



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:09 PM UTC

PDB ID : 1P9O / pdb_00001p9o
Title : Crystal Structure of Phosphopantothenoylcysteine Synthetase
Authors : Manoj, N.; Strauss, E.; Begley, T.P.; Ealick, S.E.
Deposited on : 2003-05-12
Resolution : 2.30 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

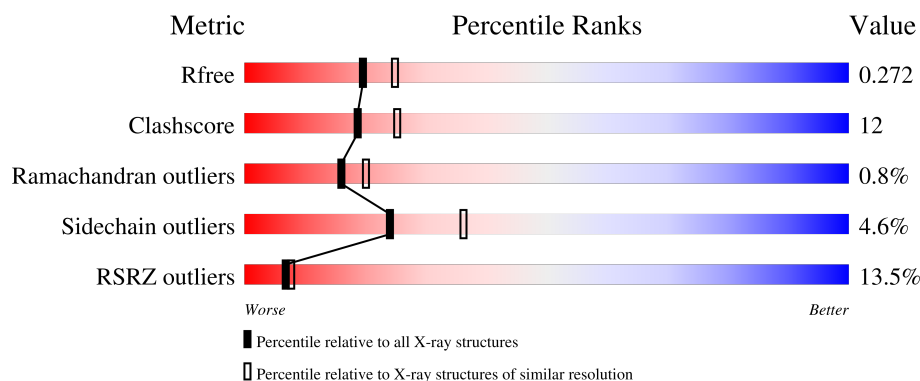
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	313	12% 62% 22% • 14%
1	B	313	12% 65% 22% • 11%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4214 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 Phosphopantothencysteine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			1984	1285	344	352	3			
1	B	280	Total	C	N	O	S	0	0	0
			2002	1302	344	353	3			

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



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

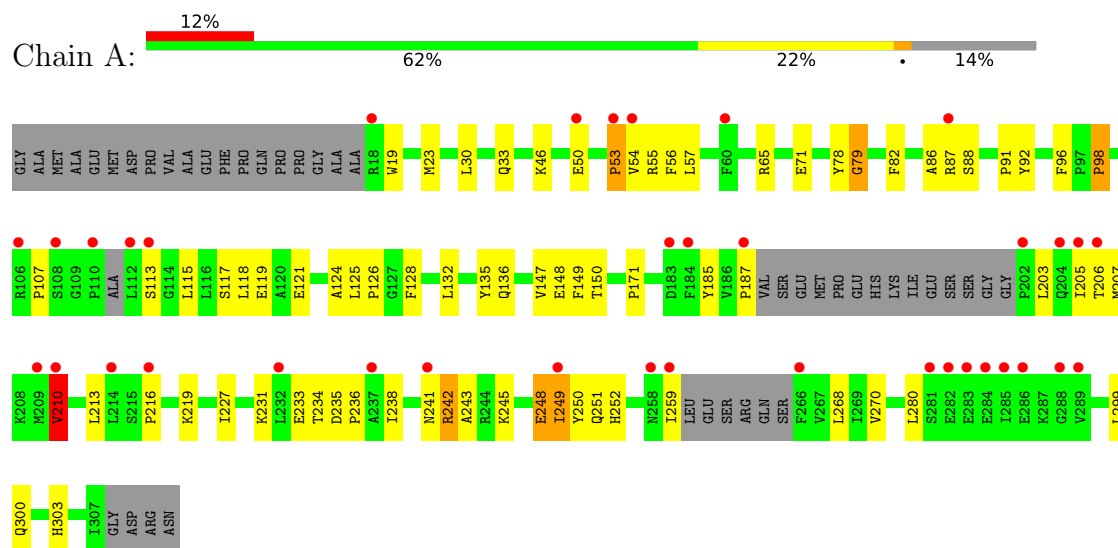
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	117	Total 117	O 117	0	0
3	B	101	Total 101	O 101	0	0

