



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:39 AM UTC

PDB ID : 6XEQ / pdb_00006xeq
Title : Crystal structure of the tetrameric 6-phosphogluconate dehydrogenase from *Gluconobacter oxidans*
Authors : Maturana, P.; Roversi, P.; Castro-Fernandez, V.; Herrera-Morande, A.; Garratt, R.C.; Cabrera, R.
Deposited on : 2020-06-13
Resolution : 3.20 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

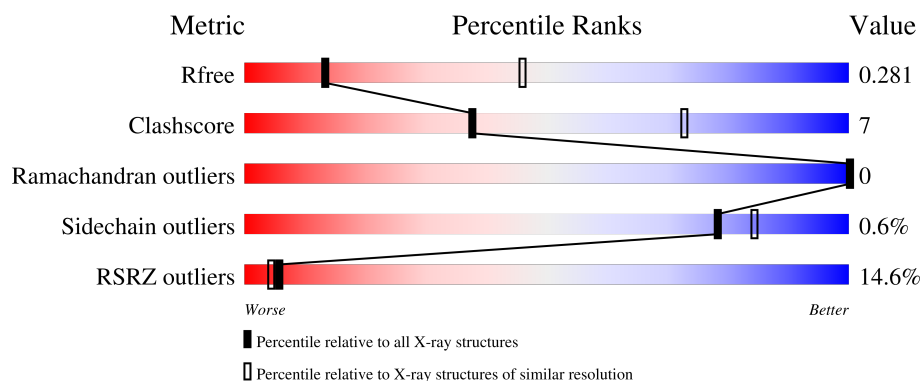
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	353	13% 76% 15% 9%
1	B	353	11% 71% 19% 10%
1	C	353	15% 74% 16% 10%
1	D	353	14% 74% 16% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9723 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 6-phosphogluconate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2424	1509	437	462	16			
1	B	318	Total	C	N	O	S	0	0	0
			2408	1497	435	460	16			
1	C	318	Total	C	N	O	S	0	0	0
			2417	1508	435	458	16			
1	D	315	Total	C	N	O	S	0	0	0
			2385	1482	432	455	16			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP G5EBD7
A	-19	GLY	-	expression tag	UNP G5EBD7
A	-18	SER	-	expression tag	UNP G5EBD7
A	-17	SER	-	expression tag	UNP G5EBD7
A	-16	HIS	-	expression tag	UNP G5EBD7
A	-15	HIS	-	expression tag	UNP G5EBD7
A	-14	HIS	-	expression tag	UNP G5EBD7
A	-13	HIS	-	expression tag	UNP G5EBD7
A	-12	HIS	-	expression tag	UNP G5EBD7
A	-11	HIS	-	expression tag	UNP G5EBD7
A	-10	SER	-	expression tag	UNP G5EBD7
A	-9	SER	-	expression tag	UNP G5EBD7
A	-8	GLY	-	expression tag	UNP G5EBD7
A	-7	GLU	-	expression tag	UNP G5EBD7
A	-6	ASN	-	expression tag	UNP G5EBD7
A	-5	LEU	-	expression tag	UNP G5EBD7
A	-4	TYR	-	expression tag	UNP G5EBD7
A	-3	PHE	-	expression tag	UNP G5EBD7
A	-2	GLN	-	expression tag	UNP G5EBD7
A	-1	GLY	-	expression tag	UNP G5EBD7
A	0	HIS	-	expression tag	UNP G5EBD7

