



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:28 AM UTC

PDB ID : 3ZGB / pdb_00003zgb
Title : Greater efficiency of photosynthetic carbon fixation due to single amino acid substitution
Authors : Paulus, J.K.; Schlieper, D.; Groth, G.
Deposited on : 2012-12-17
Resolution : 2.71 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

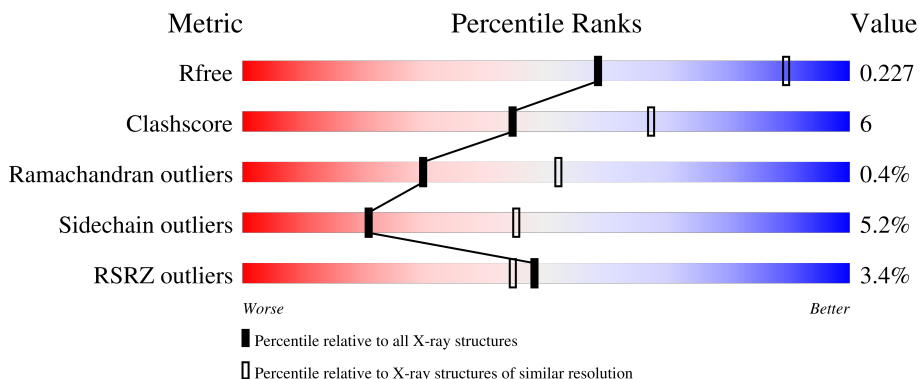
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	972	2% 78% 15% • 5%
1	B	972	4% 78% 14% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14852 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 PHOSPHOENOLPYRUVATE CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	920	Total	C	N	O	S	0	0	0
			7396	4691	1289	1382	34			
1	B	915	Total	C	N	O	S	0	0	0
			7354	4663	1282	1375	34			

There are 26 discrepancies between the modelled and reference sequences:

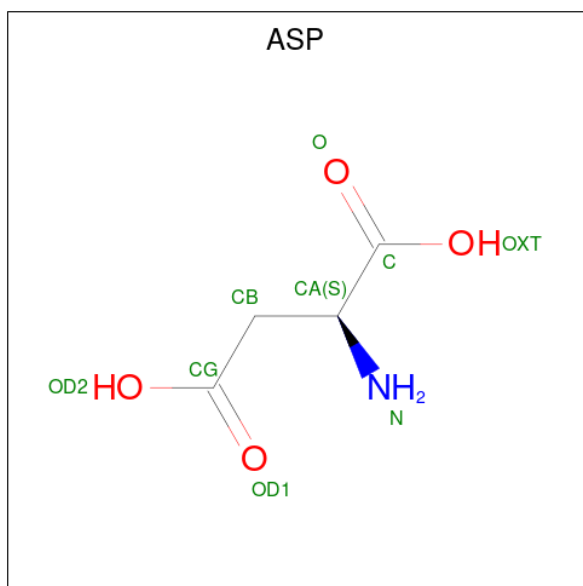
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP Q01647
A	-4	GLY	-	expression tag	UNP Q01647
A	-3	HIS	-	expression tag	UNP Q01647
A	-2	HIS	-	expression tag	UNP Q01647
A	-1	HIS	-	expression tag	UNP Q01647
A	0	HIS	-	expression tag	UNP Q01647
A	1	HIS	-	expression tag	UNP Q01647
A	2	HIS	-	expression tag	UNP Q01647
A	3	HIS	-	expression tag	UNP Q01647
A	4	HIS	-	expression tag	UNP Q01647
A	5	HIS	-	expression tag	UNP Q01647
A	?	-	LYS	SEE REMARK 999	UNP Q01647
A	291	ASN	HIS	SEE REMARK 999	UNP Q01647
B	-5	MET	-	expression tag	UNP Q01647
B	-4	GLY	-	expression tag	UNP Q01647
B	-3	HIS	-	expression tag	UNP Q01647
B	-2	HIS	-	expression tag	UNP Q01647
B	-1	HIS	-	expression tag	UNP Q01647
B	0	HIS	-	expression tag	UNP Q01647
B	1	HIS	-	expression tag	UNP Q01647
B	2	HIS	-	expression tag	UNP Q01647
B	3	HIS	-	expression tag	UNP Q01647
B	4	HIS	-	expression tag	UNP Q01647
B	5	HIS	-	expression tag	UNP Q01647
B	?	-	LYS	SEE REMARK 999	UNP Q01647

