



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2025 – 06:35 PM JST

PDB ID : 9KAO / pdb_00009kao
Title : CTP synthetase of pseudomonas aeruginosa PAO1
Authors : Wang, C.C.
Deposited on : 2024-10-29
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

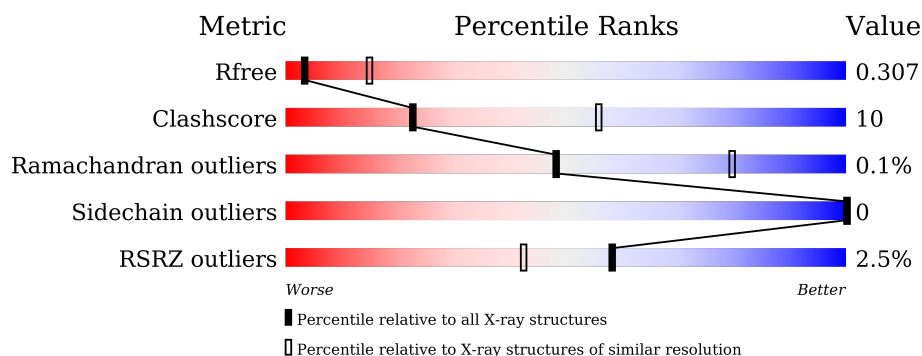
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	550	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 78% 20% . </div> </div>
1	B	550	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 1%, green 94%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 4% 72% 23% . </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8334 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 CTP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	542	Total	C	N	O	S	0	0	0
			4190	2632	736	804	18			
1	B	527	Total	C	N	O	S	0	0	0
			4085	2571	717	779	18			

There are 16 discrepancies between the modelled and reference sequences:

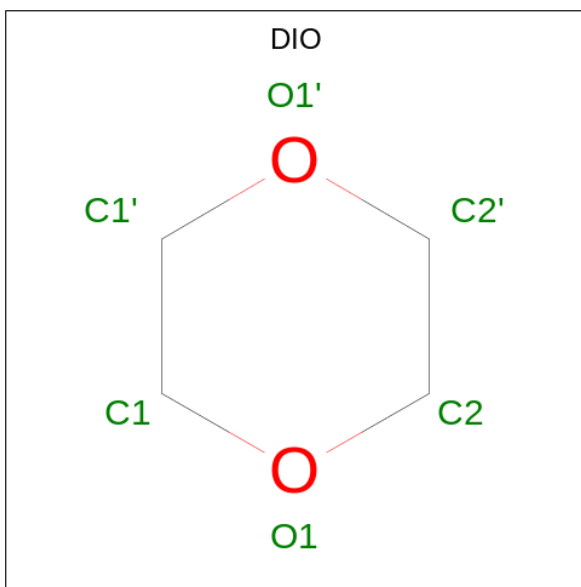
Chain	Residue	Modelled	Actual	Comment	Reference
A	543	HIS	-	expression tag	UNP Q9HXZ4
A	544	HIS	-	expression tag	UNP Q9HXZ4
A	545	HIS	-	expression tag	UNP Q9HXZ4
A	546	HIS	-	expression tag	UNP Q9HXZ4
A	547	HIS	-	expression tag	UNP Q9HXZ4
A	548	HIS	-	expression tag	UNP Q9HXZ4
A	549	HIS	-	expression tag	UNP Q9HXZ4
A	550	HIS	-	expression tag	UNP Q9HXZ4
B	543	HIS	-	expression tag	UNP Q9HXZ4
B	544	HIS	-	expression tag	UNP Q9HXZ4
B	545	HIS	-	expression tag	UNP Q9HXZ4
B	546	HIS	-	expression tag	UNP Q9HXZ4
B	547	HIS	-	expression tag	UNP Q9HXZ4
B	548	HIS	-	expression tag	UNP Q9HXZ4
B	549	HIS	-	expression tag	UNP Q9HXZ4
B	550	HIS	-	expression tag	UNP Q9HXZ4