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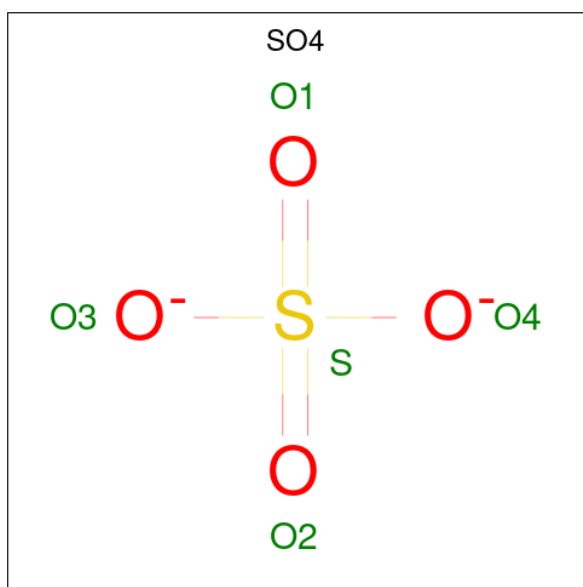
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP G5EBD7
B	-19	GLY	-	expression tag	UNP G5EBD7
B	-18	SER	-	expression tag	UNP G5EBD7
B	-17	SER	-	expression tag	UNP G5EBD7
B	-16	HIS	-	expression tag	UNP G5EBD7
B	-15	HIS	-	expression tag	UNP G5EBD7
B	-14	HIS	-	expression tag	UNP G5EBD7
B	-13	HIS	-	expression tag	UNP G5EBD7
B	-12	HIS	-	expression tag	UNP G5EBD7
B	-11	HIS	-	expression tag	UNP G5EBD7
B	-10	SER	-	expression tag	UNP G5EBD7
B	-9	SER	-	expression tag	UNP G5EBD7
B	-8	GLY	-	expression tag	UNP G5EBD7
B	-7	GLU	-	expression tag	UNP G5EBD7
B	-6	ASN	-	expression tag	UNP G5EBD7
B	-5	LEU	-	expression tag	UNP G5EBD7
B	-4	TYR	-	expression tag	UNP G5EBD7
B	-3	PHE	-	expression tag	UNP G5EBD7
B	-2	GLN	-	expression tag	UNP G5EBD7
B	-1	GLY	-	expression tag	UNP G5EBD7
B	0	HIS	-	expression tag	UNP G5EBD7
C	-20	MET	-	initiating methionine	UNP G5EBD7
C	-19	GLY	-	expression tag	UNP G5EBD7
C	-18	SER	-	expression tag	UNP G5EBD7
C	-17	SER	-	expression tag	UNP G5EBD7
C	-16	HIS	-	expression tag	UNP G5EBD7
C	-15	HIS	-	expression tag	UNP G5EBD7
C	-14	HIS	-	expression tag	UNP G5EBD7
C	-13	HIS	-	expression tag	UNP G5EBD7
C	-12	HIS	-	expression tag	UNP G5EBD7
C	-11	HIS	-	expression tag	UNP G5EBD7
C	-10	SER	-	expression tag	UNP G5EBD7
C	-9	SER	-	expression tag	UNP G5EBD7
C	-8	GLY	-	expression tag	UNP G5EBD7
C	-7	GLU	-	expression tag	UNP G5EBD7
C	-6	ASN	-	expression tag	UNP G5EBD7
C	-5	LEU	-	expression tag	UNP G5EBD7
C	-4	TYR	-	expression tag	UNP G5EBD7
C	-3	PHE	-	expression tag	UNP G5EBD7
C	-2	GLN	-	expression tag	UNP G5EBD7
C	-1	GLY	-	expression tag	UNP G5EBD7
C	0	HIS	-	expression tag	UNP G5EBD7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	initiating methionine	UNP G5EBD7
D	-19	GLY	-	expression tag	UNP G5EBD7
D	-18	SER	-	expression tag	UNP G5EBD7
D	-17	SER	-	expression tag	UNP G5EBD7
D	-16	HIS	-	expression tag	UNP G5EBD7
D	-15	HIS	-	expression tag	UNP G5EBD7
D	-14	HIS	-	expression tag	UNP G5EBD7
D	-13	HIS	-	expression tag	UNP G5EBD7
D	-12	HIS	-	expression tag	UNP G5EBD7
D	-11	HIS	-	expression tag	UNP G5EBD7
D	-10	SER	-	expression tag	UNP G5EBD7
D	-9	SER	-	expression tag	UNP G5EBD7
D	-8	GLY	-	expression tag	UNP G5EBD7
D	-7	GLU	-	expression tag	UNP G5EBD7
D	-6	ASN	-	expression tag	UNP G5EBD7
D	-5	LEU	-	expression tag	UNP G5EBD7
D	-4	TYR	-	expression tag	UNP G5EBD7
D	-3	PHE	-	expression tag	UNP G5EBD7
D	-2	GLN	-	expression tag	UNP G5EBD7
D	-1	GLY	-	expression tag	UNP G5EBD7
D	0	HIS	-	expression tag	UNP G5EBD7

