



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:38 PM UTC

PDB ID : 4NA1 / pdb_00004na1
Title : Crystal Structure of the second ketosynthase from the bacillaene polyketide synthase
Authors : Gay, D.C.; Gay, G.R.; Keatinge-Clay, A.T.
Deposited on : 2013-10-21
Resolution : 1.95 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

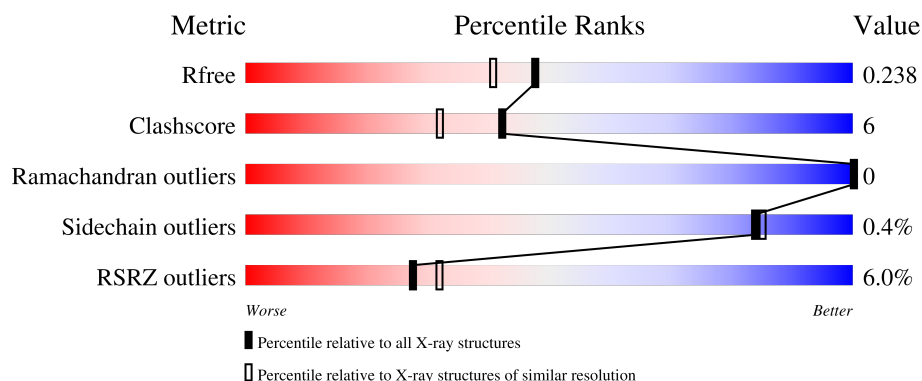
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	637	5% 81% 12% 6%
1	B	637	6% 79% 13% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9934 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 Polyketide synthase PksJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4659	2929	811	897	22			
1	B	591	Total	C	N	O	S	0	0	0
			4611	2901	808	880	22			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP P40806
A	-17	SER	-	expression tag	UNP P40806
A	-16	SER	-	expression tag	UNP P40806
A	-15	HIS	-	expression tag	UNP P40806
A	-14	HIS	-	expression tag	UNP P40806
A	-13	HIS	-	expression tag	UNP P40806
A	-12	HIS	-	expression tag	UNP P40806
A	-11	HIS	-	expression tag	UNP P40806
A	-10	HIS	-	expression tag	UNP P40806
A	-9	SER	-	expression tag	UNP P40806
A	-8	SER	-	expression tag	UNP P40806
A	-7	GLY	-	expression tag	UNP P40806
A	-6	LEU	-	expression tag	UNP P40806
A	-5	VAL	-	expression tag	UNP P40806
A	-4	PRO	-	expression tag	UNP P40806
A	-3	ARG	-	expression tag	UNP P40806
A	-2	GLY	-	expression tag	UNP P40806
A	-1	SER	-	expression tag	UNP P40806
A	0	SER	-	expression tag	UNP P40806
A	617	GLY	GLU	SEE REMARK 999	UNP P40806
B	-18	GLY	-	expression tag	UNP P40806
B	-17	SER	-	expression tag	UNP P40806
B	-16	SER	-	expression tag	UNP P40806
B	-15	HIS	-	expression tag	UNP P40806
B	-14	HIS	-	expression tag	UNP P40806

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP P40806
B	-12	HIS	-	expression tag	UNP P40806
B	-11	HIS	-	expression tag	UNP P40806
B	-10	HIS	-	expression tag	UNP P40806
B	-9	SER	-	expression tag	UNP P40806
B	-8	SER	-	expression tag	UNP P40806
B	-7	GLY	-	expression tag	UNP P40806
B	-6	LEU	-	expression tag	UNP P40806
B	-5	VAL	-	expression tag	UNP P40806
B	-4	PRO	-	expression tag	UNP P40806
B	-3	ARG	-	expression tag	UNP P40806
B	-2	GLY	-	expression tag	UNP P40806
B	-1	SER	-	expression tag	UNP P40806
B	0	SER	-	expression tag	UNP P40806
B	617	GLY	GLU	SEE REMARK 999	UNP P40806

- 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	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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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		