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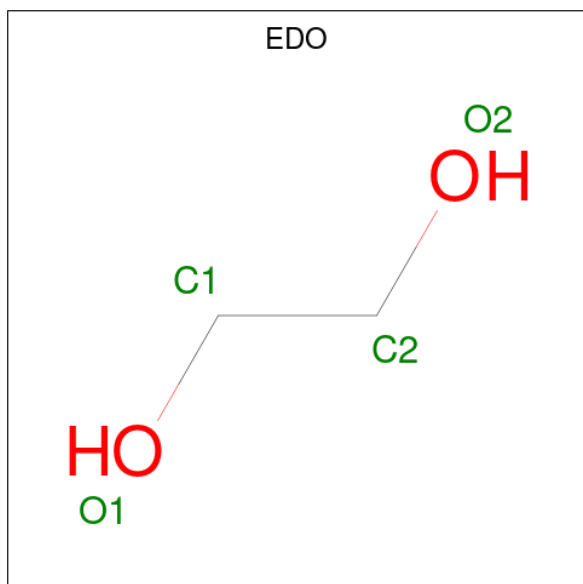
Chain	Residue	Modelled	Actual	Comment	Reference
B	291	ASN	HIS	SEE REMARK 999	UNP Q01647

- Molecule 2 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



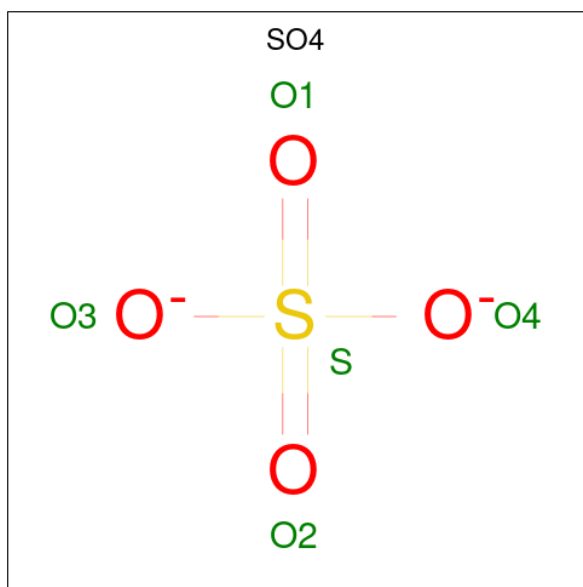
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	1	4		
2	B	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

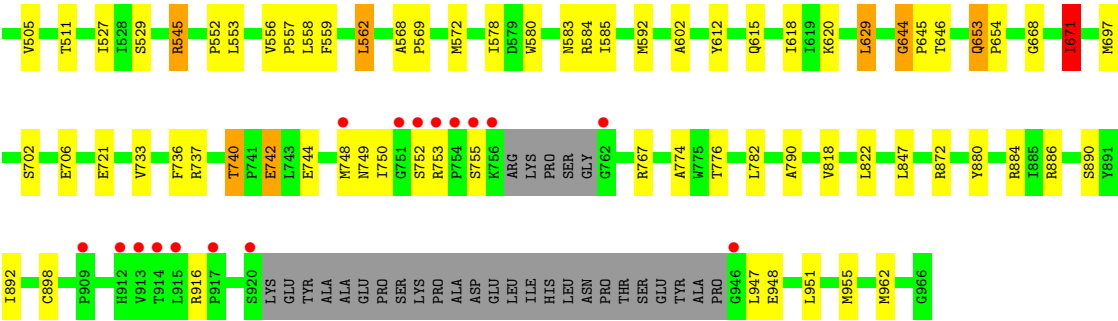
- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	35	Total O 35 35	0	0
5	B	21	Total O 21 21	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	165.55Å 121.70Å 132.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.72 – 2.71 78.72 – 2.71	Depositor EDS
% Data completeness (in resolution range)	100.0 (78.72-2.71) 100.0 (78.72-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.98 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.188 , 0.230 0.188 , 0.227	Depositor DCC
R_{free} test set	1486 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.657	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14852	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: EDO, 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	1.20	19/7549 (0.3%)	1.11	20/10205 (0.2%)
1	B	1.08	4/7506 (0.1%)	1.07	25/10148 (0.2%)
All	All	1.14	23/15055 (0.2%)	1.09	45/20353 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	659	HIS	CG-CD2	7.57	1.44	1.35
1	A	172	HIS	CG-CD2	7.22	1.43	1.35
1	A	444	LEU	N-CA	7.12	1.55	1.46
1	A	244	HIS	CG-CD2	6.62	1.43	1.35
1	A	475	TRP	NE1-CE2	-6.42	1.30	1.37
1	A	659	HIS	ND1-CE1	6.25	1.38	1.32
1	B	244	HIS	CG-CD2	6.14	1.42	1.35
1	A	659	HIS	CE1-NE2	5.71	1.38	1.32
1	A	548	HIS	CG-CD2	5.53	1.42	1.35
1	A	775	TRP	NE1-CE2	-5.49	1.31	1.37
1	A	716	VAL	CA-CB	5.42	1.60	1.54
1	A	172	HIS	CE1-NE2	5.33	1.37	1.32
1	A	647	HIS	CG-ND1	-5.29	1.32	1.38
1	A	753	ARG	CA-C	5.29	1.57	1.52
1	B	203	ASP	N-CA	5.28	1.52	1.46
1	A	455	ARG	N-CA	-5.24	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	695	HIS	CD2-NE2	-5.19	1.32	1.37
1	A	730	PRO	C-O	-5.10	1.17	1.24
1	A	385	HIS	CG-CD2	5.10	1.41	1.35
1	A	912	HIS	CG-CD2	5.07	1.41	1.35
1	B	671	ILE	CA-CB	5.06	1.60	1.54
1	B	654	PRO	CA-C	5.04	1.54	1.51
1	A	248	TRP	NE1-CE2	-5.02	1.31	1.37