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



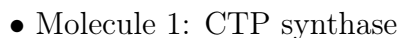
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: C₄H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	4	2		
3	A	1	Total	C	O	0	0
			6	4	2		
3	A	1	Total	C	O	0	0
			6	4	2		
3	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 1: CTP synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.66Å 143.66Å 194.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.08 – 3.20 35.08 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.9 (35.08-3.20) 95.8 (35.08-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.18Å)	Xtriage
Refinement program	PHENIX dev_5480	Depositor
R, R_{free}	0.283 , 0.308 0.283 , 0.307	Depositor DCC
R_{free} test set	2000 reflections (5.85%)	wwPDB-VP
Wilson B-factor (Å ²)	81.3	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8334	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.5061e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DIO, 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	0.19	0/4263	0.34	0/5777
1	B	0.14	0/4157	0.33	0/5632
All	All	0.17	0/8420	0.34	0/11409

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4190	0	4189	82	4
1	B	4085	0	4086	96	3
2	A	20	0	0	0	0
2	B	15	0	0	0	0
3	A	24	0	32	0	0
All	All	8334	0	8307	171	4

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 10.

All (171) 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:53:PRO:HD2	1:A:352:PHE:CZ	1.67	1.28
1:A:53:PRO:CD	1:A:352:PHE:CE1	2.21	1.24
1:A:44:ILE:HG13	1:B:112:VAL:HG13	1.24	1.17
1:A:53:PRO:HD3	1:A:352:PHE:CE1	1.86	1.10
1:A:53:PRO:HD2	1:A:352:PHE:CE1	1.91	0.98
1:A:160:ARG:NH2	1:A:165:ALA:HB2	1.82	0.94
1:B:520:THR:CG2	1:B:521:PRO:HD2	1.98	0.93
1:A:53:PRO:CD	1:A:352:PHE:CZ	2.45	0.93
1:B:520:THR:HG23	1:B:521:PRO:HD2	1.50	0.92
1:A:44:ILE:CG1	1:B:112:VAL:HG13	2.05	0.87
1:A:44:ILE:HG13	1:B:112:VAL:CG1	2.07	0.84
1:A:190:THR:HG21	1:A:223:ILE:HD11	1.60	0.82
1:B:190:THR:HG21	1:B:223:ILE:HD11	1.66	0.78
1:A:160:ARG:HH22	1:A:165:ALA:HB2	1.49	0.76
1:B:287:ARG:HB2	1:B:320:THR:HG23	1.68	0.74
1:B:28:LEU:HB3	1:B:33:LEU:HD12	1.68	0.74
1:B:294:VAL:HG21	1:B:363:THR:HG21	1.70	0.73
1:A:53:PRO:HD3	1:A:352:PHE:HE1	1.52	0.73
1:A:466:HIS:CD2	1:A:468:HIS:HE1	2.08	0.70
