



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:33 AM UTC

PDB ID : 2YOC / pdb_00002yoc
Title : Crystal structure of PulA from *Klebsiella oxytoca*
Authors : Francetic, O.; Mechaly, A.E.; Tello-Manigne, D.; Buschiazzi, A.; Bernarde, C.; Nadeau, N.; Pugsley, A.P.; Alzari, P.M.
Deposited on : 2012-10-23
Resolution : 2.88 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

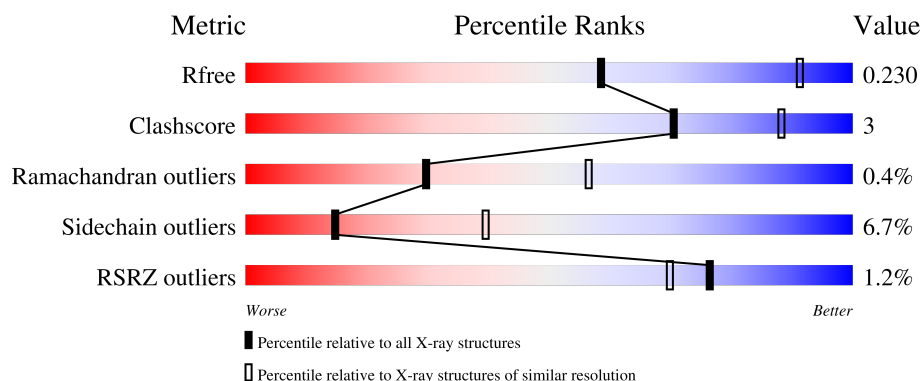
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	1078	% 82% 14% ..
1	B	1078	% 82% 14% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16490 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 PULLULANASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1051	Total	C	N	O	S	Se	0	0	0
			8030	5013	1368	1621	6	22			
1	B	1055	Total	C	N	O	S	Se	0	0	0
			8074	5043	1376	1627	6	22			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP P07206
A	1071	TYR	-	expression tag	UNP P07206
A	1072	TYR	-	expression tag	UNP P07206
A	1073	HIS	-	expression tag	UNP P07206
A	1074	HIS	-	expression tag	UNP P07206
A	1075	HIS	-	expression tag	UNP P07206
A	1076	HIS	-	expression tag	UNP P07206
A	1077	HIS	-	expression tag	UNP P07206
A	1078	HIS	-	expression tag	UNP P07206
B	1	MSE	-	expression tag	UNP P07206
B	1071	TYR	-	expression tag	UNP P07206
B	1072	TYR	-	expression tag	UNP P07206
B	1073	HIS	-	expression tag	UNP P07206
B	1074	HIS	-	expression tag	UNP P07206
B	1075	HIS	-	expression tag	UNP P07206
B	1076	HIS	-	expression tag	UNP P07206
B	1077	HIS	-	expression tag	UNP P07206
B	1078	HIS	-	expression tag	UNP P07206

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Ca	0	0
			4	4		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

