



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:20 PM UTC

PDB ID : 7PPR / pdb_00007ppr
Title : The structure of UDP-glucose pyrophosphorylase from *Aspergillus fumigatus*
Authors : Morton, S.; Raimi, O.G.; Yan, K.; van Aalten, D.M.F.
Deposited on : 2021-09-14
Resolution : 2.57 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

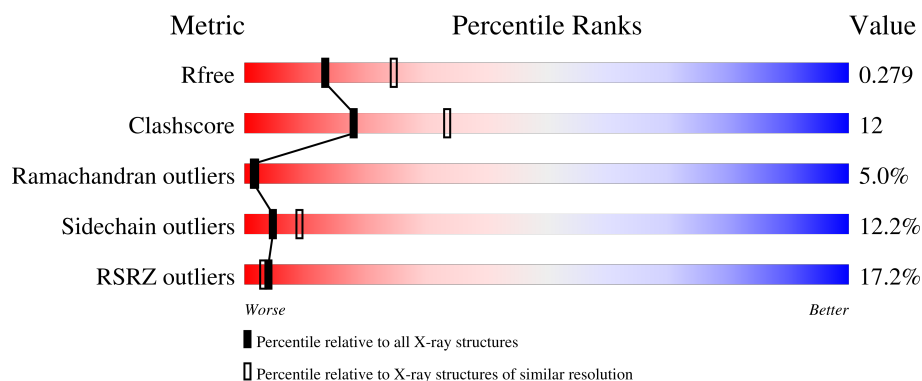
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	492	16% 63% 23% • 9%
1	B	492	16% 67% 21% 5% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7187 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.

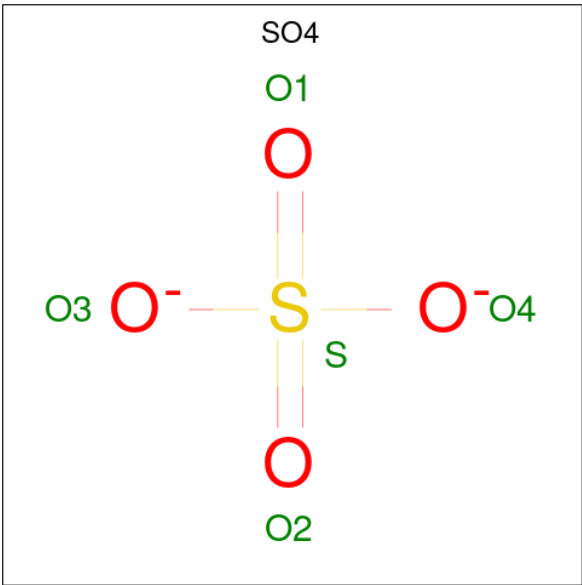
- Molecule 1 is a protein called UTP--glucose-1-phosphate uridylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	6	0
			3452	2193	606	641	12			
1	B	464	Total	C	N	O	S	0	4	0
			3527	2242	606	666	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLY	-	expression tag	UNP E9R9Z5
A	21	PRO	-	expression tag	UNP E9R9Z5
A	22	LEU	-	expression tag	UNP E9R9Z5
A	23	GLY	-	expression tag	UNP E9R9Z5
A	24	SER	-	expression tag	UNP E9R9Z5
B	20	GLY	-	expression tag	UNP E9R9Z5
B	21	PRO	-	expression tag	UNP E9R9Z5
B	22	LEU	-	expression tag	UNP E9R9Z5
B	23	GLY	-	expression tag	UNP E9R9Z5
B	24	SER	-	expression tag	UNP E9R9Z5

- 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	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		

