



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:59 AM UTC

PDB ID : 1LF6 / pdb_00001lf6
Title : CRYSTAL STRUCTURE OF BACTERIAL GLUCOAMYLASE
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Deposited on : 2002-04-10
Resolution : 2.10 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

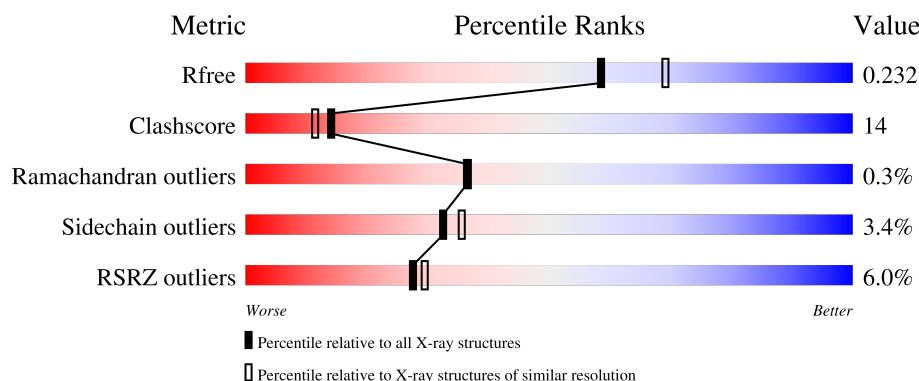
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	684	7% 72% 25% ..
1	B	684	5% 73% 24% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11584 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 glucoamylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	0	0
			5333	3385	881	1052	15			
1	B	674	Total	C	N	O	S	0	0	0
			5333	3385	881	1052	15			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	PHE	-	SEE REMARK 999	UNP O85672
A	252	GLN	GLY	conflict	UNP O85672
A	680	LYS	-	SEE REMARK 999	UNP O85672
A	681	ARG	-	SEE REMARK 999	UNP O85672
A	682	TYR	-	SEE REMARK 999	UNP O85672
A	683	VAL	-	SEE REMARK 999	UNP O85672
A	684	ALA	-	SEE REMARK 999	UNP O85672
B	125	PHE	-	SEE REMARK 999	UNP O85672
B	252	GLN	GLY	conflict	UNP O85672
B	680	LYS	-	SEE REMARK 999	UNP O85672
B	681	ARG	-	SEE REMARK 999	UNP O85672
B	682	TYR	-	SEE REMARK 999	UNP O85672
B	683	VAL	-	SEE REMARK 999	UNP O85672
B	684	ALA	-	SEE REMARK 999	UNP O85672

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

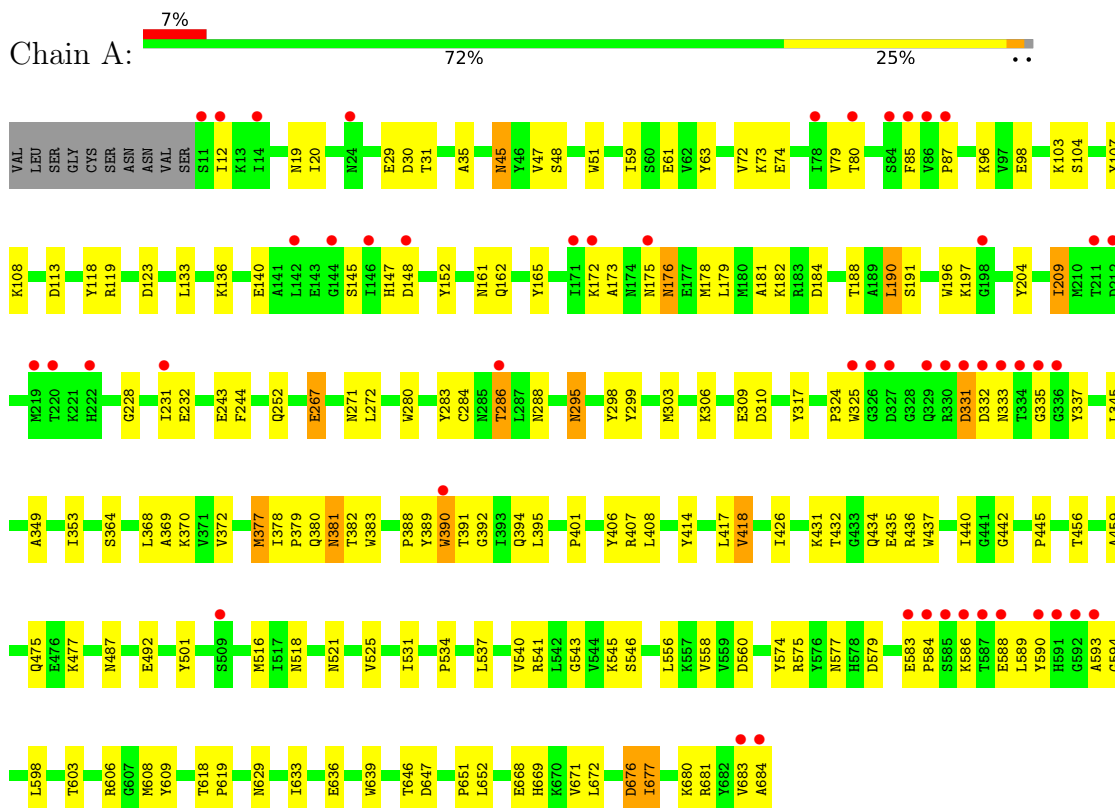
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	397	Total	O	0	0
			397	397		
3	B	511	Total	O	0	0
			511	511		

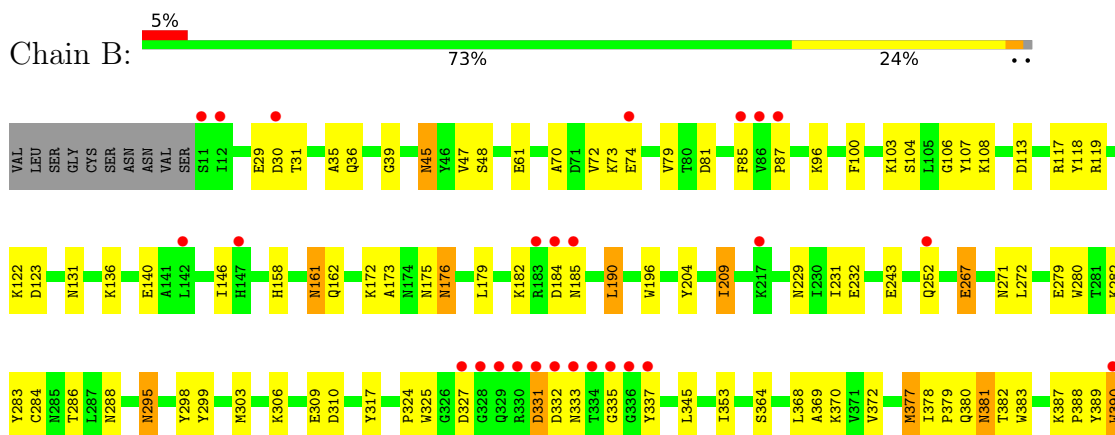
3 Residue-property plots [i](#)

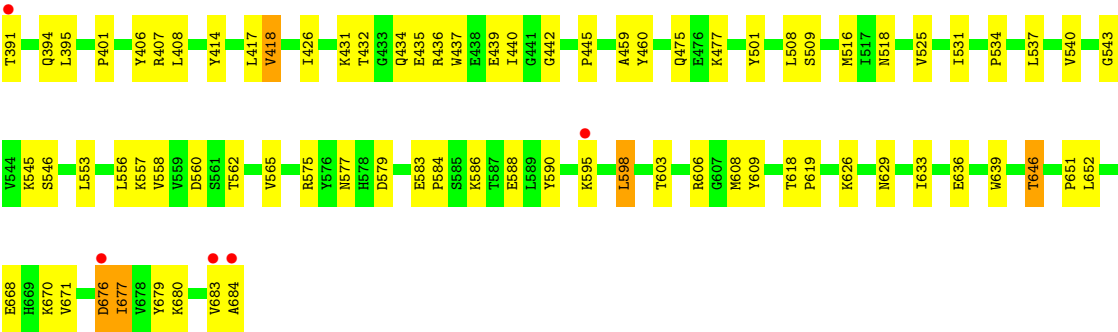
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: glucoamylase



• Molecule 1: glucoamylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.19Å 102.51Å 164.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.69 – 2.10 29.69 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.2 (29.69-2.10) 93.2 (29.69-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	20.27 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.194 , 0.232 0.194 , 0.232	Depositor DCC