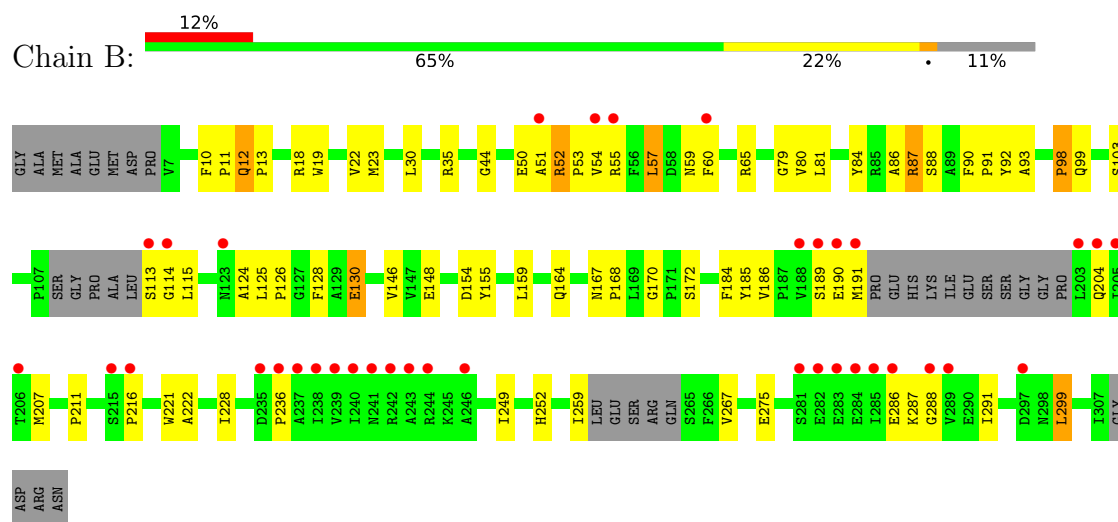
3 Residue-property plots [i](#)

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: Phosphopantothencysteine synthetase



• Molecule 1: Phosphopantothencysteine synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	73.16Å 73.16Å 281.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.32 – 2.30 45.32 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.32-2.30) 98.6 (45.32-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 2.29Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.272 0.229 , 0.272	Depositor DCC
R_{free} test set	2534 reflections (7.22%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4214	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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	0.62	0/2026	1.11	14/2756 (0.5%)
1	B	0.58	0/2048	1.10	20/2796 (0.7%)
All	All	0.60	0/4074	1.10	34/5552 (0.6%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	VAL	N-CA-C	-10.57	103.17	113.53
1	A	216	PRO	N-CA-C	-10.43	95.77	111.41
1	A	79	GLY	N-CA-C	-9.80	98.65	112.37
1	B	54	VAL	N-CA-C	-7.96	105.56	113.20
1	B	249	ILE	N-CA-C	7.80	117.75	110.42
1	B	60	PHE	N-CA-C	7.18	121.54	110.20
1	B	80	VAL	N-CA-C	6.92	117.83	107.80
1	A	57	LEU	N-CA-C	-6.74	98.24	108.96
1	A	53	PRO	N-CA-CB	6.51	110.09	103.25
1	B	88	SER	N-CA-C	-6.51	101.37	110.35
1	A	270	VAL	N-CA-C	6.32	116.96	108.11
1	A	227	ILE	N-CA-C	6.31	117.00	108.17
1	B	79	GLY	N-CA-C	-6.10	99.41	111.31
1	B	216	PRO	N-CA-CB	6.04	109.59	103.25
1	B	114	GLY	N-CA-C	-5.92	108.03	115.08
1	A	88	SER	N-CA-C	-5.89	102.92	110.53
1	B	57	LEU	N-CA-C	-5.83	99.70	108.96
1	B	52	ARG	CA-C-N	5.76	127.04	119.84
1	B	52	ARG	C-N-CA	5.76	127.04	119.84
1	B	186	VAL	CA-C-N	5.64	125.66	119.90
1	B	186	VAL	C-N-CA	5.64	125.66	119.90
1	B	222	ALA	CA-C-N	5.53	125.36	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	ALA	C-N-CA	5.53	125.36	119.28
1	B	252	HIS	N-CA-C	-5.47	103.16	110.55
1	B	170	GLY	CA-C-N	5.45	125.54	119.87
1	B	170	GLY	C-N-CA	5.45	125.54	119.87
1	B	12	GLN	CA-C-N	5.34	123.50	119.66
1	B	12	GLN	C-N-CA	5.34	123.50	119.66
1	A	33	GLN	N-CA-C	-5.32	106.56	113.16
1	A	252	HIS	N-CA-C	-5.30	103.03	110.35
1	A	96	PHE	CA-C-N	5.15	123.42	119.66
1	A	96	PHE	C-N-CA	5.15	123.42	119.66
1	A	210	VAL	CA-C-N	5.09	126.21	119.84
1	A	210	VAL	C-N-CA	5.09	126.21	119.84

