



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:44 AM UTC

PDB ID : 5OPQ / pdb_00005opq
Title : A 3,6-anhydro-D-galactosidase produced by *Zobellia galactanivorans*. This is an exo-lytic enzyme that hydrolyzes terminal 3,6-anhydro-D-galactose from the non-reducing end of carrageenan oligosaccharides.
Authors : Ficko-Blean, E.; Michel, G.; Czjzek, M.
Deposited on : 2017-08-10
Resolution : 1.70 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 ⓘ 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 ⓘ](#)) 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

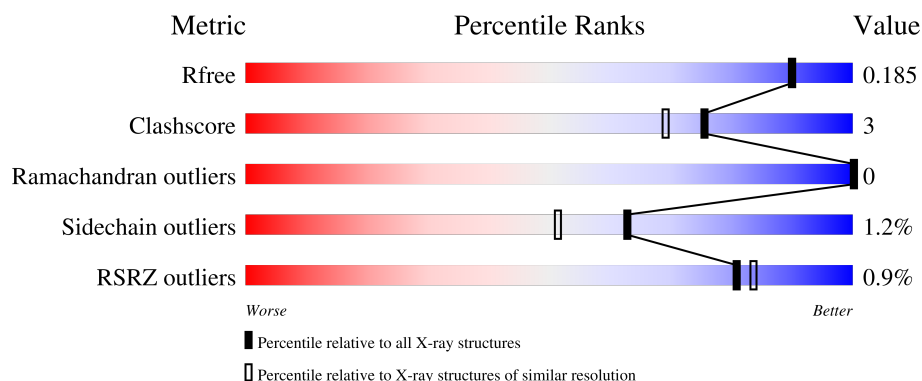
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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 $\leq 5\%$. 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	693	84% 10% • 5%
1	B	693	82% 12% • 5%
1	C	693	84% 11% 5%
1	D	693	84% 10% • 5%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPD	A	702	-	X	X	-
2	MPD	B	701	-	X	X	-
2	MPD	D	701	-	X	X	-
3	TRS	A	703[A]	-	X	-	-
3	TRS	A	703[B]	-	X	-	-
3	TRS	B	702[A]	-	X	-	-
3	TRS	C	702[A]	-	X	-	-
3	TRS	C	703	-	X	-	-
3	TRS	D	702[A]	-	X	-	-

2 Entry composition [i](#)

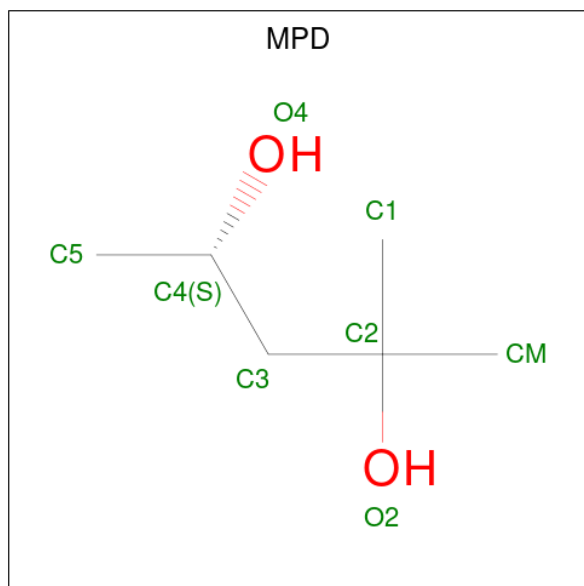
There are 5 unique types of molecules in this entry. The entry contains 23909 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3,6-anhydro-D-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	659	Total	C	N	O	S	0	6	0
			5244	3345	884	991	24			
1	B	659	Total	C	N	O	S	0	4	0
			5256	3356	892	984	24			
1	C	659	Total	C	N	O	S	0	3	0
			5224	3333	883	984	24			
1	D	658	Total	C	N	O	S	0	3	0
			5228	3337	884	983	24			

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

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

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			16	8	2	6		
3	B	1	Total	C	N	O	0	1
			16	8	2	6		
3	C	1	Total	C	N	O	0	1
			16	8	2	6		
3	C	1	Total	C	N	O	0	0
			8	4	1	3		
3	D	1	Total	C	N	O	0	1
			16	8	2	6		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0

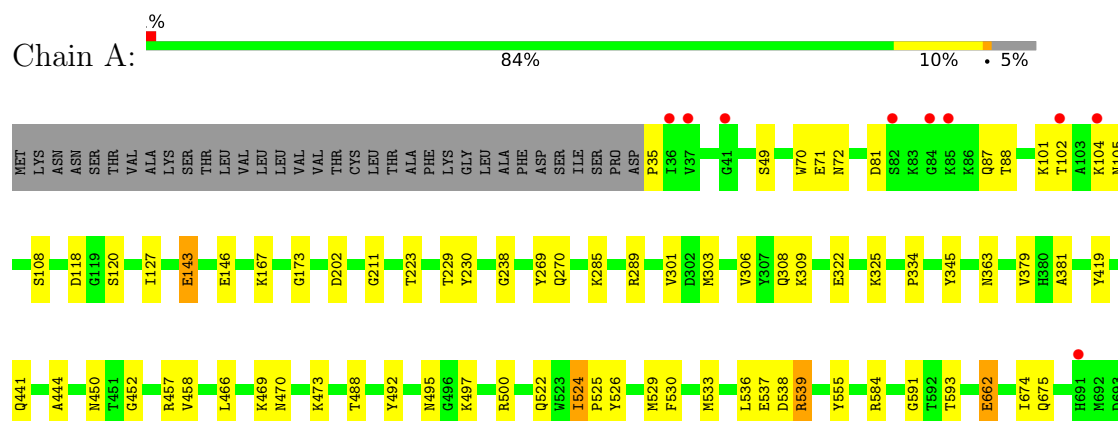
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	706	Total 718	O 718	0	12
5	B	686	Total 695	O 695	0	9
5	C	733	Total 745	O 745	0	11
5	D	669	Total 683	O 683	0	14

