



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:13 AM UTC

PDB ID : 4DLL / pdb_00004dll
Title : Crystal structure of a 2-hydroxy-3-oxopropionate reductase from *Polaromonas* sp. JS666
Authors : Agarwal, R.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; Lafleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRG)
Deposited on : 2012-02-06
Resolution : 2.11 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

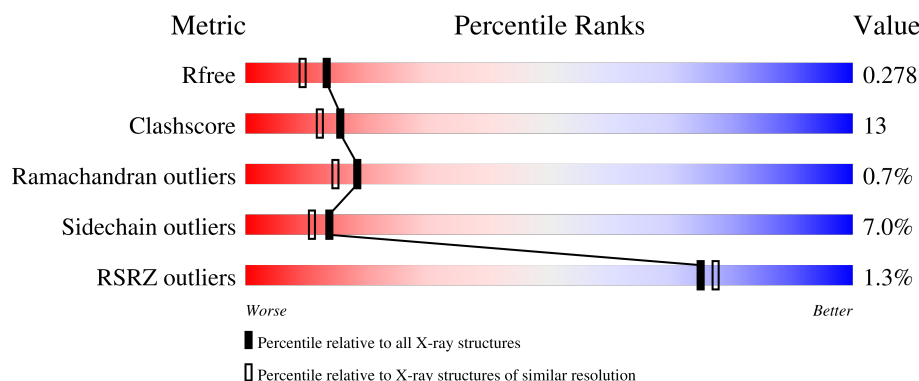
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	320	
1	B	320	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	401	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4240 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 2-hydroxy-3-oxopropionate reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	Se	0	0	0
			2081	1311	374	385	1	10			
1	B	285	Total	C	N	O	S	Se	0	0	0
			2034	1275	363	385	1	10			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q12CU4
A	2	HIS	-	expression tag	UNP Q12CU4
A	3	HIS	-	expression tag	UNP Q12CU4
A	4	HIS	-	expression tag	UNP Q12CU4
A	5	HIS	-	expression tag	UNP Q12CU4
A	6	HIS	-	expression tag	UNP Q12CU4
A	7	HIS	-	expression tag	UNP Q12CU4
A	8	SER	-	expression tag	UNP Q12CU4
A	9	SER	-	expression tag	UNP Q12CU4
A	10	GLY	-	expression tag	UNP Q12CU4
A	11	VAL	-	expression tag	UNP Q12CU4
A	12	ASP	-	expression tag	UNP Q12CU4
A	13	LEU	-	expression tag	UNP Q12CU4
A	14	GLY	-	expression tag	UNP Q12CU4
A	15	THR	-	expression tag	UNP Q12CU4
A	16	GLU	-	expression tag	UNP Q12CU4
A	17	ASN	-	expression tag	UNP Q12CU4
A	18	LEU	-	expression tag	UNP Q12CU4
A	19	TYR	-	expression tag	UNP Q12CU4
A	20	PHE	-	expression tag	UNP Q12CU4
A	21	GLN	-	expression tag	UNP Q12CU4
A	22	SER	-	expression tag	UNP Q12CU4
B	1	MSE	-	expression tag	UNP Q12CU4
B	2	HIS	-	expression tag	UNP Q12CU4
B	3	HIS	-	expression tag	UNP Q12CU4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	HIS	-	expression tag	UNP Q12CU4
B	5	HIS	-	expression tag	UNP Q12CU4
B	6	HIS	-	expression tag	UNP Q12CU4
B	7	HIS	-	expression tag	UNP Q12CU4
B	8	SER	-	expression tag	UNP Q12CU4
B	9	SER	-	expression tag	UNP Q12CU4
B	10	GLY	-	expression tag	UNP Q12CU4
B	11	VAL	-	expression tag	UNP Q12CU4
B	12	ASP	-	expression tag	UNP Q12CU4
B	13	LEU	-	expression tag	UNP Q12CU4
B	14	GLY	-	expression tag	UNP Q12CU4
B	15	THR	-	expression tag	UNP Q12CU4
B	16	GLU	-	expression tag	UNP Q12CU4
B	17	ASN	-	expression tag	UNP Q12CU4
B	18	LEU	-	expression tag	UNP Q12CU4
B	19	TYR	-	expression tag	UNP Q12CU4
B	20	PHE	-	expression tag	UNP Q12CU4
B	21	GLN	-	expression tag	UNP Q12CU4
B	22	SER	-	expression tag	UNP Q12CU4