- 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		

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

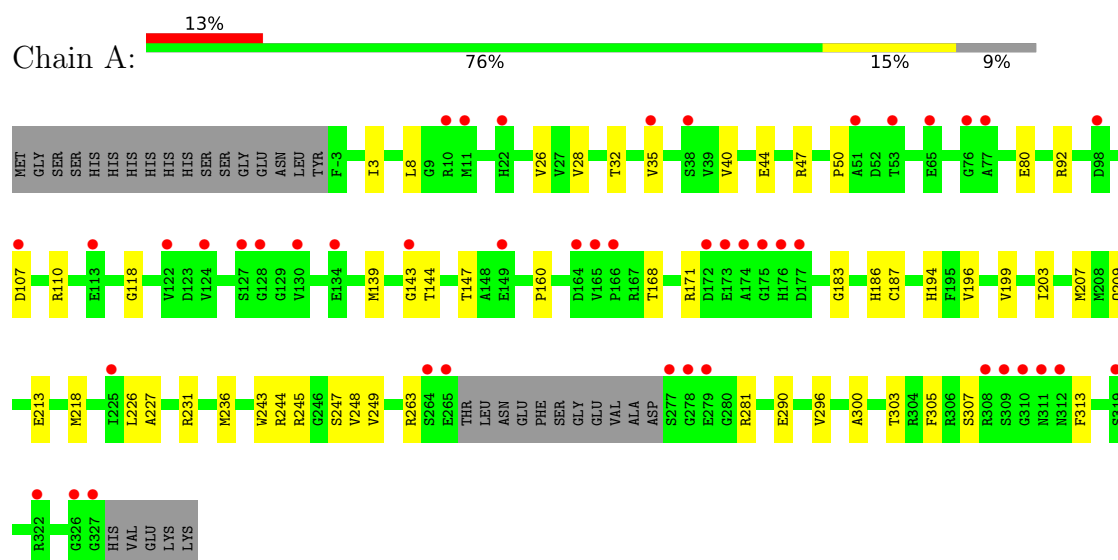
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		
3	B	19	Total	O	0	0
			19	19		
3	C	20	Total	O	0	0
			20	20		
3	D	18	Total	O	0	0
			18	18		

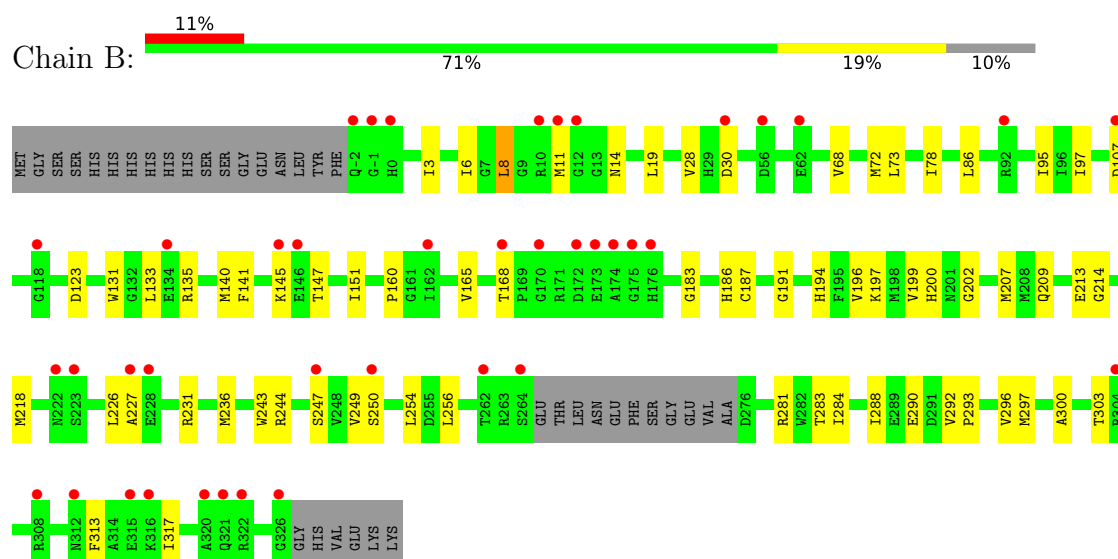
3 Residue-property plots [i](#)

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.

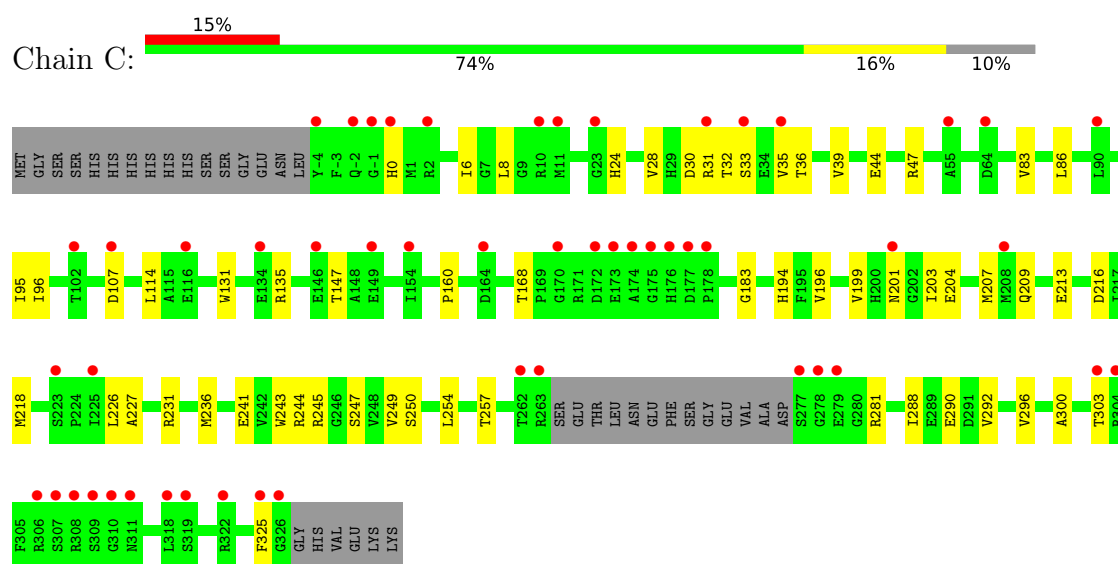
• Molecule 1: 6-phosphogluconate dehydrogenase