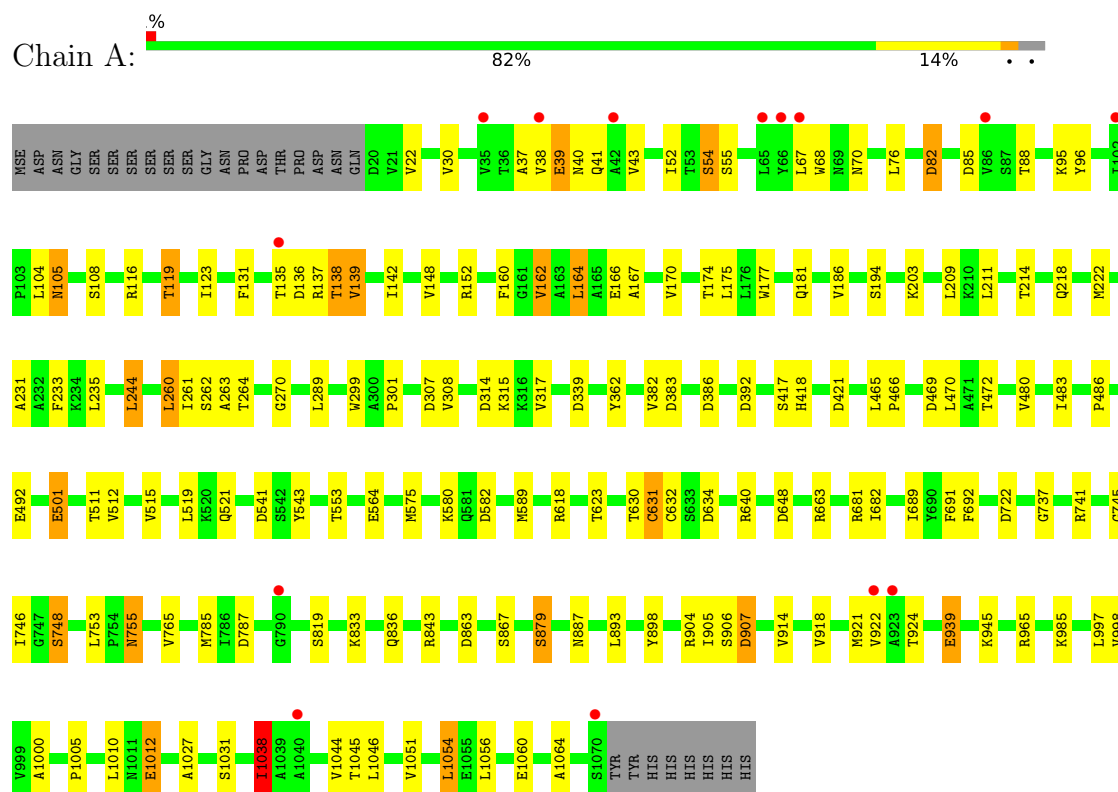
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	145	Total	O	0	0
			145	145		
4	B	163	Total	O	0	0
			163	163		

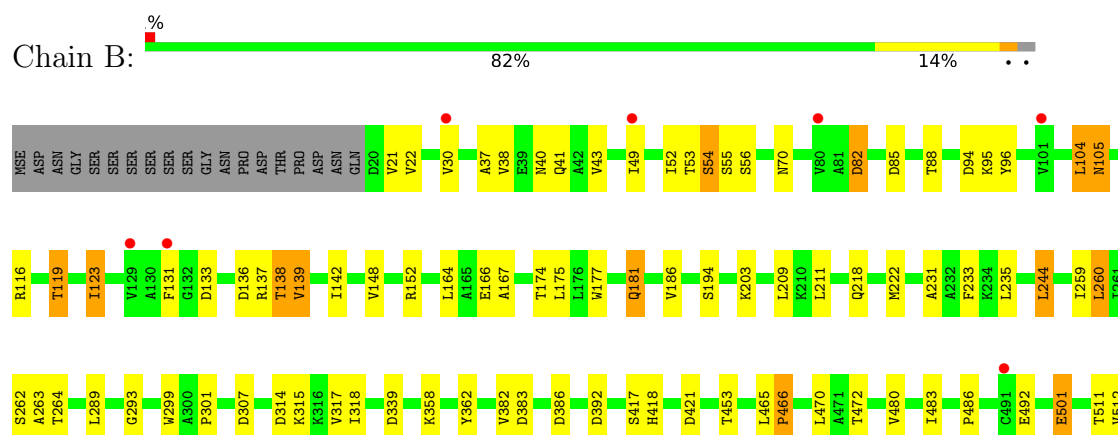
3 Residue-property plots

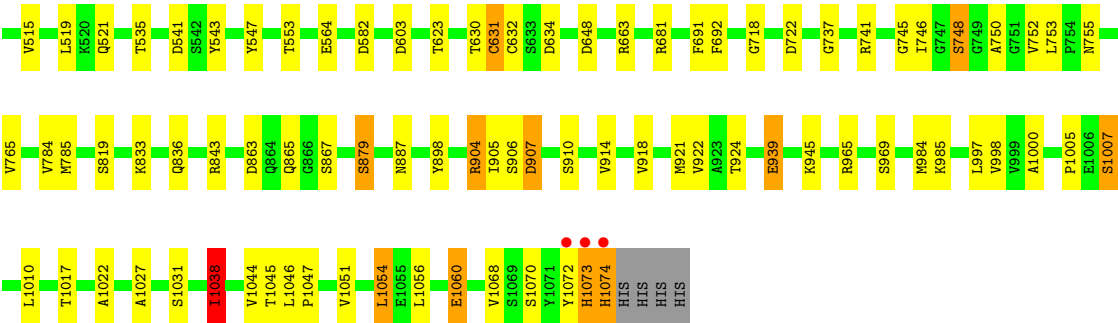
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: PULLULANASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	179.15Å 179.15Å 334.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.17 – 2.88 42.17 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.17-2.88) 99.7 (42.17-2.88)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.171 , 0.213 0.187 , 0.230	Depositor DCC
R_{free} test set	3635 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 85.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16490	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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: CA, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.84	1/8171 (0.0%)	1.36	44/11086 (0.4%)
1	B	0.84	0/8219	1.37	59/11152 (0.5%)
All	All	0.84	1/16390 (0.0%)	1.36	103/22238 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	SER	CA-C	-5.15	1.46	1.52