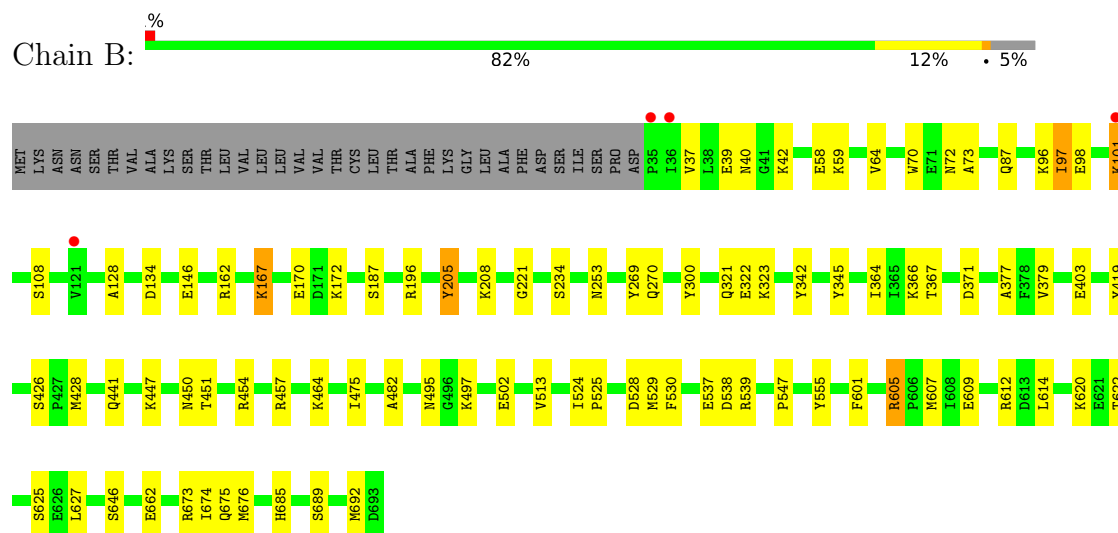
3 Residue-property plots

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.

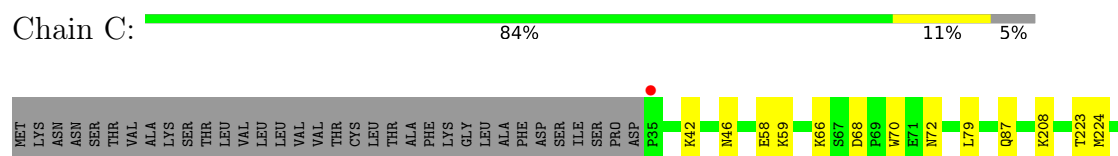
• Molecule 1: 3,6-anhydro-D-galactosidase

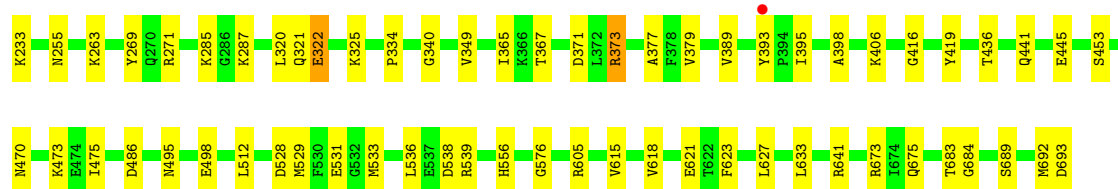


• Molecule 1: 3,6-anhydro-D-galactosidase

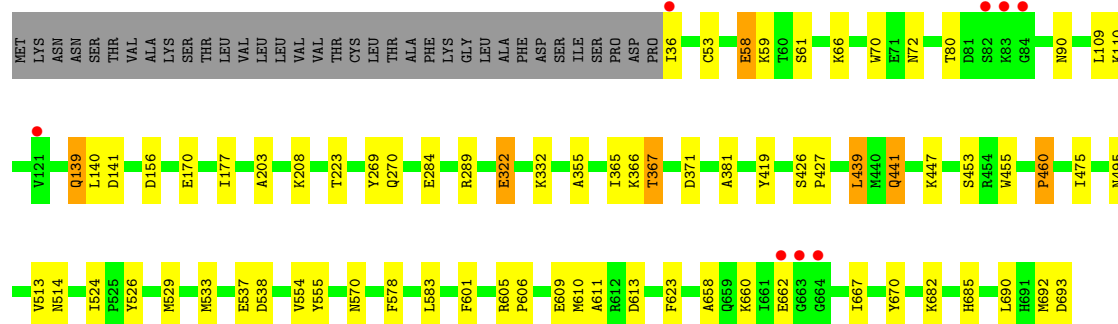
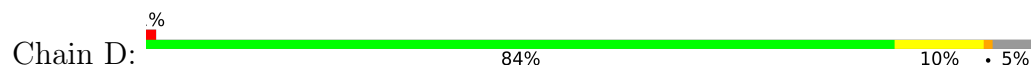


• Molecule 1: 3,6-anhydro-D-galactosidase





• Molecule 1: 3,6-anhydro-D-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	222.00Å 107.50Å 165.80Å 90.00° 114.00° 90.00°	Depositor
Resolution (Å)	46.70 – 1.70 46.70 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.70-1.70) 99.6 (46.70-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.146 , 0.176 0.158 , 0.185	Depositor DCC
R_{free} test set	19548 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	23909	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: TRS, CL, 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	1.55	31/5381 (0.6%)	1.27	15/7285 (0.2%)
1	B	1.53	33/5393 (0.6%)	1.28	18/7292 (0.2%)
1	C	1.54	30/5361 (0.6%)	1.29	10/7258 (0.1%)
1	D	1.54	38/5361 (0.7%)	1.27	24/7254 (0.3%)
All	All	1.54	132/21496 (0.6%)	1.28	67/29089 (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	B	0	1