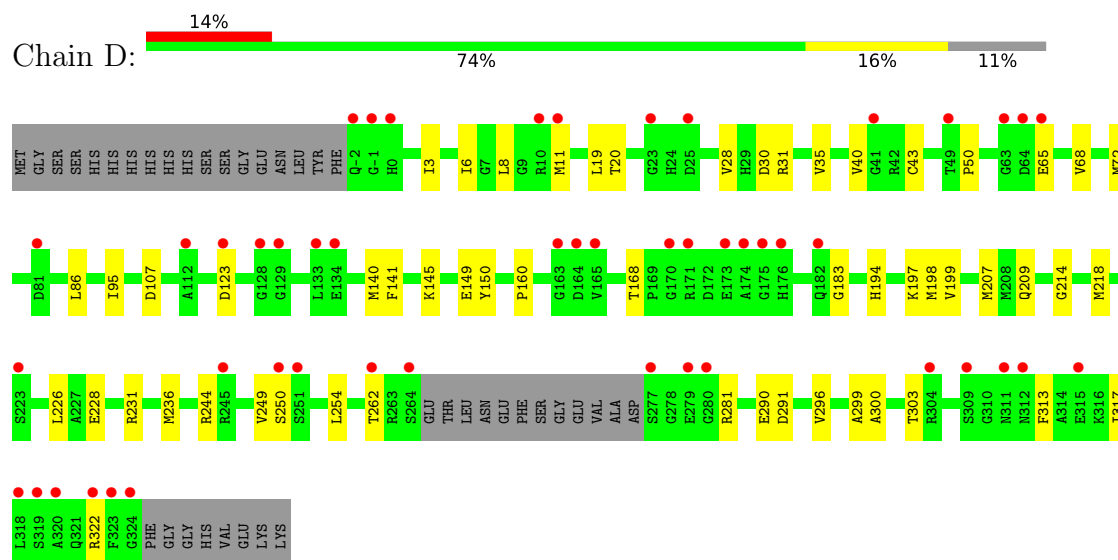
• Molecule 1: 6-phosphogluconate dehydrogenase



• Molecule 1: 6-phosphogluconate dehydrogenase



• Molecule 1: 6-phosphogluconate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.06Å 125.67Å 166.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.26 – 3.20 100.26 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.7 (100.26-3.20) 86.7 (100.26-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.246 , 0.286 0.243 , 0.281	Depositor DCC
R_{free} test set	1494 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.9	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	0.87	EDS
Total number of atoms	9723	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3044e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.11	0/2470	0.29	0/3332
1	B	0.11	0/2453	0.31	0/3310
1	C	0.11	0/2464	0.30	0/3325
1	D	0.12	0/2429	0.31	0/3278
All	All	0.11	0/9816	0.30	0/13245

There are no bond length outliers.

There are no bond angle outliers.

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	2424	0	2363	38	0
1	B	2408	0	2349	48	0
1	C	2417	0	2358	45	0
1	D	2385	0	2333	37	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	19	0	0	0	0
3	C	20	0	0	0	0
3	D	18	0	0	0	0
All	All	9723	0	9403	133	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 7.