R_{free} test set	5360 reflections (7.11%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11584	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: 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	0.37	0/5453	0.86	16/7391 (0.2%)
1	B	0.39	0/5453	0.87	14/7391 (0.2%)
All	All	0.38	0/10906	0.86	30/14782 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	418	VAL	N-CA-C	7.27	117.35	110.30
1	A	30	ASP	CA-CB-CG	7.22	119.82	112.60
1	B	331	ASP	N-CA-C	6.92	121.18	112.87
1	B	383	TRP	N-CA-C	-6.72	102.15	110.41
1	A	383	TRP	N-CA-C	-6.67	102.20	110.41
1	B	676	ASP	CA-CB-CG	6.66	119.26	112.60
1	A	531	ILE	N-CA-C	6.52	117.25	107.80
1	A	331	ASP	N-CA-C	6.46	120.63	112.87
1	B	436	ARG	N-CA-C	6.15	119.88	112.38
1	A	418	VAL	N-CA-C	6.06	116.17	110.30
1	A	436	ARG	N-CA-C	5.98	119.67	112.38
1	B	676	ASP	CA-C-N	5.85	128.78	120.53
1	B	676	ASP	C-N-CA	5.85	128.78	120.53
1	A	574	TYR	N-CA-C	-5.70	102.85	110.55
1	A	603	THR	N-CA-C	-5.70	105.15	111.36
1	B	531	ILE	N-CA-C	5.70	116.31	107.99
1	A	676	ASP	N-CA-C	5.64	118.16	111.33
1	A	184	ASP	CB-CA-C	-5.54	110.20	116.63
1	B	646	THR	N-CA-C	-5.48	101.36	109.86
1	A	161	ASN	N-CA-C	5.36	119.10	112.24
1	B	603	THR	N-CA-C	-5.32	105.56	111.36
1	A	646	THR	N-CA-C	-5.31	101.64	109.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	LYS	N-CA-C	-5.28	106.79	113.18
1	B	107	TYR	N-CA-C	5.26	117.81	109.50
1	A	107	TYR	N-CA-C	5.20	117.71	109.50
1	B	184	ASP	CB-CA-C	-5.12	110.69	116.63
1	A	672	LEU	N-CA-C	5.10	118.60	112.38
1	B	131	ASN	N-CA-C	5.10	117.49	109.39
1	A	492	GLU	N-CA-C	-5.09	105.44	113.02
1	B	161	ASN	N-CA-C	5.09	118.75	112.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5333	0	5172	153	0
1	B	5333	0	5172	152	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	397	0	0	26	0
3	B	511	0	0	24	0
All	All	11584	0	10344	300	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 14.