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	667	ILE	N-CA	-9.67	1.37	1.46
1	A	289	ARG	CD-NE	-9.35	1.33	1.46
1	D	289	ARG	CD-NE	-9.10	1.33	1.46
1	A	309	LYS	N-CA	8.16	1.56	1.46
1	B	612	ARG	N-CA	7.42	1.55	1.46
1	A	444	ALA	N-CA	7.40	1.55	1.46
1	B	322	GLU	CD-OE2	7.29	1.39	1.25
1	C	379	VAL	C-O	-7.11	1.16	1.24
1	A	452	GLY	N-CA	7.08	1.54	1.45
1	B	64	VAL	N-CA	-7.05	1.37	1.46
1	D	524	ILE	CA-C	6.98	1.60	1.52
1	A	143	GLU	N-CA	-6.95	1.37	1.46
1	A	334	PRO	CA-C	6.90	1.60	1.52
1	A	591	GLY	N-CA	-6.85	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	530	PHE	C-O	-6.73	1.16	1.24
1	A	662	GLU	N-CA	6.67	1.54	1.46
1	D	322	GLU	CD-OE1	6.54	1.37	1.25
1	D	58	GLU	C-O	-6.46	1.16	1.24
1	A	238	GLY	CA-C	-6.41	1.47	1.52
1	C	287	LYS	N-CA	-6.38	1.38	1.46
1	B	170	GLU	N-CA	6.37	1.53	1.46
1	A	458	VAL	N-CA	6.35	1.53	1.46
1	A	662	GLU	C-O	6.33	1.31	1.24
1	C	365	ILE	N-CA	-6.32	1.39	1.46
1	D	140	LEU	C-O	-6.31	1.17	1.24
1	D	670	TYR	C-N	-6.31	1.27	1.34
1	B	620	LYS	N-CA	6.29	1.53	1.46
1	B	674	ILE	C-O	-6.25	1.17	1.24
1	A	379	VAL	C-O	-6.16	1.17	1.24
1	B	674	ILE	CA-CB	-6.16	1.46	1.54
1	A	325	LYS	N-CA	6.14	1.53	1.46
1	B	614	LEU	N-CA	-6.09	1.38	1.46
1	A	81	ASP	C-O	-6.08	1.17	1.23
1	C	684	GLY	CA-C	6.08	1.58	1.51
1	C	377	ALA	C-O	-6.07	1.16	1.23
1	B	685	HIS	N-CA	6.05	1.53	1.46
1	C	398	ALA	C-O	-6.02	1.16	1.24
1	A	674	ILE	CA-CB	-6.00	1.47	1.54
1	A	146	GLU	C-O	-5.99	1.16	1.23
1	C	689	SER	CA-C	-5.99	1.45	1.52
1	D	610	MET	N-CA	-5.98	1.39	1.46
1	C	322	GLU	CD-OE1	5.97	1.36	1.25
1	D	693	ASP	CA-CB	-5.88	1.41	1.53
1	C	556	HIS	N-CA	-5.88	1.38	1.46
1	D	141	ASP	C-O	-5.87	1.16	1.23
1	D	53	CYS	N-CA	5.87	1.53	1.46
1	C	68	ASP	C-O	-5.86	1.16	1.24
1	D	332	LYS	CA-C	5.85	1.60	1.52
1	D	177	ILE	N-CA	5.84	1.50	1.45
1	C	322	GLU	N-CA	5.83	1.53	1.46
1	D	460	PRO	C-O	-5.82	1.17	1.24
1	D	554	VAL	C-O	5.82	1.30	1.24
1	A	466	LEU	N-CA	-5.80	1.39	1.46
1	D	658	ALA	CA-C	-5.80	1.45	1.52
1	B	205	TYR	N-CA	5.74	1.53	1.46
1	D	365	ILE	C-O	-5.71	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	156	ASP	N-CA	5.71	1.53	1.46
1	D	355	ALA	N-CA	5.68	1.53	1.46
1	C	627	LEU	CA-CB	5.67	1.60	1.52
1	B	662	GLU	C-O	5.66	1.31	1.24
1	C	693	ASP	CA-CB	-5.65	1.42	1.53
1	B	530	PHE	C-O	-5.63	1.17	1.24
1	D	693	ASP	N-CA	5.59	1.56	1.46
1	B	605	ARG	CA-C	-5.57	1.46	1.52
1	D	367	THR	C-O	-5.54	1.17	1.24
1	C	320	LEU	N-CA	-5.54	1.39	1.46
1	D	455	TRP	C-O	-5.52	1.16	1.24
1	B	379	VAL	C-O	-5.50	1.18	1.24
1	D	441	GLN	C-O	-5.48	1.17	1.23
1	A	105	ASN	N-CA	5.45	1.52	1.46
1	A	381	ALA	C-O	-5.44	1.17	1.24
1	C	605	ARG	CD-NE	-5.43	1.38	1.46
1	A	71	GLU	N-CA	5.43	1.52	1.46
1	A	522	GLN	N-CA	5.42	1.53	1.46
1	D	80	THR	C-O	-5.41	1.17	1.23
1	C	349	VAL	N-CA	5.41	1.52	1.46
1	A	211	GLY	C-O	-5.41	1.15	1.23
1	B	73	ALA	C-O	-5.40	1.17	1.24
1	D	139	GLN	C-O	-5.39	1.18	1.23
1	B	377	ALA	C-O	-5.39	1.17	1.23
1	D	690	LEU	N-CA	-5.39	1.39	1.46
1	A	593	THR	C-O	-5.36	1.18	1.24
1	A	308	GLN	CA-C	5.33	1.59	1.52
1	B	364	ILE	N-CA	5.33	1.52	1.46
1	B	403	GLU	CD-OE1	5.32	1.35	1.25
1	B	528	ASP	C-O	-5.31	1.17	1.24
1	B	622	THR	C-O	-5.30	1.17	1.24
1	C	528	ASP	C-O	-5.30	1.17	1.24
1	B	539	ARG	CZ-NH2	-5.29	1.26	1.33
1	A	88	THR	CA-C	-5.29	1.46	1.52
1	C	340	GLY	CA-C	-5.29	1.47	1.51
1	D	90	ASN	CA-C	-5.25	1.46	1.52
1	B	685	HIS	CA-C	-5.24	1.46	1.52
1	B	675	GLN	N-CA	5.24	1.52	1.46
1	C	395	ILE	C-O	5.23	1.29	1.24
1	D	578	PHE	CA-C	-5.22	1.46	1.52
1	A	539	ARG	N-CA	5.19	1.52	1.46
1	B	366	LYS	C-O	-5.19	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	693	ASP	CA-C	5.19	1.63	1.52
1	D	583	LEU	N-CA	-5.18	1.40	1.46
1	D	381	ALA	C-O	-5.18	1.17	1.24
1	D	61	SER	CA-C	-5.18	1.45	1.52
1	A	457	ARG	CA-CB	-5.17	1.46	1.53
1	B	321	GLN	N-CA	5.17	1.52	1.46
1	B	196	ARG	N-CA	-5.17	1.40	1.46
1	C	224	MET	CA-C	-5.17	1.47	1.52
1	C	436	THR	CB-CG2	-5.15	1.35	1.52
1	C	475	ILE	CA-CB	-5.15	1.47	1.54
1	D	660	LYS	C-O	-5.15	1.17	1.23
1	C	46	ASN	N-CA	-5.14	1.39	1.46
1	B	108	SER	CA-C	-5.14	1.46	1.52
1	B	39	GLU	CA-C	-5.12	1.46	1.52
1	A	306	VAL	C-O	5.11	1.29	1.24
1	D	606	PRO	N-CA	-5.11	1.40	1.47
1	A	49	SER	C-O	-5.11	1.17	1.24
1	C	325	LYS	N-CA	5.11	1.52	1.46
1	D	453	SER	C-O	-5.11	1.17	1.23
1	B	627	LEU	CA-CB	5.10	1.59	1.52
1	D	203	ALA	CA-C	-5.10	1.45	1.52
1	C	79	LEU	C-O	-5.09	1.17	1.23
1	B	547	PRO	CA-C	5.09	1.59	1.52
1	C	373	ARG	CA-CB	5.07	1.61	1.53
1	C	389	VAL	C-O	-5.07	1.18	1.24
1	C	618	VAL	N-CA	-5.06	1.40	1.46
1	D	109	LEU	N-CA	-5.05	1.39	1.45
1	B	447	LYS	N-CA	5.05	1.52	1.46
1	C	531	GLU	C-O	-5.03	1.17	1.24
1	D	366	LYS	C-O	-5.03	1.18	1.24
1	B	342	TYR	CA-CB	5.03	1.59	1.53
1	A	127	ILE	C-O	-5.02	1.19	1.24
1	B	475	ILE	N-CA	-5.02	1.40	1.46
1	C	416	GLY	CA-C	5.02	1.58	1.51