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



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

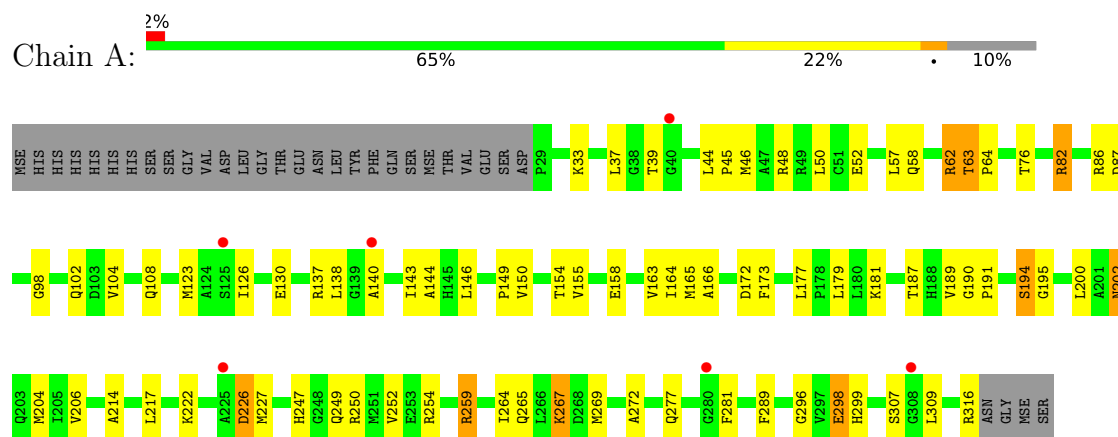
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	59	Total 59	O 59	0	0
3	B	56	Total 56	O 56	0	0

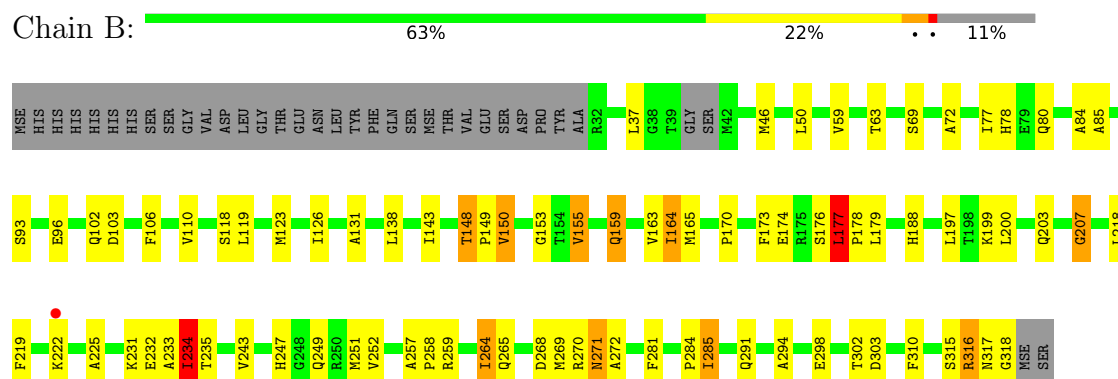
3 Residue-property plots [i](#)

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: 2-hydroxy-3-oxopropionate reductase



- Molecule 1: 2-hydroxy-3-oxopropionate reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	39.87Å 47.01Å 77.50Å 92.14° 95.30° 101.19°	Depositor
Resolution (Å)	38.52 – 2.11 38.52 – 2.11	Depositor EDS
% Data completeness (in resolution range)	93.8 (38.52-2.11) 93.7 (38.52-2.11)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.218 , 0.278 0.220 , 0.278	Depositor DCC
R_{free} test set	1591 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.7	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	0.95	EDS
Total number of atoms	4240	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.84% 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	1.20	3/2103 (0.1%)	1.24	11/2830 (0.4%)
1	B	1.12	5/2054 (0.2%)	1.29	13/2770 (0.5%)
All	All	1.16	8/4157 (0.2%)	1.27	24/5600 (0.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	ALA	C-O	-6.72	1.16	1.24
1	A	206	VAL	CA-CB	6.42	1.62	1.54
1	A	144	ALA	CA-CB	5.96	1.62	1.53
1	B	243	VAL	CA-CB	5.93	1.61	1.54
1	A	202	ASN	N-CA	5.91	1.53	1.46
1	B	252	VAL	CA-CB	5.49	1.61	1.54
1	B	235	THR	C-O	-5.21	1.17	1.23
1	B	234	ILE	C-O	-5.16	1.18	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	SER	N-CA-C	8.61	121.43	110.33
1	B	148	THR	CA-C-N	-7.67	112.84	120.21
1	B	148	THR	C-N-CA	-7.67	112.84	120.21
1	A	298	GLU	N-CA-C	-7.26	100.27	110.50
1	B	177	LEU	CA-C-N	-6.78	112.19	119.24
1	B	177	LEU	C-N-CA	-6.78	112.19	119.24
1	B	225	ALA	N-CA-C	6.73	118.99	110.24
1	A	63	THR	CA-C-N	6.33	126.53	119.32
1	A	63	THR	C-N-CA	6.33	126.53	119.32
1	B	207	GLY	N-CA-C	6.19	120.39	112.83
1	A	214	ALA	N-CA-C	-5.88	104.95	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	THR	N-CA-C	5.82	117.70	111.36
1	A	190	GLY	CA-C-N	5.76	126.22	120.52
1	A	190	GLY	C-N-CA	5.76	126.22	120.52
1	B	271	ASN	N-CA-C	-5.72	104.25	111.11
1	B	176	SER	N-CA-C	5.66	118.39	111.82
1	B	233	ALA	CA-C-N	5.57	128.10	120.46
1	B	233	ALA	C-N-CA	5.57	128.10	120.46
1	A	195	GLY	N-CA-C	-5.49	105.85	112.49
1	B	259	ARG	N-CA-C	-5.44	106.57	113.43
1	A	104	VAL	N-CA-C	5.38	116.01	110.36
1	A	86	ARG	N-CA-C	5.36	117.81	111.33
1	B	234	ILE	N-CA-C	5.17	115.90	110.62
1	A	194	SER	N-CA-C	5.15	116.90	111.28