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ASN	CA-CB-CG	8.48	121.08	112.60
1	B	105	ASN	CA-CB-CG	8.42	121.02	112.60
1	B	907	ASP	CA-CB-CG	8.35	120.95	112.60
1	A	261	ILE	N-CA-C	-7.54	104.51	111.67
1	A	748	SER	N-CA-C	-7.43	103.79	114.12
1	B	53	THR	CA-C-N	7.40	135.68	121.54
1	B	53	THR	C-N-CA	7.40	135.68	121.54
1	B	1073	HIS	CA-C-N	7.37	134.97	121.70
1	B	1073	HIS	C-N-CA	7.37	134.97	121.70
1	A	541	ASP	CA-CB-CG	7.34	119.94	112.60
1	B	82	ASP	CA-CB-CG	7.33	119.93	112.60
1	B	748	SER	N-CA-C	-7.27	104.01	114.12
1	B	631	CYS	N-CA-C	-7.14	95.59	110.80
1	A	631	CYS	N-CA-C	-7.06	95.76	110.80
1	A	630	THR	CA-C-N	6.90	134.72	121.54
1	A	630	THR	C-N-CA	6.90	134.72	121.54
1	B	541	ASP	CA-CB-CG	6.90	119.50	112.60
1	A	472	THR	N-CA-C	6.81	121.04	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	472	THR	N-CA-C	6.81	121.04	113.21
1	B	1073	HIS	CA-CB-CG	6.78	120.58	113.80
1	A	307	ASP	CA-CB-CG	6.78	119.38	112.60
1	A	907	ASP	CA-CB-CG	6.77	119.37	112.60
1	A	119	THR	CB-CA-C	6.69	120.44	111.14
1	B	630	THR	CA-C-N	6.63	134.20	121.54
1	B	630	THR	C-N-CA	6.63	134.20	121.54
1	A	82	ASP	CA-CB-CG	6.52	119.12	112.60
1	B	307	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	70	ASN	CA-CB-CG	6.50	119.10	112.60
1	B	70	ASN	CA-CB-CG	6.48	119.08	112.60
1	B	54	SER	CA-C-N	6.44	133.84	121.54
1	B	54	SER	C-N-CA	6.44	133.84	121.54
1	A	30	VAL	N-CA-CB	6.42	116.05	110.08
1	A	691	PHE	CA-CB-CG	6.30	120.10	113.80
1	A	833	LYS	N-CA-C	6.28	121.23	113.50
1	B	691	PHE	CA-CB-CG	6.25	120.05	113.80
1	B	30	VAL	N-CA-CB	6.17	115.81	110.08
1	A	55	SER	CA-C-N	6.01	132.35	122.07
1	A	55	SER	C-N-CA	6.01	132.35	122.07
1	B	833	LYS	N-CA-C	5.98	120.85	113.50
1	B	119	THR	CB-CA-C	5.92	119.37	111.14
1	A	174	THR	N-CA-C	5.79	118.40	109.07
1	B	1070	SER	N-CA-C	-5.75	103.98	111.74
1	A	634	ASP	CA-CB-CG	5.74	118.34	112.60
1	B	174	THR	N-CA-C	5.73	118.29	109.07
1	A	787	ASP	N-CA-C	5.72	117.29	110.19
1	A	386	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	634	ASP	CA-CB-CG	5.64	118.24	112.60
1	B	1060	GLU	CB-CG-CD	5.58	122.08	112.60
1	B	317	VAL	CA-C-N	5.56	128.46	121.85
1	B	317	VAL	C-N-CA	5.56	128.46	121.85
1	A	308	VAL	N-CA-CB	5.47	116.68	110.72
1	B	293	GLY	N-CA-C	5.45	117.06	111.56