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	443	SER	CA-C-N	-9.60	105.31	121.92
1	A	443	SER	C-N-CA	-9.60	105.31	121.92
1	A	200	ILE	N-CA-C	9.19	122.22	108.80
1	B	443	SER	CA-C-N	-8.54	107.14	121.92
1	B	443	SER	C-N-CA	-8.54	107.14	121.92
1	B	271	VAL	CA-C-N	-7.45	112.30	119.90
1	B	271	VAL	C-N-CA	-7.45	112.30	119.90
1	B	671	ILE	CB-CA-C	-7.26	102.34	112.14
1	A	271	VAL	CA-C-N	-6.93	112.83	119.90
1	A	271	VAL	C-N-CA	-6.93	112.83	119.90
1	A	201	THR	CA-C-N	6.75	128.28	119.84
1	A	201	THR	C-N-CA	6.75	128.28	119.84
1	B	653	GLN	CA-C-N	-6.50	114.91	119.66
1	B	653	GLN	C-N-CA	-6.50	114.91	119.66
1	A	644	GLY	CA-C-N	-6.35	112.30	119.28
1	A	644	GLY	C-N-CA	-6.35	112.30	119.28
1	B	27	ASP	CB-CA-C	-6.11	101.28	110.88
1	A	635	ARG	N-CA-C	6.02	118.54	110.35
1	B	671	ILE	N-CA-CB	5.94	118.62	110.54
1	B	271	VAL	CB-CA-C	-5.74	104.08	110.68
1	B	229	PRO	CA-C-N	5.61	126.09	120.14
1	B	229	PRO	C-N-CA	5.61	126.09	120.14
1	B	644	GLY	CA-C-N	-5.53	113.19	119.28
1	B	644	GLY	C-N-CA	-5.53	113.19	119.28
1	B	201	THR	CA-C-N	5.44	126.64	119.84
1	B	201	THR	C-N-CA	5.44	126.64	119.84
1	B	916	ARG	CA-C-N	-5.44	114.35	119.90
1	B	916	ARG	C-N-CA	-5.44	114.35	119.90
1	A	653	GLN	CA-C-N	-5.40	114.82	120.38
1	A	653	GLN	C-N-CA	-5.40	114.82	120.38
1	B	443	SER	O-C-N	-5.40	114.99	122.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	511	THR	N-CA-C	-5.36	105.35	111.14
1	A	453	SER	N-CA-C	5.34	117.85	111.71
1	A	271	VAL	CB-CA-C	-5.33	104.56	110.68
1	B	612	TYR	N-CA-C	-5.29	105.16	111.03
1	A	443	SER	O-C-N	-5.27	115.18	122.76
1	B	205	LYS	N-CA-C	5.26	117.09	111.36
1	A	584	ARG	CG-CD-NE	-5.20	100.56	112.00
1	B	203	ASP	N-CA-CB	5.18	117.82	110.16
1	A	518	LEU	CA-C-N	-5.16	114.64	119.85
1	A	518	LEU	C-N-CA	-5.16	114.64	119.85
1	B	697	MET	CG-SD-CE	-5.13	89.62	100.90
1	A	612	TYR	N-CA-C	-5.07	105.66	111.14
1	B	95	ALA	N-CA-C	-5.06	105.76	111.28
1	A	494	LEU	N-CA-C	5.03	117.88	111.69

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	229	PRO	Peptide

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	7396	0	7381	91	0
1	B	7354	0	7328	91	0
2	A	9	0	3	0	0
2	B	9	0	3	0	0
3	A	4	0	6	0	0
3	B	4	0	6	1	0
4	A	10	0	0	1	0
4	B	10	0	0	1	0
5	A	35	0	0	0	0
5	B	21	0	0	0	0
All	All	14852	0	14727	178	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 6.

