4:A:626:HOH:O	1.65	0.96
1:B:319[A]:MET:HE2	4:B:1264:HOH:O	1.66	0.94
1:B:441:TYR:CZ	3:B:503:MPD:H52	2.04	0.93
1:D:347[B]:THR:HG22	4:D:886:HOH:O	1.69	0.91
1:B:249[A]:PHE:CE2	1:B:333:ILE:CD1	2.56	0.89
1:C:97[B]:ASN:ND2	4:C:602:HOH:O	2.06	0.87
3:A:503:MPD:C5	4:A:752:HOH:O	2.22	0.87
1:B:262:MET:HE2	2:B:501:IMD:HN3	1.40	0.86
1:C:319[A]:MET:SD	4:C:1326:HOH:O	2.34	0.86
1:B:97[B]:ASN:ND2	4:B:601:HOH:O	2.09	0.84
1:B:262:MET:HE2	2:B:501:IMD:N3	1.92	0.84
1:B:262:MET:HE3	4:D:1127:HOH:O	1.77	0.84
1:B:249[A]:PHE:CE2	1:B:333:ILE:HD11	2.12	0.83
1:B:441:TYR:CE1	3:B:503:MPD:H52	2.14	0.82
1:B:3:HIS:HD2	4:B:797:HOH:O	1.61	0.81
3:A:503:MPD:H11	4:A:671:HOH:O	1.80	0.80
1:C:63[B]:ARG:NH1	4:C:601:HOH:O	1.93	0.80
1:C:433:TRP:HD1	3:C:502:MPD:H53	1.47	0.80
1:A:262[B]:MET:HE2	4:C:1122:HOH:O	1.81	0.79
1:D:97[A]:ASN:ND2	4:D:602:HOH:O	2.14	0.79
1:B:249[B]:PHE:CE1	4:B:1078:HOH:O	2.34	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:TRP:HD1	3:A:503:MPD:C5	1.92	0.78
1:B:262:MET:CE	2:B:501:IMD:HN3	1.96	0.78
3:C:502:MPD:H52	3:C:502:MPD:HM2	1.64	0.78
1:C:308[B]:HIS:CE1	4:C:667:HOH:O	2.36	0.77
1:D:403[B]:ARG:HE	1:D:478:LEU:C	1.88	0.77
3:A:503:MPD:H51	4:A:752:HOH:O	1.81	0.77
1:B:3:HIS:HE1	4:B:842:HOH:O	1.67	0.75
3:D:502:MPD:CM	4:D:973:HOH:O	2.35	0.75
1:B:180[B]:ARG:NH1	4:B:602:HOH:O	2.16	0.75
3:C:502:MPD:C1	4:C:1171:HOH:O	2.34	0.74
1:D:347[B]:THR:CG2	4:D:886:HOH:O	2.28	0.74
1:B:3:HIS:CE1	4:B:842:HOH:O	2.42	0.73
1:B:198:ASN:HD21	1:B:254:TRP:HE1	1.37	0.72
1:B:252:HIS:HD2	1:D:368:ASN:HD21	1.36	0.72
1:B:252:HIS:CD2	1:D:368:ASN:HD21	2.08	0.72
1:B:3:HIS:HA	4:B:1067:HOH:O	1.88	0.72
3:C:502:MPD:H11	4:C:1171:HOH:O	1.87	0.72
1:B:441:TYR:OH	3:B:503:MPD:HM1	1.91	0.71
1:C:321:THR:HG22	4:C:1301:HOH:O	1.91	0.70
1:A:400[A]:ASP:OD1	4:A:601:HOH:O	2.09	0.69
1:C:180:ARG:HD3	1:C:191[B]:MET:SD	2.33	0.69
1:C:198:ASN:HD21	1:C:254:TRP:HE1	1.39	0.69
1:D:286[B]:GLU:OE1	4:D:601:HOH:O	2.10	0.68
3:D:502:MPD:HM3	4:D:973:HOH:O	1.94	0.68
1:D:350:TRP:C	1:D:351[B]:ASP:CA	2.59	0.67
1:A:192:LYS:HE2	4:A:620:HOH:O	1.93	0.66
1:C:132[A]:MET:CE	4:C:1174:HOH:O	2.26	0.66
1:A:252:HIS:HD2	1:C:368:ASN:HD21	1.40	0.65
1:A:252:HIS:CD2	1:C:368:ASN:HD21	2.14	0.65
3:A:503:MPD:H53	4:A:752:HOH:O	1.89	0.65
1:D:89:PHE:CZ	1:D:96[A]:VAL:HG22	2.32	0.65
1:A:265[B]:GLN:HG3	4:C:1134:HOH:O	1.95	0.64
1:C:441:TYR:CE2	3:C:502:MPD:H13	2.32	0.64
1:B:425:TRP:CD1	3:B:503:MPD:H51	2.34	0.64