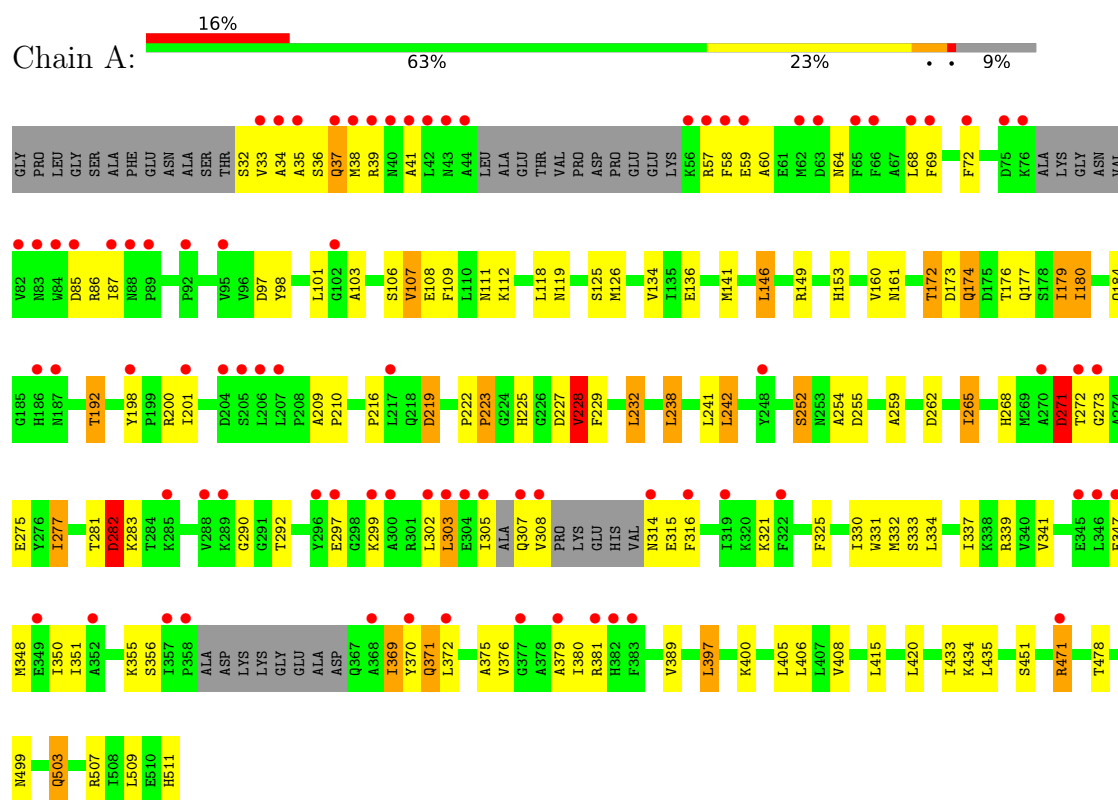
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	B	70	Total	O	0	0
			70	70		

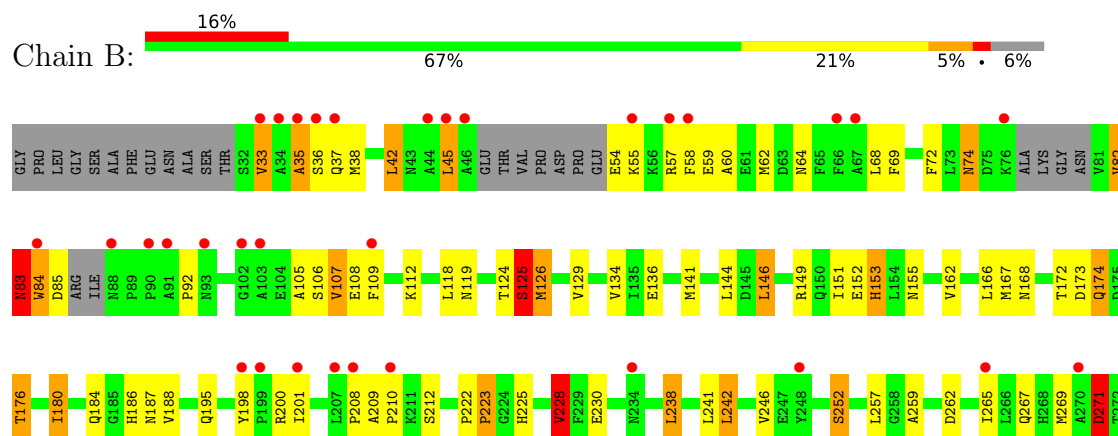
3 Residue-property plots

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: UTP--glucose-1-phosphate uridylyltransferase



- Molecule 1: UTP--glucose-1-phosphate uridylyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	134.16Å 152.61Å 160.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.00 – 2.57 80.00 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.8 (80.00-2.57) 99.8 (80.00-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.227 , 0.277 0.231 , 0.279	Depositor DCC
R_{free} test set	2699 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7187	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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, CL