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	1984	0	1940	57	0
1	B	2002	0	1894	45	0
2	B	10	0	0	1	0
3	A	117	0	0	4	0
3	B	101	0	0	2	0
All	All	4214	0	3834	93	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 (93) 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:13:PRO:HG3	1:B:154:ASP:HA	1.52	0.91
1:A:238:ILE:HG23	1:A:242:ARG:HE	1.43	0.83
1:A:259:ILE:HD11	1:A:268:LEU:HD22	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:THR:HG22	1:B:204:GLN:CB	2.21	0.70
1:B:52:ARG:N	1:B:53:PRO:HD3	2.07	0.68
1:A:233:GLU:H	1:A:233:GLU:CD	2.00	0.68
1:A:259:ILE:CD1	1:A:268:LEU:HD22	2.24	0.67
1:A:236:PRO:HG3	1:A:259:ILE:HG21	1.76	0.66
1:A:207:MET:HE1	1:B:55:ARG:HH12	1.61	0.65
1:A:245:LYS:O	1:A:249:ILE:HG22	1.98	0.64
1:A:132:LEU:O	1:A:136:GLN:HG3	1.98	0.64
1:B:86:ALA:O	1:B:87:ARG:HB2	1.97	0.63
1:B:30:LEU:HD22	1:B:35:ARG:HD2	1.81	0.62
1:A:210:VAL:HB	1:A:213:LEU:HG	1.81	0.62
1:A:248:GLU:O	1:A:251:GLN:NE2	2.32	0.62
1:A:231:LYS:HG3	3:A:423:HOH:O	1.99	0.62
1:A:171:PRO:O	1:A:303:HIS:HE1	1.85	0.60
1:A:205:ILE:O	1:B:204:GLN:HA	2.02	0.60
1:A:233:GLU:OE2	1:A:233:GLU:N	2.23	0.60
1:A:113:SER:C	1:A:115:LEU:H	2.10	0.60
1:A:55:ARG:CZ	1:B:184:PHE:HE2	2.16	0.59
1:B:125:LEU:HB3	1:B:128:PHE:HB2	1.85	0.59
1:A:46:LYS:HE2	1:A:150:THR:HG22	1.86	0.58
1:A:119:GLU:HB2	1:B:115:LEU:HD21	1.85	0.56
1:B:65:ARG:NH2	3:B:402:HOH:O	2.38	0.56
1:B:286:GLU:C	1:B:288:GLY:H	2.14	0.55
1:A:107:PRO:HA	1:A:118:LEU:HD23	1.88	0.55
1:A:259:ILE:HD11	1:A:268:LEU:CD2	2.36	0.54
1:A:78:TYR:HE1	1:A:300:GLN:HG3	1.72	0.54
1:A:23:MET:HE2	1:A:147:VAL:HG21	1.91	0.53
1:B:50:GLU:O	1:B:53:PRO:HG3	2.11	0.51
1:A:71:GLU:HG2	1:A:92:TYR:CE1	2.46	0.50
1:A:65:ARG:NH1	3:A:346:HOH:O	2.45	0.49
1:A:238:ILE:HG23	1:A:242:ARG:NE	2.21	0.49
1:B:84:TYR:CE2	1:B:148:GLU:HG3	2.48	0.48
1:A:86:ALA:O	1:A:87:ARG:HB2	2.13	0.48
1:B:185:TYR:CE2	1:B:211:PRO:HD3	2.49	0.48
1:A:234:THR:O	1:A:259:ILE:HG23	2.13	0.48
1:B:130:GLU:H	1:B:130:GLU:CD	2.21	0.48
1:A:46:LYS:HE2	1:A:150:THR:CG2	2.44	0.47
1:B:228:ILE:HD13	1:B:299:LEU:HG	1.96	0.47
1:A:91:PRO:O	1:A:92:TYR:HB2	2.15	0.47
1:B:91:PRO:O	1:B:92:TYR:HB2	2.15	0.46
1:B:164:GLN:HG2	1:B:221:TRP:CE3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:TYR:CZ	1:A:187:PRO:HG3	2.50	0.46
1:B:236:PRO:HG3	1:B:259:ILE:HG23	1.98	0.46
