



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2025 – 06:11 PM JST

PDB ID : 9J4Z / pdb_00009j4z
Title : Crystal structure of the open state of omega transaminase TA_5182 from Pseudomonas putida KT2440
Authors : Das, P.; Bhaumik, P.
Deposited on : 2024-08-10
Resolution : 3.40 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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

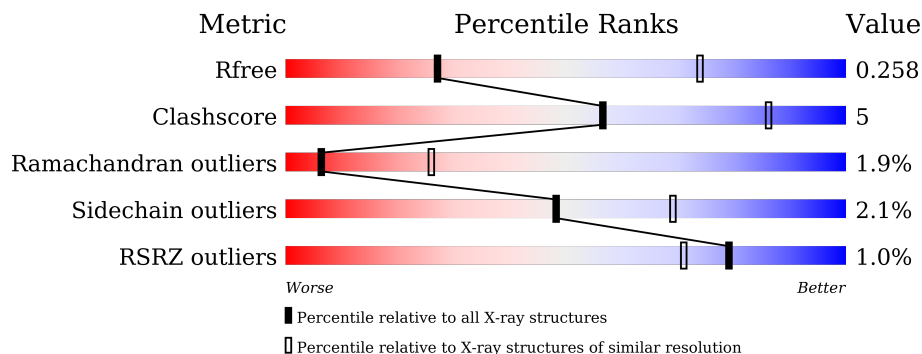
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)

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	453	
1	B	453	
1	C	453	
1	D	453	

2 Entry composition [i](#)

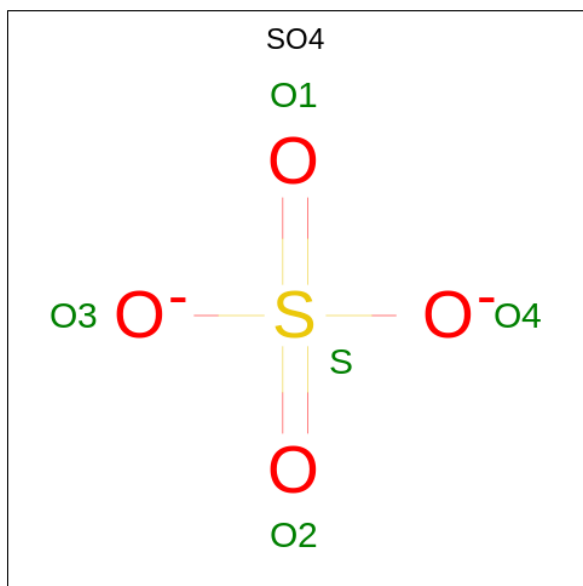
There are 2 unique types of molecules in this entry. The entry contains 12383 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Polyamine:pyruvate transaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3081	1978	526	561	16			
1	B	402	Total	C	N	O	S	0	0	0
			3123	2004	534	569	16			
1	C	397	Total	C	N	O	S	0	0	0
			3088	1981	529	562	16			
1	D	390	Total	C	N	O	S	0	0	0
			3026	1942	516	552	16			

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



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

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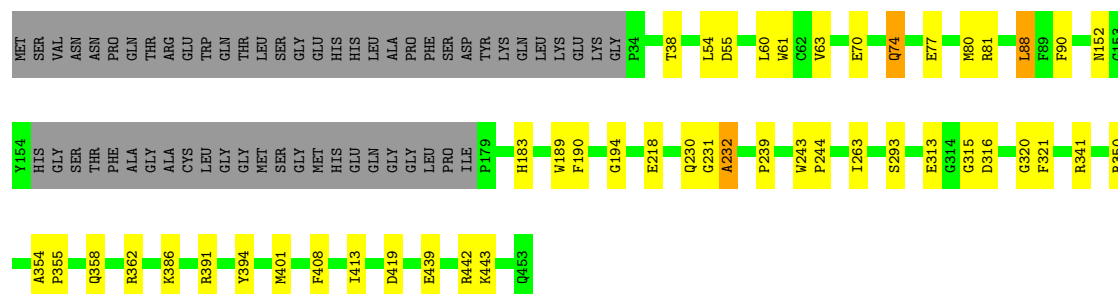
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total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

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.