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	2081	0	2079	63	0
1	B	2034	0	1999	57	0
2	A	5	0	0	2	0
2	B	5	0	0	1	0
3	A	59	0	0	2	0
3	B	56	0	0	3	0
All	All	4240	0	4078	110	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 13.

All (110) 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:207:GLY:HA3	1:B:269:MSE:HE1	1.25	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:MSE:HE2	1:A:272:ALA:HB1	1.25	1.10
1:A:62:ARG:HH11	1:A:62:ARG:HG3	1.02	1.10
1:A:222:LYS:HG3	1:B:281:PHE:HD1	1.33	0.91
1:A:204:MSE:HE2	1:A:272:ALA:CB	2.00	0.91
1:A:62:ARG:HG3	1:A:62:ARG:NH1	1.81	0.87
1:B:207:GLY:HA3	1:B:269:MSE:CE	2.04	0.86
1:A:217:LEU:HD13	1:A:227:MSE:HE3	1.60	0.83
1:A:222:LYS:HG3	1:B:281:PHE:CD1	2.13	0.83
1:A:166:ALA:O	1:A:189:VAL:HG22	1.80	0.81
1:A:62:ARG:HH11	1:A:62:ARG:CG	1.91	0.81
1:A:281:PHE:CD1	1:B:222:LYS:HG3	2.16	0.80
1:B:318:GLY:C	3:B:510:HOH:O	2.28	0.74
1:A:281:PHE:HD1	1:B:222:LYS:HG3	1.53	0.73
1:B:258:PRO:HG3	1:B:303:ASP:O	1.89	0.72
1:B:155:VAL:O	1:B:159:GLN:HG2	1.89	0.72
1:B:50:LEU:HD11	1:B:179:LEU:HD11	1.73	0.70
1:A:50:LEU:HD11	1:A:179:LEU:HD11	1.72	0.70
1:A:204:MSE:HE1	1:B:219:PHE:CE2	2.27	0.69
1:B:294:ALA:O	1:B:298:GLU:HG3	1.97	0.64
1:B:102:GLN:HG3	1:B:106:PHE:HD2	1.63	0.64
1:B:155:VAL:O	1:B:159:GLN:CG	2.47	0.63
1:B:265:GLN:HE21	1:B:269:MSE:HE2	1.64	0.63
1:A:298:GLU:CB	3:A:505:HOH:O	2.46	0.63
1:A:63:THR:HG22	2:A:401:SO4:O2	2.01	0.61
1:A:204:MSE:HE1	1:B:219:PHE:CZ	2.38	0.59
1:B:302:THR:HG22	3:B:538:HOH:O	2.01	0.58
1:A:227:MSE:HE2	1:A:252:VAL:HG22	1.84	0.58
1:B:218:LEU:O	1:B:222:LYS:HG2	2.05	0.57
1:A:50:LEU:HD11	1:A:179:LEU:CD1	2.35	0.57
1:A:177:LEU:HG	1:A:181:LYS:HE2	1.87	0.57
1:A:189:VAL:HG23	1:A:194:SER:HB3	1.87	0.57
1:A:146:LEU:HD12	1:A:146:LEU:N	2.21	0.56
1:A:200:LEU:C	1:A:204:MSE:HE3	2.30	0.56
1:A:58:GLN:OE1	1:A:76:THR:HB	2.06	0.56
1:B:265:GLN:HE21	1:B:269:MSE:CE	2.18	0.56
1:A:137:ARG:O	1:A:140:ALA:HB3	2.06	0.56
1:B:138:LEU:HB3	1:B:143:ILE:HB	1.88	0.55
1:B:46:MSE:HE1	1:B:123:MSE:SE	2.57	0.55
1:B:78:HIS:HB2	1:B:84:ALA:HB2	1.89	0.55
1:A:247:HIS:HB3	1:A:307:SER:HB3	1.87	0.55
1:B:85:ALA:CB	1:B:110:VAL:HG13	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LEU:O	1:A:181:LYS:HG2	2.07	0.54
1:B:200:LEU:HD13	1:B:272:ALA:HA	1.89	0.54
1:B:247:HIS:O	1:B:251:MSE:HG3	2.08	0.54
1:A:45:PRO:HB3	1:A:158:GLU:HG2	1.90	0.53
1:B:291:GLN:HA	1:B:291:GLN:OE1	2.10	0.52
1:A:62:ARG:NH1	1:A:62:ARG:CG	2.58	0.52
1:B:203:GLN:HG3	1:B:268:ASP:OD2	2.10	0.52
1:B:123:MSE:HG2	1:B:148:THR:O	2.09	0.52
1:A:166:ALA:O	1:A:189:VAL:CG2	2.57	0.51
1:A:265:GLN:NE2	1:A:269:MSE:HE3	2.26	0.50
1:A:98:GLY:HA3	1:A:130:GLU:OE2	2.12	0.50
1:A:82:ARG:HG2	1:A:108:GLN:O	2.11	0.49