1:B:249[B]:PHE:CD1	4:B:1078:HOH:O	2.51	0.63
1:C:433:TRP:CD1	3:C:502:MPD:H53	2.32	0.63
1:D:198:ASN:HD21	1:D:254:TRP:HE1	1.45	0.63
1:A:433:TRP:H	3:A:503:MPD:H53	1.64	0.63
1:A:441:TYR:CE2	3:A:503:MPD:H13	2.34	0.62
1:B:249[A]:PHE:CD2	1:B:333:ILE:CD1	2.82	0.62
3:B:503:MPD:HM1	3:B:503:MPD:H52	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265[B]:GLN:HG2	4:A:935:HOH:O	1.99	0.62
1:A:245:ASN:HD22	1:C:364:ARG:HH22	1.48	0.61
1:C:238[B]:GLU:OE2	1:C:308[B]:HIS:CE1	2.53	0.61
1:A:198:ASN:HD21	1:A:254:TRP:HE1	1.47	0.61
1:C:307:GLU:OE2	1:D:214:HIS:HD2	1.83	0.61
1:B:7:LYS:HD2	4:B:1033:HOH:O	1.99	0.61
1:B:112[B]:ARG:NH1	4:B:605:HOH:O	2.26	0.61
1:B:262:MET:CE	2:B:501:IMD:N3	2.60	0.61
1:A:63[B]:ARG:CZ	4:A:643:HOH:O	2.48	0.60
1:A:368:ASN:HD21	1:C:252:HIS:HD2	1.49	0.59
1:A:110:GLU:O	1:A:114:HIS:HD2	1.84	0.59
3:A:503:MPD:C1	4:A:671:HOH:O	2.42	0.59
1:C:99[A]:LYS:HE3	4:C:847:HOH:O	2.01	0.59
1:A:245:ASN:ND2	1:C:364:ARG:HH22	2.00	0.59
1:B:265:GLN:HE21	1:B:269:ASN:ND2	2.00	0.59
3:B:503:MPD:H12	4:B:1178:HOH:O	2.02	0.59
1:C:99[A]:LYS:HE2	4:C:775:HOH:O	2.03	0.58
1:B:249[A]:PHE:CE2	1:B:333:ILE:HD13	2.38	0.58
1:C:265:GLN:HE21	1:C:269:ASN:HD21	1.51	0.58
1:B:319[A]:MET:CE	4:B:1264:HOH:O	2.37	0.58
1:B:368[B]:ASN:HD22	1:B:369:ARG:N	2.00	0.58
1:C:432:SER:HA	3:C:502:MPD:H32	1.85	0.58
1:A:262[A]:MET:HE3	4:C:1122:HOH:O	2.02	0.58
1:D:469:ARG:NH2	1:D:477[B]:GLU:OE1	2.37	0.57
1:B:12[A]:GLU:CD	1:B:12[A]:GLU:H	2.06	0.57
1:D:349:ASN:CG	4:D:628:HOH:O	2.43	0.57
1:A:433:TRP:CD1	3:A:503:MPD:C5	2.74	0.57
1:C:110:GLU:O	1:C:114:HIS:HD2	1.89	0.56
1:C:308[A]:HIS:ND1	4:C:610:HOH:O	2.33	0.56
1:C:291:ALA:HB1	4:C:853:HOH:O	2.04	0.56
1:A:438:GLN:NE2	4:A:604:HOH:O	2.38	0.56
1:C:286:GLU:HG2	4:C:1218:HOH:O	2.06	0.56
1:A:252:HIS:HE1	4:A:824:HOH:O	1.87	0.55
1:B:93:ASN:C	1:B:93:ASN:HD22	2.10	0.55
1:A:93:ASN:HD22	1:A:93:ASN:C	2.09	0.55
1:C:180:ARG:CD	1:C:191[B]:MET:SD	2.94	0.55
1:B:249[A]:PHE:CD2	1:B:333:ILE:HD11	2.42	0.55
1:A:368:ASN:HD21	1:C:252:HIS:CD2	2.24	0.55
1:B:262:MET:CE	4:D:1127:HOH:O	2.42	0.54
1:C:265:GLN:HE21	1:C:269:ASN:ND2	2.05	0.54
1:C:114:HIS:CE1	4:C:1095:HOH:O	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477[B]:GLU:HG2	4:B:654:HOH:O	2.07	0.54
1:D:292:LYS:HB3	4:D:902:HOH:O	2.08	0.54
1:A:112:ARG:HG2	4:A:982:HOH:O	2.06	0.54
3:B:503:MPD:H13	4:B:1016:HOH:O	2.07	0.54
1:B:368[A]:ASN:OD1	1:D:369:ARG:NH1	2.38	0.54