1	B	543	TYR	N-CA-C	5.44	117.60	108.73
1	B	386	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	722	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	123	ILE	CA-C-N	5.40	127.83	120.54
1	B	123	ILE	C-N-CA	5.40	127.83	120.54
1	B	1073	HIS	N-CA-C	5.38	116.25	108.34
1	A	836	GLN	CA-C-N	5.38	128.48	120.31
1	A	836	GLN	C-N-CA	5.38	128.48	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	VAL	CA-C-N	5.36	128.23	121.85
1	A	317	VAL	C-N-CA	5.36	128.23	121.85
1	B	54	SER	N-CA-C	5.34	122.18	110.80
1	B	318	ILE	N-CA-CB	-5.32	105.00	112.35
1	A	904	ARG	CA-C-N	5.31	127.45	120.60
1	A	904	ARG	C-N-CA	5.31	127.45	120.60
1	A	1038	ILE	N-CA-CB	5.30	118.58	111.90
1	B	1038	ILE	N-CA-CB	5.30	118.56	112.15
1	B	752	VAL	N-CA-C	5.29	116.02	110.62
1	B	1022	ALA	CA-C-N	5.27	127.39	120.60
1	B	1022	ALA	C-N-CA	5.27	127.39	120.60
1	B	836	GLN	CA-C-N	5.26	128.30	120.31
1	B	836	GLN	C-N-CA	5.26	128.30	120.31
1	A	543	TYR	N-CA-C	5.25	117.29	108.73
1	A	1012	GLU	CB-CG-CD	5.25	121.52	112.60
1	B	746	ILE	N-CA-C	-5.23	99.94	107.37
1	A	162	VAL	N-CA-CB	5.23	117.45	111.39
1	B	939	GLU	CA-C-N	5.23	127.28	120.28
1	B	939	GLU	C-N-CA	5.23	127.28	120.28
1	B	1017	THR	CB-CA-C	5.23	120.19	111.30
1	B	21	VAL	N-CA-C	5.22	116.13	109.30
1	A	755	ASN	CA-CB-CG	5.21	117.81	112.60
1	B	648	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	746	ILE	N-CA-C	-5.15	100.06	107.37
1	A	939	GLU	CA-C-N	5.14	127.17	120.28
1	A	939	GLU	C-N-CA	5.14	127.17	120.28
1	B	94	ASP	CA-CB-CG	5.13	117.73	112.60
1	B	133	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	648	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	580	LYS	N-CA-C	5.12	116.94	111.36
1	A	640	ARG	N-CA-C	5.09	117.22	111.11
1	B	466	PRO	N-CA-C	5.08	122.93	112.47
1	B	1068	VAL	CA-C-N	5.07	127.08	120.28
1	B	1068	VAL	C-N-CA	5.07	127.08	120.28
1	A	722	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	259	ILE	N-CA-CB	5.07	116.05	110.53
1	A	765	VAL	N-CA-CB	5.05	118.15	110.58
1	A	1064	ALA	N-CA-C	-5.02	102.28	110.20
1	B	547	TYR	CA-C-N	5.02	128.06	122.74
1	B	547	TYR	C-N-CA	5.02	128.06	122.74
1	B	904	ARG	CA-C-N	5.01	127.60	120.53
1	B	904	ARG	C-N-CA	5.01	127.60	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	ASP	N-CA-C	5.00	116.64	108.63