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	692	MET	CA-C-N	11.14	141.75	121.70
1	D	692	MET	C-N-CA	11.14	141.75	121.70
1	A	289	ARG	NE-CZ-NH2	-9.82	110.36	119.20
1	D	289	ARG	NE-CZ-NH2	-8.79	111.29	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	692	MET	CA-C-N	8.27	136.59	121.70
1	C	692	MET	C-N-CA	8.27	136.59	121.70
1	A	289	ARG	NE-CZ-NH1	7.92	129.41	121.50
1	B	162	ARG	NE-CZ-NH2	7.52	125.97	119.20
1	A	289	ARG	CB-CG-CD	-7.10	94.98	111.30
1	B	134	ASP	CA-C-N	-6.98	112.51	119.56
1	B	134	ASP	C-N-CA	-6.98	112.51	119.56
1	D	692	MET	O-C-N	6.94	131.13	123.22
1	B	162	ARG	NE-CZ-NH1	-6.64	114.86	121.50
1	C	576	GLY	CA-C-O	6.53	127.14	122.37
1	C	59	LYS	N-CA-C	6.49	120.45	112.54
1	A	555	TYR	N-CA-C	6.28	121.71	113.30
1	A	675	GLN	CB-CG-CD	6.26	123.24	112.60
1	D	284	GLU	N-CA-C	6.21	118.71	109.59
1	D	270	GLN	CB-CG-CD	6.18	123.11	112.60
1	D	623	PHE	N-CA-C	6.08	118.40	111.11
1	B	37	VAL	N-CA-C	6.06	116.59	108.11
1	D	59	LYS	N-CA-C	6.05	119.92	112.54
1	C	621	GLU	N-CA-C	5.93	117.74	111.28
1	A	301	VAL	N-CA-C	-5.93	104.96	110.53
1	B	555	TYR	N-CA-C	5.92	120.51	112.88
1	D	555	TYR	N-CA-C	5.85	120.42	112.88
1	D	475	ILE	O-C-N	5.83	127.62	121.91
1	A	285	LYS	CA-C-N	-5.82	116.51	122.27
1	A	285	LYS	C-N-CA	-5.82	116.51	122.27
1	D	692	MET	CA-C-O	-5.80	114.15	120.36
1	C	436	THR	OG1-CB-CG2	-5.77	97.77	109.30
1	C	321	GLN	N-CA-C	-5.74	104.94	111.14
1	B	345	TYR	N-CA-C	-5.70	101.71	110.32
1	A	345	TYR	N-CA-C	-5.65	101.79	110.32
1	D	289	ARG	CB-CG-CD	-5.62	98.36	111.30
1	B	97	ILE	CB-CA-C	-5.58	102.18	110.33
1	D	289	ARG	NE-CZ-NH1	5.58	127.08	121.50
1	A	72	ASN	N-CA-CB	-5.51	103.64	111.84
1	B	300	TYR	N-CA-C	5.40	117.92	111.71
1	B	607	MET	O-C-N	5.38	127.82	122.12
1	A	526	TYR	N-CA-C	5.36	119.97	113.38
1	D	610	MET	N-CA-C	5.34	117.10	111.28
1	B	601	PHE	N-CA-C	5.32	117.50	111.11
1	B	609	GLU	N-CA-C	5.31	117.07	111.28
1	D	613	ASP	N-CA-C	5.30	117.13	111.36
1	C	453	SER	CB-CA-C	-5.28	104.55	112.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	692	MET	O-C-N	5.25	129.23	122.93
1	D	203	ALA	N-CA-C	5.25	117.75	111.71
1	D	609	GLU	N-CA-C	5.25	116.69	111.07
1	B	221	GLY	N-CA-C	5.25	120.28	112.41
1	A	524	ILE	CA-C-N	-5.21	114.24	119.56
1	A	524	ILE	C-N-CA	-5.21	114.24	119.56
1	B	676	MET	CA-C-N	5.20	127.50	120.38
1	B	676	MET	C-N-CA	5.20	127.50	120.38
1	A	584	ARG	NE-CZ-NH2	-5.18	114.54	119.20
1	A	303	MET	N-CA-C	5.18	116.61	111.07
1	B	689	SER	CA-CB-OG	-5.13	100.84	111.10
1	D	526	TYR	N-CA-C	5.09	119.64	113.38
1	D	514	ASN	N-CA-C	5.08	117.10	109.23
1	B	323	LYS	N-CA-C	5.07	117.54	111.71
1	D	513	VAL	N-CA-C	-5.07	102.15	108.84
1	B	426	SER	N-CA-C	5.07	121.01	109.81
1	D	605	ARG	N-CA-C	5.05	120.47	113.45
1	C	615	VAL	N-CA-C	5.04	116.50	111.00
1	D	601	PHE	N-CA-C	5.04	117.16	111.11
1	D	611	ALA	O-C-N	5.04	127.26	122.07
1	D	570	ASN	N-CA-C	5.04	119.30	113.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	205	TYR	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	5244	0	5064	29	0
1	B	5256	0	5129	35	0
1	C	5224	0	5055	30	0
1	D	5228	0	5070	21	0
2	A	16	0	27	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8	0	12	7	0
2	C	8	0	14	0	0
2	D	8	0	12	8	0
3	A	16	0	23	0	0
3	B	16	0	24	2	0
3	C	24	0	36	2	0
3	D	16	0	24	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	718	0	0	13	1
5	B	695	0	0	9	0
5	C	745	0	0	17	1
5	D	683	0	0	6	0
All	All	23909	0	20490	125	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 3.