1:C:321:THR:CG2	4:C:1301:HOH:O	2.52	0.54
1:C:477:GLU:HG2	4:C:609:HOH:O	2.07	0.54
1:A:192:LYS:CE	4:A:620:HOH:O	2.53	0.53
4:A:1086:HOH:O	1:C:262[B]:MET:CE	2.56	0.53
1:B:441:TYR:CE1	3:B:503:MPD:C5	2.91	0.53
1:C:441:TYR:HE2	3:C:502:MPD:H13	1.74	0.52
1:C:99[A]:LYS:CE	4:C:775:HOH:O	2.57	0.52
1:A:312:ASP:HB2	4:A:1070:HOH:O	2.10	0.52
1:C:192:LYS:NZ	4:C:618:HOH:O	2.43	0.52
1:D:252:HIS:HE1	4:D:804:HOH:O	1.92	0.52
1:D:93:ASN:HD22	1:D:93:ASN:C	2.13	0.52
1:D:96[B]:VAL:HG13	4:D:986:HOH:O	2.11	0.51
1:B:368[A]:ASN:HD21	1:D:252:HIS:CD2	2.28	0.50
1:B:441:TYR:OH	3:B:503:MPD:CM	2.58	0.50
1:B:368[A]:ASN:HD21	1:D:252:HIS:HD2	1.57	0.50
1:B:425:TRP:NE1	3:B:503:MPD:H51	2.27	0.50
1:D:403[B]:ARG:NE	1:D:478:LEU:O	2.45	0.50
1:B:319[A]:MET:HE3	4:B:1206:HOH:O	2.11	0.50
1:D:89:PHE:CZ	1:D:96[B]:VAL:HG12	2.46	0.49
1:B:252:HIS:HE1	4:B:1045:HOH:O	1.95	0.49
1:B:308[B]:HIS:CE1	4:B:712:HOH:O	2.65	0.49
3:B:503:MPD:H11	4:B:1061:HOH:O	2.13	0.49
1:C:252:HIS:HE1	4:C:997:HOH:O	1.95	0.49
3:B:503:MPD:C1	4:B:1016:HOH:O	2.59	0.49
1:C:43:LYS:HE3	4:C:846:HOH:O	2.12	0.49
1:C:349:ASN:CB	4:C:608:HOH:O	2.60	0.49
3:D:502:MPD:C1	4:D:1039:HOH:O	2.61	0.49
1:A:232:PRO:HG2	1:C:232:PRO:HG2	1.93	0.49
1:A:89:PHE:CZ	1:A:96:VAL:HG22	2.48	0.48
1:C:291:ALA:CB	4:C:853:HOH:O	2.60	0.48
1:A:156:GLN:NE2	1:A:157[A]:ARG:HE	2.12	0.48
3:B:503:MPD:H53	4:B:998:HOH:O	2.12	0.48
1:B:7:LYS:NZ	4:B:620:HOH:O	2.46	0.48
1:C:349:ASN:HB2	4:C:608:HOH:O	2.13	0.48
1:B:352:TRP:HH2	3:B:503:MPD:H32	1.78	0.48
1:B:149[B]:ARG:NH2	4:B:622:HOH:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:PRO:HG2	4:C:818:HOH:O	2.13	0.47
1:C:262[A]:MET:HE2	4:C:971:HOH:O	2.13	0.47
1:A:194[B]:MET:CE	1:A:195:TYR:CE2	2.97	0.47
1:B:108:ILE:O	1:B:112[B]:ARG:HG2	2.15	0.47
1:B:44:GLN:NE2	4:B:625:HOH:O	2.47	0.47
1:D:286[A]:GLU:HG2	4:D:601:HOH:O	2.15	0.47
1:B:441:TYR:CE1	3:B:503:MPD:HM1	2.50	0.47
1:A:433:TRP:N	3:A:503:MPD:H53	2.31	0.46
1:D:286[A]:GLU:HG2	4:D:736:HOH:O	2.14	0.46
1:B:441:TYR:OH	3:B:503:MPD:H52	2.15	0.46
1:C:30[A]:GLU:HG3	4:C:629:HOH:O	2.16	0.46
1:C:319[B]:MET:HB2	1:C:319[B]:MET:HE2	1.59	0.46
1:C:99[A]:LYS:HG3	4:C:847:HOH:O	2.15	0.46
2:D:501:IMD:H2	4:D:1067:HOH:O	2.15	0.46
1:A:262[A]:MET:HE2	4:C:1267:HOH:O	2.15	0.46
4:A:1086:HOH:O	1:C:262[B]:MET:HE1	2.15	0.46
1:D:265:GLN:HE21	1:D:269:ASN:ND2	2.13	0.46
1:D:89:PHE:CE1	1:D:96[B]:VAL:HG12	2.51	0.45
1:A:245:ASN:HD21	1:C:364:ARG:HH12	1.65	0.45