1:B:96:MET:HE3	1:B:100:ARG:HE	1.57	0.69
1:B:237:LEU:HD11	1:B:246:ILE:HG12	1.74	0.69
1:B:381:MET:HA	1:B:510:ALA:HB1	1.74	0.69
1:B:533:ASN:HA	1:B:536:LEU:HD12	1.75	0.69
1:A:41:ASP:HB2	1:A:90:THR:HG22	1.74	0.69
1:A:340:LEU:HD11	1:A:363:THR:HG23	1.73	0.68
1:B:381:MET:SD	1:B:512:GLN:HB2	2.34	0.67
1:B:466:HIS:HB3	1:B:468:HIS:CE1	2.30	0.67
1:A:347:LEU:HD11	1:A:375:LEU:HD23	1.76	0.66
1:A:405:LYS:HE2	1:A:429:THR:HA	1.75	0.65
1:A:287:ARG:HB2	1:A:320:THR:HG23	1.78	0.65
1:A:466:HIS:CD2	1:A:468:HIS:CE1	2.84	0.65
1:B:520:THR:HG22	1:B:521:PRO:HD2	1.77	0.65
1:A:197:LEU:HD23	1:A:204:PRO:HD3	1.79	0.64
1:B:520:THR:CG2	1:B:521:PRO:CD	2.76	0.61
1:B:171:MET:HG3	1:B:206:VAL:HB	1.82	0.61
1:B:41:ASP:HB2	1:B:90:THR:HG22	1.83	0.60
1:A:364:VAL:HG11	1:A:384:ALA:HA	1.85	0.59
1:B:243:ILE:HA	1:B:246:ILE:HD12	1.84	0.59
1:B:298:MET:HE3	1:B:298:MET:HA	1.85	0.58
1:A:278:VAL:HA	1:A:316:ILE:HD11	1.86	0.57
1:B:256:ASP:O	1:B:260:VAL:HG22	2.04	0.57
1:B:274:GLU:O	1:B:278:VAL:HG23	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:ARG:HB2	1:B:468:HIS:O	2.04	0.57
1:B:210:ARG:HD3	1:B:237:LEU:HD23	1.87	0.56
1:B:159:LEU:O	1:B:163:ILE:HG12	2.05	0.56
1:B:300:LEU:HD12	1:B:301:LEU:H	1.69	0.56
1:A:159:LEU:O	1:A:163:ILE:HG12	2.05	0.56
1:B:35:ILE:HD12	1:B:135:VAL:HB	1.88	0.56
1:B:520:THR:HG22	1:B:521:PRO:CD	2.36	0.56
1:A:381:MET:HA	1:A:510:ALA:HB1	1.87	0.55
1:A:35:ILE:HD12	1:A:135:VAL:HB	1.88	0.55
1:B:357:VAL:HG21	1:B:403:PHE:CE1	2.41	0.55
1:A:11:VAL:HG12	1:A:12:VAL:HG13	1.89	0.55
1:A:293:MET:HE2	1:A:298:MET:HE1	1.88	0.55
1:A:382:GLN:O	1:A:386:ILE:HG13	2.07	0.54
1:A:489:GLY:HA3	1:A:499:VAL:HG22	1.89	0.54
1:B:170:LEU:HB3	1:B:204:PRO:HA	1.89	0.54
1:A:414:LEU:HD12	1:A:432:SER:HB3	1.88	0.54
1:A:53:PRO:CG	1:A:352:PHE:CE1	2.90	0.54
1:B:24:LEU:O	1:B:28:LEU:HG	2.07	0.54
1:A:123:LYS:O	1:A:127:ILE:HG13	2.08	0.54
1:B:197:LEU:HD23	1:B:204:PRO:HD3	1.90	0.53
1:B:489:GLY:HA3	1:B:499:VAL:HG22	1.90	0.53
1:A:75:TYR:HB3	1:A:83:MET:HE3	1.89	0.52
1:B:75:TYR:HB3	1:B:83:MET:HE3	1.92	0.52
1:A:375:LEU:HA	1:A:509:VAL:O	2.09	0.52
1:B:314:ALA:HB2	1:B:528:PHE:HB3	1.91	0.52
1:B:357:VAL:HG21	1:B:403:PHE:CZ	2.44	0.51
1:A:314:ALA:HB2	1:A:528:PHE:HB3	1.93	0.51
1:A:415:ILE:HG22	1:A:419:GLN:HG3	1.92	0.51
1:A:38:LEU:HD21	1:A:129:GLY:HA3	1.92	0.51
1:B:40:LEU:HD11	1:B:126:ILE:HD11	1.91	0.51