All (300) 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:516:MET:H	1:B:518:ASN:HD21	1.11	0.94
1:A:518:ASN:HD21	1:B:516:MET:H	1.18	0.88
1:B:353:ILE:HD11	1:B:408:LEU:HD21	1.55	0.86
1:B:280:TRP:HB3	1:B:303:MET:HE1	1.57	0.86
1:A:353:ILE:HD11	1:A:408:LEU:HD21	1.56	0.85
1:B:96:LYS:HD3	3:B:1237:HOH:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:MET:HE3	1:A:525:VAL:HG12	1.62	0.81
1:B:288:ASN:HB3	3:B:963:HOH:O	1.78	0.80
1:B:73:LYS:HD3	1:B:74:GLU:HG3	1.63	0.80
1:B:146:ILE:HB	3:B:1403:HOH:O	1.81	0.80
1:A:73:LYS:HD3	1:A:74:GLU:HG3	1.63	0.79
1:B:283:TYR:O	1:B:286:THR:HG22	1.83	0.79
1:B:516:MET:HE3	1:B:525:VAL:HG12	1.65	0.79
1:A:380:GLN:HE21	1:A:392:GLY:H	1.32	0.78
1:B:79:VAL:HG13	1:B:87:PRO:HG2	1.65	0.77
1:A:280:TRP:CE3	1:A:303:MET:HE2	2.20	0.77
1:A:79:VAL:O	1:A:87:PRO:HD2	1.85	0.77
1:A:280:TRP:HB3	1:A:303:MET:HE1	1.65	0.75
1:A:45:ASN:HD21	1:A:48:SER:H	1.33	0.75
1:A:309:GLU:HB2	1:A:317:TYR:CE1	2.20	0.75
1:A:283:TYR:O	1:A:286:THR:HG22	1.86	0.74
1:B:546:SER:HA	1:B:683:VAL:HG13	1.69	0.74
1:A:475:GLN:HB3	3:A:1212:HOH:O	1.87	0.74
1:A:540:VAL:HG21	1:A:609:TYR:HD2	1.53	0.74
1:B:540:VAL:HG21	1:B:609:TYR:HD2	1.52	0.74
1:A:381:ASN:HD21	1:A:390:TRP:H	1.34	0.74
1:B:280:TRP:HB3	1:B:303:MET:CE	2.17	0.74
1:A:589:LEU:HD13	3:A:1228:HOH:O	1.88	0.73
1:B:162:GLN:HA	1:B:331:ASP:O	1.89	0.73
1:A:79:VAL:HG13	1:A:87:PRO:HG2	1.69	0.72
1:B:79:VAL:O	1:B:87:PRO:HD2	1.88	0.72
1:A:147:HIS:HB2	3:A:1229:HOH:O	1.89	0.72
1:B:280:TRP:CE3	1:B:303:MET:HE2	2.25	0.71
1:B:284:CYS:SG	1:B:303:MET:HE3	2.30	0.71
1:A:381:ASN:ND2	1:A:389:TYR:HB3	2.06	0.71
1:B:575:ARG:HD3	1:B:579:ASP:OD2	1.90	0.70
1:A:426:ILE:HG23	1:A:477:LYS:HE3	1.73	0.70
1:A:546:SER:HA	1:A:683:VAL:HG13	1.72	0.70
1:A:459:ALA:CB	1:A:475:GLN:HG2	2.22	0.70
1:B:377:MET:HG2	1:B:378:ILE:N	2.06	0.70
1:B:381:ASN:ND2	1:B:389:TYR:HB3	2.07	0.70
1:A:172:LYS:HE2	1:A:175:ASN:HA	1.75	0.69
1:B:309:GLU:HB2	1:B:317:TYR:CE1	2.29	0.68
1:B:345:LEU:HD11	1:B:364:SER:HB2	1.76	0.68
1:B:680:LYS:HA	1:B:684:ALA:HB2	1.76	0.68
1:A:345:LEU:HD11	1:A:364:SER:HB2	1.75	0.68
1:A:575:ARG:HD3	1:A:579:ASP:OD2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:MET:HG2	1:A:378:ILE:N	2.08	0.67
1:B:406:TYR:CZ	1:B:677:ILE:HG22	2.30	0.67
1:A:390:TRP:HA	1:A:390:TRP:CE3	2.28	0.66
1:B:626:LYS:HE3	3:B:1304:HOH:O	1.94	0.66
1:B:172:LYS:HE2	1:B:175:ASN:HA	1.77	0.66
1:A:590:TYR:HE1	3:A:1176:HOH:O	1.78	0.66
1:B:390:TRP:HA	1:B:390:TRP:CE3	2.30	0.66
1:A:280:TRP:HB3	1:A:303:MET:CE	2.25	0.66
1:B:633:ILE:HG23	1:B:651:PRO:HB3	1.78	0.66
1:B:509:SER:HB2	3:B:1399:HOH:O	1.95	0.66
1:B:584:PRO:HG2	1:B:588:GLU:HB2	1.79	0.65
1:A:390:TRP:HA	1:A:390:TRP:HE3	1.61	0.65
1:B:381:ASN:HD21	1:B:390:TRP:H	1.41	0.65
1:B:390:TRP:HA	1:B:390:TRP:HE3	1.62	0.64
1:A:96:LYS:HD3	3:A:1325:HOH:O	1.96	0.64