There are no chirality outliers.

There are no planarity outliers.

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	8030	0	7714	57	0
1	B	8074	0	7746	52	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	20	0	0	0	0
3	B	50	0	0	0	0
4	A	145	0	0	0	0
4	B	163	0	0	0	0
All	All	16490	0	15460	107	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 3.

All (107) 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:A:52:ILE:HD11	1:A:160:PHE:CZ	2.02	0.93
1:A:52:ILE:HD11	1:A:160:PHE:HZ	1.38	0.84
1:A:54:SER:O	1:A:95:LYS:NZ	2.24	0.70
1:B:483:ILE:HA	1:B:512:VAL:HB	1.80	0.63
1:A:483:ILE:HA	1:A:512:VAL:HB	1.81	0.63
1:B:218:GLN:O	1:B:222:MSE:HG2	1.99	0.63
1:A:289:LEU:HD23	1:A:383:ASP:HB2	1.81	0.62
1:B:289:LEU:HD23	1:B:383:ASP:HB2	1.81	0.61
1:B:784:VAL:HG21	1:B:1072:TYR:HB2	1.83	0.61
1:B:843:ARG:HH22	1:B:921:MSE:HE3	1.67	0.60
1:A:965:ARG:HG2	1:A:1012:GLU:CD	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LEU:HD13	1:B:137:ARG:HH12	1.67	0.59
1:A:843:ARG:HH22	1:A:921:MSE:HE3	1.68	0.58
1:A:745:GLY:H	1:A:748:SER:HB2	1.68	0.57
1:B:745:GLY:H	1:B:748:SER:HB2	1.69	0.56
1:A:218:GLN:O	1:A:222:MSE:HG2	2.05	0.56
1:B:315:LYS:NZ	1:B:564:GLU:OE2	2.36	0.54
1:A:82:ASP:HB3	1:A:85:ASP:HB2	1.90	0.54
1:B:82:ASP:HB3	1:B:85:ASP:HB2	1.89	0.54
1:B:1073:HIS:CG	1:B:1074:HIS:H	2.27	0.53
1:B:1038:ILE:HG23	1:B:1044:VAL:HG22	1.90	0.52
1:A:1038:ILE:HG23	1:A:1044:VAL:HG22	1.91	0.52
1:B:37:ALA:HB2	1:B:43:VAL:HG12	1.91	0.52
1:A:37:ALA:HB2	1:A:43:VAL:HG12	1.92	0.51
1:B:918:VAL:HA	1:B:921:MSE:HG3	1.92	0.51
1:A:164:LEU:HD22	1:A:623:THR:HG22	1.92	0.51
1:B:939:GLU:OE1	1:B:1031:SER:HA	2.11	0.51
1:B:753:LEU:HB2	1:B:1005:PRO:HG3	1.92	0.51
1:A:753:LEU:HB2	1:A:1005:PRO:HG3	1.92	0.51
1:B:52:ILE:CG2	1:B:96:TYR:HA	2.42	0.50
1:A:315:LYS:NZ	1:A:564:GLU:OE2	2.34	0.50
1:A:939:GLU:OE1	1:A:1031:SER:HA	2.11	0.50
1:A:918:VAL:HA	1:A:921:MSE:HG3	1.94	0.50
1:B:167:ALA:HB1	1:B:175:LEU:HD21	1.93	0.50
1:B:209:LEU:HD11	1:B:244:LEU:HD21	1.94	0.50
1:A:486:PRO:HA	1:A:511:THR:HA	1.94	0.50
1:A:136:ASP:HB2	1:A:138:THR:HG23	1.94	0.49
1:A:167:ALA:HB1	1:A:175:LEU:HD21	1.93	0.49
1:B:737:GLY:C	1:B:914:VAL:HG21	2.37	0.49
1:A:214:THR:OG1	1:B:181:GLN:HG2	2.12	0.49
1:A:299:TRP:CZ2	1:A:301:PRO:HG3	2.48	0.49
1:B:486:PRO:HA	1:B:511:THR:HA	1.95	0.48
1:B:741:ARG:NH2	1:B:755:ASN:HB2	2.28	0.48
1:B:136:ASP:HB2	1:B:138:THR:HG23	1.95	0.48
1:A:737:GLY:C	1:A:914:VAL:HG21	2.38	0.48
1:B:104:LEU:HD13	1:B:137:ARG:NH1	2.27	0.48
1:B:535:THR:HG23	1:B:904:ARG:CZ	2.44	0.48
1:B:299:TRP:CZ2	1:B:301:PRO:HG3	2.49	0.48
1:A:879:SER:HB2	1:A:887:ASN:HD21	1.78	0.47
1:A:52:ILE:CG2	1:A:96:TYR:HA	2.44	0.47
1:A:741:ARG:NH2	1:A:755:ASN:HB2	2.29	0.47
1:B:164:LEU:HD22	1:B:623:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:879:SER:HB2	1:B:887:ASN:HD21	1.79	0.47