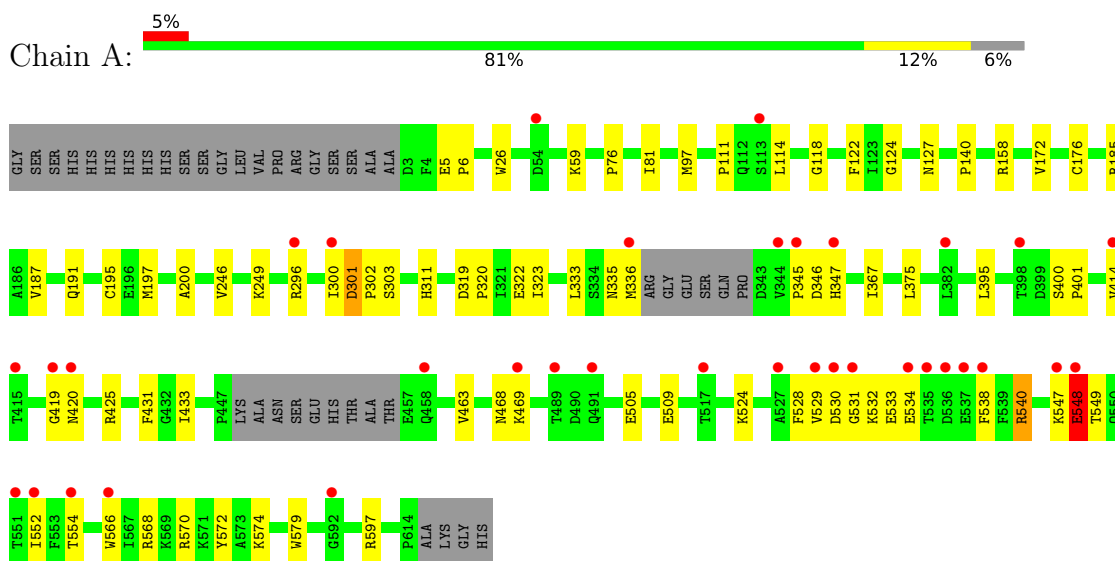
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	330	Total	O	0	0
			330	330		
3	B	304	Total	O	0	0
			304	304		

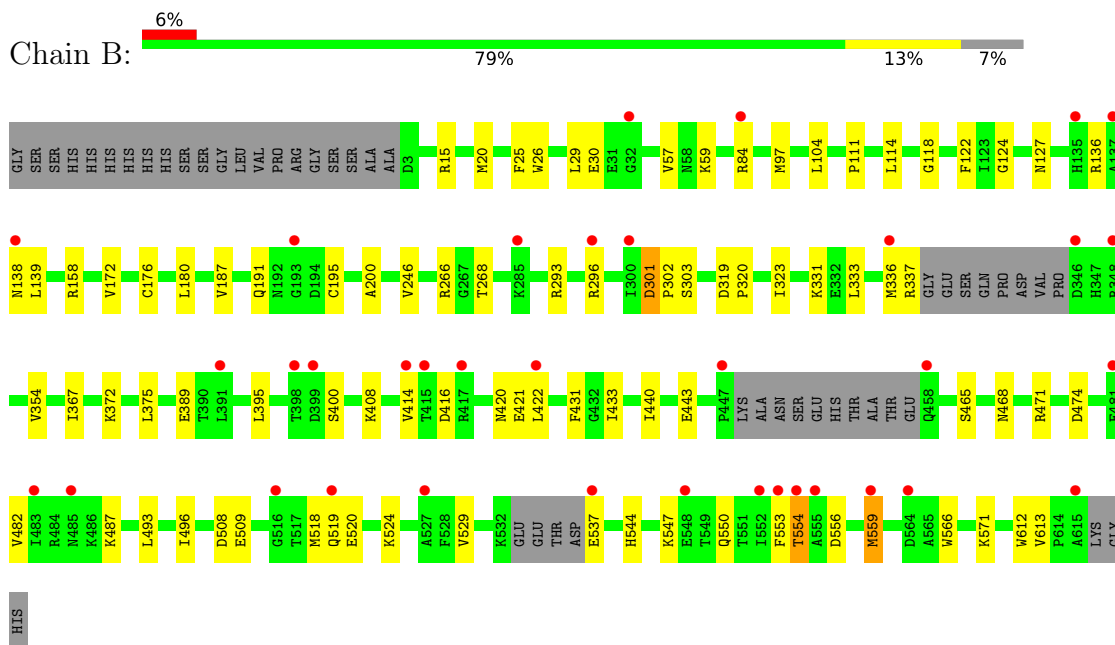
3 Residue-property plots [i](#)