3:A:503:MPD:H4	3:A:503:MPD:HM2	1.72	0.45
1:A:234:ASP:HA	1:C:234:ASP:HA	1.98	0.45
1:A:238[A]:GLU:HG3	4:A:1140:HOH:O	2.15	0.45
1:A:432:SER:HA	3:A:503:MPD:H32	1.99	0.45
1:A:441:TYR:HE2	3:A:503:MPD:H13	1.79	0.45
1:B:441:TYR:CZ	3:B:503:MPD:HM1	2.52	0.45
1:C:99[B]:LYS:NZ	4:C:625:HOH:O	2.49	0.45
1:D:89:PHE:CE1	1:D:96[A]:VAL:HG22	2.51	0.44
1:A:378:GLU:HG3	1:A:425:TRP:HB2	1.99	0.44
3:A:503:MPD:H11	3:A:503:MPD:O4	2.16	0.44
1:A:192:LYS:NZ	4:A:620:HOH:O	2.51	0.44
1:D:378:GLU:HG3	1:D:425:TRP:HB2	2.00	0.44
1:D:347[A]:THR:CG2	4:D:1037:HOH:O	2.65	0.44
1:B:166:VAL:HA	1:B:222:GLY:O	2.19	0.43
1:D:433:TRP:CD1	3:D:502:MPD:H31	2.53	0.43
1:B:92:GLY:HA2	1:B:128:PRO:HG2	2.01	0.43
3:B:503:MPD:C1	4:B:1061:HOH:O	2.66	0.43
1:A:99[A]:LYS:CE	4:A:626:HOH:O	2.39	0.43
1:B:438:GLN:NE2	1:B:449:ASP:HB2	2.34	0.43
1:B:149[A]:ARG:NH2	4:B:628:HOH:O	2.52	0.43
1:C:319[B]:MET:HB3	1:C:319[B]:MET:HE3	1.63	0.43
1:B:234:ASP:HA	1:D:234:ASP:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400[B]:ASP:OD2	4:D:605:HOH:O	2.21	0.42
1:B:157:ARG:HG3	1:B:158:PHE:CE1	2.54	0.42
1:C:433:TRP:CD1	3:C:502:MPD:H31	2.54	0.42
1:C:166:VAL:HA	1:C:222:GLY:O	2.20	0.42
1:D:349:ASN:ND2	4:D:628:HOH:O	2.53	0.42
1:B:441:TYR:CZ	3:B:503:MPD:C5	2.90	0.42
1:B:368[A]:ASN:OD1	1:D:369:ARG:NH2	2.52	0.42
1:C:385:ASP:HB2	1:C:440:ARG:HD2	2.01	0.42
1:D:166:VAL:HA	1:D:222:GLY:O	2.20	0.42
1:A:262[A]:MET:CE	4:C:1122:HOH:O	2.63	0.42
1:B:198:ASN:ND2	1:B:254:TRP:HE1	2.10	0.42
1:D:61:TYR:OH	4:D:604:HOH:O	2.20	0.42
1:C:7:LYS:HE3	1:C:7:LYS:HB3	1.90	0.41
1:C:112[B]:ARG:NH2	4:C:614:HOH:O	2.41	0.41
1:B:400:ASP:OD2	4:B:603:HOH:O	2.21	0.41
1:B:403:ARG:HD2	4:B:618:HOH:O	2.20	0.41
1:D:175:ILE:CG2	1:D:194[B]:MET:HG2	2.50	0.41
1:B:238[A]:GLU:HG3	4:B:1121:HOH:O	2.19	0.41
1:B:249[B]:PHE:HZ	1:B:270:TYR:HB3	1.86	0.41
1:B:477[B]:GLU:CG	4:B:654:HOH:O	2.66	0.41
1:D:350:TRP:CH2	1:D:384:PHE:CE2	3.08	0.41
1:D:430:LEU:HD12	1:D:430:LEU:C	2.41	0.41
1:A:7:LYS:HE3	1:A:7:LYS:HB3	1.86	0.41
1:C:378:GLU:HG3	1:C:425:TRP:HB2	2.02	0.41
1:D:403[B]:ARG:NH2	4:D:618:HOH:O	2.43	0.41
1:B:171:GLN:HA	1:B:174:PHE:CE2	2.56	0.41
1:B:368[A]:ASN:CG	1:D:369:ARG:HH22	2.24	0.41
1:C:174:PHE:HA	4:C:619:HOH:O	2.22	0.40
1:D:265:GLN:HE21	1:D:269:ASN:HD21	1.69	0.40
1:D:149:ARG:HD3	4:D:1004:HOH:O	2.20	0.40
1:C:338[A]:LYS:HE2	4:C:1009:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:935:HOH:O	4:D:863:HOH:O[1_545]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	497/485 (102%)	478 (96%)	19 (4%)	0	100	100