1:A:203:LEU:HD21	1:A:205:ILE:HD11	1.98	0.45
1:B:84:TYR:CZ	1:B:148:GLU:HG3	2.51	0.45
1:B:52:ARG:N	1:B:53:PRO:CD	2.76	0.45
1:B:12:GLN:HA	1:B:13:PRO:HD3	1.88	0.44
1:A:206:THR:HA	1:B:204:GLN:HA	1.99	0.44
1:A:135:TYR:HE2	1:B:103:SER:HB3	1.83	0.44
1:A:236:PRO:HG3	1:A:259:ILE:HD13	2.00	0.44
1:B:124:ALA:C	1:B:126:PRO:HD3	2.43	0.44
1:A:235:ASP:OD2	1:A:238:ILE:HG13	2.18	0.43
1:A:19:TRP:O	1:A:23:MET:HG3	2.19	0.43
1:A:249:ILE:HG23	1:A:250:TYR:H	1.83	0.43
1:B:51:ALA:C	1:B:53:PRO:HD3	2.44	0.43
1:B:236:PRO:HG3	1:B:259:ILE:CG2	2.48	0.43
1:B:19:TRP:O	1:B:23:MET:HG3	2.18	0.43
1:B:44:GLY:HA3	1:B:59:ASN:O	2.18	0.43
1:A:87:ARG:NH2	3:A:403:HOH:O	2.47	0.43
1:A:113:SER:C	1:A:115:LEU:N	2.75	0.43
1:A:231:LYS:HB3	1:A:233:GLU:OE2	2.19	0.42
1:A:124:ALA:C	1:A:126:PRO:HD3	2.44	0.42
1:B:189:SER:C	1:B:191:MET:H	2.27	0.42
1:B:65:ARG:HD3	2:B:400:SO4:O1	2.19	0.42
1:A:149:PHE:CD1	1:A:149:PHE:C	2.97	0.42
1:A:238:ILE:O	1:A:242:ARG:HB2	2.20	0.42
1:A:250:TYR:O	1:A:251:GLN:HB2	2.20	0.42
1:A:125:LEU:HB3	1:A:128:PHE:HB2	2.01	0.42
1:B:10:PHE:HA	1:B:11:PRO:HD3	1.91	0.42
1:B:113:SER:C	1:B:115:LEU:H	2.27	0.42
1:A:82:PHE:CE2	1:A:91:PRO:HD3	2.55	0.41
1:A:46:LYS:HE3	1:A:56:PHE:CE1	2.54	0.41
1:A:219:LYS:HE2	1:A:251:GLN:HB2	2.03	0.41
1:B:57:LEU:HD12	1:B:57:LEU:HA	1.76	0.41
1:B:99:GLN:HG3	3:B:403:HOH:O	2.20	0.41
1:B:18:ARG:O	1:B:22:VAL:HG23	2.20	0.41
1:A:210:VAL:HB	1:A:213:LEU:CG	2.49	0.41
1:B:286:GLU:C	1:B:288:GLY:N	2.78	0.41
1:A:30:LEU:HD13	1:A:79:GLY:HA3	2.03	0.41
1:A:219:LYS:HE2	1:A:251:GLN:CB	2.51	0.41
1:B:286:GLU:O	1:B:288:GLY:N	2.53	0.41
1:B:167:ASN:HB3	1:B:168:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:VAL:CG2	1:B:291:ILE:HG12	2.51	0.41
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.85	0.41
1:B:90:PHE:CZ	1:B:146:VAL:HG21	2.56	0.41
1:A:243:ALA:HA	3:A:347:HOH:O	2.20	0.40
1:A:86:ALA:HB2	1:A:148:GLU:HG2	2.02	0.40
1:A:203:LEU:HB3	1:B:207:MET:HB2	2.02	0.40
1:B:155:TYR:CZ	1:B:159:LEU:HD22	2.57	0.40
1:A:98:PRO:HB3	1:B:93:ALA:CB	2.51	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	261/313 (83%)	257 (98%)	3 (1%)	1 (0%)	30	38
1	B	272/313 (87%)	258 (95%)	11 (4%)	3 (1%)	11	13
All	All	533/626 (85%)	515 (97%)	14 (3%)	4 (1%)	16	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	PRO
1	B	287	LYS
1	B	190	GLU
1	B	98	PRO