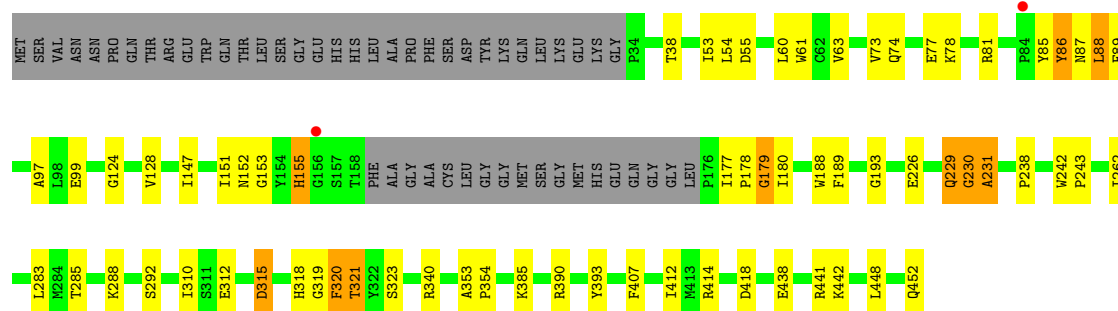
• Molecule 1: Polyamine:pyruvate transaminase

Chain A: 



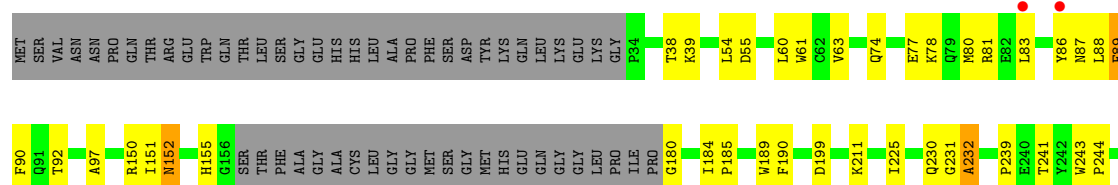
• Molecule 1: Polyamine:pyruvate transaminase

Chain B: 



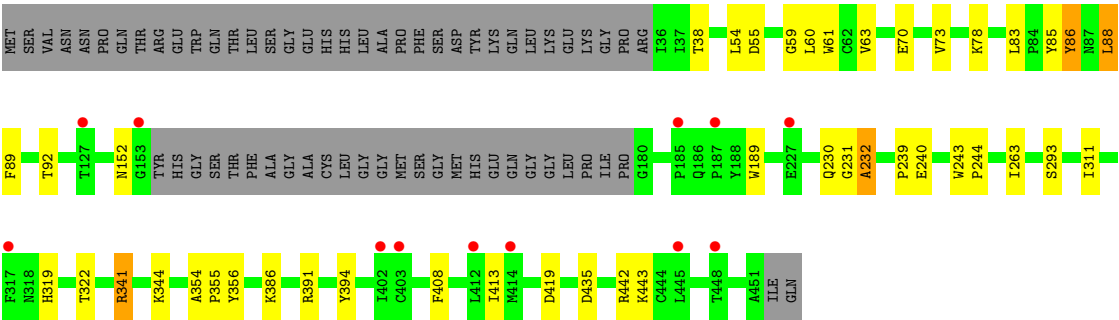
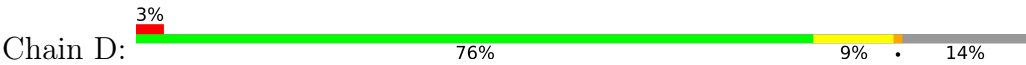
• Molecule 1: Polyamine:pyruvate transaminase

Chain C: 





● Molecule 1: Polyamine:pyruvate transaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.03Å 151.34Å 156.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.02 – 3.40 48.02 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.02-3.40) 99.9 (48.02-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.206 , 0.258 0.208 , 0.258	Depositor DCC
R_{free} test set	1588 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	79.2	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12383	wwPDB-VP
Average B, all atoms (Å ²)	93.0	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 [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	0.54	0/3153	1.05	4/4266 (0.1%)
1	B	0.54	0/3197	1.05	6/4327 (0.1%)
1	C	0.52	0/3160	1.05	8/4275 (0.2%)
1	D	0.51	0/3095	1.03	3/4189 (0.1%)
All	All	0.53	0/12605	1.04	21/17057 (0.1%)