1	B	497/485 (102%)	482 (97%)	15 (3%)	0	100	100
1	C	502/485 (104%)	482 (96%)	20 (4%)	0	100	100
1	D	471/485 (97%)	454 (96%)	17 (4%)	0	100	100
All	All	1967/1940 (101%)	1896 (96%)	71 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	426/412 (103%)	422 (99%)	4 (1%)	84	57
1	B	426/412 (103%)	421 (99%)	5 (1%)	78	46
1	C	431/412 (105%)	427 (99%)	4 (1%)	84	57
1	D	407/412 (99%)	405 (100%)	2 (0%)	92	75
All	All	1690/1648 (102%)	1675 (99%)	15 (1%)	84	57

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	93	ASN

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Mol	Chain	Res	Type
1	A	430	LEU
1	A	452	SER
1	B	12[A]	GLU
1	B	12[B]	GLU
1	B	93	ASN
1	B	269	ASN
1	B	430	LEU
1	C	6	LEU
1	C	93	ASN
1	C	324	LYS
1	C	430	LEU
1	D	93	ASN
1	D	430	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	114	HIS
1	A	129	GLN
1	A	156	GLN
1	A	171	GLN
1	A	198	ASN
1	A	202	ASN
1	A	205	ASN
1	A	245	ASN
1	A	251	ASN
1	A	252	HIS
1	A	349	ASN
1	A	379	ASN
1	A	438	GLN
1	B	3	HIS
1	B	44	GLN
1	B	93	ASN
1	B	129	GLN
1	B	171	GLN
1	B	198	ASN
1	B	202	ASN
1	B	205	ASN
1	B	251	ASN
1	B	252	HIS
1	B	269	ASN

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Mol	Chain	Res	Type
1	B	349	ASN
1	B	379	ASN
1	B	394	ASN
1	C	93	ASN
1	C	114	HIS
1	C	129	GLN
1	C	171	GLN
1	C	198	ASN
1	C	202	ASN
1	C	205	ASN
1	C	251	ASN
1	C	252	HIS
1	C	269	ASN
1	C	349	ASN
1	C	379	ASN
1	C	394	ASN
1	C	435	ASN
1	D	93	ASN
1	D	129	GLN
1	D	171	GLN
1	D	198	ASN
1	D	202	ASN
1	D	205	ASN
1	D	214	HIS
1	D	251	ASN
1	D	252	HIS
1	D	269	ASN
1	D	349	ASN
1	D	379	ASN
1	D	394	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

10 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	IMD	A	501	-	3,5,5	0.38	0	4,5,5	0.65	0
2	IMD	A	502	-	3,5,5	0.56	0	4,5,5	0.67	0
3	MPD	A	503	-	6,7,7	0.80	0	6,10,10	1.30	1 (16%)
2	IMD	B	501	-	3,5,5	0.36	0	4,5,5	1.04	0
2	IMD	B	502	-	3,5,5	0.57	0	4,5,5	0.99	0
3	MPD	B	503	-	6,7,7	1.07	1 (16%)	6,10,10	2.21	2 (33%)
2	IMD	C	501	-	3,5,5	0.53	0	4,5,5	1.08	0
3	MPD	C	502	-	6,7,7	2.11	2 (33%)	6,10,10	2.25	2 (33%)
2	IMD	D	501	-	3,5,5	0.41	0	4,5,5	1.04	0
3	MPD	D	502	-	6,7,7	0.96	0	6,10,10	2.59	2 (33%)

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
2	IMD	A	501	-	-	0/0/0/0	0/1/1/1
2	IMD	A	502	-	-	0/0/0/0	0/1/1/1
3	MPD	A	503	-	-	0/5/5/5	0/0/0/0
2	IMD	B	501	-	-	0/0/0/0	0/1/1/1