1:B:150:VAL:HG22	1:B:164:ILE:HD13	1.94	0.49
1:B:63:THR:HG23	2:B:401:SO4:O2	2.13	0.49
1:B:218:LEU:HD21	1:B:310:PHE:CZ	2.47	0.49
1:B:150:VAL:O	1:B:199:LYS:NZ	2.31	0.49
1:A:33:LYS:NZ	1:A:87:ASP:OD2	2.46	0.49
1:A:50:LEU:HD23	1:A:57:LEU:HD13	1.95	0.49
1:A:298:GLU:O	1:A:299:HIS:HB2	2.13	0.48
1:B:126:ILE:HD11	1:B:131:ALA:HB2	1.95	0.48
1:B:80:GLN:HG3	3:B:532:HOH:O	2.14	0.48
1:A:146:LEU:HD21	1:A:173:PHE:HA	1.95	0.48
1:B:231:LYS:NZ	1:B:249:GLN:HE21	2.11	0.48
1:B:69:SER:O	1:B:72:ALA:HB3	2.14	0.48
1:A:82:ARG:HG3	3:A:529:HOH:O	2.14	0.47
1:A:146:LEU:HD11	1:A:172:ASP:HB3	1.96	0.47
1:A:227:MSE:HE2	1:A:252:VAL:HA	1.96	0.47
1:A:265:GLN:HE21	1:A:269:MSE:HE3	1.80	0.47
1:B:59:VAL:HB	1:B:77:ILE:CD1	2.45	0.47
1:B:247:HIS:H	1:B:247:HIS:CD2	2.33	0.47
1:A:249:GLN:NE2	1:A:249:GLN:HA	2.30	0.46
1:A:63:THR:HA	1:A:64:PRO:HD3	1.81	0.46
1:A:204:MSE:CE	1:A:272:ALA:HB1	2.18	0.46
1:A:187:THR:HG23	1:B:232:GLU:OE2	2.16	0.46
1:A:289:PHE:CZ	1:B:285:ILE:HD12	2.49	0.46
1:A:150:VAL:HG12	1:A:164:ILE:HG12	1.97	0.46
1:B:177:LEU:O	1:B:178:PRO:C	2.56	0.45
1:A:316:ARG:NH2	1:B:284:PRO:HG3	2.32	0.45
1:A:39:THR:OG1	2:A:401:SO4:O2	2.33	0.45
1:A:149:PRO:O	1:A:165:MSE:HE3	2.17	0.44
1:A:307:SER:C	1:A:309:LEU:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:GLY:C	1:B:155:VAL:N	2.75	0.44
1:A:149:PRO:HD2	1:A:165:MSE:O	2.18	0.44
1:B:265:GLN:HG3	1:B:269:MSE:HE2	1.99	0.44
1:B:231:LYS:HZ1	1:B:249:GLN:HE21	1.66	0.44
1:A:267:LYS:HB3	1:A:267:LYS:HE3	1.87	0.43
1:A:46:MSE:HE1	1:A:123:MSE:SE	2.68	0.43
1:A:202:ASN:HD22	1:B:234:ILE:HG12	1.84	0.43
1:A:298:GLU:O	1:A:299:HIS:CB	2.67	0.43
1:B:264:ILE:H	1:B:264:ILE:HG12	1.52	0.43
1:A:50:LEU:HA	1:A:50:LEU:HD12	1.72	0.43
1:B:170:PRO:O	1:B:174:GLU:HG2	2.18	0.43
1:B:270:ARG:O	1:B:271:ASN:C	2.61	0.43
1:A:191:PRO:O	1:A:194:SER:HB2	2.20	0.42
1:B:149:PRO:HD2	1:B:165:MSE:O	2.19	0.42
1:A:48:ARG:HG2	1:A:52:GLU:OE2	2.20	0.42
1:A:200:LEU:O	1:A:204:MSE:HE3	2.20	0.42
1:A:138:LEU:HB3	1:A:143:ILE:HB	2.02	0.42
1:B:315:SER:C	1:B:317:ASN:N	2.76	0.42
1:A:250:ARG:NH2	1:A:259:ARG:HG3	2.36	0.41
1:B:59:VAL:HB	1:B:77:ILE:HD12	2.03	0.41
1:A:296:GLY:C	1:A:298:GLU:O	2.64	0.41
1:B:315:SER:O	1:B:317:ASN:N	2.54	0.41
1:B:257:ALA:HA	1:B:258:PRO:HD3	1.87	0.41
1:B:315:SER:O	1:B:316:ARG:C	2.62	0.41
1:B:173:PHE:CE1	1:B:188:HIS:HB2	2.55	0.40
1:B:50:LEU:HD11	1:B:179:LEU:CD1	2.47	0.40
1:A:82:ARG:HG3	1:A:82:ARG:H	1.59	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	286/320 (89%)	274 (96%)	10 (4%)	2 (1%)	18	15
1	B	281/320 (88%)	269 (96%)	10 (4%)	2 (1%)	18	15
All	All	567/640 (89%)	543 (96%)	20 (4%)	4 (1%)	18	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	ARG
1	B	316	ARG
1	A	226	ASP
1	B	103	ASP