1:B:118:ILE:O	1:B:122:ILE:HG13	2.10	0.51
1:A:160:ARG:NH1	1:A:165:ALA:N	2.59	0.51
1:B:123:LYS:O	1:B:127:ILE:HG13	2.11	0.51
1:A:194:VAL:HG11	1:A:227:THR:HB	1.93	0.50
1:B:72:LEU:O	1:B:75:TYR:HB2	2.11	0.50
1:B:90:THR:O	1:B:94:VAL:HG23	2.12	0.50
1:B:98:VAL:HG21	1:B:118:ILE:HD13	1.93	0.50
1:A:103:ARG:HH22	1:B:47:ASP:CG	2.20	0.49
1:A:53:PRO:HD2	1:A:352:PHE:HZ	1.61	0.49
1:B:112:VAL:HG23	1:B:117:HIS:CD2	2.48	0.49
1:B:287:ARG:HH11	1:B:536:LEU:HD13	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:VAL:HG21	1:B:384:ALA:HA	1.93	0.48
1:A:54:PHE:HE1	1:A:352:PHE:HE2	1.61	0.48
1:A:499:VAL:HG12	1:A:511:CYS:HA	1.95	0.48
1:B:466:HIS:HB3	1:B:468:HIS:HE1	1.76	0.48
1:B:28:LEU:HB2	1:B:35:ILE:HG13	1.94	0.48
1:A:3:ARG:HD3	1:A:263:PHE:HB3	1.96	0.48
1:A:77:ARG:HD3	1:A:313:HIS:HE1	1.78	0.48
1:A:96:MET:HB2	1:B:99:LEU:HD13	1.96	0.48
1:B:63:GLN:HB2	1:B:465:ARG:HH21	1.79	0.47
1:A:103:ARG:HA	1:A:103:ARG:HD3	1.62	0.47
1:A:375:LEU:HB2	1:A:507:TRP:HZ3	1.79	0.47
1:B:27:ILE:HG22	1:B:28:LEU:HD23	1.96	0.47
1:A:53:PRO:HG3	1:A:352:PHE:CD1	2.50	0.47
1:A:466:HIS:HD2	1:A:468:HIS:CE1	2.33	0.47
1:B:313:HIS:O	1:B:316:ILE:HG22	2.13	0.47
1:B:289:VAL:HG21	1:B:535:ALA:HB1	1.97	0.47
1:A:23:SER:O	1:A:27:ILE:HG13	2.16	0.46
1:A:148:GLU:HG2	1:B:113:GLN:OE1	2.15	0.46
1:B:414:LEU:HB2	1:B:470:TYR:HE1	1.79	0.46
1:A:73:GLY:O	1:A:77:ARG:HG3	2.16	0.46
1:A:405:LYS:HD3	1:A:429:THR:HG22	1.97	0.46
1:A:179:ILE:HG12	1:A:186:LYS:HG2	1.98	0.46
1:B:77:ARG:HD3	1:B:313:HIS:HE1	1.80	0.46
1:A:220:ARG:HA	1:A:223:ILE:HG22	1.98	0.46
1:B:511:CYS:HB2	1:B:513:PHE:CE1	2.51	0.46
1:B:27:ILE:HD11	1:B:247:PRO:O	2.15	0.45
1:B:291:ILE:HG12	1:B:345:ALA:HB3	1.99	0.45
1:B:414:LEU:HB2	1:B:470:TYR:CE1	2.51	0.45
1:B:360:LYS:O	1:B:364:VAL:HG12	2.17	0.45
1:B:516:GLU:HG2	1:B:517:PHE:CD1	2.52	0.45
1:A:335:GLN:HB2	1:A:339:LEU:HD11	1.99	0.45
1:B:97:ASP:O	1:B:101:LYS:HG3	2.16	0.45
1:A:98:VAL:HG21	1:A:118:ILE:HD13	1.99	0.45
1:B:174:THR:HG21	1:B:190:THR:HG23	1.98	0.45
1:A:499:VAL:HA	1:A:510:ALA:O	2.17	0.45
1:B:449:THR:HA	1:B:454:HIS:ND1	2.32	0.45
1:B:381:MET:SD	1:B:512:GLN:OE1	2.76	0.44
1:B:402:GLU:HG3	1:B:470:TYR:HE2	1.82	0.44
1:A:300:LEU:HD12	1:A:301:LEU:H	1.83	0.44
1:B:179:ILE:HG22	1:B:182:ALA:H	1.82	0.44
1:A:410:PRO:HG3	1:A:427:ILE:HD11	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:VAL:O	1:B:316:ILE:HD11	2.17	0.44