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	1.12	0/3518	1.48	13/4765 (0.3%)
1	B	1.13	0/3596	1.48	12/4882 (0.2%)
All	All	1.12	0/7114	1.48	25/9647 (0.3%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	ASP	CB-CA-C	-10.49	91.23	110.63
1	A	271	ASP	CA-CB-CG	8.04	120.64	112.60
1	B	271	ASP	CA-CB-CG	7.61	120.21	112.60
1	B	290	GLY	CA-C-N	6.69	126.45	120.10
1	B	290	GLY	C-N-CA	6.69	126.45	120.10
1	A	290	GLY	CA-C-N	6.62	126.39	120.10
1	A	290	GLY	C-N-CA	6.62	126.39	120.10
1	A	271	ASP	CB-CA-C	6.35	120.89	111.17
1	B	271	ASP	CB-CA-C	6.33	123.02	110.42
1	A	325	PHE	CA-C-N	5.71	129.47	121.24
1	A	325	PHE	C-N-CA	5.71	129.47	121.24
1	A	228	VAL	N-CA-CB	5.65	116.78	110.51
1	B	325	PHE	CA-C-N	5.64	129.36	121.24
1	B	325	PHE	C-N-CA	5.64	129.36	121.24
1	A	227	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	228	VAL	N-CA-CB	5.46	116.57	110.51
1	A	282	ASP	CA-CB-CG	5.40	118.00	112.60
1	B	186	HIS	CA-C-O	-5.37	116.37	122.01
1	B	92	PRO	CA-C-N	5.31	127.66	120.44
1	B	92	PRO	C-N-CA	5.31	127.66	120.44
1	A	254	ALA	CA-C-N	5.21	127.78	120.28
1	A	254	ALA	C-N-CA	5.21	127.78	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	282	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	126	MET	N-CA-C	-5.10	107.22	112.93
1	A	255	ASP	CA-CB-CG	5.02	117.62	112.60

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	3452	0	3361	79	0
1	B	3527	0	3428	91	0
2	A	45	0	0	2	0
2	B	30	0	0	1	0
3	B	2	0	0	0	0
4	A	61	0	0	0	0
4	B	70	0	0	0	0
All	All	7187	0	6789	169	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 12.