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	A	0	3
1	C	0	1
All	All	0	4

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	PHE	CA-CB-CG	8.12	121.92	113.80
1	B	407	PHE	CA-CB-CG	7.89	121.69	113.80
1	A	38	THR	CA-CB-OG1	-7.26	98.71	109.60
1	C	38	THR	CA-CB-OG1	-7.19	98.82	109.60
1	D	38	THR	CA-CB-OG1	-6.95	99.18	109.60
1	D	408	PHE	CA-CB-CG	6.77	120.57	113.80
1	B	38	THR	CA-CB-OG1	-6.63	99.65	109.60
1	B	418	ASP	CA-CB-CG	6.33	118.93	112.60
1	C	419	ASP	CA-CB-CG	6.05	118.65	112.60
1	C	89	PHE	CA-CB-CG	5.92	119.72	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	419	ASP	CA-CB-CG	5.57	118.17	112.60
1	C	316	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	419	ASP	CA-CB-CG	5.40	118.00	112.60
1	C	408	PHE	CB-CA-C	5.32	119.23	110.88
1	C	439	GLU	N-CA-CB	-5.24	102.48	110.07
1	A	439	GLU	N-CA-CB	-5.19	102.55	110.07
1	B	155	HIS	CB-CA-C	5.15	120.66	110.42
1	B	315	ASP	CA-CB-CG	5.10	117.70	112.60
1	C	317	PHE	CA-CB-CG	5.08	118.88	113.80
1	B	438	GLU	N-CA-CB	-5.07	102.72	110.07
1	A	321	PHE	CA-CB-CG	5.04	118.84	113.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	341	ARG	Sidechain
1	A	350	ARG	Sidechain
1	A	81	ARG	Sidechain
1	C	150	ARG	Sidechain

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	3081	0	3085	27	0
1	B	3123	0	3125	42	0
1	C	3088	0	3087	32	0
1	D	3026	0	3028	23	0
2	A	15	0	0	1	0
2	B	30	0	0	1	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
All	All	12383	0	12325	112	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 5.