1:A:663:ARG:HA	1:A:692:PHE:O	2.15	0.47
1:B:1010:LEU:HB2	1:B:1044:VAL:HB	1.97	0.47
1:A:22:VAL:HG11	1:A:203:LYS:HD3	1.97	0.46
1:A:209:LEU:HD11	1:A:244:LEU:HD21	1.96	0.46
1:B:260:LEU:HD11	1:B:263:ALA:HB2	1.97	0.46
1:B:663:ARG:HA	1:B:692:PHE:O	2.15	0.46
1:A:1010:LEU:HB2	1:A:1044:VAL:HB	1.97	0.46
1:B:1000:ALA:HB1	1:B:1046:LEU:HD11	1.97	0.45
1:A:1000:ALA:HB1	1:A:1046:LEU:HD11	1.98	0.45
1:B:515:VAL:O	1:B:519:LEU:HG	2.16	0.45
1:A:260:LEU:HD11	1:A:263:ALA:HB2	1.99	0.45
1:B:131:PHE:CD1	1:B:137:ARG:HG2	2.51	0.45
1:B:166:GLU:HB2	1:B:264:THR:HG21	1.98	0.45
1:A:515:VAL:O	1:A:519:LEU:HG	2.16	0.45
1:B:863:ASP:OD2	1:B:867:SER:HB2	2.17	0.45
1:A:38:VAL:HG22	1:A:39:GLU:H	1.83	0.45
1:B:116:ARG:HH11	1:B:119:THR:HA	1.82	0.45
1:A:131:PHE:CD1	1:A:137:ARG:HG2	2.53	0.44
1:B:418:HIS:HB3	1:B:421:ASP:HB2	1.98	0.44
1:B:898:TYR:HB3	1:B:924:THR:HG23	1.99	0.44
1:A:863:ASP:OD2	1:A:867:SER:HB2	2.17	0.44
1:B:998:VAL:HB	1:B:1054:LEU:HB2	1.99	0.44
1:A:186:VAL:HG12	1:A:211:LEU:HB2	2.00	0.44
1:A:965:ARG:HD2	1:A:965:ARG:HA	1.73	0.44
1:B:54:SER:HB3	1:B:55:SER:H	1.58	0.44
1:A:116:ARG:HH11	1:A:119:THR:HA	1.82	0.44
1:A:998:VAL:HB	1:A:1054:LEU:HB2	2.00	0.44
1:A:418:HIS:HB3	1:A:421:ASP:HB2	1.99	0.44
1:A:1027:ALA:HB3	1:A:1031:SER:HB2	2.00	0.43
1:A:166:GLU:HB2	1:A:264:THR:HG21	2.00	0.43
1:B:177:TRP:O	1:B:231:ALA:HB3	2.19	0.43
1:B:186:VAL:HG12	1:B:211:LEU:HB2	2.00	0.43
1:A:52:ILE:HA	1:A:95:LYS:HE3	2.01	0.43
1:A:898:TYR:HB3	1:A:924:THR:HG23	2.00	0.43
1:B:1027:ALA:HB3	1:B:1031:SER:HB2	2.00	0.43
1:A:68:TRP:HZ3	1:B:82:ASP:OD1	2.01	0.42
1:B:139:VAL:HG13	1:B:148:VAL:HG13	2.01	0.42
1:A:67:LEU:HB3	1:A:76:LEU:CD2	2.50	0.42
1:A:879:SER:HB2	1:A:887:ASN:ND2	2.34	0.42
1:B:211:LEU:HB3	1:B:233:PHE:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:879:SER:HB2	1:B:887:ASN:ND2	2.35	0.42
1:B:22:VAL:HG11	1:B:203:LYS:HD3	2.01	0.42
1:A:52:ILE:HD12	1:A:52:ILE:C	2.45	0.41
1:A:52:ILE:CD1	1:A:160:PHE:CZ	2.91	0.41
1:A:139:VAL:HG13	1:A:148:VAL:HG13	2.01	0.41
1:B:692:PHE:HA	1:B:718:GLY:O	2.21	0.41
1:B:750:ALA:O	1:B:765:VAL:HG21	2.20	0.41
1:A:211:LEU:HB3	1:A:233:PHE:HB3	2.01	0.41
1:A:575:MSE:HE2	1:A:575:MSE:HB3	2.02	0.41
1:A:170:VAL:HA	1:A:270:GLY:HA3	2.03	0.40
1:A:682:ILE:HG22	1:A:689:ILE:HG21	2.02	0.40
1:A:177:TRP:O	1:A:231:ALA:HB3	2.21	0.40
1:A:618:ARG:HH11	1:A:618:ARG:HD2	1.78	0.40
1:B:1007:SER:HB2	1:B:1047:PRO:HA	2.04	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	1049/1078 (97%)	987 (94%)	58 (6%)	4 (0%)	30	56
1	B	1053/1078 (98%)	986 (94%)	63 (6%)	4 (0%)	30	56
All	All	2102/2156 (98%)	1973 (94%)	121 (6%)	8 (0%)	30	56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	631	CYS
1	B	631	CYS
1	A	466	PRO
1	B	466	PRO