All (169) 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:B:112:LYS:O	1:B:246:VAL:O	1.60	1.17
1:B:57[B]:ARG:HG2	1:B:57[B]:ARG:HH11	1.12	1.07
1:A:119:ASN:O	1:A:172:THR:HG21	1.60	1.01
1:A:111:ASN:OD1	1:A:160:VAL:HG13	1.62	0.97
1:B:57[B]:ARG:HH11	1:B:57[B]:ARG:CG	1.83	0.92
1:A:60:ALA:O	1:A:64:ASN:ND2	2.09	0.86
1:B:60:ALA:O	1:B:64:ASN:ND2	2.09	0.86
1:A:200:ARG:NH1	1:A:371:GLN:OE1	2.12	0.83
1:B:200:ARG:HE	1:B:371:GLN:HE21	1.28	0.82
1:B:362[B]:LYS:HE3	1:B:362[B]:LYS:HA	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ASN:HD21	1:B:162:VAL:H	1.32	0.78
1:B:57[B]:ARG:HG2	1:B:57[B]:ARG:NH1	1.94	0.77
1:A:106:SER:O	1:A:107:VAL:HG23	1.85	0.76
1:A:57:ARG:O	1:A:59:GLU:N	2.20	0.75
1:B:200:ARG:HE	1:B:371:GLN:NE2	1.83	0.75
1:A:225[B]:HIS:CD2	1:A:376:VAL:H	2.06	0.73
1:A:111:ASN:OD1	1:A:160:VAL:CG1	2.36	0.72
1:B:262:ASP:O	1:B:265:ILE:HG22	1.90	0.71
1:A:229:PHE:HE1	1:A:332:MET:CE	2.03	0.70
1:B:106:SER:O	1:B:107:VAL:HG23	1.92	0.70
1:B:74:ASN:HD22	1:B:74:ASN:N	1.90	0.69
1:A:271:ASP:O	1:A:271:ASP:OD1	2.11	0.69
1:B:271:ASP:O	1:B:271:ASP:OD1	2.11	0.69
1:A:153:HIS:ND1	2:A:602:SO4:O1	2.24	0.67
1:B:507:ARG:NH1	2:B:602:SO4:O3	2.27	0.67
1:B:83:ASN:O	1:B:85:ASP:N	2.27	0.67
1:B:241:LEU:O	1:B:246:VAL:HG13	1.95	0.67
1:A:229:PHE:CE1	1:A:332:MET:CE	2.79	0.66
1:A:229:PHE:CE1	1:A:332:MET:HE1	2.30	0.66
1:A:201:ILE:HG23	1:A:370:TYR:HB2	1.78	0.65
1:A:198:TYR:CD2	1:A:223:PRO:HG3	2.32	0.64
1:B:105:ALA:HA	1:B:267:GLN:HE21	1.62	0.64
1:B:198:TYR:CD2	1:B:223:PRO:HG3	2.33	0.64
1:A:98:TYR:HA	1:A:101:LEU:HD13	1.80	0.63
1:B:83:ASN:O	1:B:83:ASN:ND2	2.24	0.62
1:B:284:THR:O	1:B:285[B]:LYS:HG3	2.00	0.62
1:A:406:LEU:HD22	1:A:433:ILE:HD13	1.82	0.61
1:B:35:ALA:O	1:B:38:MET:N	2.35	0.59
1:B:337:ILE:O	1:B:341:VAL:CG1	2.50	0.59
1:A:355:LYS:HB2	1:A:369:ILE:HD11	1.84	0.58
1:B:126:MET:HE2	1:B:400:LYS:C	2.28	0.58
1:B:362[B]:LYS:HE3	1:B:362[B]:LYS:CA	2.32	0.57
1:B:351:ILE:O	1:B:372:LEU:HA	2.04	0.57
1:B:151:ILE:O	1:B:153:HIS:O	2.21	0.57
1:B:57[B]:ARG:CG	1:B:57[B]:ARG:NH1	2.50	0.57
1:A:272:THR:O	1:A:272:THR:HG22	2.03	0.57
1:B:172:THR:O	1:B:176:THR:CG2	2.53	0.56
1:A:37:GLN:O	1:A:39:ARG:N	2.38	0.56
1:B:124:THR:O	1:B:125:SER:HB3	2.05	0.56
1:B:337:ILE:O	1:B:341:VAL:HG12	2.05	0.56
1:A:252:SER:OG	1:A:259:ALA:HB1	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:MET:HE2	1:A:400:LYS:C	2.32	0.55
1:A:141:MET:HB3	1:A:146:LEU:HD13	1.89	0.55
1:B:252:SER:OG	1:B:259:ALA:HB1	2.07	0.54
1:A:160:VAL:HG12	1:A:161:ASN:H	1.72	0.54
1:A:173:ASP:O	1:A:174:GLN:CB	2.55	0.54
1:A:511:HIS:OXT	1:B:460:HIS:HE1	1.89	0.54
1:B:152:GLU:C	1:B:153:HIS:O	2.45	0.54
1:B:141:MET:HB3	1:B:146:LEU:HD13	1.88	0.54
1:A:32:SER:O	1:A:34:ALA:N	2.41	0.54
1:B:265:ILE:CG2	1:B:331:TRP:CZ2	2.91	0.53
1:B:173:ASP:O	1:B:174:GLN:CB	2.56	0.52
1:A:305:ILE:HD12	1:A:305:ILE:O	2.10	0.52
1:A:225[A]:HIS:O	1:A:228:VAL:HG22	2.10	0.52
1:B:238:LEU:CD1	1:B:334:LEU:HG	2.40	0.52
1:B:487:SER:HB3	1:B:505:SER:OG	2.10	0.52
1:B:241:LEU:HB3	1:B:246:VAL:HG21	1.92	0.51
1:A:149:ARG:NH2	2:A:603:SO4:O2	2.44	0.51
1:B:58:PHE:HD2	1:B:62:MET:HE3	1.74	0.51
1:A:337:ILE:O	1:A:341:VAL:HG23	2.11	0.51
1:A:238:LEU:HD13	1:A:334:LEU:HD11	1.93	0.50
1:A:265:ILE:HD11	1:A:331:TRP:NE1	2.25	0.50
1:A:332:MET:HE2	1:A:337:ILE:HD11	1.92	0.50
1:A:379:ALA:O	1:A:381:ARG:N	2.45	0.50
1:B:200:ARG:HH21	1:B:371:GLN:HE22	1.60	0.50
1:B:379:ALA:O	1:B:381:ARG:N	2.45	0.50
1:A:225[B]:HIS:O	1:A:228:VAL:HG22	2.12	0.50
1:A:200:ARG:HD3	1:A:369:ILE:HG13	1.93	0.49
1:A:238:LEU:CD1	1:A:334:LEU:HG	2.41	0.49
1:B:105:ALA:CA	1:B:267:GLN:HG2	2.42	0.49
1:B:172:THR:O	1:B:176:THR:HG23	2.11	0.49
1:B:64:ASN:O	1:B:68:LEU:HD13	2.13	0.49
1:B:225:HIS:O	1:B:228:VAL:HG22	2.12	0.49
1:A:160:VAL:HG12	1:A:161:ASN:N	2.28	0.49
1:B:74:ASN:N	1:B:74:ASN:ND2	2.61	0.49