2	IMD	B	502	-	-	0/0/0/0	0/1/1/1
3	MPD	B	503	-	-	0/5/5/5	0/0/0/0
2	IMD	C	501	-	-	0/0/0/0	0/1/1/1
3	MPD	C	502	-	-	0/5/5/5	0/0/0/0
2	IMD	D	501	-	-	0/0/0/0	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	D	502	-	-	0/5/5/5	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	MPD	C3-C4	2.15	1.63	1.51
3	B	503	MPD	O2-C2	2.42	1.51	1.44
3	C	502	MPD	O2-C2	4.21	1.56	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	MPD	O4-C4-C5	-3.70	91.00	109.47
3	B	503	MPD	CM-C2-C1	-3.15	102.90	110.41
3	D	502	MPD	O2-C2-CM	-2.70	98.09	108.01
3	A	503	MPD	O4-C4-C5	-2.24	98.31	109.47
3	C	502	MPD	CM-C2-C1	3.44	118.62	110.41
3	B	503	MPD	O2-C2-CM	4.03	122.83	108.01
3	D	502	MPD	CM-C2-C1	5.08	122.52	110.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	MPD	16	0
2	B	501	IMD	5	0
3	B	503	MPD	19	0
3	C	502	MPD	10	0
2	D	501	IMD	1	0
3	D	502	MPD	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	387:LEU	C	388:GLU	N	1.19
1	A	160:ASP	C	161:ARG	N	0.98

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	474/485 (97%)	-0.16	4 (0%) 87 89	10, 15, 28, 61	0
1	B	476/485 (98%)	-0.11	6 (1%) 79 82	11, 17, 29, 62	2 (0%)
1	C	474/485 (97%)	-0.18	9 (1%) 70 72	10, 15, 27, 66	0
1	D	455/485 (93%)	-0.18	9 (1%) 68 71	10, 15, 27, 73	7 (1%)
All	All	1879/1940 (96%)	-0.16	28 (1%) 76 78	10, 16, 28, 73	9 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	HIS	4.9
1	D	330	SER	4.8
1	D	350	TRP	4.2
1	D	347[A]	THR	4.1
1	D	5	HIS	3.8
1	C	312	ASP	3.7
1	C	313	GLY	3.6
1	C	311	PRO	3.4
1	B	5	HIS	3.2
1	A	321	THR	3.1
1	A	5	HIS	2.9
1	D	331	SER	2.8
1	C	5	HIS	2.8
1	D	352	TRP	2.5
1	D	310	PRO	2.5
1	B	218	ASP	2.5
1	C	350	TRP	2.4
1	C	322	THR	2.3
1	A	217	PRO	2.3
1	C	314	VAL	2.3
1	A	318	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	347	THR	2.1
1	B	160	ASP	2.1
1	B	389	PRO	2.1
1	D	282	PRO	2.1
1	B	4	ARG	2.0
1	C	324	LYS	2.0
1	D	351[A]	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	MPD	C	502	8/8	0.90	0.21	14.24	12,19,22,32	8
3	MPD	B	503	8/8	0.88	0.20	9.20	14,25,35,41	0
3	MPD	A	503	8/8	0.93	0.14	5.29	16,25,35,41	1
3	MPD	D	502	8/8	0.90	0.13	3.98	16,23,36,41	0
2	IMD	B	502	5/5	0.94	0.06	0.43	21,22,26,27	0
2	IMD	D	501	5/5	0.78	0.21	-	26,35,37,37	0
2	IMD	A	502	5/5	0.85	0.14	-	31,33,38,38	5
2	IMD	B	501	5/5	0.86	0.20	-	28,28,39,42	0
2	IMD	A	501	5/5	0.78	0.21	-	63,63,70,74	0
2	IMD	C	501	5/5	0.84	0.29	-	30,37,41,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.