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Mol	Chain	Res	Type
1	A	501	GLU
1	B	501	GLU
1	B	879	SER
1	A	879	SER

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	861/863 (100%)	807 (94%)	54 (6%)	16	42
1	B	865/863 (100%)	804 (93%)	61 (7%)	13	37
All	All	1726/1726 (100%)	1611 (93%)	115 (7%)	15	39

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	40	ASN
1	A	41	GLN
1	A	88	THR
1	A	104	LEU
1	A	105	ASN
1	A	108	SER
1	A	123	ILE
1	A	135	THR
1	A	138	THR
1	A	139	VAL
1	A	142	ILE
1	A	152	ARG
1	A	162	VAL
1	A	164	LEU
1	A	181	GLN
1	A	194	SER
1	A	235	LEU
1	A	244	LEU

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Mol	Chain	Res	Type
1	A	260	LEU
1	A	262	SER
1	A	314	ASP
1	A	339	ASP
1	A	362	TYR
1	A	382	VAL
1	A	392	ASP
1	A	417	SER
1	A	465	LEU
1	A	470	LEU
1	A	480	VAL
1	A	492	GLU
1	A	501	GLU
1	A	521	GLN
1	A	553	THR
1	A	582	ASP
1	A	589	MSE
1	A	632	CYS
1	A	681	ARG
1	A	785	MSE
1	A	819	SER
1	A	893	LEU
1	A	905	ILE
1	A	906	SER
1	A	907	ASP
1	A	922	VAL
1	A	945	LYS
1	A	985	LYS
1	A	997	LEU
1	A	1038	ILE
1	A	1045	THR
1	A	1051	VAL
1	A	1054	LEU
1	A	1056	LEU
1	A	1060	GLU
1	B	38	VAL
1	B	40	ASN
1	B	41	GLN
1	B	49	ILE
1	B	56	SER
1	B	88	THR
1	B	95	LYS

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Mol	Chain	Res	Type
1	B	104	LEU
1	B	105	ASN
1	B	123	ILE
1	B	138	THR
1	B	139	VAL
1	B	142	ILE
1	B	152	ARG
1	B	181	GLN
1	B	194	SER
1	B	235	LEU
1	B	244	LEU
1	B	260	LEU
1	B	262	SER
1	B	314	ASP
1	B	339	ASP
1	B	358	LYS
1	B	362	TYR
1	B	382	VAL
1	B	392	ASP
1	B	417	SER
1	B	453	THR
1	B	465	LEU
1	B	470	LEU
1	B	480	VAL
1	B	492	GLU
1	B	501	GLU
1	B	521	GLN
1	B	553	THR
1	B	582	ASP
1	B	603	ASP
1	B	632	CYS
1	B	681	ARG
1	B	785	MSE
1	B	819	SER
1	B	865	GLN
1	B	905	ILE
1	B	906	SER
1	B	907	ASP
1	B	910	SER
1	B	922	VAL
1	B	945	LYS
1	B	965	ARG

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Mol	Chain	Res	Type
1	B	969	SER
1	B	984	MSE
1	B	985	LYS
1	B	997	LEU
1	B	1007	SER
1	B	1038	ILE
1	B	1045	THR
1	B	1051	VAL
1	B	1054	LEU
1	B	1056	LEU
1	B	1060	GLU
1	B	1074	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	ASN
1	A	304	GLN
1	A	370	HIS
1	A	484	GLN
1	A	577	GLN
1	A	617	GLN
1	A	742	GLN
1	A	864	GLN
1	A	887	ASN
1	A	894	GLN
1	A	899	ASN
1	A	932	GLN
1	A	972	GLN
1	B	240	ASN
1	B	265	GLN
1	B	370	HIS
1	B	617	GLN
1	B	742	GLN
1	B	864	GLN
1	B	887	ASN
1	B	894	GLN
1	B	899	ASN
1	B	932	GLN