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	197/225 (88%)	184 (93%)	13 (7%)	15	12
1	B	191/225 (85%)	177 (93%)	14 (7%)	13	10
All	All	388/450 (86%)	361 (93%)	27 (7%)	14	11

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	44	LEU
1	A	62	ARG
1	A	82	ARG
1	A	102	GLN
1	A	126	ILE
1	A	155	VAL
1	A	163	VAL
1	A	226	ASP
1	A	259	ARG
1	A	264	ILE
1	A	267	LYS

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Mol	Chain	Res	Type
1	A	277	GLN
1	B	37	LEU
1	B	93	SER
1	B	96	GLU
1	B	119	LEU
1	B	150	VAL
1	B	155	VAL
1	B	159	GLN
1	B	163	VAL
1	B	164	ILE
1	B	177	LEU
1	B	197	LEU
1	B	234	ILE
1	B	264	ILE
1	B	285	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	HIS
1	A	192	HIS
1	A	196	GLN
1	A	202	ASN
1	A	247	HIS
1	A	265	GLN
1	A	299	HIS
1	A	306	GLN
1	B	80	GLN
1	B	102	GLN
1	B	196	GLN
1	B	245	GLN
1	B	247	HIS
1	B	249	GLN
1	B	265	GLN
1	B	306	GLN

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	A	401	-	4,4,4	0.28	0	6,6,6	0.57	0
2	SO4	B	401	-	4,4,4	0.28	0	6,6,6	0.29	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SO4	2	0
2	B	401	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	278/320 (86%)	0.34	6 (2%) 62 65	20, 39, 52, 60	0
1	B	275/320 (85%)	0.46	1 (0%) 88 90	23, 43, 54, 60	0
All	All	553/640 (86%)	0.40	7 (1%) 75 77	20, 41, 54, 60	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	ALA	2.8
1	A	225	ALA	2.8
1	B	222	LYS	2.7
1	A	125	SER	2.4
1	A	40	GLY	2.2
1	A	280	GLY	2.1
1	A	308	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($\text{\AA}^2$)	Q<0.9
2	SO4	A	401	5/5	0.96	0.07	43,44,47,47	0
2	SO4	B	401	5/5	0.98	0.07	52,52,53,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.