All (178) 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:806:LEU:HA	1:A:809:MET:HE2	1.31	1.12
1:A:240:MET:HE2	1:A:284:MET:HE1	1.46	0.98
1:A:748:MET:HE1	1:A:948:GLU:HB3	1.47	0.96
1:B:273:TYR:OH	1:B:411:GLU:OE2	1.90	0.90
1:A:806:LEU:HD23	1:A:809:MET:HE1	1.51	0.88
1:A:273:TYR:OH	1:A:411:GLU:OE2	1.92	0.86
1:A:322:MET:HE1	1:A:373:ARG:HD3	1.59	0.84
1:B:488:LEU:O	1:B:545:ARG:NH2	2.11	0.83
1:B:379:THR:HA	1:B:399:VAL:HG22	1.64	0.78
1:A:615:GLN:HE22	1:A:653:GLN:HE22	1.31	0.77
1:B:615:GLN:HE22	1:B:653:GLN:HE22	1.30	0.77
1:A:240:MET:CE	1:A:284:MET:HE1	2.15	0.76
1:A:806:LEU:HD23	1:A:809:MET:CE	2.14	0.76
1:B:318:ILE:CG2	1:B:373:ARG:HG3	2.16	0.76
1:A:178:ARG:NH1	4:A:1969:SO4:O2	2.21	0.74
1:A:200:ILE:HG22	1:A:201:THR:H	1.53	0.74
1:B:615:GLN:HE22	1:B:653:GLN:NE2	1.85	0.73
1:A:318:ILE:CG2	1:A:373:ARG:HG3	2.18	0.73
1:A:615:GLN:HE22	1:A:653:GLN:NE2	1.90	0.69
1:A:120:LYS:NZ	1:B:24:VAL:HG23	2.08	0.69
1:A:618:ILE:HG22	1:A:629:LEU:HD22	1.74	0.68
1:B:618:ILE:HG22	1:B:629:LEU:HD22	1.76	0.68
1:A:240:MET:CE	1:A:284:MET:CE	2.72	0.67
1:B:557:PRO:HG3	1:B:572:MET:HE1	1.77	0.66
1:A:29:LYS:H	1:A:112:GLN:HE22	1.43	0.66
1:B:289:ASP:O	1:B:767:ARG:NH1	2.27	0.66
1:A:359:VAL:HG13	1:A:360:PRO:HD2	1.77	0.66
1:B:240:MET:HE2	1:B:284:MET:HE1	1.77	0.65
1:B:222:THR:HG22	1:B:222:THR:O	1.96	0.65
1:A:289:ASP:O	1:A:767:ARG:NH1	2.28	0.65
1:B:62:GLU:O	1:B:66:GLU:HG2	2.00	0.62
1:B:562:LEU:HD13	1:B:602:ALA:CB	2.30	0.61
1:B:736:PHE:O	1:B:740:THR:HB	2.01	0.61
1:B:379:THR:CA	1:B:399:VAL:HG22	2.32	0.60
1:B:29:LYS:H	1:B:112:GLN:HE22	1.47	0.59
1:A:379:THR:HA	1:A:399:VAL:HG22	1.83	0.59
1:B:19:LEU:HD11	1:B:68:GLU:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:ALA:HB3	1:B:569:PRO:HD3	1.84	0.59
1:A:226:ARG:NH1	1:A:228:THR:OG1	2.36	0.59
1:B:273:TYR:CE1	1:B:274:ASN:HB3	2.39	0.58
1:A:145:LEU:HD23	1:A:149:LEU:HD13	1.86	0.58
1:A:736:PHE:O	1:A:740:THR:HB	2.03	0.58
1:B:240:MET:HE2	1:B:284:MET:CE	2.34	0.57
1:A:248:TRP:HE1	1:A:317:GLN:HE21	1.52	0.57
1:A:740:THR:HG22	1:A:742:GLU:H	1.69	0.56
1:B:178:ARG:NH1	4:B:1969:SO4:O1	2.37	0.56
1:B:240:MET:HE1	1:B:445:VAL:HG21	1.87	0.56
1:B:951:LEU:HG	1:B:955:MET:HE2	1.88	0.56
1:A:414:TYR:CE1	1:A:426:ALA:HB1	2.41	0.56
1:A:414:TYR:CD1	1:A:426:ALA:HB1	2.41	0.56
1:A:618:ILE:HG22	1:A:629:LEU:CD2	2.35	0.55
1:A:139:GLU:OE2	1:A:143:LYS:NZ	2.40	0.55
1:A:806:LEU:HA	1:A:809:MET:CE	2.20	0.55
1:B:552:PRO:HB2	1:B:584:ARG:NH2	2.22	0.54
1:A:638:THR:HG21	1:A:818:VAL:HG13	1.89	0.54
1:B:12:ILE:HD12	1:B:12:ILE:H	1.72	0.54
1:A:240:MET:CB	1:A:309:MET:HE1	2.38	0.54
1:A:24:VAL:HG12	1:B:120:LYS:NZ	2.23	0.53
1:B:440:PHE:HB3	1:B:444:LEU:HD23	1.89	0.53
1:A:318:ILE:HG21	1:A:373:ARG:HG3	1.91	0.53