All (133) 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:296:VAL:HG13	1:D:296:VAL:HG13	1.74	0.70
1:B:160:PRO:HD2	1:B:183:GLY:HA3	1.73	0.69
1:B:207:MET:HE1	1:C:249:VAL:HA	1.76	0.68
1:A:249:VAL:HA	1:D:207:MET:HE1	1.77	0.67
1:A:307:SER:HB2	1:B:293:PRO:HD2	1.77	0.67
1:B:296:VAL:HG13	1:C:296:VAL:HG13	1.77	0.66
1:B:68:VAL:HG12	1:B:95:ILE:HB	1.78	0.66
1:A:290:GLU:HG2	1:D:226:LEU:HD11	1.77	0.66
1:A:160:PRO:HD2	1:A:183:GLY:HA3	1.78	0.65
1:D:68:VAL:HG12	1:D:95:ILE:HB	1.78	0.65
1:B:226:LEU:HD11	1:C:290:GLU:HG2	1.79	0.65
1:B:249:VAL:HA	1:C:207:MET:HE1	1.80	0.62
1:C:95:ILE:HD13	1:C:147:THR:HG23	1.81	0.62
1:C:244:ARG:HB2	1:C:245:ARG:HH11	1.66	0.60
1:B:107:ASP:OD2	1:B:194:HIS:ND1	2.28	0.60
1:C:131:TRP:HB3	1:C:135:ARG:HD3	1.83	0.60
1:D:3:ILE:HD13	1:D:19:LEU:HD13	1.84	0.60
1:A:203:ILE:HD11	1:D:214:GLY:HA3	1.83	0.59
1:D:228:GLU:HA	1:D:231:ARG:HD3	1.85	0.59
1:D:160:PRO:HD2	1:D:183:GLY:HA3	1.85	0.59
1:B:300:ALA:O	1:B:303:THR:OG1	2.21	0.59
1:C:288:ILE:O	1:D:281:ARG:NH2	2.36	0.59
1:D:107:ASP:OD2	1:D:194:HIS:ND1	2.30	0.59
1:D:145:LYS:NZ	1:D:149:GLU:OE2	2.37	0.58
1:B:140:MET:HE1	1:B:197:LYS:HD3	1.84	0.58
1:B:168:THR:OG1	1:C:241:GLU:OE2	2.19	0.58
1:A:8:LEU:HD21	1:A:28:VAL:HB	1.85	0.58
1:C:8:LEU:HD12	1:C:30:ASP:HB2	1.87	0.57
1:A:107:ASP:OD2	1:A:194:HIS:ND1	2.32	0.56
1:D:300:ALA:O	1:D:303:THR:OG1	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:TRP:O	1:A:247:SER:OG	2.21	0.55
1:B:8:LEU:HD21	1:B:28:VAL:HB	1.86	0.55
1:A:207:MET:HE1	1:D:249:VAL:HA	1.89	0.55
1:C:107:ASP:OD2	1:C:194:HIS:ND1	2.34	0.55
1:C:201:ASN:ND2	1:C:204:GLU:OE1	2.39	0.55
1:B:214:GLY:HA3	1:C:203:ILE:HD11	1.89	0.54
1:B:14:ASN:HB3	1:B:133:LEU:HB2	1.90	0.54
1:B:131:TRP:HB3	1:B:135:ARG:HD2	1.91	0.53
1:B:281:ARG:O	1:B:284:ILE:HG12	2.08	0.53
1:C:300:ALA:O	1:C:303:THR:OG1	2.25	0.52
1:A:313:PHE:HZ	1:C:257:THR:HG23	1.73	0.52
1:C:160:PRO:HD2	1:C:183:GLY:HA3	1.92	0.51
1:B:218:MET:HE3	1:C:199:VAL:HB	1.93	0.51
1:B:290:GLU:HG2	1:C:226:LEU:HD11	1.93	0.51
1:C:281:ARG:NH2	1:D:291:ASP:OD1	2.44	0.51
1:D:140:MET:HE1	1:D:197:LYS:HD3	1.91	0.51
1:D:30:ASP:OD1	1:D:31:ARG:N	2.43	0.51
1:A:199:VAL:HB	1:D:218:MET:HE3	1.93	0.51
1:A:209:GLN:O	1:A:213:GLU:HG2	2.10	0.50