1:A:584:PRO:HG2	1:A:588:GLU:HB2	1.80	0.64
1:A:434:GLN:HA	1:A:440:ILE:O	1.98	0.63
1:B:45:ASN:HD21	1:B:48:SER:H	1.45	0.63
1:A:377:MET:HE1	3:B:1162:HOH:O	1.99	0.63
1:A:381:ASN:ND2	1:A:390:TRP:H	1.95	0.63
1:A:593:ALA:HA	3:A:1176:HOH:O	1.97	0.63
1:B:45:ASN:HD22	1:B:47:VAL:H	1.46	0.62
1:B:434:GLN:HA	1:B:440:ILE:O	1.99	0.62
1:A:45:ASN:ND2	1:A:48:SER:H	1.97	0.62
1:B:381:ASN:ND2	1:B:390:TRP:H	1.97	0.62
1:A:407:ARG:HD3	3:A:1073:HOH:O	1.99	0.62
1:B:306:LYS:HD3	3:B:974:HOH:O	1.99	0.62
1:B:381:ASN:C	1:B:381:ASN:HD22	2.08	0.62
1:B:426:ILE:HG23	1:B:477:LYS:HE3	1.82	0.62
1:A:391:THR:HG22	3:A:1220:HOH:O	1.99	0.62
1:B:459:ALA:CB	1:B:475:GLN:HG2	2.31	0.61
1:A:381:ASN:C	1:A:381:ASN:HD22	2.08	0.60
1:A:19:ASN:C	1:A:20:ILE:HG13	2.25	0.60
1:A:295:ASN:ND2	1:A:298:TYR:H	1.99	0.60
1:A:45:ASN:HD22	1:A:47:VAL:H	1.48	0.59
1:B:407:ARG:HD3	3:B:1252:HOH:O	2.01	0.59
1:A:633:ILE:HG23	1:A:651:PRO:HB3	1.84	0.59
1:A:179:LEU:HD23	1:A:232:GLU:HB3	1.83	0.59
1:A:681:ARG:NH1	3:A:1212:HOH:O	2.36	0.59
1:A:204:TYR:HD1	1:A:231:ILE:HD11	1.68	0.58
1:A:380:GLN:NE2	1:A:390:TRP:HB3	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLU:HG2	3:A:1201:HOH:O	2.04	0.58
1:A:85:PHE:HD1	1:A:87:PRO:HD3	1.69	0.58
1:B:119:ARG:HD2	1:B:140:GLU:OE2	2.05	0.57
1:B:534:PRO:HD2	1:B:575:ARG:O	2.04	0.57
1:A:295:ASN:C	1:A:295:ASN:HD22	2.12	0.56
1:A:136:LYS:HE2	1:A:243:GLU:OE1	2.05	0.56
1:A:324:PRO:HG3	1:A:337:TYR:CE1	2.41	0.56
1:A:487:ASN:HB2	3:A:1139:HOH:O	2.06	0.56
1:A:516:MET:H	1:B:518:ASN:ND2	1.94	0.56
1:A:173:ALA:O	1:A:176:ASN:HB2	2.06	0.56
1:A:545:LYS:C	1:A:683:VAL:HG22	2.31	0.56
1:B:267:GLU:HG3	3:B:1434:HOH:O	2.05	0.55
1:A:372:VAL:HG21	1:A:417:LEU:HD22	1.87	0.55
1:A:537:LEU:O	1:A:540:VAL:HG22	2.06	0.55
1:A:284:CYS:SG	1:A:303:MET:HE3	2.46	0.55
1:A:204:TYR:CD1	1:A:231:ILE:HD11	2.42	0.55
1:B:179:LEU:HD23	1:B:232:GLU:HB3	1.89	0.55
1:A:309:GLU:HG2	1:A:310:ASP:O	2.06	0.54
1:B:252:GLN:O	1:B:252:GLN:HG2	2.07	0.54
1:B:557:LYS:HG2	3:B:1361:HOH:O	2.06	0.54
1:B:676:ASP:HB3	3:B:1352:HOH:O	2.06	0.54
1:A:417:LEU:C	1:A:417:LEU:HD13	2.33	0.54
1:B:445:PRO:HG2	3:B:1016:HOH:O	2.06	0.54
1:A:636:GLU:HA	1:A:652:LEU:HD22	1.88	0.54
1:B:173:ALA:O	1:B:176:ASN:HB2	2.08	0.53
1:A:534:PRO:HD2	1:A:575:ARG:O	2.09	0.53
1:B:85:PHE:HD1	1:B:87:PRO:HD3	1.73	0.53
1:A:104:SER:HA	1:A:303:MET:HE1	1.88	0.53
1:A:431:LYS:HD2	1:A:442:GLY:HA2	1.89	0.53
1:A:543:GLY:O	1:A:683:VAL:HG23	2.09	0.53
1:B:560:ASP:OD1	1:B:606:ARG:NH1	2.42	0.53
1:A:560:ASP:OD1	1:A:606:ARG:NH1	2.42	0.53
1:A:113:ASP:HB2	1:A:118:TYR:CE1	2.44	0.53
1:B:317:TYR:HB2	1:B:345:LEU:HD13	1.91	0.53
1:A:45:ASN:HD22	1:A:47:VAL:N	2.06	0.53
1:B:39:GLY:HA2	1:B:633:ILE:HD11	1.90	0.52
1:A:288:ASN:ND2	3:A:1171:HOH:O	2.40	0.52
1:B:460:TYR:HB2	1:B:677:ILE:CD1	2.40	0.52