1:B:58:PHE:CD2	1:B:62:MET:HE3	2.48	0.48
1:A:225[B]:HIS:CD2	1:A:375:ALA:HA	2.48	0.48
1:B:119:ASN:HD22	1:B:168:ASN:ND2	2.12	0.48
1:A:64:ASN:O	1:A:68:LEU:HD13	2.13	0.48
1:B:238:LEU:HD13	1:B:334:LEU:HD11	1.95	0.47
1:A:177:GLN:OE1	1:A:192:THR:HG21	2.13	0.47
1:A:265:ILE:HD11	1:A:331:TRP:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ILE:HG21	1:B:331:TRP:CZ2	2.49	0.47
1:A:478:THR:H	1:A:499:ASN:HD22	1.62	0.47
1:A:101:LEU:HD23	1:A:268:HIS:HB2	1.96	0.47
1:A:225[B]:HIS:HD2	1:A:376:VAL:H	1.55	0.47
1:A:307:GLN:O	1:A:308:VAL:CB	2.63	0.47
1:A:262:ASP:HB3	1:A:265:ILE:HG23	1.96	0.47
1:A:503:GLN:O	1:A:503:GLN:HG2	2.12	0.47
1:A:177:GLN:O	1:A:180:ILE:HG22	2.16	0.46
1:A:176:THR:O	1:A:180:ILE:HB	2.16	0.46
1:A:209:ALA:N	1:A:210:PRO:HD2	2.31	0.45
1:A:351:ILE:O	1:A:372:LEU:HA	2.16	0.45
1:B:311:GLU:O	1:B:312:HIS:HB2	2.16	0.45
1:A:108:GLU:O	1:A:112:LYS:HD2	2.17	0.45
1:B:242:LEU:HD13	1:B:334:LEU:HD23	1.99	0.45
1:B:105:ALA:HA	1:B:267:GLN:HG2	1.98	0.45
1:B:172:THR:O	1:B:176:THR:HG22	2.16	0.45
1:B:406:LEU:C	1:B:406:LEU:HD23	2.42	0.45
1:A:507[A]:ARG:CZ	1:A:509:LEU:HD21	2.46	0.45
1:A:406:LEU:C	1:A:406:LEU:HD23	2.41	0.45
1:A:216:PRO:O	1:A:219:ASP:OD1	2.34	0.44
1:A:275:GLU:OE1	1:A:339:ARG:NH2	2.51	0.44
1:B:176:THR:O	1:B:180:ILE:HB	2.17	0.44
1:B:222:PRO:O	1:B:223:PRO:O	2.36	0.44
1:A:209:ALA:N	1:A:210:PRO:CD	2.81	0.44
1:A:303:LEU:HD22	1:A:303:LEU:C	2.43	0.44
1:A:222:PRO:O	1:A:223:PRO:O	2.35	0.44
1:A:201:ILE:CG2	1:A:370:TYR:HB2	2.46	0.43
1:B:369:ILE:HD12	1:B:369:ILE:C	2.43	0.43
1:B:82:VAL:O	1:B:84:TRP:N	2.51	0.43
1:B:246:VAL:CG2	1:B:334:LEU:HD22	2.48	0.43
1:B:277:ILE:HG23	1:B:389:VAL:HG23	2.00	0.43
1:B:42:LEU:HD12	1:B:42:LEU:HA	1.80	0.43
1:B:200:ARG:HH21	1:B:371:GLN:NE2	2.15	0.43
1:B:167:MET:HE3	1:B:195:GLN:HB3	2.00	0.43
1:B:275:GLU:OE1	1:B:339:ARG:NH2	2.51	0.43
1:B:406:LEU:HD22	1:B:433:ILE:HD13	2.01	0.43
1:B:35:ALA:O	1:B:37:GLN:N	2.52	0.43
1:B:124:THR:O	1:B:125:SER:CB	2.66	0.43
1:A:252:SER:OG	1:A:259:ALA:CB	2.67	0.43
1:B:108:GLU:O	1:B:112:LYS:HD2	2.19	0.43
1:B:209:ALA:N	1:B:210:PRO:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:GLN:O	1:B:372:LEU:HG	2.19	0.42
1:A:173:ASP:O	1:A:174:GLN:HB2	2.19	0.42
1:B:277:ILE:CG2	1:B:389:VAL:HG23	2.48	0.42
1:B:285[B]:LYS:HE2	1:B:285[B]:LYS:HB2	1.87	0.42
1:B:109:PHE:O	1:B:112:LYS:HB2	2.19	0.42
1:A:69:PHE:O	1:A:72:PHE:HB3	2.19	0.42
1:B:209:ALA:N	1:B:210:PRO:CD	2.82	0.42
1:B:144:LEU:HD23	1:B:144:LEU:HA	1.78	0.42
1:B:242:LEU:HD12	1:B:242:LEU:HA	1.89	0.42
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.89	0.42
1:A:471[A]:ARG:H	1:A:471[A]:ARG:HG3	1.56	0.42
1:A:348:MET:O	1:A:350:ILE:HD12	2.19	0.41
1:A:415:LEU:HD12	1:A:415:LEU:HA	1.89	0.41
1:B:69:PHE:O	1:B:72:PHE:HB3	2.21	0.41
1:B:415:LEU:HD12	1:B:415:LEU:HA	1.87	0.41
1:A:277:ILE:HG23	1:A:389:VAL:HG23	2.02	0.41
1:B:83:ASN:HD22	1:B:83:ASN:C	2.23	0.41
1:A:281:THR:O	1:A:282:ASP:CB	2.68	0.41
1:B:269:MET:HE1	1:B:332:MET:C	2.46	0.41
1:A:109:PHE:O	1:A:112:LYS:HB2	2.21	0.41
1:A:232:LEU:HD12	1:A:232:LEU:HA	1.90	0.41
1:B:38:MET:SD	1:B:208:PRO:HD3	2.61	0.41
1:B:320:LYS:O	1:B:321:LYS:HB2	2.21	0.41
1:B:345:GLU:O	1:B:345:GLU:HG3	2.20	0.41
1:B:167:MET:HE3	1:B:195:GLN:CB	2.51	0.41
1:A:106:SER:O	1:A:107:VAL:CG2	2.62	0.40
1:A:161:ASN:OD1	1:A:161:ASN:C	2.64	0.40
1:B:334:LEU:HD12	1:B:334:LEU:HA	1.92	0.40
1:B:151:ILE:C	1:B:153:HIS:O	2.64	0.40
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.90	0.40
1:A:330:ILE:HG22	1:A:332:MET:SD	2.61	0.40
1:B:281:THR:O	1:B:282:ASP:CB	2.69	0.40
1:A:478:THR:H	1:A:499:ASN:ND2	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	443/492 (90%)	387 (87%)	38 (9%)	18 (4%)	2	2
1	B	457/492 (93%)	390 (85%)	38 (8%)	29 (6%)	1	1
All	All	900/984 (92%)	777 (86%)	76 (8%)	47 (5%)	1	1