1:B:250:SER:HA	1:B:254:LEU:HD23	1.93	0.50
1:A:300:ALA:O	1:A:303:THR:OG1	2.30	0.50
1:A:281:ARG:NH1	1:B:288:ILE:O	2.44	0.50
1:B:283:THR:HG21	1:B:297:MET:HE1	1.94	0.50
1:A:218:MET:HE3	1:D:199:VAL:HB	1.94	0.49
1:C:243:TRP:O	1:C:247:SER:OG	2.25	0.49
1:B:3:ILE:HD13	1:B:19:LEU:HD13	1.95	0.49
1:B:199:VAL:HB	1:C:218:MET:HE3	1.93	0.49
1:A:244:ARG:HB2	1:A:245:ARG:HH11	1.78	0.48
1:B:209:GLN:O	1:B:213:GLU:HG2	2.13	0.48
1:B:202:GLY:HA3	1:B:297:MET:HE3	1.95	0.48
1:D:65:GLU:HB3	1:D:150:TYR:OH	2.14	0.48
1:B:243:TRP:O	1:B:247:SER:OG	2.28	0.48
1:A:32:THR:HB	1:A:35:VAL:HG22	1.96	0.48
1:C:32:THR:HB	1:C:35:VAL:HG22	1.95	0.48
1:A:307:SER:OG	1:C:216:ASP:OD2	2.31	0.48
1:C:30:ASP:OD1	1:C:31:ARG:N	2.46	0.48
1:C:209:GLN:O	1:C:213:GLU:HG2	2.13	0.48
1:A:226:LEU:HD11	1:D:290:GLU:HG2	1.96	0.47
1:D:8:LEU:HD11	1:D:28:VAL:HB	1.96	0.47
1:B:244:ARG:NH1	1:C:168:THR:HG23	2.30	0.47
1:D:218:MET:HB3	1:D:236:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:HG3	1:A:118:GLY:HA3	1.97	0.47
1:C:8:LEU:HD13	1:C:39:VAL:HG21	1.97	0.47
1:C:83:VAL:HG22	1:C:96:ILE:HD11	1.96	0.46
1:B:183:GLY:HA2	1:C:245:ARG:HB2	1.96	0.46
1:A:40:VAL:HG21	1:A:50:PRO:HB3	1.97	0.46
1:A:218:MET:HB3	1:A:236:MET:HE1	1.98	0.46
1:A:263:ARG:HH11	1:C:325:PHE:HD1	1.64	0.46
1:B:145:LYS:HD2	1:B:186:HIS:CE1	2.51	0.46
1:D:123:ASP:O	1:D:141:PHE:HA	2.16	0.46
1:D:40:VAL:HG21	1:D:50:PRO:HB3	1.98	0.45
1:A:244:ARG:NH1	1:D:168:THR:HG23	2.31	0.45
1:A:80:GLU:OE1	1:A:110:ARG:NE	2.45	0.45
1:A:139:MET:HE3	1:A:139:MET:HB2	1.88	0.45
1:A:168:THR:OG1	1:D:244:ARG:NH1	2.50	0.45
1:B:296:VAL:HG21	1:C:209:GLN:HB3	1.99	0.45
1:D:6:ILE:HD12	1:D:86:LEU:HD11	1.99	0.45
1:D:20:THR:HG21	1:D:43:CYS:HB3	1.99	0.45
1:D:299:ALA:O	1:D:303:THR:HG23	2.17	0.44
1:C:96:ILE:HG21	1:C:114:LEU:HD13	1.99	0.44
1:C:218:MET:HE1	1:C:243:TRP:CZ2	2.53	0.43
1:D:250:SER:HA	1:D:254:LEU:HD23	1.99	0.43
1:A:143:GLY:O	1:A:186:HIS:NE2	2.44	0.43
1:A:144:THR:OG1	1:A:147:THR:HG22	2.18	0.43
1:A:44:GLU:HB2	1:A:47:ARG:HD2	2.01	0.43
1:C:6:ILE:HD12	1:C:86:LEU:HD11	2.00	0.43
1:B:218:MET:HE1	1:C:196:VAL:HG13	2.01	0.43
1:A:218:MET:HE1	1:A:243:TRP:CZ2	2.54	0.43
1:A:305:PHE:HB2	1:B:293:PRO:HG3	2.01	0.43
1:B:165:VAL:HG11	1:C:245:ARG:CD	2.49	0.43
1:C:204:GLU:HA	1:C:207:MET:HE2	2.01	0.43