1:A:394:GLN:CG	1:A:434:GLN:HG3	2.40	0.52
1:A:456:THR:HG23	1:A:475:GLN:OE1	2.09	0.52
1:A:680:LYS:HA	1:A:684:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1060:HOH:O	1:B:377:MET:HE1	2.10	0.51
1:B:353:ILE:CD1	1:B:408:LEU:HD21	2.34	0.51
1:A:368:LEU:HD13	1:A:401:PRO:HB3	1.91	0.51
1:A:406:TYR:OH	1:A:677:ILE:CG2	2.58	0.51
1:B:372:VAL:HG21	1:B:417:LEU:HD22	1.92	0.51
1:A:283:TYR:CZ	1:A:306:LYS:HG3	2.46	0.51
1:B:431:LYS:HD2	1:B:442:GLY:HA2	1.93	0.50
1:B:583:GLU:OE2	1:B:646:THR:HB	2.10	0.50
1:A:681:ARG:CZ	3:A:1212:HOH:O	2.58	0.50
1:B:501:TYR:CD1	1:B:558:VAL:HG21	2.45	0.50
1:B:417:LEU:HD13	1:B:417:LEU:C	2.36	0.50
1:B:30:ASP:OD2	1:B:158:HIS:NE2	2.42	0.50
1:B:104:SER:HA	1:B:303:MET:HE1	1.93	0.50
1:B:394:GLN:CG	1:B:434:GLN:HG3	2.42	0.50
1:B:546:SER:HA	1:B:683:VAL:CG1	2.39	0.50
1:B:45:ASN:HD22	1:B:47:VAL:N	2.10	0.50
1:B:668:GLU:HG3	1:B:670:LYS:HE2	1.93	0.50
1:B:282:LYS:HG2	3:B:1333:HOH:O	2.11	0.49
1:B:651:PRO:HG2	3:B:998:HOH:O	2.12	0.49
1:B:209:ILE:HD13	1:B:209:ILE:O	2.13	0.49
1:A:190:LEU:HD22	1:A:196:TRP:CZ2	2.48	0.49
1:B:295:ASN:C	1:B:295:ASN:HD22	2.19	0.49
1:A:136:LYS:HE3	3:A:990:HOH:O	2.12	0.49
1:A:518:ASN:ND2	1:B:516:MET:H	1.99	0.49
1:B:45:ASN:ND2	1:B:48:SER:H	2.11	0.49
1:B:267:GLU:HG2	1:B:272:LEU:HG	1.92	0.49
1:B:382:THR:HG22	1:B:388:PRO:HA	1.94	0.49
1:B:537:LEU:O	1:B:540:VAL:HG22	2.12	0.49
1:A:445:PRO:HG2	3:A:973:HOH:O	2.12	0.48
1:B:103:LYS:O	1:B:303:MET:HE1	2.12	0.48
1:B:545:LYS:C	1:B:683:VAL:HG22	2.38	0.48
1:A:309:GLU:HB2	1:A:317:TYR:CZ	2.49	0.48
1:B:560:ASP:CG	1:B:606:ARG:HH12	2.22	0.48
1:A:325:TRP:CD1	1:A:647:ASP:HB3	2.48	0.48
1:A:618:THR:N	1:A:619:PRO:HD2	2.29	0.48
1:B:636:GLU:HA	1:B:652:LEU:HD22	1.95	0.48
1:A:608:MET:HE3	1:A:671:VAL:HG13	1.96	0.47
1:A:325:TRP:CD2	1:A:590:TYR:HB3	2.49	0.47
1:A:546:SER:HA	1:A:683:VAL:CG1	2.41	0.47
1:B:618:THR:N	1:B:619:PRO:HD2	2.29	0.47
1:A:51:TRP:HB2	1:A:63:TYR:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:LYS:HE2	3:A:1120:HOH:O	2.14	0.47
1:A:676:ASP:OD2	1:A:676:ASP:N	2.47	0.47
1:B:391:THR:HG22	3:B:1177:HOH:O	2.13	0.47
1:A:12:ILE:HD11	1:A:173:ALA:HB1	1.96	0.47
1:A:629:ASN:HB2	3:A:1157:HOH:O	2.13	0.47
1:A:103:LYS:O	1:A:303:MET:HE1	2.13	0.47
1:A:379:PRO:O	1:A:380:GLN:C	2.57	0.47
1:B:31:THR:O	1:B:73:LYS:HE3	2.15	0.47
1:B:70:ALA:H	1:B:161:ASN:HD21	1.63	0.47
1:A:306:LYS:HD3	3:A:998:HOH:O	2.14	0.47
1:A:546:SER:CA	1:A:683:VAL:HG13	2.43	0.47
1:B:295:ASN:ND2	1:B:298:TYR:H	2.13	0.46
1:A:518:ASN:HD21	1:B:516:MET:N	2.00	0.46
1:A:560:ASP:CG	1:A:606:ARG:HH12	2.24	0.46
1:A:668:GLU:O	1:A:669:HIS:HB2	2.15	0.46
1:B:324:PRO:HG3	1:B:337:TYR:CE1	2.51	0.46
1:B:379:PRO:O	1:B:380:GLN:C	2.58	0.46
1:B:608:MET:HE3	1:B:671:VAL:HG13	1.98	0.46
1:A:59:ILE:HD13	1:A:133:LEU:HD21	1.98	0.46