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ALA
1	A	37	GLN
1	A	38	MET
1	A	58	PHE
1	A	107	VAL
1	A	174	GLN
1	A	282	ASP
1	A	380	ILE
1	B	33	VAL
1	B	35	ALA
1	B	36	SER
1	B	84	TRP
1	B	107	VAL
1	B	174	GLN
1	B	187	ASN
1	B	282	ASP
1	A	41	ALA
1	A	103	ALA
1	A	223	PRO
1	A	321	LYS
1	B	83	ASN
1	B	125	SER
1	B	223	PRO
1	B	285[A]	LYS
1	B	285[B]	LYS

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Mol	Chain	Res	Type
1	B	314	ASN
1	B	380	ILE
1	B	385	ASN
1	A	85	ASP
1	A	87	ILE
1	A	347	GLU
1	B	45[A]	LEU
1	B	45[B]	LEU
1	B	55	LYS
1	B	153	HIS
1	B	297	GLU
1	B	321	LYS
1	B	372	LEU
1	B	384	LYS
1	A	33	VAL
1	B	312	HIS
1	B	347	GLU
1	A	273	GLY
1	A	297	GLU
1	B	188	VAL
1	B	273	GLY
1	B	313	VAL

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	354/425 (83%)	309 (87%)	45 (13%)	4	8
1	B	366/425 (86%)	323 (88%)	43 (12%)	5	10
All	All	720/850 (85%)	632 (88%)	88 (12%)	5	9

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	SER

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Mol	Chain	Res	Type
1	A	86	ARG
1	A	97	ASP
1	A	118	LEU
1	A	125	SER
1	A	134	VAL
1	A	136	GLU
1	A	146	LEU
1	A	172	THR
1	A	179	ILE
1	A	180	ILE
1	A	184	GLN
1	A	192	THR
1	A	219	ASP
1	A	228	VAL
1	A	232	LEU
1	A	238	LEU
1	A	241	LEU
1	A	242	LEU
1	A	252	SER
1	A	265	ILE
1	A	271	ASP
1	A	277	ILE
1	A	283	LYS
1	A	292	THR
1	A	299	LYS
1	A	302	LEU
1	A	303	LEU
1	A	314	ASN
1	A	315	GLU
1	A	316	PHE
1	A	333	SER
1	A	356	SER
1	A	369	ILE
1	A	371	GLN
1	A	397	LEU
1	A	405	LEU
1	A	408	VAL
1	A	420	LEU
1	A	434	LYS
1	A	435	LEU
1	A	451	SER
1	A	471[A]	ARG

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Mol	Chain	Res	Type
1	A	471[B]	ARG
1	A	503	GLN
1	B	33	VAL
1	B	42	LEU
1	B	54	GLU
1	B	59	GLU
1	B	74	ASN
1	B	82	VAL
1	B	83	ASN
1	B	118	LEU
1	B	125	SER
1	B	129	VAL
1	B	134	VAL
1	B	136	GLU
1	B	146	LEU
1	B	149	ARG
1	B	166	LEU
1	B	176	THR
1	B	180	ILE
1	B	184	GLN
1	B	201	ILE
1	B	212	SER
1	B	228	VAL
1	B	230	GLU
1	B	238	LEU
1	B	242	LEU
1	B	252	SER
1	B	257	LEU
1	B	271	ASP
1	B	283	LYS
1	B	284	THR
1	B	302	LEU
1	B	305	ILE
1	B	312	HIS
1	B	321	LYS
1	B	333	SER
1	B	340	VAL
1	B	341	VAL
1	B	345	GLU
1	B	372	LEU
1	B	405	LEU
1	B	408	VAL