1:A:359:VAL:CG1	1:A:360:PRO:HD2	2.39	0.53
1:B:359:VAL:HG13	1:B:360:PRO:HD2	1.90	0.53
1:B:736:PHE:CE2	1:B:742:GLU:HG2	2.43	0.52
1:B:822:LEU:HD11	3:B:1968:EDO:H22	1.91	0.52
1:A:25:SER:HB2	1:A:27:ASP:OD1	2.09	0.52
1:A:736:PHE:CE2	1:A:742:GLU:HG2	2.44	0.52
1:B:880:TYR:O	1:B:884:ARG:HG3	2.09	0.52
1:B:318:ILE:HG21	1:B:373:ARG:HG3	1.89	0.52
1:A:880:TYR:O	1:A:884:ARG:HG3	2.10	0.52
1:A:319:GLU:OE2	1:A:373:ARG:HD2	2.10	0.51
1:B:319:GLU:OE2	1:B:373:ARG:HD2	2.10	0.51
1:A:463:ILE:HG21	1:A:494:LEU:HD13	1.92	0.51
1:B:488:LEU:C	1:B:545:ARG:HH22	2.19	0.51
1:B:277:LEU:HD12	1:B:277:LEU:N	2.25	0.51
1:A:619:ILE:HD12	1:A:629:LEU:HD22	1.93	0.51
1:A:552:PRO:HB2	1:A:584:ARG:NH2	2.25	0.51
1:B:488:LEU:HD22	1:B:580:TRP:CZ2	2.45	0.51
1:A:200:ILE:HB	1:A:205:LYS:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:MET:HB3	1:A:309:MET:HE1	1.91	0.50
1:B:488:LEU:HD22	1:B:580:TRP:CH2	2.46	0.50
1:A:740:THR:CG2	1:A:742:GLU:HB3	2.42	0.50
1:A:359:VAL:HG12	1:A:360:PRO:N	2.27	0.50
1:A:581:TYR:CZ	1:A:585:ILE:HD13	2.47	0.50
1:A:568:ALA:HB3	1:A:569:PRO:HD3	1.95	0.49
1:A:733:VAL:O	1:A:737:ARG:HG3	2.13	0.49
1:A:273:TYR:CE1	1:A:274:ASN:HB3	2.47	0.49
1:B:748:MET:HE1	1:B:948:GLU:HB3	1.94	0.49
1:B:733:VAL:O	1:B:737:ARG:HG3	2.13	0.48
1:B:414:TYR:CD1	1:B:426:ALA:HB1	2.49	0.48
1:A:951:LEU:HG	1:A:955:MET:HE2	1.95	0.48
1:A:53:LEU:HD13	1:A:920:SER:HB3	1.96	0.48
1:B:234:ASP:OD1	1:B:237:ARG:NH2	2.47	0.48
1:B:618:ILE:HG22	1:B:629:LEU:CD2	2.41	0.48
1:A:379:THR:CA	1:A:399:VAL:HG22	2.44	0.47
1:A:822:LEU:C	1:A:822:LEU:HD23	2.39	0.47
1:A:120:LYS:HZ1	1:B:24:VAL:HG23	1.78	0.47
1:B:143:LYS:O	1:B:147:LEU:HD23	2.14	0.47
1:B:740:THR:CG2	1:B:774:ALA:HB1	2.44	0.47
1:B:359:VAL:CG1	1:B:360:PRO:HD2	2.43	0.47
1:B:558:LEU:HD13	1:B:592:MET:HG2	1.95	0.47
1:A:113:ILE:HG22	1:A:680:LEU:HD21	1.96	0.47
1:B:142:PHE:HB3	1:B:265:ILE:HD13	1.96	0.47
1:A:288:ARG:NH2	1:A:299:THR:OG1	2.33	0.47
1:B:88:PRO:O	1:B:92:ILE:HD13	2.14	0.47
1:B:98:PHE:CE1	1:B:101:MET:HE1	2.49	0.47
1:B:283:TRP:CH2	1:B:592:MET:HE1	2.50	0.47
1:B:28:ASP:HA	1:B:112:GLN:HE22	1.80	0.47
1:A:234:ASP:OD1	1:A:237:ARG:NH2	2.48	0.46
1:A:222:THR:HG22	1:A:222:THR:O	2.15	0.46
1:B:562:LEU:HD13	1:B:602:ALA:HB3	1.96	0.46
1:A:283:TRP:CH2	1:A:592:MET:HE1	2.51	0.46
1:A:740:THR:CG2	1:A:742:GLU:H	2.28	0.46
1:A:527:ILE:HD13	1:A:556:VAL:HB	1.97	0.46
1:B:175:GLN:OE1	1:B:750:ILE:HG23	2.16	0.46
1:B:343:ARG:O	1:B:345:ALA:N	2.49	0.46
1:B:344:THR:O	1:B:346:ARG:N	2.49	0.46
1:B:740:THR:CG2	1:B:742:GLU:HB3	2.46	0.46
1:A:744:GLU:O	1:A:748:MET:HG3	2.16	0.45
1:B:744:GLU:O	1:B:748:MET:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:LEU:HD23	1:B:460:LEU:HA	1.70	0.45
1:B:205:LYS:O	1:B:206:GLN:C	2.60	0.45