All (112) 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:C:151:ILE:O	1:C:152:ASN:HB2	1.79	0.80
1:B:177:ILE:O	1:B:179:GLY:N	2.14	0.76
1:C:321:PHE:O	1:C:322:THR:HG23	1.84	0.76
1:B:147:ILE:HB	1:B:180:ILE:HD13	1.70	0.74
1:B:85:TYR:O	1:B:86:TYR:CB	2.36	0.72
1:D:85:TYR:O	1:D:86:TYR:CB	2.41	0.68
1:A:77:GLU:HG3	1:B:73:VAL:CG1	2.29	0.62
1:B:85:TYR:O	1:B:86:TYR:HB3	2.01	0.60
1:C:86:TYR:OH	1:C:97:ALA:HB2	2.01	0.59
1:A:88:LEU:HD21	1:B:414:ARG:HB2	1.86	0.57
1:C:151:ILE:HG13	1:C:184:ILE:O	2.05	0.57
1:B:310:ILE:O	1:B:318:HIS:HB2	2.06	0.56
1:B:128:VAL:HG13	1:B:283:LEU:HD22	1.86	0.56
1:D:88:LEU:O	1:D:89:PHE:HB2	2.06	0.55
1:B:128:VAL:HG21	1:B:285:THR:CG2	2.35	0.55
1:C:151:ILE:HD12	1:C:185:PRO:HA	1.88	0.55
1:B:320:PHE:O	1:B:321:THR:C	2.49	0.55
1:C:80:MET:SD	1:D:73:VAL:HA	2.46	0.54
1:A:90:PHE:CE2	1:B:53:ILE:HD13	2.42	0.54
1:C:312:SER:HA	1:C:319:HIS:NE2	2.23	0.54
1:B:88:LEU:O	1:B:89:PHE:HB2	2.07	0.54
1:B:97:ALA:HB1	1:B:323:SER:HB2	1.89	0.54
1:C:87:ASN:HD21	1:D:59:GLY:HA2	1.73	0.54
1:B:128:VAL:HG21	1:B:285:THR:HG23	1.88	0.53
1:D:85:TYR:O	1:D:86:TYR:HB3	2.07	0.53
1:B:321:THR:C	1:B:323:SER:H	2.16	0.53
1:A:60:LEU:O	1:A:61:TRP:HB2	2.10	0.52
1:C:189:TRP:CZ2	1:C:391:ARG:NH1	2.77	0.51
1:B:321:THR:C	1:B:323:SER:N	2.69	0.51
1:A:183:HIS:N	2:A:503:SO4:O1	2.44	0.50
1:A:189:TRP:CZ2	1:A:391:ARG:NH1	2.80	0.50
1:B:124:GLY:O	1:B:128:VAL:HG23	2.11	0.50
1:B:319:GLY:O	1:B:320:PHE:C	2.55	0.49
1:B:85:TYR:O	1:B:86:TYR:HB2	2.12	0.49
1:C:354:ALA:HB3	1:C:355:PRO:HD3	1.94	0.49
1:B:60:LEU:O	1:B:61:TRP:HB2	2.12	0.48
1:D:189:TRP:CZ2	1:D:391:ARG:NH1	2.80	0.48
1:B:188:TRP:CZ2	1:B:390:ARG:NH1	2.81	0.48
1:C:60:LEU:O	1:C:61:TRP:HB2	2.13	0.48
1:C:386:LYS:HA	1:C:394:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:C	1:A:54:LEU:HD23	2.38	0.48
1:A:70:GLU:CD	1:B:81:ARG:HH21	2.22	0.48
1:D:60:LEU:O	1:D:61:TRP:HB2	2.14	0.48
1:C:54:LEU:C	1:C:54:LEU:HD23	2.38	0.48
1:D:231:GLY:O	1:D:232:ALA:C	2.58	0.47
1:D:354:ALA:HB3	1:D:355:PRO:HD3	1.96	0.47
1:A:55:ASP:HA	1:A:413:ILE:HB	1.97	0.47
1:C:231:GLY:O	1:C:232:ALA:C	2.58	0.47
1:A:354:ALA:HB3	1:A:355:PRO:HD3	1.96	0.47
1:A:231:GLY:O	1:A:232:ALA:C	2.57	0.47
1:B:54:LEU:C	1:B:54:LEU:HD23	2.39	0.47
1:B:97:ALA:HB1	1:B:323:SER:CB	2.45	0.47
1:B:353:ALA:HB3	1:B:354:PRO:HD3	1.96	0.46
1:A:313:GLU:OE1	1:C:180:GLY:N	2.49	0.46
1:B:315:ASP:HA	1:B:318:HIS:HB3	1.98	0.46
1:D:54:LEU:C	1:D:54:LEU:HD23	2.40	0.46
1:A:70:GLU:OE2	1:B:81:ARG:NH2	2.50	0.45
1:B:385:LYS:HA	1:B:393:TYR:CE1	2.51	0.45
1:C:83:LEU:HD22	1:C:92:THR:HG23	1.99	0.44