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Mol	Chain	Res	Type
1	B	484	THR
1	B	505	SER
1	B	507	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	A	268	HIS
1	A	307	GLN
1	A	344	ASN
1	A	419	GLN
1	A	499	ASN
1	A	511	HIS
1	B	74	ASN
1	B	150	GLN
1	B	155	ASN
1	B	168	ASN
1	B	267	GLN
1	B	367	GLN
1	B	371	GLN
1	B	390	ASN
1	B	460	HIS
1	B	468	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

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	$\# Z > 2$
2	SO4	A	605	-	4,4,4	0.31	0	6,6,6	0.15	0
2	SO4	A	606	-	4,4,4	0.29	0	6,6,6	0.11	0
2	SO4	A	608	-	4,4,4	0.31	0	6,6,6	0.11	0
2	SO4	A	604	-	4,4,4	0.29	0	6,6,6	0.20	0
2	SO4	A	603	-	4,4,4	0.33	0	6,6,6	0.15	0
2	SO4	B	606	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	B	604	-	4,4,4	0.29	0	6,6,6	0.11	0
2	SO4	B	605	-	4,4,4	0.29	0	6,6,6	0.14	0
2	SO4	B	602	-	4,4,4	0.23	0	6,6,6	0.17	0
2	SO4	B	603	-	4,4,4	0.42	0	6,6,6	0.18	0
2	SO4	B	601	-	4,4,4	0.28	0	6,6,6	0.07	0
2	SO4	A	602	-	4,4,4	0.33	0	6,6,6	0.15	0
2	SO4	A	607	-	4,4,4	0.31	0	6,6,6	0.07	0
2	SO4	A	609	-	4,4,4	0.34	0	6,6,6	0.12	0
2	SO4	A	601	-	4,4,4	0.31	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	SO4	1	0
2	B	602	SO4	1	0
2	A	602	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	450/492 (91%)	0.79	80 (17%) 4 3	20, 65, 134, 160	6 (1%)
1	B	464/492 (94%)	0.88	77 (16%) 4 3	30, 71, 141, 190	4 (0%)
All	All	914/984 (92%)	0.84	157 (17%) 4 3	20, 69, 138, 190	10 (1%)