1:A:581:TYR:CZ	1:A:585:ILE:CD1	2.99	0.45
1:B:740:THR:HG22	1:B:742:GLU:H	1.81	0.45
1:A:322:MET:HE1	1:A:373:ARG:CD	2.37	0.45
1:B:553:LEU:HD12	1:B:553:LEU:N	2.31	0.45
1:A:62:GLU:O	1:A:66:GLU:HG3	2.17	0.45
1:B:527:ILE:HD13	1:B:556:VAL:HB	1.99	0.45
1:A:445:VAL:HG23	1:A:445:VAL:O	2.17	0.44
1:B:559:PHE:CZ	1:B:572:MET:HE3	2.52	0.44
1:B:748:MET:O	1:B:749:ASN:C	2.60	0.44
1:B:847:LEU:HD23	1:B:847:LEU:HA	1.87	0.44
1:A:271:VAL:O	1:A:272:PRO:C	2.58	0.44
1:A:318:ILE:HG23	1:A:373:ARG:HG3	1.99	0.43
1:A:913:VAL:HG12	1:A:914:THR:N	2.32	0.43
1:A:406:PHE:CE2	1:A:437:VAL:HG22	2.54	0.43
1:A:740:THR:CG2	1:A:774:ALA:HB1	2.49	0.43
1:B:459:VAL:HG22	1:B:505:VAL:HG13	1.99	0.43
1:B:83:LEU:HD13	1:B:898:CYS:HB2	2.00	0.43
1:B:72:ASP:OD1	1:B:72:ASP:C	2.62	0.43
1:A:174:THR:HA	1:A:750:ILE:HG22	2.00	0.43
1:B:782:LEU:C	1:B:782:LEU:HD23	2.44	0.43
1:A:440:PHE:HB3	1:A:444:LEU:HD23	2.01	0.42
1:A:782:LEU:HB3	1:A:783:PRO:HD3	2.01	0.42
1:B:668:GLY:O	1:B:671:ILE:HG13	2.18	0.42
1:A:273:TYR:C	1:A:273:TYR:CD1	2.96	0.42
1:A:767:ARG:O	1:A:770:PRO:HD2	2.19	0.42
1:B:70:LYS:O	1:B:71:HIS:HB2	2.19	0.42
1:B:553:LEU:N	1:B:553:LEU:CD1	2.82	0.42
1:A:166:ASP:OD1	1:A:281:SER:OG	2.36	0.42
1:A:553:LEU:N	1:A:553:LEU:CD1	2.83	0.42
1:B:644:GLY:O	1:B:645:PRO:C	2.61	0.42
1:B:776:THR:HG22	1:B:962:MET:HG3	2.02	0.42
1:B:334:LEU:CD2	1:B:364:PRO:HB2	2.50	0.42
1:A:88:PRO:O	1:A:92:ILE:HD13	2.20	0.42
1:B:721:GLU:CD	1:B:790:ALA:HB2	2.45	0.42
1:A:793:LYS:NZ	1:A:860:GLU:OE1	2.52	0.41
1:A:600:LYS:NZ	1:A:763:ILE:O	2.52	0.41
1:A:748:MET:O	1:A:749:ASN:C	2.64	0.41
1:B:485:LEU:HD21	1:B:578:ILE:HG21	2.02	0.41
1:B:668:GLY:HA2	1:B:671:ILE:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:892:ILE:HD13	1:B:962:MET:HE2	2.02	0.41
1:A:515:LEU:HD13	1:A:553:LEU:HD22	2.03	0.41
1:A:240:MET:HE3	1:A:284:MET:HE3	2.02	0.41
1:A:718:ALA:HB2	1:A:791:ALA:HB2	2.03	0.41
1:B:271:VAL:O	1:B:272:PRO:C	2.57	0.41
1:B:359:VAL:HG12	1:B:360:PRO:N	2.35	0.41
1:A:181:LEU:HD12	1:A:181:LEU:HA	1.82	0.41
1:B:562:LEU:HD13	1:B:602:ALA:HB2	2.03	0.41
1:A:101:MET:HE3	1:A:891:TYR:HE1	1.86	0.40
1:B:318:ILE:HG23	1:B:373:ARG:HG3	2.01	0.40
1:A:120:LYS:HZ3	1:B:24:VAL:HG23	1.82	0.40
1:A:277:LEU:HD12	1:A:277:LEU:N	2.36	0.40
1:B:706:GLU:H	1:B:706:GLU:CD	2.29	0.40
1:A:101:MET:HE3	1:A:891:TYR:CE1	2.56	0.40
1:B:143:LYS:O	1:B:147:LEU:CD2	2.70	0.40
1:B:408:GLU:HB3	1:B:409:PRO:CD	2.52	0.40
1:B:559:PHE:CE2	1:B:572:MET:HE3	2.56	0.40
1:B:273:TYR:CD1	1:B:273:TYR:C	3.00	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	912/972 (94%)	879 (96%)	30 (3%)	3 (0%)	36	59
1	B	905/972 (93%)	873 (96%)	27 (3%)	5 (1%)	21	42
All	All	1817/1944 (94%)	1752 (96%)	57 (3%)	8 (0%)	30	52