1:C:218:MET:HB3	1:C:236:MET:HE1	2.01	0.43
1:B:313:PHE:O	1:B:317:ILE:HG12	2.19	0.42
1:B:6:ILE:HD12	1:B:86:LEU:HD11	2.01	0.42
1:C:250:SER:HA	1:C:254:LEU:HD23	2.01	0.42
1:D:322:ARG:HD3	1:D:322:ARG:HA	1.89	0.42
1:A:187:CYS:SG	1:A:196:VAL:HG21	2.58	0.42
1:B:131:TRP:CH2	1:B:256:LEU:HD21	2.54	0.42
1:B:95:ILE:HD13	1:B:147:THR:HG23	2.02	0.42
1:B:73:LEU:HD13	1:B:78:ILE:HG22	2.02	0.42
1:C:33:SER:HA	1:C:36:THR:HG22	2.02	0.42
1:B:187:CYS:SG	1:B:196:VAL:HG21	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:LEU:HD11	1:C:28:VAL:HB	2.01	0.42
1:A:196:VAL:HG12	1:D:218:MET:HE2	2.01	0.42
1:B:123:ASP:CG	1:B:191:GLY:H	2.28	0.42
1:D:11:MET:HG2	1:D:72:MET:HE1	2.01	0.42
1:C:44:GLU:HB2	1:C:47:ARG:HD2	2.02	0.41
1:C:0:HIS:HB2	1:C:24:HIS:HA	2.02	0.41
1:A:227:ALA:O	1:A:231:ARG:HG3	2.19	0.41
1:B:200:HIS:HB2	1:C:243:TRP:CZ2	2.56	0.41
1:B:123:ASP:O	1:B:141:PHE:HA	2.21	0.41
1:B:218:MET:HB3	1:B:236:MET:HE1	2.01	0.41
1:B:145:LYS:HD2	1:B:186:HIS:HE1	1.85	0.41
1:A:171:ARG:HD3	1:D:262:THR:HG21	2.02	0.41
1:B:11:MET:HE3	1:B:72:MET:HE1	2.02	0.41
1:B:97:ILE:HD11	1:B:151:ILE:HG12	2.03	0.41
1:D:72:MET:HE2	1:D:72:MET:HB3	1.94	0.41
1:B:8:LEU:HB2	1:B:30:ASP:HB2	2.03	0.40
1:D:198:MET:HE2	1:D:198:MET:HB3	1.97	0.40
1:C:227:ALA:O	1:C:231:ARG:HG3	2.22	0.40
1:A:3:ILE:O	1:A:26:VAL:HA	2.22	0.40
1:D:313:PHE:O	1:D:317:ILE:HG12	2.21	0.40
1:B:227:ALA:O	1:B:231:ARG:HG3	2.21	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	316/353 (90%)	311 (98%)	5 (2%)	0	100	100
1	B	314/353 (89%)	307 (98%)	7 (2%)	0	100	100
1	C	314/353 (89%)	305 (97%)	9 (3%)	0	100	100
1	D	311/353 (88%)	303 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1255/1412 (89%)	1226 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	247/276 (90%)	246 (100%)	1 (0%)	84	86
1	B	246/276 (89%)	244 (99%)	2 (1%)	73	82
1	C	246/276 (89%)	245 (100%)	1 (0%)	84	86
1	D	244/276 (88%)	242 (99%)	2 (1%)	73	82
All	All	983/1104 (89%)	977 (99%)	6 (1%)	78	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	VAL
1	B	8	LEU
1	B	292	VAL
1	C	292	VAL
1	D	35	VAL
1	D	209	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	C	101	ASN
1	C	182	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](#)