All (125) 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:406:LYS:HE2	5:C:1079:HOH:O	1.37	1.24
2:B:701:MPD:H51	5:B:1334:HOH:O	1.49	1.13
2:D:701:MPD:H12	2:D:701:MPD:H52	1.21	1.10
1:C:498:GLU:OE1	5:C:801:HOH:O	1.71	1.09
1:C:233:LYS:HE2	5:C:1349:HOH:O	1.51	1.08
1:D:538:ASP:H	2:D:701:MPD:H51	1.13	1.08
1:C:393:TYR:CD2	1:C:470[B]:ASN:ND2	2.23	1.07
1:A:537:GLU:H	2:A:702:MPD:H51	0.94	1.06
1:A:537:GLU:N	2:A:702:MPD:H51	1.72	1.04
2:A:702:MPD:H52	5:A:1089:HOH:O	1.63	0.98
1:A:35:PRO:N	5:A:801:HOH:O	1.95	0.98
1:A:537:GLU:H	2:A:702:MPD:C5	1.83	0.91
3:C:703:TRS:H12	5:C:986:HOH:O	1.69	0.91
2:D:701:MPD:H12	2:D:701:MPD:C5	1.84	0.88
1:C:322:GLU:HG2	5:C:1414:HOH:O	1.75	0.86
2:B:701:MPD:H11	5:B:990:HOH:O	1.80	0.81
1:B:441:GLN:HE22	1:B:495:ASN:HD21	1.31	0.78
1:C:486:ASP:OD2	3:C:702[A]:TRS:O2	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:THR:HG21	1:A:108[B]:SER:OG	1.85	0.77
1:B:457[A]:ARG:HG2	1:B:457[A]:ARG:HH11	1.51	0.76
1:C:538:ASP:OD1	1:D:538:ASP:OD1	2.05	0.75
1:A:202:ASP:OD2	3:B:702[B]:TRS:O2	2.04	0.75
1:B:367:THR:HG21	1:B:605:ARG:HH22	1.51	0.75
1:D:538:ASP:N	2:D:701:MPD:H51	1.96	0.75
1:D:322:GLU:HG2	5:D:1342:HOH:O	1.85	0.74
2:B:701:MPD:H52	5:B:1393:HOH:O	1.85	0.74
1:D:441:GLN:HE22	1:D:495:ASN:HD21	1.35	0.73
1:C:393:TYR:CE2	1:C:470[B]:ASN:ND2	2.56	0.73
1:B:96:LYS:HE3	1:B:98:GLU:OE2	1.90	0.72
1:B:537:GLU:H	2:B:701:MPD:C1	2.07	0.68
1:A:538:ASP:OD1	1:B:538:ASP:OD1	2.11	0.68
1:B:208:LYS:HE2	5:B:1084:HOH:O	1.94	0.67
1:A:143:GLU:OE2	5:A:802:HOH:O	2.13	0.66
1:C:512:LEU:O	5:C:802:HOH:O	2.14	0.65
5:C:1187[B]:HOH:O	1:D:685:HIS:HD2	1.79	0.64
2:A:702:MPD:O4	2:A:702:MPD:H12	1.68	0.64
1:A:539:ARG:NH1	5:A:805:HOH:O	2.30	0.64
1:B:454:ARG:HA	1:B:457[A]:ARG:NE	2.12	0.64
3:B:702[B]:TRS:O1	3:B:702[B]:TRS:O3	1.95	0.64
5:C:1364:HOH:O	2:D:701:MPD:C1	2.47	0.63
1:B:167:LYS:HZ1	1:B:270:GLN:HG3	1.64	0.62
1:A:363[B]:ASN:ND2	5:A:806:HOH:O	2.34	0.61
1:A:322:GLU:HG3	5:A:1343:HOH:O	1.99	0.61
1:D:170[B]:GLU:HG3	5:D:1176:HOH:O	2.01	0.60
1:D:537:GLU:HB2	2:D:701:MPD:H53	1.84	0.60
1:C:441:GLN:HE22	1:C:495:ASN:HD21	1.50	0.60
1:B:428:MET:O	1:B:457[A]:ARG:HD2	2.01	0.59
1:B:537:GLU:H	2:B:701:MPD:H13	1.68	0.59
1:A:118:ASP:OD1	1:A:120:SER:OG	2.18	0.58
1:D:439:LEU:HB2	5:D:819:HOH:O	2.04	0.57
1:C:673:ARG:HG2	1:C:683:THR:HG22	1.87	0.56
1:A:441:GLN:HE22	1:A:495:ASN:HD21	1.52	0.56
5:C:1364:HOH:O	2:D:701:MPD:H11	2.05	0.56
1:B:451:THR:HA	1:B:457[A]:ARG:HH12	1.71	0.56
1:B:208:LYS:CE	5:B:1084:HOH:O	2.53	0.56
1:D:36:ILE:N	5:D:812:HOH:O	2.41	0.54
1:A:104:LYS:NZ	5:A:803:HOH:O	2.17	0.54
1:C:42:LYS:NZ	5:C:807:HOH:O	2.40	0.53
1:A:492:TYR:OH	1:A:497:LYS:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457[A]:ARG:HG2	1:B:457[A]:ARG:NH1	2.23	0.52
1:C:66:LYS:HE2	5:C:820:HOH:O	2.08	0.52
1:A:469:LYS:HD2	5:A:1185:HOH:O	2.09	0.52
1:C:675:GLN:HG2	5:C:1354:HOH:O	2.10	0.52
1:D:367:THR:HG23	1:D:371:ASP:OD2	2.10	0.52
1:B:367:THR:HG23	1:B:371:ASP:OD2	2.10	0.50
1:A:101:LYS:CE	5:A:1392:HOH:O	2.59	0.50
1:A:223:THR:HG21	1:A:533:MET:SD	2.52	0.50
1:B:101:LYS:NZ	1:B:101:LYS:HB3	2.26	0.49
1:D:223:THR:HG21	1:D:533:MET:SD	2.53	0.49
1:B:40:ASN:O	1:B:59:LYS:NZ	2.44	0.48
1:C:470[A]:ASN:OD1	1:C:473:LYS:HD2	2.13	0.48
1:B:625[A]:SER:OG	1:B:646:SER:HB3	2.14	0.48
1:C:367:THR:HG23	1:C:371:ASP:OD2	2.14	0.48
1:B:537:GLU:HB2	2:B:701:MPD:H13	1.95	0.48
1:A:101:LYS:HE2	5:A:1392:HOH:O	2.14	0.48
1:A:470:ASN:OD1	1:A:473:LYS:HD2	2.14	0.47
1:A:450:ASN:ND2	5:A:810:HOH:O	2.46	0.47
1:B:367:THR:HG21	1:B:605:ARG:NH2	2.25	0.47
1:A:173:GLY:HA3	1:A:230:TYR:O	2.15	0.47
5:A:1066:HOH:O	1:B:692:MET:HE3	2.15	0.47
1:A:488:THR:O	1:A:500:ARG:HD3	2.15	0.46
1:D:426:SER:N	1:D:427:PRO:HD3	2.29	0.46
1:B:419:TYR:CD1	1:B:419:TYR:C	2.93	0.46
1:A:363[B]:ASN:CG	5:A:806:HOH:O	2.58	0.46
1:B:464:LYS:HD2	1:B:502:GLU:HG2	1.98	0.45
1:B:482:ALA:HA	1:B:513:VAL:O	2.15	0.45
1:B:497:LYS:HE2	5:B:806:HOH:O	2.16	0.45
1:D:70:TRP:CD1	1:D:269:TYR:HB3	2.51	0.45
1:C:536:LEU:O	1:C:539:ARG:NH1	2.47	0.45
1:B:70:TRP:CD1	1:B:269:TYR:HB3	2.52	0.45
1:C:70:TRP:CD1	1:C:269:TYR:HB3	2.52	0.45
1:C:675:GLN:CG	5:C:1354:HOH:O	2.65	0.45
1:D:426:SER:H	1:D:427:PRO:HD3	1.82	0.44
1:B:450:ASN:O	1:B:457[A]:ARG:NH1	2.51	0.44
1:C:223:THR:HG21	1:C:533:MET:SD	2.57	0.44
2:A:702:MPD:H12	2:A:702:MPD:H4	1.10	0.44
1:C:66:LYS:CE	5:C:820:HOH:O	2.64	0.44
1:B:58:GLU:OE2	1:B:234:SER:HB3	2.18	0.43
1:D:426:SER:N	1:D:427:PRO:CD	2.82	0.43
1:A:70:TRP:CD1	1:A:269:TYR:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LYS:HZ1	1:A:270:GLN:HG3	1.84	0.43
1:B:187:SER:HA	1:B:253:ASN:HD21	1.83	0.43
1:D:419:TYR:CD1	1:D:419:TYR:C	2.96	0.43
1:C:334:PRO:HG3	1:C:623:PHE:CD2	2.54	0.43
1:C:233:LYS:CD	5:C:1349:HOH:O	2.65	0.43
1:B:42:LYS:HD3	5:B:1455:HOH:O	2.19	0.43
1:D:208[B]:LYS:NZ	5:D:821:HOH:O	2.52	0.43
1:C:393:TYR:CG	1:C:470[B]:ASN:ND2	2.85	0.42
1:A:536:LEU:HD22	2:A:702:MPD:H53	2.01	0.42
1:C:263:LYS:O	1:D:447:LYS:HD2	2.20	0.42
1:B:428:MET:O	1:B:457[A]:ARG:CD	2.68	0.42
1:B:673:ARG:HD3	5:B:810:HOH:O	2.19	0.42
1:B:524:ILE:N	1:B:525:PRO:CD	2.83	0.42
1:C:208:LYS:HE2	5:C:1364:HOH:O	2.20	0.42
1:D:682:LYS:HE3	5:D:916:HOH:O	2.17	0.42
1:D:537:GLU:HB2	2:D:701:MPD:C5	2.50	0.42
1:C:419:TYR:CD1	1:C:419:TYR:C	2.98	0.41
1:A:524:ILE:N	1:A:525:PRO:CD	2.84	0.41
1:C:373:ARG:HD2	5:C:1009:HOH:O	2.19	0.41
1:C:255:ASN:HB3	1:C:271:ARG:HG3	2.03	0.41
1:C:633:LEU:HD11	1:C:641:ARG:HB2	2.01	0.41
1:B:128:ALA:HB3	1:B:146:GLU:CG	2.51	0.40
1:A:419:TYR:CD1	1:A:419:TYR:C	2.99	0.40
2:B:701:MPD:HM2	5:B:844:HOH:O	2.21	0.40
1:B:457[A]:ARG:NH1	1:B:457[A]:ARG:CG	2.77	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)
5:A:1240:HOH:O	5:C:806:HOH:O[2_556]	2.02	0.18