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 22 ligands modelled in this entry, 8 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	SO4	A	2078	-	4,4,4	0.49	0	6,6,6	0.15	0
3	SO4	B	2083	-	4,4,4	0.44	0	6,6,6	0.11	0
3	SO4	B	2079	-	4,4,4	0.42	0	6,6,6	0.17	0
3	SO4	A	2076	-	4,4,4	0.41	0	6,6,6	0.35	0
3	SO4	B	2082	-	4,4,4	0.40	0	6,6,6	0.25	0
3	SO4	B	2084	-	4,4,4	0.48	0	6,6,6	0.16	0
3	SO4	A	2075	-	4,4,4	0.57	0	6,6,6	0.34	0
3	SO4	B	2080	-	4,4,4	0.42	0	6,6,6	0.20	0
3	SO4	B	2081	-	4,4,4	0.56	0	6,6,6	0.16	0
3	SO4	B	2085	-	4,4,4	0.39	0	6,6,6	0.24	0
3	SO4	B	2087	-	4,4,4	0.44	0	6,6,6	0.22	0
3	SO4	A	2077	-	4,4,4	0.34	0	6,6,6	0.19	0
3	SO4	B	2086	-	4,4,4	0.36	0	6,6,6	0.19	0
3	SO4	B	2088	-	4,4,4	0.29	0	6,6,6	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1029/1078 (95%)	-0.18	14 (1%) 73 66	43, 77, 128, 162	0
1	B	1033/1078 (95%)	-0.18	10 (0%) 79 73	41, 74, 141, 170	0
All	All	2062/2156 (95%)	-0.18	24 (1%) 76 70	41, 76, 136, 170	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	VAL	3.9
1	B	101	VAL	3.5
1	B	1072	TYR	3.4
1	A	35	VAL	3.1
1	B	49	ILE	3.0
1	A	790	GLY	3.0
1	A	86	VAL	2.9
1	A	1040	ALA	2.9
1	A	1070	SER	2.9
1	A	38	VAL	2.7
1	A	922	VAL	2.6
1	B	1073	HIS	2.5
1	B	30	VAL	2.5
1	B	491	CYS	2.4
1	A	102	ILE	2.3
1	B	80	VAL	2.3
1	A	42	ALA	2.2
1	B	131	PHE	2.2
1	A	65	LEU	2.2
1	B	1074	HIS	2.2
1	A	135	THR	2.1
1	A	67	LEU	2.1
1	A	66	TYR	2.1
1	A	923	ALA	2.1

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($\text{\AA}^2$)	Q<0.9
3	SO4	B	2086	5/5	0.74	0.13	156,161,162,162	0
3	SO4	B	2082	5/5	0.78	0.17	141,145,146,147	0
3	SO4	B	2083	5/5	0.80	0.13	156,159,161,162	0
3	SO4	B	2084	5/5	0.84	0.09	147,152,152,154	0
3	SO4	A	2077	5/5	0.85	0.12	135,139,141,142	0
3	SO4	B	2081	5/5	0.85	0.11	145,149,151,151	0
2	CA	B	2078	1/1	0.87	0.16	106,106,106,106	0
3	SO4	B	2080	5/5	0.88	0.08	130,133,135,137	0
3	SO4	B	2088	5/5	0.88	0.12	142,146,147,147	0
3	SO4	B	2079	5/5	0.90	0.12	106,111,111,112	0
3	SO4	B	2087	5/5	0.90	0.07	131,135,136,137	0
3	SO4	A	2078	5/5	0.90	0.10	154,158,159,159	0
3	SO4	B	2085	5/5	0.91	0.06	124,128,130,130	0
3	SO4	A	2076	5/5	0.91	0.10	130,133,136,137	0
3	SO4	A	2075	5/5	0.94	0.09	78,82,83,85	0
2	CA	A	2074	1/1	0.94	0.07	106,106,106,106	0
2	CA	A	2073	1/1	0.96	0.05	123,123,123,123	0
2	CA	B	2076	1/1	0.97	0.06	106,106,106,106	0
2	CA	A	2072	1/1	0.97	0.13	140,140,140,140	0
2	CA	B	2077	1/1	0.98	0.05	78,78,78,78	0
2	CA	B	2075	1/1	0.99	0.06	58,58,58,58	0
2	CA	A	2071	1/1	0.99	0.04	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.