1:D:55:ASP:HA	1:D:413:ILE:HB	2.00	0.44
1:D:83:LEU:HD22	1:D:92:THR:HG23	1.99	0.44
1:B:74:GLN:NE2	1:B:77:GLU:OE1	2.51	0.44
1:B:448:LEU:O	1:B:452:GLN:OE1	2.35	0.44
1:A:243:TRP:N	1:A:244:PRO:HD2	2.32	0.43
1:D:386:LYS:HA	1:D:394:TYR:CE1	2.52	0.43
1:B:230:GLY:O	1:B:231:ALA:HB2	2.17	0.43
1:B:63:VAL:HA	1:B:292:SER:O	2.17	0.43
1:C:63:VAL:HA	1:C:293:SER:O	2.18	0.43
1:A:63:VAL:HA	1:A:293:SER:O	2.18	0.43
1:B:288:LYS:HA	2:B:501:SO4:O2	2.18	0.43
1:C:89:PHE:HB2	1:C:90:PHE:CD2	2.54	0.43
1:A:190:PHE:CE1	1:A:391:ARG:HD2	2.54	0.43
1:D:63:VAL:HA	1:D:293:SER:O	2.19	0.43
1:A:386:LYS:HA	1:A:394:TYR:CE1	2.54	0.42
1:C:243:TRP:N	1:C:244:PRO:HD2	2.34	0.42
1:C:77:GLU:HG3	1:D:73:VAL:CG1	2.50	0.42
1:A:243:TRP:N	1:A:244:PRO:CD	2.82	0.42
1:A:442:ARG:O	1:A:443:LYS:C	2.63	0.42
1:A:408:PHE:N	1:A:408:PHE:CD1	2.87	0.42
1:C:55:ASP:HA	1:C:413:ILE:HB	2.01	0.42
1:D:311:ILE:HG22	1:D:311:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:LEU:O	1:C:453:GLN:OE1	2.37	0.41
1:C:81:ARG:HH21	1:D:70:GLU:CD	2.28	0.41
1:C:414:MET:HG2	1:C:423:ILE:CG2	2.51	0.41
1:B:55:ASP:HA	1:B:412:ILE:HB	2.02	0.41
1:B:193:GLY:O	1:B:390:ARG:NH2	2.53	0.41
1:D:243:TRP:N	1:D:244:PRO:HD2	2.35	0.41
1:D:356:TYR:OH	1:D:435:ASP:OD1	2.38	0.41
1:C:408:PHE:CD1	1:C:408:PHE:N	2.87	0.41
1:D:442:ARG:O	1:D:443:LYS:C	2.63	0.41
1:B:242:TRP:N	1:B:243:PRO:HD2	2.35	0.41
1:C:243:TRP:N	1:C:244:PRO:CD	2.84	0.41
1:A:218:GLU:N	1:C:395:GLU:OE2	2.50	0.41
1:A:401:MET:HE2	1:A:401:MET:HB2	1.81	0.41
1:C:311:ILE:O	1:C:311:ILE:HG22	2.20	0.41
1:C:442:ARG:O	1:C:443:LYS:C	2.63	0.41
1:A:313:GLU:C	1:A:315:GLY:H	2.27	0.41
1:B:242:TRP:N	1:B:243:PRO:CD	2.84	0.41
1:A:77:GLU:HG3	1:B:73:VAL:HG11	1.99	0.41
1:A:80:MET:HE3	1:A:80:MET:HB2	1.98	0.41
1:B:151:ILE:HD13	1:B:151:ILE:HA	1.96	0.41
1:B:226:GLU:OE2	1:B:229:GLN:O	2.38	0.41
1:D:85:TYR:O	1:D:86:TYR:HB2	2.17	0.41
1:B:189:PHE:CE1	1:B:390:ARG:HD2	2.55	0.41
1:D:243:TRP:N	1:D:244:PRO:CD	2.84	0.41
1:C:190:PHE:CE1	1:C:391:ARG:HD2	2.56	0.40
1:C:199:ASP:HB3	1:C:241:THR:HG21	2.02	0.40
1:B:441:ARG:O	1:B:442:LYS:C	2.63	0.40
1:D:341:ARG:O	1:D:344:LYS:HE3	2.21	0.40
1:A:70:GLU:OE2	1:A:74:GLN:NE2	2.55	0.40
1:A:358:GLN:HB3	1:A:362:ARG:NH1	2.37	0.40
1:C:323:TYR:HD1	1:C:323:TYR:HA	1.84	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	392/453 (86%)	359 (92%)	27 (7%)	6 (2%)	8	30
1	B	398/453 (88%)	356 (89%)	29 (7%)	13 (3%)	3	18
1	C	393/453 (87%)	360 (92%)	27 (7%)	6 (2%)	8	30
1	D	386/453 (85%)	354 (92%)	27 (7%)	5 (1%)	10	33
All	All	1569/1812 (87%)	1429 (91%)	110 (7%)	30 (2%)	6	26

