



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:41 PM UTC

PDB ID : 6P1J / pdb_00006p1j
Title : The structure of condensation and adenylation domains of teixobactin-producing nonribosomal peptide synthetase Txo2 serine module
Authors : Tan, K.; Zhou, M.; Jedrzejczak, R.; Babnigg, G.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2019-05-20
Resolution : 2.95 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

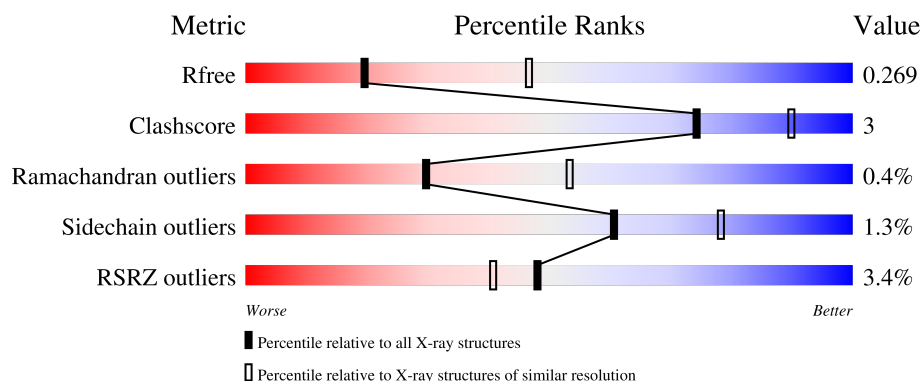
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

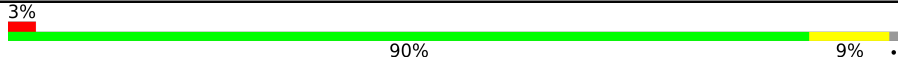
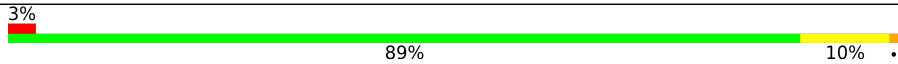
The reported resolution of this entry is 2.95 Å.

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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	964	
1	B	964	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 15057 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.

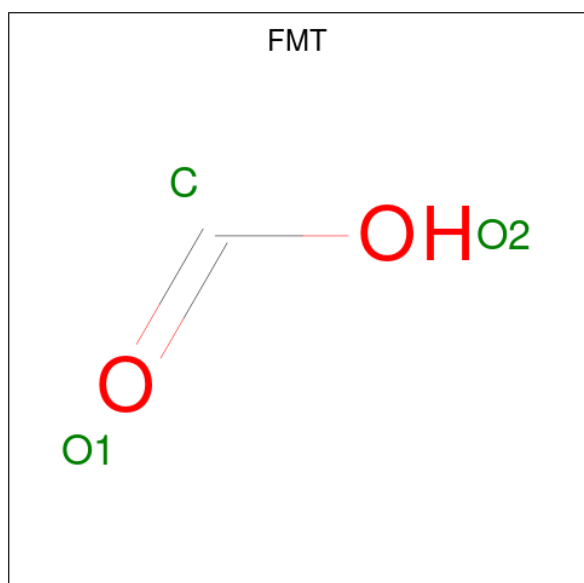
- Molecule 1 is a protein called Txo2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	958	Total	C	N	O	S	0	1	0
			7432	4692	1363	1354	23			
1	B	957	Total	C	N	O	S	0	2	0
			7444	4698	1364	1359	23			

There are 6 discrepancies between the modelled and reference sequences:

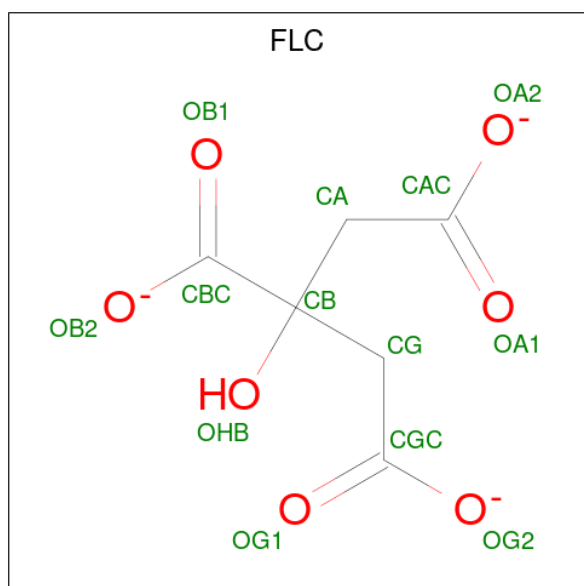
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	SER	-	expression tag	UNP A0A0B5H0S3
A	43	ASN	-	expression tag	UNP A0A0B5H0S3
A	44	ALA	-	expression tag	UNP A0A0B5H0S3
B	42	SER	-	expression tag	UNP A0A0B5H0S3
B	43	ASN	-	expression tag	UNP A0A0B5H0S3
B	44	ALA	-	expression tag	UNP A0A0B5H0S3

- Molecule 2 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



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

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).