1:B:472:VAL:HB	1:B:497:VAL:HB	1.99	0.44
1:A:94:VAL:HG22	1:A:125:ARG:HE	1.83	0.44
1:A:293:MET:HG2	1:A:347:LEU:HB3	2.00	0.44
1:B:507:TRP:CD1	1:B:534:ALA:HB2	2.53	0.43
1:B:73:GLY:O	1:B:77:ARG:HG3	2.19	0.43
1:A:361:ILE:HD11	1:A:386:ILE:HB	2.00	0.43
1:B:38:LEU:HG	1:B:87:ASN:HA	2.00	0.43
1:B:51:MET:HE3	1:B:51:MET:HB2	1.89	0.43
1:B:375:LEU:HA	1:B:509:VAL:O	2.19	0.43
1:A:408:GLY:HA2	1:A:425:THR:OG1	2.18	0.43
1:A:63:GLN:OE1	1:A:82:THR:HG21	2.19	0.43
1:A:152:PHE:O	1:A:156:ILE:HG23	2.19	0.43
1:A:7:VAL:HG21	1:A:21:SER:HB2	2.00	0.42
1:A:294:VAL:HA	1:A:327:ILE:O	2.19	0.42
1:B:513:PHE:H	1:B:513:PHE:HD1	1.67	0.42
1:B:39:LYS:C	1:B:40:LEU:HD23	2.45	0.42
1:B:9:GLY:O	1:B:144:VAL:HG13	2.20	0.42
1:A:438:MET:HE2	1:A:438:MET:HB2	1.93	0.42
1:B:520:THR:HG22	1:B:521:PRO:N	2.35	0.42
1:A:210:ARG:HD2	1:A:237:LEU:O	2.19	0.41
1:A:427:ILE:HG22	1:A:429:THR:H	1.84	0.41
1:A:434:LEU:HB3	1:A:437:THR:HG23	2.01	0.41
1:B:443:GLN:HB3	1:B:466:HIS:CD2	2.55	0.41
1:B:330:GLU:O	1:B:334:GLN:HG3	2.19	0.41
1:B:466:HIS:ND1	1:B:513:PHE:HB3	2.35	0.41
1:A:207:LEU:HD23	1:A:207:LEU:HA	1.96	0.41
1:B:393:LEU:HD23	1:B:393:LEU:HA	1.86	0.41
1:B:438:MET:H	1:B:469:ARG:HG3	1.84	0.41
1:B:447:LEU:HD12	1:B:447:LEU:H	1.84	0.41
1:A:63:GLN:HG3	1:A:442:ALA:HB2	2.03	0.41
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.89	0.41
1:A:188:LYS:HE2	1:A:188:LYS:HB2	1.87	0.41
1:B:412:VAL:HG22	1:B:472:VAL:HA	2.02	0.41
1:A:446:GLN:HG2	1:A:491:SER:O	2.21	0.41
1:B:220:ARG:O	1:B:223:ILE:HG22	2.20	0.41
1:B:368:ARG:HE	1:B:368:ARG:HB2	1.77	0.41
1:B:292:ALA:HB2	1:B:343:VAL:HG11	2.02	0.40
1:B:23:SER:OG	1:B:246:ILE:HG22	2.21	0.40
1:B:72:LEU:HA	1:B:75:TYR:CD2	2.57	0.40
1:A:292:ALA:HB2	1:A:343:VAL:HG11	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ASP:HA	1:A:538:TYR:CD1	2.56	0.40
1:B:173:LEU:HG	1:B:208:VAL:HB	2.02	0.40
1:B:331:ASP:O	1:B:335:GLN:HB2	2.21	0.40
1:B:390:ARG:HG2	1:B:395:TRP:O	2.21	0.40
1:A:46:VAL:HB	1:B:103:ARG:CZ	2.52	0.40
1:A:54:PHE:HZ	1:A:297:TYR:CZ	2.40	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:NH2	1:A:482:GLN:NE2[4_545]	1.67	0.53
1:A:420:ASP:OD2	1:B:355:ARG:CD[3_444]	2.07	0.13
1:A:196:GLU:OE2	1:B:195:LYS:NZ[8_555]	2.12	0.08
1:A:195:LYS:NZ	1:B:196:GLU:OE2[8_555]	2.16	0.04