1:A:252:GLN:O	1:A:252:GLN:HG2	2.14	0.46
1:B:283:TYR:CZ	1:B:306:LYS:HG3	2.50	0.46
1:A:31:THR:O	1:A:73:LYS:HE3	2.15	0.46
1:A:145:SER:HB3	3:A:1229:HOH:O	2.16	0.46
1:A:406:TYR:CZ	1:A:677:ILE:HG23	2.51	0.46
1:B:325:TRP:CD2	1:B:590:TYR:HB3	2.50	0.46
1:A:406:TYR:OH	1:A:677:ILE:HG23	2.16	0.46
1:B:390:TRP:CD1	3:B:1325:HOH:O	2.69	0.46
1:B:543:GLY:O	1:B:683:VAL:HG23	2.15	0.46
1:B:36:GLN:HA	1:B:36:GLN:HE21	1.81	0.46
1:B:81:ASP:HB3	1:B:85:PHE:CZ	2.50	0.46
1:A:79:VAL:CG1	1:A:87:PRO:HG2	2.43	0.46
1:A:369:ALA:HA	1:A:417:LEU:HD23	1.97	0.46
1:B:30:ASP:HB2	1:B:229:ASN:HD22	1.81	0.46
1:A:349:ALA:O	1:A:353:ILE:HG12	2.16	0.46
1:A:353:ILE:CD1	1:A:408:LEU:HD21	2.37	0.46
1:B:35:ALA:HB2	1:B:324:PRO:HA	1.97	0.46
1:A:61:GLU:HA	1:A:72:VAL:O	2.15	0.45
1:B:309:GLU:HG2	1:B:310:ASP:O	2.16	0.45
1:B:79:VAL:CG1	1:B:87:PRO:HG2	2.41	0.45
1:A:280:TRP:CD2	1:A:303:MET:HE2	2.50	0.45
1:A:306:LYS:HD2	3:A:1144:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:TYR:HB2	1:A:345:LEU:HD13	1.98	0.45
1:A:594:GLY:N	3:A:1176:HOH:O	2.47	0.45
1:A:593:ALA:CA	3:A:1176:HOH:O	2.61	0.45
1:B:395:LEU:HD23	1:B:432:THR:HA	1.99	0.45
1:B:540:VAL:HG21	1:B:609:TYR:CD2	2.42	0.45
1:A:475:GLN:HG3	3:A:1310:HOH:O	2.15	0.45
1:B:394:GLN:HG3	1:B:434:GLN:HG3	1.99	0.45
1:B:79:VAL:HG11	1:B:118:TYR:CE1	2.52	0.44
1:B:595:LYS:HG2	3:B:1326:HOH:O	2.16	0.44
1:B:35:ALA:CB	1:B:324:PRO:HA	2.46	0.44
1:A:283:TYR:CE1	1:A:306:LYS:HG3	2.52	0.44
1:A:521:ASN:HB3	3:A:1176:HOH:O	2.17	0.44
1:A:113:ASP:HB2	1:A:118:TYR:CD1	2.52	0.44
1:B:327:ASP:HB3	3:B:1392:HOH:O	2.18	0.44
1:B:406:TYR:CZ	1:B:677:ILE:CG2	2.99	0.44
1:A:267:GLU:HG2	1:A:272:LEU:HG	1.99	0.44
1:A:98:GLU:OE1	1:A:108:LYS:HD3	2.18	0.44
1:B:136:LYS:HE2	1:B:243:GLU:OE1	2.18	0.44
1:B:369:ALA:HA	1:B:417:LEU:HD23	1.99	0.43
1:B:387:LYS:HG3	1:B:388:PRO:HD2	1.99	0.43
1:A:295:ASN:ND2	1:A:295:ASN:C	2.75	0.43
1:B:546:SER:CA	1:B:683:VAL:HG13	2.42	0.43
1:A:162:GLN:HA	1:A:331:ASP:O	2.18	0.43
1:A:119:ARG:HD2	1:A:140:GLU:OE2	2.19	0.43
1:A:145:SER:HB3	1:A:148:ASP:OD2	2.18	0.43
1:A:586:LYS:HA	1:A:639:TRP:CH2	2.53	0.43
1:A:103:LYS:C	1:A:303:MET:HE1	2.43	0.43
1:A:231:ILE:HG21	3:A:1234:HOH:O	2.19	0.43
1:B:204:TYR:CD1	1:B:231:ILE:HD11	2.54	0.43
1:A:501:TYR:CD1	1:A:558:VAL:HG21	2.54	0.43
1:B:30:ASP:HB2	1:B:229:ASN:ND2	2.33	0.43
1:B:327:ASP:CB	3:B:1392:HOH:O	2.67	0.43
1:A:382:THR:HG22	1:A:388:PRO:HA	2.01	0.43
1:B:283:TYR:CE1	1:B:306:LYS:HG3	2.54	0.43
1:B:508:LEU:HB2	3:B:1435:HOH:O	2.18	0.43
1:B:61:GLU:HA	1:B:72:VAL:O	2.18	0.42
1:B:190:LEU:HD22	1:B:196:TRP:CZ2	2.54	0.42
1:A:35:ALA:CB	1:A:324:PRO:HA	2.50	0.42
1:A:165:TYR:HA	1:A:228:GLY:HA2	2.01	0.42
1:B:475:GLN:HA	1:B:475:GLN:NE2	2.34	0.42
1:A:377:MET:HG2	1:A:378:ILE:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ASP:HB2	1:B:118:TYR:CE1	2.54	0.42