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	188/249 (76%)	178 (95%)	10 (5%)	20	30
1	B	178/249 (72%)	171 (96%)	7 (4%)	28	43
All	All	366/498 (74%)	349 (95%)	17 (5%)	24	36

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	GLU
1	A	98	PRO
1	A	117	SER
1	A	121	GLU
1	A	210	VAL
1	A	241	ASN
1	A	242	ARG
1	A	248	GLU
1	A	249	ILE
1	A	299	LEU
1	B	81	LEU
1	B	87	ARG
1	B	98	PRO
1	B	130	GLU
1	B	172	SER
1	B	275	GLU
1	B	299	LEU

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	164	GLN
1	A	303	HIS
1	B	167	ASN

5.3.3 RNA ⓘ

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](#)

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	400	-	4,4,4	0.31	0	6,6,6	0.24	0
2	SO4	B	401	-	4,4,4	0.33	0	6,6,6	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	SO4	1	0

5.7 Other polymers [i](#)

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	269/313 (85%)	0.68	37 (13%) 6 7	22, 36, 76, 101	0
1	B	280/313 (89%)	0.81	37 (13%) 7 8	23, 42, 78, 96	0
All	All	549/626 (87%)	0.74	74 (13%) 7 8	22, 39, 77, 101	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	241	ASN	7.8
1	A	282	GLU	6.2
1	B	284	GLU	5.7
1	A	202	PRO	5.4
1	A	110	PRO	5.3
1	B	285	ILE	5.2
1	B	238	ILE	5.1
1	A	237	ALA	4.8
1	B	203	LEU	4.7
1	B	237	ALA	4.7
1	B	283	GLU	4.4
1	B	113	SER	4.4
1	A	259	ILE	4.2
1	B	240	ILE	4.2
1	B	188	VAL	4.2
1	B	204	GLN	4.1
1	B	282	GLU	4.1
1	A	108	SER	4.0
1	A	281	SER	3.9
1	B	189	SER	3.8
1	B	281	SER	3.8
1	B	191	MET	3.7
1	A	204	GLN	3.6
1	A	288	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	206	THR	3.6
1	A	283	GLU	3.5
1	B	215	SER	3.5
1	A	285	ILE	3.5
1	B	54	VAL	3.4
1	B	60	PHE	3.3
1	B	205	ILE	3.3
1	A	284	GLU	3.3
1	A	113	SER	3.3
1	A	241	ASN	3.2
1	A	205	ILE	3.2
1	B	235	ASP	3.1
1	B	289	VAL	3.1
1	A	232	LEU	3.0
1	B	236	PRO	3.0
1	A	210	VAL	2.9
1	A	214	LEU	2.9
1	A	249	ILE	2.9
1	B	286	GLU	2.9
1	A	206	THR	2.9
1	B	288	GLY	2.8
1	A	184	PHE	2.8
1	B	244	ARG	2.8
1	A	53	PRO	2.8
1	A	54	VAL	2.8
1	B	216	PRO	2.7
1	A	112	LEU	2.6
1	A	87	ARG	2.6
1	A	266	PHE	2.6
1	A	289	VAL	2.6
1	A	187	PRO	2.5
1	A	216	PRO	2.5
1	A	60	PHE	2.4
1	A	258	ASN	2.4
1	B	246	ALA	2.4
1	A	209	MET	2.4
1	A	183	ASP	2.3
1	B	123	ASN	2.3
1	B	55	ARG	2.3
1	A	18	ARG	2.2
1	B	243	ALA	2.2
1	B	239	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	50	GLU	2.2
1	B	114	GLY	2.2
1	B	242	ARG	2.1
1	B	297	ASP	2.1
1	A	106	ARG	2.1
1	A	286	GLU	2.1
1	B	51	ALA	2.0
1	B	190	GLU	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	B	400	5/5	0.89	0.17	64,64,76,78	0
2	SO4	B	401	5/5	0.90	0.12	66,69,76,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.