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	540/550 (98%)	521 (96%)	18 (3%)	1 (0%)	44	75
1	B	523/550 (95%)	506 (97%)	17 (3%)	0	100	100
All	All	1063/1100 (97%)	1027 (97%)	35 (3%)	1 (0%)	48	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	VAL

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	451/459 (98%)	451 (100%)	0	100	100
1	B	441/459 (96%)	441 (100%)	0	100	100
All	All	892/918 (97%)	892 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	313	HIS
1	A	335	GLN
1	A	468	HIS
1	A	474	ASN
1	B	313	HIS

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](#)

11 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	$\# Z > 2$
3	DIO	A	606	-	6,6,6	0.44	0	6,6,6	0.22	0
2	SO4	A	603	-	4,4,4	0.56	0	6,6,6	0.07	0
3	DIO	A	608	-	6,6,6	0.44	0	6,6,6	0.16	0
3	DIO	A	605	-	6,6,6	0.43	0	6,6,6	0.21	0
2	SO4	B	603	-	4,4,4	0.57	0	6,6,6	0.04	0
3	DIO	A	607	-	6,6,6	0.45	0	6,6,6	0.19	0
2	SO4	A	601	-	4,4,4	0.53	0	6,6,6	0.05	0
2	SO4	B	601	-	4,4,4	0.56	0	6,6,6	0.06	0
2	SO4	B	602	-	4,4,4	0.54	0	6,6,6	0.06	0
2	SO4	A	604	-	4,4,4	0.56	0	6,6,6	0.06	0
2	SO4	A	602	-	4,4,4	0.55	0	6,6,6	0.05	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	DIO	A	608	-	-	-	0/1/1/1
3	DIO	A	606	-	-	-	0/1/1/1
3	DIO	A	607	-	-	-	0/1/1/1
3	DIO	A	605	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	542/550 (98%)	0.10	7 (1%) 74 60	44, 67, 98, 151	0
1	B	527/550 (95%)	0.39	20 (3%) 44 30	62, 113, 159, 172	0
All	All	1069/1100 (97%)	0.25	27 (2%) 58 42	44, 82, 151, 172	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	528	PHE	4.0
1	A	445	CYS	3.7
1	B	294	VAL	3.7
1	A	542	ALA	3.7
1	B	295	GLY	3.7
1	B	415	ILE	3.3
1	A	425	THR	3.2
1	B	314	ALA	3.2
1	B	352	PHE	3.2
1	A	352	PHE	3.2
1	B	457	TYR	3.1
1	B	350	GLY	3.1
1	B	393	LEU	2.9
1	B	360	LYS	2.6
1	B	293	MET	2.4
1	B	500	VAL	2.3
1	B	502	ALA	2.2
1	A	533	ASN	2.2
1	B	400	SER	2.2
1	B	476	LEU	2.1
1	B	351	GLY	2.1
1	B	517	PHE	2.1
1	B	301	LEU	2.1
1	B	382	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	434	LEU	2.1
1	A	429	THR	2.1
1	A	537	LYS	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(Å ²)	Q<0.9
3	DIO	A	606	6/6	0.35	0.21	84,90,96,100	0
2	SO4	B	603	5/5	0.61	0.12	94,102,125,128	0
3	DIO	A	607	6/6	0.66	0.25	73,75,80,87	0
3	DIO	A	605	6/6	0.71	0.29	67,69,77,81	0
2	SO4	A	603	5/5	0.72	0.14	95,111,116,118	0
3	DIO	A	608	6/6	0.73	0.24	67,76,85,86	0
2	SO4	A	604	5/5	0.74	0.13	80,84,104,109	0
2	SO4	B	601	5/5	0.76	0.11	73,77,101,103	0
2	SO4	B	602	5/5	0.82	0.10	69,76,82,95	0
2	SO4	A	602	5/5	0.86	0.11	72,75,92,92	0
2	SO4	A	601	5/5	0.87	0.10	55,67,69,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.