1:B:309:GLU:HB2	1:B:317:TYR:CZ	2.54	0.42
1:B:324:PRO:HB2	1:B:325:TRP:CE3	2.55	0.42
1:B:679:TYR:CD1	1:B:683:VAL:HB	2.55	0.42
1:A:324:PRO:HB2	1:A:325:TRP:CE3	2.55	0.42
1:A:394:GLN:HG3	1:A:434:GLN:HG3	2.01	0.42
1:B:100:PHE:CD1	1:B:106:GLY:HA3	2.54	0.42
1:A:299:TYR:O	1:A:303:MET:HG3	2.20	0.42
1:B:317:TYR:HB2	1:B:345:LEU:CD1	2.49	0.42
1:B:460:TYR:HB2	1:B:677:ILE:HD12	2.01	0.42
1:A:459:ALA:HB1	1:A:475:GLN:HG2	1.99	0.42
1:B:108:LYS:HA	1:B:122:LYS:O	2.20	0.42
1:B:185:ASN:O	1:B:252:GLN:HA	2.20	0.42
1:B:204:TYR:HD1	1:B:231:ILE:HD11	1.85	0.42
1:A:123:ASP:HB2	1:A:136:LYS:HB3	2.01	0.42
1:A:395:LEU:HD23	1:A:432:THR:HA	2.02	0.41
1:B:671:VAL:HG21	3:B:1147:HOH:O	2.20	0.41
1:B:29:GLU:HG2	3:B:1175:HOH:O	2.19	0.41
1:B:299:TYR:O	1:B:303:MET:HG3	2.19	0.41
1:B:406:TYR:OH	1:B:677:ILE:HG22	2.20	0.41
1:A:178:MET:HG2	1:A:191:SER:HB3	2.01	0.41
1:B:368:LEU:HD13	1:B:401:PRO:HB3	2.01	0.41
1:B:437:TRP:O	1:B:439:GLU:HG3	2.20	0.41
1:A:181:ALA:HB3	1:A:188:THR:OG1	2.20	0.41
1:B:553:LEU:N	1:B:553:LEU:HD22	2.36	0.41
1:B:683:VAL:HG11	3:B:1112:HOH:O	2.21	0.41
1:A:79:VAL:HG11	1:A:118:TYR:CE1	2.55	0.41
1:A:209:ILE:HD13	1:A:209:ILE:O	2.20	0.41
1:B:565:VAL:HB	1:B:598:LEU:HD21	2.02	0.41
1:A:80:THR:HG22	1:A:152:TYR:HE1	1.85	0.41
1:B:103:LYS:C	1:B:303:MET:HE1	2.46	0.41
1:B:295:ASN:C	1:B:295:ASN:ND2	2.79	0.41
1:B:295:ASN:ND2	1:B:295:ASN:H	2.19	0.41
1:B:414:TYR:HA	1:B:418:VAL:HB	2.03	0.41
1:B:558:VAL:O	1:B:562:THR:HG23	2.21	0.41
1:A:79:VAL:HG13	1:A:87:PRO:CG	2.47	0.41
1:A:540:VAL:HG23	1:A:541:ARG:N	2.36	0.41
1:B:70:ALA:H	1:B:161:ASN:ND2	2.19	0.41
1:B:434:GLN:HE21	1:B:434:GLN:HB3	1.73	0.41
1:B:586:LYS:HA	1:B:639:TRP:CH2	2.56	0.41
1:A:244:PHE:CD1	1:A:244:PHE:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ASP:HB2	1:B:136:LYS:HB3	2.03	0.40
1:A:437:TRP:HB3	1:A:575:ARG:NH1	2.35	0.40
1:B:85:PHE:CG	1:B:117:ARG:NH1	2.90	0.40
1:A:414:TYR:HA	1:A:418:VAL:HB	2.03	0.40
1:B:629:ASN:HB2	3:B:1058:HOH:O	2.21	0.40
1:A:345:LEU:CD1	1:A:364:SER:HB2	2.49	0.40
1:A:317:TYR:HB2	1:A:345:LEU:CD1	2.50	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	672/684 (98%)	631 (94%)	39 (6%)	2 (0%)	36	36
1	B	672/684 (98%)	633 (94%)	37 (6%)	2 (0%)	36	36
All	All	1344/1368 (98%)	1264 (94%)	76 (6%)	4 (0%)	36	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	ASN
1	B	333	ASN
1	A	335	GLY
1	B	335	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	566/575 (98%)	546 (96%)	20 (4%)	32	35
1	B	566/575 (98%)	547 (97%)	19 (3%)	32	35
All	All	1132/1150 (98%)	1093 (97%)	39 (3%)	32	35

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	176	ASN
1	A	182	LYS
1	A	190	LEU
1	A	209	ILE
1	A	267	GLU
1	A	271	ASN
1	A	286	THR
1	A	295	ASN
1	A	332	ASP
1	A	370	LYS
1	A	377	MET
1	A	381	ASN
1	A	390	TRP
1	A	435	GLU
1	A	556	LEU