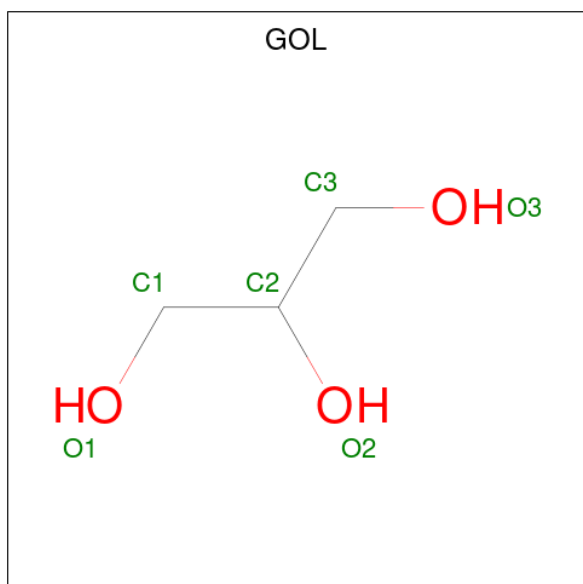


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

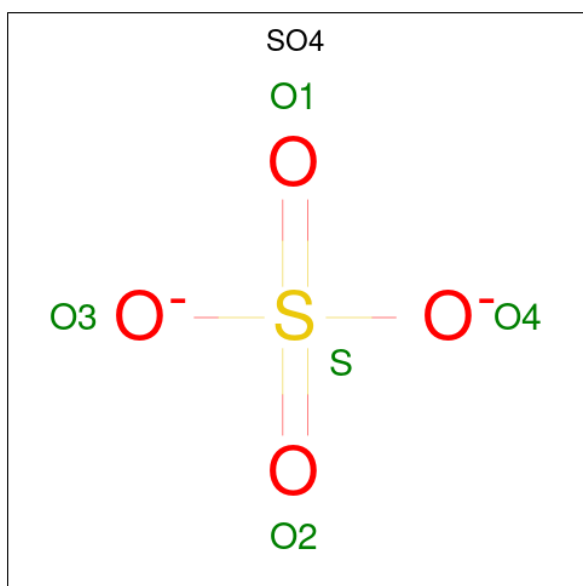
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	Cl	0	0
			6	6		
5	B	13	Total	Cl	0	0
			13	13		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

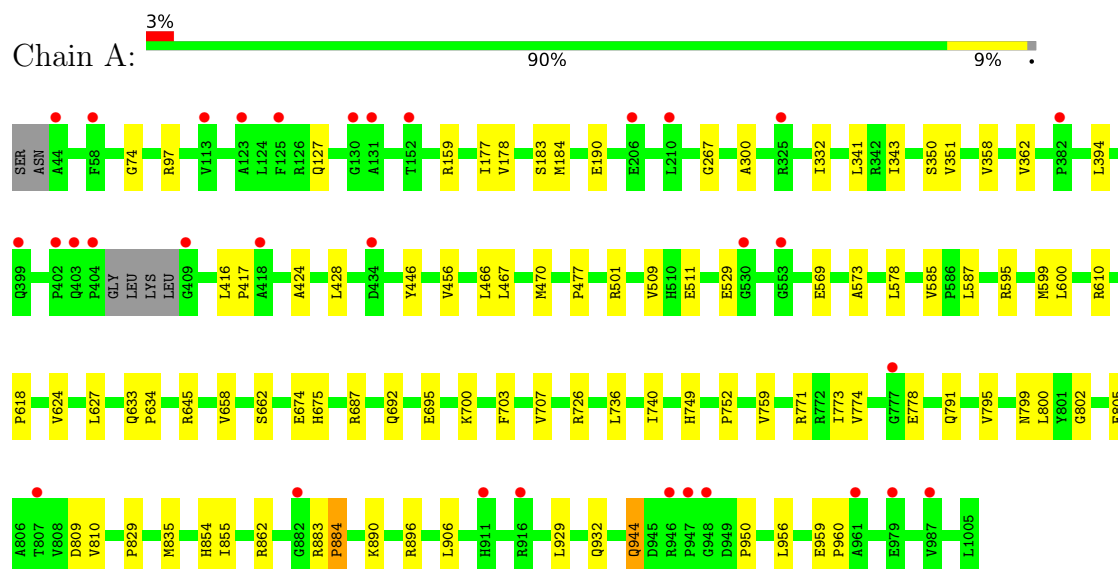
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	37	Total O 37 37	0	0
8	B	40	Total O 40 40	0	0