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: Polyketide synthase PksJ



• Molecule 1: Polyketide synthase PksJ



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.86Å 113.09Å 96.48Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	30.71 – 1.95 30.71 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.71-1.95) 98.9 (30.71-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.210 , 0.240 0.208 , 0.238	Depositor DCC
R_{free} test set	5862 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.1	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	0.96	EDS
Total number of atoms	9934	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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 32.34 % 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 9.5427e-04. 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: 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	0.72	0/4759	0.91	6/6442 (0.1%)
1	B	0.74	0/4709	0.89	6/6370 (0.1%)
All	All	0.73	0/9468	0.90	12/12812 (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	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	549	THR	N-CA-C	-13.86	96.08	113.55
1	A	548	GLU	CB-CA-C	-10.31	95.21	110.06
1	B	301	ASP	CA-C-N	7.57	128.25	119.47
1	B	301	ASP	C-N-CA	7.57	128.25	119.47
1	A	419	GLY	N-CA-C	6.02	122.77	115.31
1	B	553	PHE	N-CA-C	5.90	120.17	112.92
1	B	554	THR	N-CA-C	5.80	118.94	109.59
1	B	547	LYS	N-CA-C	-5.60	106.29	113.23
1	A	420	ASN	N-CA-C	5.51	118.22	109.24
1	A	301	ASP	CA-C-N	5.43	125.77	119.47
1	A	301	ASP	C-N-CA	5.43	125.77	119.47
1	B	559	MET	CG-SD-CE	-5.12	89.64	100.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	548	GLU	Mainchain

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	4659	0	4550	50	1
1	B	4611	0	4518	67	1
2	A	10	0	0	1	0
2	B	20	0	0	0	0
3	A	330	0	0	7	0
3	B	304	0	0	9	0
All	All	9934	0	9068	116	1