4 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	C	401	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	401	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	D	401	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	B	401	-	4,4,4	0.23	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 [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	320/353 (90%)	1.01	45 (14%) 6 5	19, 41, 87, 116	0
1	B	318/353 (90%)	0.90	40 (12%) 8 6	21, 38, 73, 115	0
1	C	318/353 (90%)	1.11	52 (16%) 4 3	20, 44, 86, 117	0
1	D	315/353 (89%)	0.98	49 (15%) 5 4	19, 42, 81, 116	0
All	All	1271/1412 (90%)	1.00	186 (14%) 6 4	19, 42, 82, 117	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-1	GLY	7.2
1	A	277	SER	5.9
1	D	-2	GLN	5.7
1	D	319	SER	5.2
1	A	278	GLY	4.8
1	D	174	ALA	4.6
1	A	175	GLY	4.6
1	C	277	SER	4.5
1	C	175	GLY	4.4
1	C	310	GLY	4.4
1	A	310	GLY	4.2
1	C	-2	GLN	4.2
1	B	134	GLU	4.2
1	C	262	THR	4.1
1	C	319	SER	4.1
1	D	264	SER	4.1
1	B	176	HIS	4.1
1	D	64	ASP	4.1
1	B	264	SER	4.0
1	A	322	ARG	4.0
1	C	279	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	265	GLU	4.0
1	B	-2	GLN	3.9
1	B	174	ALA	3.9
1	C	-4	TYR	3.9
1	D	11	MET	3.9
1	C	23	GLY	3.7
1	C	326	GLY	3.7
1	D	10	ARG	3.6
1	B	326	GLY	3.6
1	C	116	GLU	3.6
1	A	98	ASP	3.6
1	A	308	ARG	3.6
1	D	170	GLY	3.6
1	D	324	GLY	3.5
1	A	149	GLU	3.5
1	C	149	GLU	3.5
1	A	327	GLY	3.5
1	C	278	GLY	3.5
1	D	250	SER	3.5
1	B	173	GLU	3.4
1	C	174	ALA	3.4
1	D	318	LEU	3.4
1	C	10	ARG	3.4
1	A	134	GLU	3.4
1	B	247	SER	3.3
1	D	128	GLY	3.3
1	A	176	HIS	3.3
1	D	173	GLU	3.3
1	A	264	SER	3.3
1	D	322	ARG	3.2
1	B	56	ASP	3.2
1	D	251	SER	3.2
1	A	174	ALA	3.2
1	A	53	THR	3.1
1	A	177	ASP	3.1
1	D	-1	GLY	3.1
1	C	31	ARG	3.1
1	C	307	SER	3.1
1	D	315	GLU	3.1
1	C	172	ASP	3.0
1	D	164	ASP	3.0
1	C	170	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	262	THR	3.0
1	A	10	ARG	2.9
1	B	304	ARG	2.9
1	C	173	GLU	2.9
1	B	170	GLY	2.9
1	B	322	ARG	2.9
1	C	0	HIS	2.9
1	B	312	ASN	2.9
1	D	134	GLU	2.9
1	A	172	ASP	2.8
1	D	133	LEU	2.8
1	C	33	SER	2.8
1	D	223	SER	2.8
1	B	262	THR	2.8
1	A	164	ASP	2.8
1	A	122	VAL	2.8
1	C	2	ARG	2.7
1	A	77	ALA	2.7
1	C	154	ILE	2.7
1	D	309	SER	2.7
1	B	118	GLY	2.6
1	D	280	GLY	2.6
1	A	38	SER	2.6
1	C	311	ASN	2.6
1	D	129	GLY	2.6
1	B	223	SER	2.6
1	C	134	GLU	2.6
1	B	162	ILE	2.6
1	C	303	THR	2.6
1	D	23	GLY	2.5
1	B	107	ASP	2.5
1	C	107	ASP	2.5
1	B	168	THR	2.5
1	B	250	SER	2.5
1	D	41	GLY	2.5
1	C	263	ARG	2.5
1	C	304	ARG	2.5
1	D	304	ARG	2.5
1	B	145	LYS	2.5
1	B	315	GLU	2.5
1	A	165	VAL	2.5
1	C	309	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	279	GLU	2.5
1	A	143	GLY	2.5
1	A	279	GLU	2.4
1	C	11	MET	2.4
1	D	63	GLY	2.4
1	D	65	GLU	2.4
1	A	76	GLY	2.4
1	A	113	GLU	2.4
1	C	223	SER	2.4
1	B	228	GLU	2.4
1	D	175	GLY	2.4
1	D	311	ASN	2.4
1	A	107	ASP	2.3
1	D	25	ASP	2.3
1	B	146	GLU	2.3
1	A	127	SER	2.3
1	D	277	SER	2.3
1	C	176	HIS	2.3
1	D	176	HIS	2.3
1	B	11	MET	2.3
1	C	318	LEU	2.3
1	A	65	GLU	2.3
1	C	308	ARG	2.3
1	C	322	ARG	2.3
1	B	175	GLY	2.3
1	D	312	ASN	2.3
1	D	182	GLN	2.3
1	A	130	VAL	2.3
1	B	92	ARG	2.3
1	C	-1	GLY	2.3
1	D	323	PHE	2.3
1	C	64	ASP	2.3
1	B	316	LYS	2.2
1	C	35	VAL	2.2
1	B	30	ASP	2.2
1	C	177	ASP	2.2
1	D	123	ASP	2.2
1	D	112	ALA	2.2
1	D	163	GLY	2.2
1	B	172	ASP	2.2
1	D	171	ARG	2.2
1	D	49	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	51	ALA	2.2
1	B	0	HIS	2.2
1	C	225	ILE	2.1
1	C	146	GLU	2.1
1	A	312	ASN	2.1
1	B	222	ASN	2.1
1	C	201	ASN	2.1
1	D	0	HIS	2.1
1	B	10	ARG	2.1
1	B	227	ALA	2.1
1	A	22	HIS	2.1
1	C	208	MET	2.1
1	A	128	GLY	2.1
1	A	326	GLY	2.1
1	D	165	VAL	2.1
1	A	225	ILE	2.1
1	C	102	THR	2.1
1	B	320	ALA	2.1
1	C	55	ALA	2.1
1	C	325	PHE	2.1
1	C	90	LEU	2.1
1	D	245	ARG	2.1
1	C	164	ASP	2.1
1	D	320	ALA	2.1
1	A	173	GLU	2.1
1	A	319	SER	2.0
1	A	11	MET	2.0
1	D	81	ASP	2.0
1	A	166	PRO	2.0
1	A	35	VAL	2.0
1	A	124	VAL	2.0
1	A	309	SER	2.0
1	A	311	ASN	2.0
1	B	12	GLY	2.0
1	B	321	GLN	2.0
1	C	178	PRO	2.0
1	B	62	GLU	2.0
1	B	308	ARG	2.0
1	C	306	ARG	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	401	5/5	0.72	0.20	101,102,103,107	0
2	SO4	C	401	5/5	0.76	0.20	85,85,91,92	0
2	SO4	B	401	5/5	0.88	0.10	94,96,98,101	0
2	SO4	D	401	5/5	0.89	0.14	78,84,84,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.