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	752	SER
1	B	752	SER
1	A	22	GLY
1	B	22	GLY
1	B	498	ASP
1	B	345	ALA
1	A	175	GLN
1	B	175	GLN

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	802/848 (95%)	759 (95%)	43 (5%)	20	43
1	B	797/848 (94%)	756 (95%)	41 (5%)	21	46
All	All	1599/1696 (94%)	1515 (95%)	84 (5%)	21	44

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	16	LEU
1	A	17	ARG
1	A	18	LEU
1	A	25	SER
1	A	26	GLU
1	A	53	LEU
1	A	92	ILE
1	A	94	ILE
1	A	99	SER
1	A	158	ASP
1	A	178	ARG
1	A	200	ILE
1	A	205	LYS
1	A	209	ASP
1	A	225	ILE

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Mol	Chain	Res	Type
1	A	228	THR
1	A	268	ASN
1	A	326	SER
1	A	327	MET
1	A	343	ARG
1	A	344	THR
1	A	383	SER
1	A	399	VAL
1	A	529	SER
1	A	583	ASN
1	A	585	ILE
1	A	619	ILE
1	A	620	LYS
1	A	646	THR
1	A	664	VAL
1	A	670	VAL
1	A	701	ILE
1	A	702	SER
1	A	740	THR
1	A	742	GLU
1	A	753	ARG
1	A	755	SER
1	A	809	MET
1	A	818	VAL
1	A	872	ARG
1	A	890	SER
1	A	947	LEU
1	B	12	ILE
1	B	15	GLN
1	B	17	ARG
1	B	24	VAL
1	B	25	SER
1	B	26	GLU
1	B	66	GLU
1	B	94	ILE
1	B	99	SER
1	B	121	LEU
1	B	178	ARG
1	B	200	ILE
1	B	207	GLU
1	B	209	ASP
1	B	225	ILE

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Mol	Chain	Res	Type
1	B	228	THR
1	B	327	MET
1	B	343	ARG
1	B	344	THR
1	B	375	LYS
1	B	383	SER
1	B	399	VAL
1	B	529	SER
1	B	545	ARG
1	B	562	LEU
1	B	583	ASN
1	B	585	ILE
1	B	620	LYS
1	B	629	LEU
1	B	646	THR
1	B	671	ILE
1	B	702	SER
1	B	740	THR
1	B	742	GLU
1	B	753	ARG
1	B	755	SER
1	B	818	VAL
1	B	872	ARG
1	B	886	ARG
1	B	890	SER
1	B	947	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	58	GLN
1	A	112	GLN
1	A	317	GLN
1	A	653	GLN
1	A	673	GLN
1	A	698	ASN
1	A	713	GLN
1	A	781	HIS
1	A	899	GLN
1	A	963	GLN
1	B	49	HIS