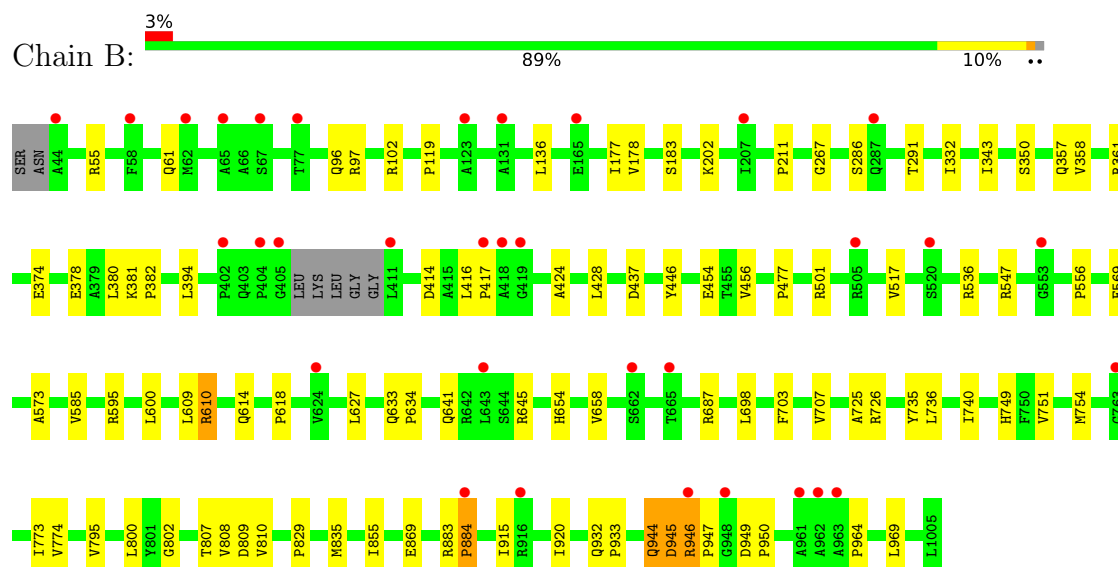
3 Residue-property plots [i](#)

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: Txo2



• Molecule 1: Txo2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	110.86Å 399.88Å 144.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.20 – 2.95 47.20 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.5 (47.20-2.95) 97.4 (47.20-2.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.96Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.226 , 0.267 0.228 , 0.269	Depositor DCC
R_{free} test set	3249 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	58.8	Xtrriage
Anisotropy	0.717	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15057	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.17 % 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 1.1893e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, FLC, ACT, CL, FMT

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	0.09	0/7599	0.29	0/10345
1	B	0.09	0/7611	0.28	0/10361
All	All	0.09	0/15210	0.29	0/20706

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 [i](#)

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	7432	0	7410	49	0
1	B	7444	0	7424	44	0
2	A	3	0	1	0	0
2	B	12	0	4	0	0
3	A	13	0	5	0	0
3	B	13	0	5	1	0
4	A	4	0	3	0	0
5	A	6	0	0	0	0
5	B	13	0	0	0	0
6	A	30	0	40	0	0
7	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	37	0	0	0	0
8	B	40	0	0	0	0
All	All	15057	0	14892	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 3.