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 (116) 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:296:ARG:NH2	1:A:336:MET:O	2.08	0.86
1:B:301:ASP:OD1	1:B:337:ARG:NH1	2.11	0.83
1:A:531:GLY:HA3	1:A:532:LYS:C	2.04	0.82
1:B:301:ASP:OD2	1:B:303:SER:OG	1.96	0.81
1:A:301:ASP:OD2	1:A:303:SER:OG	2.02	0.74
1:B:111:PRO:HG2	3:B:1066:HOH:O	1.87	0.74
1:A:547:LYS:O	1:A:548:GLU:HB2	1.89	0.72
1:B:296:ARG:NH1	1:B:336:MET:SD	2.60	0.72
1:A:414:VAL:HG22	3:A:951:HOH:O	1.92	0.69
1:A:127:ASN:OD1	1:B:127:ASN:ND2	2.30	0.65
1:A:469:LYS:HE2	3:A:1006:HOH:O	1.97	0.64
2:A:702:SO4:O1	3:A:1042:HOH:O	2.14	0.63
1:A:323:ILE:HG13	1:A:395:LEU:HD22	1.82	0.62
1:B:496:ILE:HD12	1:B:518:MET:HE1	1.82	0.62
1:B:331:LYS:NZ	3:B:968:HOH:O	2.20	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:SER:HB2	1:A:401:PRO:HD2	1.83	0.60
1:A:118:GLY:O	1:A:195:CYS:HB2	2.02	0.59
1:A:548:GLU:O	1:A:552:ILE:HG13	2.01	0.59
1:B:268:THR:HG22	1:B:440:ILE:HG12	1.86	0.58
1:A:300:ILE:HD12	1:A:425:ARG:HD3	1.86	0.58
1:B:26:TRP:HB2	1:B:375:LEU:HD13	1.85	0.57
1:B:139:LEU:CD1	1:B:613:VAL:HG13	2.34	0.57
1:A:468:ASN:HA	1:A:509:GLU:HG3	1.86	0.57
1:A:319:ASP:HB2	1:A:320:PRO:HD3	1.88	0.56
1:B:468:ASN:HA	1:B:509:GLU:HG3	1.88	0.55
1:A:566:TRP:CE2	1:A:574:LYS:HE3	2.42	0.55
1:B:176:CYS:HB2	1:B:431:PHE:O	2.06	0.55
1:A:122:PHE:CD1	1:A:185:ARG:HG2	2.42	0.54
1:B:266:ARG:NH1	1:B:443:GLU:OE1	2.41	0.54
1:A:528:PHE:CE1	1:A:540:ARG:HD2	2.43	0.54
1:A:531:GLY:CA	1:A:532:LYS:C	2.80	0.54
1:B:296:ARG:NH2	1:B:336:MET:HB2	2.22	0.53
1:B:84:ARG:HG3	3:B:1034:HOH:O	2.08	0.53
1:B:187:VAL:O	1:B:191:GLN:HG2	2.08	0.53
1:A:524:LYS:NZ	3:A:995:HOH:O	2.40	0.53
1:B:180:LEU:HG	1:B:440:ILE:HD12	1.90	0.53
1:A:246:VAL:HG13	1:A:367:ILE:HD11	1.90	0.52
1:B:519:GLN:OE1	1:B:519:GLN:N	2.43	0.52
1:B:400:SER:O	3:B:1070:HOH:O	2.19	0.52
1:A:176:CYS:HB2	1:A:431:PHE:O	2.10	0.51
1:B:136:ARG:C	1:B:138:ASN:H	2.18	0.51
1:B:139:LEU:HD11	1:B:613:VAL:HG13	1.93	0.51
1:B:537:GLU:N	1:B:537:GLU:OE1	2.44	0.51
1:A:124:GLY:HA2	1:A:172:VAL:O	2.11	0.51
1:A:335:ASN:O	1:A:336:MET:HB2	2.10	0.51
1:B:57:VAL:O	1:B:59:LYS:HG2	2.11	0.51
1:B:550:GLN:O	1:B:554:THR:OG1	2.18	0.51
1:B:118:GLY:O	1:B:195:CYS:HB2	2.11	0.50
1:A:530:ASP:HB2	1:A:533:GLU:OE1	2.10	0.50
1:B:414:VAL:HG23	1:B:422:LEU:HD12	1.94	0.50
1:B:508:ASP:OD2	1:B:544:HIS:ND1	2.42	0.50
1:B:139:LEU:HD11	1:B:613:VAL:CG1	2.42	0.50
1:A:187:VAL:O	1:A:191:GLN:HG2	2.13	0.49
1:B:471:ARG:NH1	1:B:474:ASP:OD1	2.45	0.49
1:B:389:GLU:CD	3:B:1079:HOH:O	2.56	0.49
1:B:97:MET:SD	1:B:158:ARG:HD2	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:CYS:SG	1:B:433:ILE:HG23	2.54	0.48