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	ILE	6.5
1	B	45[A]	LEU	5.9
1	B	33	VAL	5.9
1	B	34	ALA	5.7
1	A	44	ALA	5.6
1	B	305	ILE	5.0
1	A	76[A]	LYS	5.0
1	A	319	ILE	4.9
1	A	33	VAL	4.6
1	B	44	ALA	4.6
1	B	316	PHE	4.6
1	A	82	VAL	4.5
1	B	66	PHE	4.3
1	A	347	GLU	4.2
1	B	46	ALA	4.2
1	B	362[A]	LYS	4.2
1	A	288	VAL	4.2
1	B	57[A]	ARG	4.2
1	A	382	HIS	4.1
1	B	285[A]	LYS	4.1
1	A	308	VAL	4.1
1	B	372	LEU	4.1
1	B	288	VAL	4.0
1	B	248	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	345	GLU	3.9
1	B	88	ASN	3.7
1	A	205	SER	3.6
1	B	102	GLY	3.6
1	A	322	PHE	3.6
1	B	485	GLU	3.5
1	A	289	LYS	3.4
1	B	358	PRO	3.4
1	A	38	MET	3.3
1	A	65	PHE	3.3
1	A	56	LYS	3.3
1	B	199	PRO	3.3
1	B	284	THR	3.3
1	B	304	GLU	3.3
1	B	307	GLN	3.3
1	B	84	TRP	3.2
1	B	308	VAL	3.1
1	A	270	ALA	3.1
1	A	358	PRO	3.1
1	A	206	LEU	3.1
1	A	217	LEU	3.1
1	B	93	ASN	3.1
1	B	377	GLY	3.1
1	B	365	ALA	3.1
1	B	312	HIS	3.1
1	A	87	ILE	3.1
1	A	72	PHE	3.1
1	A	75	ASP	3.1
1	A	83	ASN	3.1
1	B	314	ASN	3.1
1	A	300	ALA	3.0
1	B	321	LYS	3.0
1	B	302	LEU	3.0
1	A	349	GLU	3.0
1	A	42	LEU	3.0
1	A	57	ARG	3.0
1	B	301	ARG	2.9
1	A	41	ALA	2.9
1	B	207	LEU	2.9
1	A	58	PHE	2.9
1	A	357	ILE	2.9
1	B	265	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	58	PHE	2.9
1	B	309	PRO	2.9
1	B	210	PRO	2.8
1	A	35	ALA	2.8
1	A	352	ALA	2.8
1	B	35	ALA	2.8
1	B	299	LYS	2.8
1	B	370	TYR	2.8
1	B	322	PHE	2.8
1	A	273	GLY	2.8
1	A	95	VAL	2.7
1	B	103	ALA	2.7
1	B	306	ALA	2.6
1	A	69	PHE	2.6
1	B	109	PHE	2.6
1	A	88	ASN	2.6
1	A	303	LEU	2.6
1	B	319	ILE	2.6
1	B	208	PRO	2.6
1	B	201	ILE	2.6
1	A	316	PHE	2.5
1	B	91	ALA	2.5
1	A	204	ASP	2.5
1	A	304	GLU	2.5
1	A	43	ASN	2.5
1	A	471[A]	ARG	2.5
1	B	298	GLY	2.5
1	B	349	GLU	2.5
1	A	34	ALA	2.5
1	B	270	ALA	2.5
1	A	370	TYR	2.4
1	A	307	GLN	2.4
1	A	66	PHE	2.4
1	A	368	ALA	2.4
1	B	36	SER	2.4
1	A	285	LYS	2.4
1	B	37	GLN	2.4
1	B	286	ALA	2.4
1	B	293	ILE	2.4
1	A	296	TYR	2.4
1	A	383	PHE	2.4
1	B	198	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	299	LYS	2.4
1	B	67	ALA	2.4
1	A	187	ASN	2.3
1	A	297	GLU	2.3
1	B	303	LEU	2.3
1	B	296	TYR	2.3
1	A	381	ARG	2.3
1	A	84	TRP	2.3
1	A	207	LEU	2.3
1	B	315	GLU	2.3
1	A	92	PRO	2.3
1	A	379	ALA	2.3
1	A	186[A]	HIS	2.3
1	A	248	TYR	2.3
1	A	314	ASN	2.2
1	B	273	GLY	2.2
1	B	76	LYS	2.2
1	B	234	ASN	2.2
1	A	198	TYR	2.2
1	A	37	GLN	2.2
1	A	68	LEU	2.2
1	A	372	LEU	2.2
1	B	294	ILE	2.2
1	A	272	THR	2.2
1	A	302	LEU	2.2
1	A	39	ARG	2.2
1	B	300	ALA	2.2
1	B	292	THR	2.2
1	B	290	GLY	2.2
1	A	63	ASP	2.2
1	A	85	ASP	2.2
1	B	317	LYS	2.2
1	A	62	MET	2.1
1	B	346	LEU	2.1
1	B	350	ILE	2.1
1	A	346	LEU	2.1
1	B	374	THR	2.1
1	B	55	LYS	2.1
1	B	368	ALA	2.1
1	B	326	ASN	2.1
1	A	40	ASN	2.1
1	A	59	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	201	ILE	2.1
1	B	283	LYS	2.1
1	A	89	PRO	2.1
1	B	427	PHE	2.0
1	B	90	PRO	2.0
1	A	102	GLY	2.0
1	A	377	GLY	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	SO4	A	607	5/5	0.40	0.13	168,169,185,186	0
2	SO4	A	601	5/5	0.51	0.18	118,127,141,145	0
2	SO4	A	609	5/5	0.65	0.14	130,130,150,155	0
2	SO4	B	606	5/5	0.66	0.10	112,133,146,147	0
2	SO4	B	601	5/5	0.68	0.13	112,114,119,125	0
2	SO4	A	603	5/5	0.68	0.11	110,134,142,144	0
2	SO4	A	608	5/5	0.71	0.12	133,135,143,145	0
2	SO4	A	605	5/5	0.80	0.10	94,95,110,116	0
2	SO4	B	604	5/5	0.81	0.12	120,127,139,141	0
2	SO4	A	604	5/5	0.83	0.10	69,84,104,107	0
2	SO4	A	602	5/5	0.83	0.09	109,111,125,129	0
3	CL	B	608	1/1	0.84	0.20	100,100,100,100	0
2	SO4	A	606	5/5	0.89	0.09	90,97,105,108	0
2	SO4	B	602	5/5	0.91	0.15	60,74,90,97	0
3	CL	B	607	1/1	0.92	0.09	72,72,72,72	0
2	SO4	B	605	5/5	0.94	0.14	70,75,85,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	603	5/5	0.97	0.08	60,61,71,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.