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	663/693 (96%)	637 (96%)	26 (4%)	0	100	100
1	B	661/693 (95%)	637 (96%)	24 (4%)	0	100	100
1	C	660/693 (95%)	639 (97%)	21 (3%)	0	100	100
1	D	659/693 (95%)	631 (96%)	28 (4%)	0	100	100
All	All	2643/2772 (95%)	2544 (96%)	99 (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	558/592 (94%)	554 (99%)	4 (1%)	76	69
1	B	562/592 (95%)	555 (99%)	7 (1%)	63	51
1	C	556/592 (94%)	550 (99%)	6 (1%)	65	54
1	D	556/592 (94%)	547 (98%)	9 (2%)	55	41
All	All	2232/2368 (94%)	2206 (99%)	26 (1%)	63	51

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	229	THR
1	A	529	MET
1	A	662	GLU
1	B	72	ASN
1	B	87	GLN
1	B	97	ILE
1	B	101	LYS
1	B	167	LYS
1	B	172	LYS

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Mol	Chain	Res	Type
1	B	529	MET
1	C	58	GLU
1	C	72	ASN
1	C	87	GLN
1	C	285	LYS
1	C	445	GLU
1	C	529	MET
1	D	58	GLU
1	D	66	LYS
1	D	72	ASN
1	D	110	LYS
1	D	139	GLN
1	D	439	LEU
1	D	460	PRO
1	D	529	MET
1	D	662	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	63	HIS
1	A	105	ASN
1	A	151	ASN
1	A	283	GLN
1	A	308	GLN
1	A	331	ASN
1	A	387	ASN
1	A	450	ASN
1	A	463	GLN
1	A	495	ASN
1	A	691	HIS
1	B	46	ASN
1	B	147	HIS
1	B	253	ASN
1	B	387	ASN
1	B	470	ASN
1	B	495	ASN
1	C	46	ASN
1	C	151	ASN
1	C	331	ASN
1	C	387	ASN

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Mol	Chain	Res	Type
1	C	463	GLN
1	C	495	ASN
1	D	44	ASN
1	D	151	ASN
1	D	283	GLN
1	D	308	GLN
1	D	331	ASN
1	D	387	ASN
1	D	495	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	TRS	D	702[B]	-	7,7,7	0.91	0	9,9,9	1.75	4 (44%)
3	TRS	A	703[A]	-	7,7,7	0.78	0	9,9,9	2.75	5 (55%)
2	MPD	C	701	-	7,7,7	0.83	0	9,10,10	1.12	0
2	MPD	B	701	-	7,7,7	2.60	2 (28%)	9,10,10	7.62	6 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TRS	B	702[B]	-	7,7,7	1.04	0	9,9,9	1.81	3 (33%)
2	MPD	A	702	-	7,7,7	3.30	5 (71%)	9,10,10	3.88	6 (66%)
2	MPD	A	701	-	7,7,7	0.96	0	9,10,10	0.95	0
2	MPD	D	701	-	7,7,7	2.31	5 (71%)	9,10,10	3.19	6 (66%)
3	TRS	D	702[A]	-	7,7,7	1.08	1 (14%)	9,9,9	2.13	3 (33%)
3	TRS	C	702[B]	-	7,7,7	1.00	0	9,9,9	3.57	4 (44%)
3	TRS	B	702[A]	-	7,7,7	1.25	1 (14%)	9,9,9	3.10	5 (55%)
3	TRS	A	703[B]	-	7,7,7	2.65	3 (42%)	9,9,9	4.75	7 (77%)
3	TRS	C	702[A]	-	7,7,7	2.01	3 (42%)	9,9,9	2.80	6 (66%)
3	TRS	C	703	-	7,7,7	2.61	2 (28%)	9,9,9	6.12	7 (77%)