1:A:176:CYS:SG	1:A:433:ILE:HG23	2.54	0.47
1:B:554:THR:O	3:B:1041:HOH:O	2.20	0.47
1:B:296:ARG:HH21	1:B:333:LEU:HA	1.80	0.47
1:B:482:VAL:CG2	1:B:487:LYS:HD2	2.45	0.47
1:B:15:ARG:NH2	1:B:20:MET:HE3	2.30	0.46
1:B:508:ASP:CG	1:B:544:HIS:HD1	2.23	0.46
1:A:597:ARG:NH2	3:A:1042:HOH:O	2.48	0.46
1:A:347:HIS:ND1	3:A:992:HOH:O	2.20	0.46
1:A:302:PRO:HG3	1:A:333:LEU:HB3	1.98	0.45
1:B:612:TRP:CG	1:B:613:VAL:H	2.35	0.45
1:A:463:VAL:HB	1:A:579:TRP:CH2	2.50	0.45
1:B:246:VAL:HG13	1:B:367:ILE:HD11	1.98	0.45
1:A:463:VAL:HB	1:A:579:TRP:CZ3	2.51	0.45
1:B:293:ARG:HD2	3:B:1045:HOH:O	2.17	0.45
1:A:528:PHE:HE1	1:A:540:ARG:HD2	1.81	0.45
1:A:534:GLU:OE1	1:A:534:GLU:N	2.50	0.45
1:B:389:GLU:OE1	3:B:1079:HOH:O	2.21	0.45
1:A:122:PHE:O	1:A:200:ALA:HA	2.18	0.44
1:A:538:PHE:CD1	1:A:538:PHE:C	2.96	0.44
1:B:30:GLU:OE2	1:B:408:LYS:NZ	2.42	0.44
1:A:59:LYS:NZ	3:A:957:HOH:O	2.50	0.44
1:B:30:GLU:O	1:B:408:LYS:HE2	2.18	0.44
1:B:559:MET:HE2	1:B:559:MET:N	2.33	0.44
1:B:416:ASP:OD1	1:B:420:ASN:N	2.48	0.43
1:B:559:MET:HE2	1:B:559:MET:HA	2.00	0.43
1:B:319:ASP:HB2	1:B:320:PRO:HD3	1.99	0.43
1:B:520:GLU:HG2	1:B:524:LYS:HE3	2.01	0.43
1:A:97:MET:SD	1:A:158:ARG:HD2	2.58	0.43
1:B:302:PRO:HG3	1:B:333:LEU:HB3	2.00	0.43
1:B:122:PHE:O	1:B:200:ALA:HA	2.18	0.43
1:A:26:TRP:HB2	1:A:375:LEU:HD13	2.00	0.43
1:B:296:ARG:HE	1:B:333:LEU:HD23	1.84	0.43
1:B:465:SER:HA	1:B:509:GLU:O	2.18	0.43
1:A:111:PRO:CG	1:A:505:GLU:HB2	2.49	0.43
1:B:421:GLU:OE1	1:B:421:GLU:N	2.43	0.42
1:B:471:ARG:HA	1:B:471:ARG:HD3	1.90	0.42
1:B:124:GLY:HA2	1:B:172:VAL:O	2.18	0.42
1:B:559:MET:HE2	1:B:559:MET:CA	2.49	0.42
1:A:5:GLU:HA	1:A:6:PRO:HD2	1.91	0.42
1:B:468:ASN:CA	1:B:509:GLU:HG3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:MET:HG2	1:A:249:LYS:HG2	2.01	0.42
1:A:554:THR:O	1:A:554:THR:HG22	2.20	0.42
1:A:570:ARG:HB3	1:A:572:TYR:CZ	2.54	0.42
1:B:25:PHE:O	1:B:29:LEU:HG	2.20	0.42
1:B:104:LEU:HD22	1:B:114:LEU:HD11	2.02	0.42
1:B:493:LEU:O	1:B:493:LEU:HG	2.19	0.42
1:B:566:TRP:CD1	1:B:571:LYS:HD2	2.55	0.42
1:B:354:VAL:HB	1:B:372:LYS:HD3	2.02	0.41
1:B:520:GLU:O	1:B:524:LYS:HG3	2.19	0.41
1:A:531:GLY:HA3	1:A:532:LYS:HB2	2.02	0.41
1:B:556:ASP:N	3:B:982:HOH:O	2.51	0.41
1:B:323:ILE:HG13	1:B:395:LEU:HD22	2.03	0.41
1:A:76:PRO:HB2	1:A:81:ILE:O	2.21	0.41
1:A:568:ARG:HH11	1:A:568:ARG:HG2	1.85	0.41
1:A:111:PRO:HG3	1:A:505:GLU:HB2	2.03	0.41
1:A:345:PRO:O	1:A:346:ASP:HB2	2.20	0.41
1:B:493:LEU:HD12	1:B:518:MET:HE2	2.03	0.41
1:A:140:PRO:HB3	1:B:57:VAL:HG13	2.02	0.40
1:A:311:HIS:N	1:A:322:GLU:OE2	2.53	0.40