1	A	577	ASN
1	A	583	GLU
1	A	598	LEU
1	A	677	ILE
1	B	45	ASN
1	B	176	ASN
1	B	182	LYS
1	B	190	LEU
1	B	209	ILE
1	B	267	GLU
1	B	271	ASN
1	B	279	GLU
1	B	295	ASN
1	B	332	ASP
1	B	370	LYS
1	B	377	MET
1	B	381	ASN

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Mol	Chain	Res	Type
1	B	390	TRP
1	B	435	GLU
1	B	556	LEU
1	B	577	ASN
1	B	598	LEU
1	B	677	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	56	ASN
1	A	161	ASN
1	A	216	ASN
1	A	218	GLN
1	A	295	ASN
1	A	313	ASN
1	A	380	GLN
1	A	381	ASN
1	A	464	GLN
1	A	493	ASN
1	A	500	GLN
1	A	518	ASN
1	A	554	ASN
1	A	666	ASN
1	B	45	ASN
1	B	56	ASN
1	B	161	ASN
1	B	218	GLN
1	B	229	ASN
1	B	270	ASN
1	B	275	ASN
1	B	295	ASN
1	B	381	ASN
1	B	464	GLN
1	B	493	ASN
1	B	518	ASN
1	B	554	ASN
1	B	666	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	SO4	B	951	-	4,4,4	0.39	0	6,6,6	0.10	0
2	SO4	A	950	-	4,4,4	0.41	0	6,6,6	0.07	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	674/684 (98%)	0.28	50 (7%)	20 22	11, 24, 50, 66	0
1	B	674/684 (98%)	0.01	31 (4%)	37 39	11, 20, 41, 64	0
All	All	1348/1368 (98%)	0.14	81 (6%)	27 29	11, 22, 46, 66	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	GLY	5.6
1	B	331	ASP	5.6
1	A	333	ASN	5.3
1	A	84	SER	5.2
1	B	334	THR	5.0
1	B	87	PRO	4.9
1	A	335	GLY	4.8
1	A	331	ASP	4.7
1	B	333	ASN	4.7
1	A	593	ALA	4.6
1	A	327	ASP	4.4
1	A	590	TYR	4.3
1	A	585	SER	4.3
1	A	334	THR	4.2
1	A	584	PRO	4.2
1	B	327	ASP	4.2
1	B	336	GLY	4.0
1	A	325	TRP	4.0
1	A	85	PHE	4.0
1	B	332	ASP	3.9
1	A	326	GLY	3.9
1	B	330	ARG	3.8
1	B	252	GLN	3.7
1	A	87	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	336	GLY	3.4
1	A	330	ARG	3.4
1	A	146	ILE	3.4
1	B	683	VAL	3.4
1	A	211	THR	3.3
1	A	591	HIS	3.3
1	A	220	THR	3.2
1	A	14	ILE	3.1
1	A	332	ASP	3.1
1	B	185	ASN	3.0
1	B	85	PHE	3.0
1	B	329	GLN	3.0
1	A	231	ILE	2.9
1	A	586	LYS	2.9
1	A	587	THR	2.9
1	B	30	ASP	2.8
1	B	86	VAL	2.8
1	B	684	ALA	2.7
1	A	329	GLN	2.6
1	B	595	LYS	2.6
1	A	11	SER	2.6
1	B	183	ARG	2.5
1	B	184	ASP	2.4
1	B	11	SER	2.4
1	B	217	LYS	2.4
1	A	588	GLU	2.4
1	A	286	THR	2.4
1	A	592	GLY	2.4
1	B	337	TYR	2.3
1	A	86	VAL	2.3
1	B	147	HIS	2.3
1	A	684	ALA	2.3
1	A	198	GLY	2.3
1	A	148	ASP	2.3
1	A	172	LYS	2.3
1	A	144	GLY	2.3
1	A	222	HIS	2.3
1	A	219	MET	2.3
1	A	78	ILE	2.2
1	B	74	GLU	2.2
1	A	171	ILE	2.2
1	A	583	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	390	TRP	2.2
1	B	390	TRP	2.2
1	A	80	THR	2.2
1	A	24	ASN	2.1
1	B	676	ASP	2.1
1	B	391	THR	2.1
1	B	12	ILE	2.1
1	B	328	GLY	2.1
1	A	175	ASN	2.1
1	A	683	VAL	2.1
1	A	509	SER	2.1
1	A	142	LEU	2.0
1	A	212	ASP	2.0
1	A	12	ILE	2.0
1	B	142	LEU	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($\text{\AA}^2$)	Q<0.9
2	SO4	A	950	5/5	0.89	0.17	54,54,55,56	0
2	SO4	B	951	5/5	0.92	0.15	50,51,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.