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	TRS	D	702[B]	-	-	0/9/9/9	-
3	TRS	A	703[A]	-	-	7/9/9/9	-
2	MPD	C	701	-	-	0/5/5/5	-
2	MPD	B	701	-	-	4/5/5/5	-
3	TRS	B	702[B]	-	-	5/9/9/9	-
2	MPD	A	702	-	-	3/5/5/5	-
2	MPD	A	701	-	-	0/5/5/5	-
2	MPD	D	701	-	-	4/5/5/5	-
3	TRS	D	702[A]	-	-	6/9/9/9	-
3	TRS	C	702[B]	-	-	5/9/9/9	-
3	TRS	B	702[A]	-	-	9/9/9/9	-
3	TRS	A	703[B]	-	-	7/9/9/9	-
3	TRS	C	702[A]	-	-	5/9/9/9	-
3	TRS	C	703	-	-	6/9/9/9	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	703	TRS	C3-C	5.73	1.68	1.53
2	A	702	MPD	C3-C2	-5.64	1.37	1.54
2	B	701	MPD	O2-C2	5.57	1.58	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703[B]	TRS	O2-C2	4.26	1.55	1.42
2	A	702	MPD	C5-C4	-3.85	1.35	1.51
3	A	703[B]	TRS	C2-C	3.77	1.63	1.53
2	B	701	MPD	C1-C2	3.37	1.62	1.52
2	A	702	MPD	C1-C2	3.36	1.62	1.52
3	C	702[A]	TRS	C2-C	-3.21	1.44	1.53
3	C	703	TRS	O2-C2	3.20	1.52	1.42
2	D	701	MPD	C5-C4	-3.11	1.38	1.51
2	A	702	MPD	CM-C2	3.10	1.61	1.52
3	C	702[A]	TRS	C-N	3.09	1.59	1.49
2	D	701	MPD	C3-C2	-2.81	1.45	1.54
2	D	701	MPD	CM-C2	2.78	1.60	1.52
3	A	703[B]	TRS	C1-C	-2.59	1.46	1.53
2	D	701	MPD	C1-C2	2.37	1.59	1.52
2	A	702	MPD	O2-C2	2.28	1.50	1.44
3	C	702[A]	TRS	O3-C3	2.18	1.49	1.42
2	D	701	MPD	O4-C4	-2.14	1.34	1.43
3	D	702[A]	TRS	O1-C1	2.10	1.49	1.42
3	B	702[A]	TRS	C2-C	-2.07	1.47	1.53

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	MPD	CM-C2-C1	15.57	145.50	110.63
2	B	701	MPD	O2-C2-C1	-14.52	62.73	107.99
3	C	703	TRS	C2-C-C1	-10.33	83.14	110.66
3	C	703	TRS	C1-C-N	-9.96	82.78	108.17
3	A	703[B]	TRS	C3-C-C1	-9.59	85.12	110.66
3	C	702[B]	TRS	C2-C-N	7.87	128.24	108.17
2	A	702	MPD	O4-C4-C3	7.74	142.14	111.35
3	C	703	TRS	O3-C3-C	-7.61	89.66	110.88
3	A	703[B]	TRS	O1-C1-C	-7.13	90.99	110.88
2	D	701	MPD	C1-C2-C3	-6.90	80.43	110.20
2	B	701	MPD	O2-C2-CM	-6.08	89.03	107.99
3	B	702[A]	TRS	C3-C-C1	5.12	124.30	110.66
3	B	702[A]	TRS	C3-C-C2	-5.11	97.06	110.66
3	C	702[A]	TRS	C1-C-N	4.99	120.90	108.17
3	A	703[A]	TRS	C2-C-N	-4.97	95.50	108.17
3	C	702[B]	TRS	C3-C-C2	-4.94	97.50	110.66
2	A	702	MPD	C5-C4-C3	-4.73	89.69	111.67
3	A	703[B]	TRS	O2-C2-C	4.71	124.01	110.88
2	A	702	MPD	O2-C2-CM	4.65	122.49	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	703	TRS	C3-C-C2	4.52	122.70	110.66
3	C	703	TRS	C2-C-N	4.50	119.64	108.17
3	C	703	TRS	O2-C2-C	4.29	122.84	110.88
3	D	702[A]	TRS	C2-C-C1	4.06	121.46	110.66
3	B	702[A]	TRS	C2-C-C1	-3.92	100.21	110.66
3	A	703[A]	TRS	C3-C-C2	-3.89	100.29	110.66
3	C	702[B]	TRS	O3-C3-C	-3.88	100.05	110.88
2	B	701	MPD	C5-C4-C3	3.86	129.60	111.67
3	C	702[A]	TRS	C3-C-C1	-3.83	100.46	110.66
3	A	703[B]	TRS	C3-C-N	3.73	117.69	108.17
2	D	701	MPD	O4-C4-C3	-3.68	96.69	111.35
2	A	702	MPD	C1-C2-C3	-3.49	95.14	110.20
2	D	701	MPD	CM-C2-C1	3.47	118.39	110.63
3	C	703	TRS	C3-C-N	3.43	116.92	108.17
3	C	702[A]	TRS	C2-C-C1	-3.39	101.62	110.66
3	C	702[B]	TRS	C3-C-N	-3.35	99.64	108.17
3	D	702[B]	TRS	O2-C2-C	-3.22	101.90	110.88
3	B	702[B]	TRS	O1-C1-C	-3.22	101.91	110.88
3	D	702[A]	TRS	C3-C-C1	-3.16	102.23	110.66
3	A	703[B]	TRS	C2-C-N	3.11	116.11	108.17
3	A	703[B]	TRS	C2-C-C1	3.04	118.74	110.66
2	A	702	MPD	O2-C2-C3	-2.80	98.78	109.27
3	D	702[A]	TRS	C3-C-N	2.78	115.26	108.17
2	B	701	MPD	O2-C2-C3	2.75	119.55	109.27
2	D	701	MPD	O4-C4-C5	2.74	121.26	109.45
3	A	703[A]	TRS	O1-C1-C	2.74	118.52	110.88
3	D	702[B]	TRS	C2-C-N	-2.59	101.56	108.17
2	B	701	MPD	CM-C2-C3	-2.50	99.39	110.20
3	B	702[A]	TRS	O2-C2-C	-2.45	104.04	110.88
3	A	703[A]	TRS	C3-C-N	2.44	114.39	108.17
3	C	702[A]	TRS	O3-C3-C	2.43	117.64	110.88
3	B	702[B]	TRS	O2-C2-C	-2.36	104.28	110.88
3	D	702[B]	TRS	C3-C-C1	2.36	116.94	110.66
3	B	702[A]	TRS	C3-C-N	2.34	114.13	108.17
3	C	702[A]	TRS	C3-C-N	2.32	114.10	108.17
3	B	702[B]	TRS	C3-C-N	2.30	114.04	108.17
2	D	701	MPD	O2-C2-CM	2.26	115.04	107.99
2	A	702	MPD	O2-C2-C1	2.25	115.01	107.99
3	A	703[A]	TRS	C1-C-N	2.20	113.78	108.17
3	A	703[B]	TRS	C1-C-N	-2.12	102.76	108.17
3	C	702[A]	TRS	O2-C2-C	-2.07	105.11	110.88
2	D	701	MPD	O2-C2-C3	2.04	116.89	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702[B]	TRS	O3-C3-C	-2.02	105.23	110.88