All (1) 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:566:TRP:CZ2	1:B:559:MET:CE[1_454]	2.01	0.19

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	591/637 (93%)	577 (98%)	14 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	583/637 (92%)	566 (97%)	17 (3%)	0	100	100
All	All	1174/1274 (92%)	1143 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	497/527 (94%)	494 (99%)	3 (1%)	78	79
1	B	490/527 (93%)	489 (100%)	1 (0%)	87	89
All	All	987/1054 (94%)	983 (100%)	4 (0%)	84	85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	LEU
1	A	529	VAL
1	A	540	ARG
1	B	529	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	347	HIS
1	A	409	GLN
1	A	437	ASN
1	A	501	GLN
1	A	526	GLN
1	A	588	ASN
1	B	92	GLN
1	B	204	ASN

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Mol	Chain	Res	Type
1	B	437	ASN
1	B	501	GLN
1	B	526	GLN
1	B	588	ASN

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](#)

6 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	701	-	4,4,4	0.21	0	6,6,6	0.23	0
2	SO4	A	701	-	4,4,4	0.38	0	6,6,6	0.31	0
2	SO4	B	704	-	4,4,4	0.31	0	6,6,6	0.56	0
2	SO4	B	703	-	4,4,4	0.38	0	6,6,6	0.11	0
2	SO4	A	702	-	4,4,4	0.29	0	6,6,6	0.19	0
2	SO4	B	702	-	4,4,4	0.29	0	6,6,6	0.20	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	A	702	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	597/637 (93%)	0.38	35 (5%) 28 32	24, 38, 71, 95	0
1	B	591/637 (92%)	0.45	36 (6%) 27 31	24, 40, 63, 98	0
All	All	1188/1274 (93%)	0.41	71 (5%) 27 32	24, 39, 67, 98	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	554	THR	5.8
1	A	535	THR	5.3
1	B	559	MET	4.7
1	A	548	GLU	4.4
1	B	458	GLN	4.3
1	A	536	ASP	4.3
1	A	552	ILE	4.3
1	A	566	TRP	4.2
1	B	346	ASP	4.0
1	B	300	ILE	3.8
1	A	414	VAL	3.8
1	B	615	ALA	3.7
1	B	417	ARG	3.4
1	B	84	ARG	3.3
1	A	458	GLN	3.3
1	B	553	PHE	3.2
1	B	336	MET	3.2
1	A	592	GLY	3.2
1	A	336	MET	3.1
1	A	534	GLU	3.1
1	A	527	ALA	3.1
1	B	135	HIS	3.1
1	A	529	VAL	3.1
1	A	530	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	447	PRO	3.0
1	A	345	PRO	3.0
1	B	137	ALA	2.9
1	B	399	ASP	2.9
1	A	419	GLY	2.9
1	B	32	GLY	2.9
1	B	415	THR	2.9
1	B	537	GLU	2.9
1	B	398	THR	2.8
1	A	517	THR	2.7
1	A	537	GLU	2.6
1	B	481	GLU	2.6
1	B	548	GLU	2.6
1	B	348	ARG	2.6
1	A	344	VAL	2.6
1	A	554	THR	2.5
1	B	296	ARG	2.5
1	B	138	ASN	2.5
1	B	485	ASN	2.5
1	B	391	LEU	2.5
1	A	113	SER	2.5
1	A	547	LYS	2.4
1	A	415	THR	2.4
1	B	516	GLY	2.4
1	A	491	GLN	2.3
1	A	398	THR	2.3
1	A	489	THR	2.3
1	A	296	ARG	2.2
1	A	54	ASP	2.2
1	B	527	ALA	2.2
1	B	555	ALA	2.2
1	A	420	ASN	2.2
1	A	531	GLY	2.2
1	A	538	PHE	2.2
1	A	551	THR	2.2
1	B	193	GLY	2.1
1	B	519	GLN	2.1
1	A	300	ILE	2.1
1	A	469	LYS	2.1
1	B	564	ASP	2.1
1	B	552	ILE	2.0
1	A	347	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	382	LEU	2.0
1	B	422	LEU	2.0
1	B	285	LYS	2.0
1	B	483	ILE	2.0
1	B	414	VAL	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
2	SO4	B	702	5/5	0.79	0.12	68,70,73,87	0
2	SO4	B	703	5/5	0.82	0.12	42,54,69,72	0
2	SO4	B	704	5/5	0.83	0.12	44,49,66,67	0
2	SO4	B	701	5/5	0.89	0.07	55,68,69,70	0
2	SO4	A	702	5/5	0.89	0.07	64,67,75,81	0
2	SO4	A	701	5/5	0.90	0.08	38,46,61,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.