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	155	HIS
1	B	320	PHE
1	C	152	ASN
1	A	232	ALA
1	A	320	GLY
1	B	86	TYR
1	B	88	LEU
1	B	231	ALA
1	B	321	THR
1	C	232	ALA
1	D	86	TYR
1	D	88	LEU
1	D	232	ALA
1	A	152	ASN
1	B	152	ASN
1	B	153	GLY
1	B	230	GLY
1	C	321	PHE
1	C	322	THR
1	A	316	ASP
1	B	178	PRO
1	D	152	ASN
1	B	312	GLU
1	B	179	GLY
1	B	238	PRO
1	C	319	HIS
1	D	239	PRO
1	A	239	PRO
1	C	239	PRO
1	A	194	GLY

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	318/363 (88%)	314 (99%)	4 (1%)	65	78
1	B	323/363 (89%)	317 (98%)	6 (2%)	52	71
1	C	318/363 (88%)	308 (97%)	10 (3%)	35	60
1	D	312/363 (86%)	305 (98%)	7 (2%)	47	68
All	All	1271/1452 (88%)	1244 (98%)	27 (2%)	48	69

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

Mol	Chain	Res	Type
1	A	74	GLN
1	A	88	LEU
1	A	230	GLN
1	A	263	ILE
1	B	78	LYS
1	B	87	ASN
1	B	99	GLU
1	B	229	GLN
1	B	262	ILE
1	B	340	ARG
1	C	39	LYS
1	C	74	GLN
1	C	78	LYS
1	C	88	LEU
1	C	155	HIS
1	C	211	LYS
1	C	225	ILE
1	C	230	GLN
1	C	322	THR
1	C	386	LYS
1	D	78	LYS
1	D	230	GLN
1	D	240	GLU
1	D	263	ILE

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Mol	Chain	Res	Type
1	D	319	HIS
1	D	322	THR
1	D	341	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	91	GLN
1	A	134	HIS
1	A	143	HIS
1	A	152	ASN
1	A	230	GLN
1	A	431	HIS
1	B	74	GLN
1	B	143	HIS
1	B	229	GLN
1	B	318	HIS
1	B	452	GLN
1	C	41	GLN
1	C	87	ASN
1	C	134	HIS
1	C	143	HIS
1	C	183	HIS
1	C	230	GLN
1	C	431	HIS
1	C	453	GLN
1	D	134	HIS
1	D	152	ASN
1	D	230	GLN
1	D	431	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

13 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	503	-	4,4,4	0.38	0	6,6,6	0.07	0
2	SO4	D	502	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SO4	A	503	-	4,4,4	0.31	0	6,6,6	0.17	0
2	SO4	B	502	-	4,4,4	0.36	0	6,6,6	0.18	0
2	SO4	B	505	-	4,4,4	0.34	0	6,6,6	0.10	0
2	SO4	D	501	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	B	501	-	4,4,4	0.33	0	6,6,6	0.12	0
2	SO4	C	502	-	4,4,4	0.38	0	6,6,6	0.12	0
2	SO4	B	504	-	4,4,4	0.34	0	6,6,6	0.11	0
2	SO4	B	506	-	4,4,4	0.38	0	6,6,6	0.11	0
2	SO4	C	501	-	4,4,4	0.38	0	6,6,6	0.10	0
2	SO4	A	502	-	4,4,4	0.36	0	6,6,6	0.14	0
2	SO4	A	501	-	4,4,4	0.34	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	SO4	1	0
2	B	501	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	396/453 (87%)	-0.61	0 100 100	43, 65, 105, 185	0
1	B	402/453 (88%)	-0.52	2 (0%) 87 83	46, 69, 129, 199	0
1	C	397/453 (87%)	-0.34	2 (0%) 87 83	54, 87, 154, 207	0
1	D	390/453 (86%)	0.30	12 (3%) 51 44	74, 129, 187, 242	0
All	All	1585/1812 (87%)	-0.30	16 (1%) 79 71	43, 81, 166, 242	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	414	MET	3.2
1	D	153	GLY	3.2
1	D	403	CYS	2.9
1	D	127	THR	2.7
1	C	86	TYR	2.6
1	D	185	PRO	2.6
1	D	445	LEU	2.4
1	D	448	THR	2.4
1	D	412	LEU	2.4
1	D	402	ILE	2.3
1	D	317	PHE	2.3
1	B	84	PRO	2.2
1	B	156	GLY	2.1
1	D	227	GLU	2.1
1	C	83	LEU	2.0
1	D	187	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	D	502	5/5	0.73	0.07	167,173,191,209	0
2	SO4	D	501	5/5	0.74	0.14	164,177,188,190	0
2	SO4	B	504	5/5	0.78	0.10	143,144,149,149	0
2	SO4	A	501	5/5	0.81	0.09	108,133,141,162	0
2	SO4	B	506	5/5	0.82	0.12	174,183,190,206	0
2	SO4	B	503	5/5	0.83	0.08	130,149,158,171	0
2	SO4	C	502	5/5	0.87	0.10	120,123,130,131	0
2	SO4	A	503	5/5	0.87	0.14	94,104,107,111	0
2	SO4	A	502	5/5	0.87	0.10	111,121,142,143	0
2	SO4	B	505	5/5	0.88	0.13	111,122,128,148	0
2	SO4	B	501	5/5	0.89	0.21	107,117,137,159	0
2	SO4	C	501	5/5	0.91	0.10	109,109,116,121	0
2	SO4	B	502	5/5	0.91	0.13	100,129,137,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.