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Mol	Chain	Res	Type
1	B	112	GLN
1	B	150	ASN
1	B	358	GLN
1	B	389	HIS
1	B	589	GLN
1	B	653	GLN
1	B	673	GLN
1	B	781	HIS
1	B	963	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](#)

8 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$
4	SO4	B	1970	-	4,4,4	0.63	0	6,6,6	0.61	0
2	ASP	A	1967	-	7,8,8	1.43	2 (28%)	6,10,10	1.05	0
4	SO4	A	1969	-	4,4,4	0.39	0	6,6,6	1.26	1 (16%)
4	SO4	A	1970	-	4,4,4	0.55	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	1968	-	3,3,3	0.61	0	2,2,2	0.24	0
2	ASP	B	1967	-	7,8,8	1.32	0	6,10,10	1.22	1 (16%)
3	EDO	A	1968	-	3,3,3	0.89	0	2,2,2	0.44	0
4	SO4	B	1969	-	4,4,4	0.56	0	6,6,6	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	1968	-	-	1/1/1/1	-
2	ASP	A	1967	-	-	0/8/8/8	-
3	EDO	B	1968	-	-	1/1/1/1	-
2	ASP	B	1967	-	-	0/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1967	ASP	OXT-C	-2.23	1.23	1.30
2	A	1967	ASP	CB-CG	-2.05	1.45	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1967	ASP	OD1-CG-CB	-2.28	115.86	122.84
4	A	1969	SO4	O4-S-O3	2.00	119.59	108.54

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1968	EDO	O1-C1-C2-O2
3	B	1968	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1969	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1968	EDO	1	0
4	B	1969	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	920/972 (94%)	-0.27	24 (2%) 57 54	23, 39, 78, 116	0
1	B	915/972 (94%)	-0.12	39 (4%) 40 36	29, 46, 88, 135	0
All	All	1835/1944 (94%)	-0.19	63 (3%) 48 44	23, 43, 83, 135	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	LEU	5.3
1	A	24	VAL	5.1
1	A	199	ASP	5.1
1	B	24	VAL	4.8
1	B	754	PRO	4.8
1	A	751	GLY	4.8
1	B	12	ILE	4.6
1	B	225	ILE	4.5
1	B	391	ILE	4.4
1	A	225	ILE	4.2
1	A	200	ILE	4.1
1	B	25	SER	4.0
1	B	21	PRO	4.0
1	A	754	PRO	4.0
1	B	909	PRO	3.9
1	A	750	ILE	3.6
1	B	10	ALA	3.5
1	A	23	LYS	3.4
1	A	752	SER	3.4
1	A	912	HIS	3.4
1	B	18	LEU	3.4
1	A	753	ARG	3.3
1	A	22	GLY	3.3
1	B	23	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	753	ARG	3.2
1	A	19	LEU	3.2
1	B	917	PRO	3.1
1	B	913	VAL	3.1
1	B	914	THR	3.1
1	B	751	GLY	3.1
1	A	8	LYS	3.0
1	A	18	LEU	2.9
1	B	912	HIS	2.8
1	B	226	ARG	2.8
1	B	946	GLY	2.8
1	B	228	THR	2.8
1	A	20	VAL	2.8
1	B	915	LEU	2.8
1	A	21	PRO	2.7
1	B	920	SER	2.7
1	B	346	ARG	2.7
1	A	761	GLY	2.7
1	B	345	ALA	2.6
1	B	752	SER	2.5
1	B	203	ASP	2.5
1	B	342	TYR	2.5
1	B	343	ARG	2.5
1	B	20	VAL	2.4
1	B	756	LYS	2.3
1	A	227	ARG	2.3
1	A	9	LEU	2.3
1	B	22	GLY	2.2
1	B	748	MET	2.2
1	B	762	GLY	2.2
1	B	358	GLN	2.1
1	A	391	ILE	2.1
1	B	755	SER	2.1
1	A	224	GLU	2.0
1	A	25	SER	2.0
1	B	88	PRO	2.0
1	B	229	PRO	2.0
1	B	74	LYS	2.0
1	B	15	GLN	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
4	SO4	B	1970	5/5	0.87	0.18	60,72,86,87	0
4	SO4	A	1970	5/5	0.90	0.12	63,64,80,87	0
4	SO4	B	1969	5/5	0.90	0.15	55,64,69,76	0
3	EDO	A	1968	4/4	0.90	0.14	27,29,32,37	0
3	EDO	B	1968	4/4	0.94	0.12	31,36,37,39	0
4	SO4	A	1969	5/5	0.95	0.10	40,52,55,59	0
2	ASP	A	1967	9/9	0.95	0.09	37,39,46,47	0
2	ASP	B	1967	9/9	0.96	0.08	34,41,46,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.