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	MPD	C2-C3-C4-C5
2	D	701	MPD	C2-C3-C4-C5
3	A	703[A]	TRS	C1-C-C2-O2
3	A	703[A]	TRS	C3-C-C2-O2
3	A	703[A]	TRS	N-C-C2-O2
3	A	703[B]	TRS	C2-C-C1-O1
3	A	703[B]	TRS	C3-C-C1-O1
3	A	703[B]	TRS	N-C-C1-O1
3	B	702[A]	TRS	C2-C-C1-O1
3	B	702[A]	TRS	C3-C-C1-O1
3	B	702[A]	TRS	N-C-C1-O1
3	B	702[A]	TRS	C1-C-C2-O2
3	B	702[A]	TRS	C3-C-C2-O2
3	B	702[A]	TRS	N-C-C2-O2
3	B	702[B]	TRS	N-C-C1-O1
3	C	702[A]	TRS	C2-C-C1-O1
3	C	702[A]	TRS	C3-C-C1-O1
3	C	702[A]	TRS	N-C-C1-O1
3	C	702[B]	TRS	C1-C-C2-O2
3	C	702[B]	TRS	C3-C-C2-O2
3	C	702[B]	TRS	N-C-C2-O2
3	C	702[B]	TRS	N-C-C3-O3
3	C	703	TRS	C1-C-C2-O2
3	C	703	TRS	C3-C-C2-O2
3	D	702[A]	TRS	C1-C-C2-O2
3	D	702[A]	TRS	C3-C-C2-O2
3	D	702[A]	TRS	N-C-C2-O2
3	A	703[A]	TRS	C3-C-C1-O1
3	A	703[B]	TRS	C1-C-C2-O2
3	C	702[A]	TRS	C2-C-C3-O3
3	D	702[A]	TRS	C2-C-C3-O3
3	A	703[A]	TRS	C2-C-C1-O1
3	A	703[B]	TRS	N-C-C2-O2
3	B	702[B]	TRS	C3-C-C1-O1
3	B	702[B]	TRS	N-C-C2-O2
3	C	702[A]	TRS	N-C-C3-O3

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Mol	Chain	Res	Type	Atoms
3	C	703	TRS	N-C-C2-O2
3	C	703	TRS	C2-C-C3-O3
3	D	702[A]	TRS	C1-C-C3-O3
3	D	702[A]	TRS	N-C-C3-O3
2	A	702	MPD	CM-C2-C3-C4
2	B	701	MPD	C1-C2-C3-C4
3	A	703[B]	TRS	C1-C-C3-O3
3	A	703[B]	TRS	C2-C-C3-O3
3	B	702[A]	TRS	C2-C-C3-O3
3	A	703[A]	TRS	N-C-C1-O1
3	B	702[A]	TRS	N-C-C3-O3
3	C	702[B]	TRS	C2-C-C1-O1
3	B	702[A]	TRS	C1-C-C3-O3
3	B	702[B]	TRS	C2-C-C1-O1
3	B	702[B]	TRS	C1-C-C3-O3
3	C	703	TRS	C2-C-C1-O1
3	C	703	TRS	C1-C-C3-O3
2	B	701	MPD	O2-C2-C3-C4
2	D	701	MPD	O2-C2-C3-C4
2	A	702	MPD	C2-C3-C4-O4
2	B	701	MPD	C2-C3-C4-O4
2	D	701	MPD	C2-C3-C4-O4
2	A	702	MPD	C1-C2-C3-C4
2	D	701	MPD	C1-C2-C3-C4
3	A	703[A]	TRS	N-C-C3-O3

There are no ring outliers.

6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	MPD	7	0
3	B	702[B]	TRS	2	0
2	A	702	MPD	7	0
2	D	701	MPD	8	0
3	C	702[A]	TRS	1	0
3	C	703	TRS	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	659/693 (95%)	-0.31	9 (1%)	73 77	8, 17, 36, 60	6 (0%)
1	B	659/693 (95%)	-0.29	4 (0%)	85 88	7, 18, 37, 57	4 (0%)
1	C	659/693 (95%)	-0.32	2 (0%)	90 91	8, 18, 36, 56	3 (0%)
1	D	658/693 (94%)	-0.22	8 (1%)	76 80	7, 19, 37, 57	3 (0%)
All	All	2635/2772 (95%)	-0.29	23 (0%)	81 83	7, 18, 37, 60	16 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	663	GLY	3.6
1	C	35	PRO	3.3
1	B	101	LYS	3.0
1	A	36	ILE	2.9
1	B	36	ILE	2.9
1	B	35	PRO	2.6
1	D	82	SER	2.6
1	D	36	ILE	2.6
1	A	85	LYS	2.5
1	A	104	LYS	2.5
1	D	84	GLY	2.5
1	B	121	VAL	2.5
1	D	662	GLU	2.4
1	A	82	SER	2.4
1	A	102	THR	2.4
1	C	393	TYR	2.4
1	A	41	GLY	2.3
1	A	37	VAL	2.3
1	D	664	GLY	2.3
1	A	84	GLY	2.2
1	D	83	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	691	HIS	2.1
1	D	121	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 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
2	MPD	D	701	8/8	0.79	0.14	21,25,31,32	0
3	TRS	C	702[A]	8/8	0.81	0.14	9,17,19,24	8
3	TRS	C	702[B]	8/8	0.81	0.14	16,22,23,28	8
3	TRS	C	703	8/8	0.81	0.15	21,28,30,40	0
2	MPD	A	702	8/8	0.83	0.14	14,24,31,31	0
2	MPD	B	701	8/8	0.84	0.12	14,21,30,34	0
3	TRS	D	702[A]	8/8	0.85	0.15	15,25,27,30	8
3	TRS	D	702[B]	8/8	0.85	0.15	13,16,19,28	8
2	MPD	C	701	8/8	0.89	0.13	29,35,39,40	0
2	MPD	A	701	8/8	0.90	0.13	30,35,38,38	0
3	TRS	A	703[B]	8/8	0.91	0.13	12,15,18,19	8
3	TRS	B	702[A]	8/8	0.91	0.10	10,17,18,20	8
3	TRS	B	702[B]	8/8	0.91	0.10	13,24,31,35	8
3	TRS	A	703[A]	8/8	0.91	0.13	19,21,23,25	8
4	CL	C	704	1/1	0.98	0.09	24,24,24,24	0
4	CL	D	703	1/1	0.98	0.06	24,24,24,24	0
4	CL	A	704	1/1	0.99	0.07	21,21,21,21	0
4	CL	B	703	1/1	0.99	0.05	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.