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:547:ARG:NH1	1:B:641:GLN:O	2.29	0.66
1:A:127:GLN:OE1	1:A:159:ARG:NH1	2.34	0.61
1:B:610:ARG:HD3	1:B:614:GLN:HB2	1.82	0.60
1:B:97:ARG:NH2	1:B:211:PRO:O	2.36	0.58
1:B:177:ILE:HG23	1:B:178:VAL:HG13	1.85	0.58
1:A:343:ILE:HD12	1:A:358:VAL:HG22	1.86	0.56
1:A:959:GLU:HG3	1:A:960:PRO:HD2	1.87	0.56
1:B:573:ALA:HB2	1:B:627:LEU:HD11	1.86	0.56
1:A:341:LEU:HD22	1:A:362:VAL:HG22	1.88	0.56
1:A:183:SER:HB3	1:A:332:ILE:HG23	1.88	0.55
1:A:573:ALA:HB2	1:A:627:LEU:HD11	1.88	0.55
1:A:569:GLU:HB3	1:A:627:LEU:HG	1.88	0.54
1:B:774:VAL:HG13	1:B:800:LEU:HD13	1.89	0.54
1:A:600:LEU:HD21	1:A:618:PRO:HB3	1.90	0.54
1:A:511:GLU:OE2	1:A:645:ARG:NH1	2.42	0.53
1:B:569:GLU:N	1:B:569:GLU:OE1	2.42	0.53
1:A:529:GLU:OE2	1:A:726:ARG:NE	2.38	0.53
1:B:883:ARG:HB3	1:B:884:PRO:HD2	1.90	0.53
1:A:466:LEU:HG	1:A:470:MET:HE2	1.91	0.52
1:B:183:SER:HB3	1:B:332:ILE:HG23	1.90	0.52
1:B:609:LEU:HB3	1:B:627:LEU:HD13	1.91	0.52
1:A:692:GLN:HB2	1:A:695:GLU:HG3	1.90	0.51
1:B:374:GLU:O	1:B:378:GLU:HG2	2.09	0.51
1:A:707:VAL:HG11	1:A:749:HIS:CE1	2.45	0.51
1:A:633:GLN:N	1:A:634:PRO:HD2	2.24	0.51
1:A:774:VAL:HG13	1:A:800:LEU:HD13	1.91	0.51
1:A:736:LEU:O	1:A:740:ILE:HG12	2.12	0.50
1:A:267:GLY:HA3	1:A:424:ALA:HB2	1.93	0.50
1:A:467:LEU:HA	1:A:470:MET:HE3	1.94	0.49
1:A:569:GLU:OE1	1:A:569:GLU:N	2.45	0.49
1:B:751:VAL:HG22	1:B:754:MET:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:LEU:HD12	1:B:417:PRO:HD2	1.95	0.48
1:B:915:ILE:HG12	1:B:920:ILE:HG13	1.95	0.48
1:A:177:ILE:HG23	1:A:178:VAL:HG23	1.94	0.48
1:A:585:VAL:HG22	1:A:658:VAL:HB	1.95	0.48
1:A:810:VAL:HG21	1:A:855:ILE:HD13	1.96	0.48
1:B:517:VAL:HG12	1:B:536:ARG:HH21	1.79	0.48
1:A:350:SER:HA	1:A:477:PRO:HA	1.96	0.47
1:A:416:LEU:HD12	1:A:417:PRO:HD2	1.96	0.47
1:A:446:TYR:CG	1:A:456:VAL:HG21	2.49	0.47
1:B:357:GLN:HG2	1:B:361:ARG:HD2	1.97	0.47
1:B:698:LEU:HD11	1:B:725:ALA:HB2	1.97	0.47
1:B:810:VAL:HG21	1:B:855:ILE:HD13	1.96	0.47
1:A:929:LEU:HD23	1:A:956:LEU:HD11	1.97	0.47
1:A:351:VAL:HG13	1:A:470:MET:HG2	1.97	0.47
1:B:726:ARG:HG2	1:B:735:TYR:CZ	2.49	0.47
1:A:394:LEU:HD22	1:A:428:LEU:HB2	1.96	0.47
1:B:707:VAL:HG11	1:B:749:HIS:CE1	2.49	0.46
1:B:932:GLN:HG2	1:B:969:LEU:HD23	1.97	0.46
1:A:773:ILE:HG13	1:A:795:VAL:HG21	1.97	0.46
1:B:633:GLN:N	1:B:634:PRO:HD2	2.31	0.46
1:B:350:SER:HA	1:B:477:PRO:HA	1.97	0.46
1:B:446:TYR:CG	1:B:456:VAL:HG21	2.50	0.45
1:B:394:LEU:HD22	1:B:428:LEU:HB2	1.97	0.45
1:A:805:GLU:OE1	1:A:805:GLU:N	2.46	0.45
1:A:883:ARG:HB3	1:A:884:PRO:HD2	1.98	0.45
1:B:585:VAL:HG22	1:B:658:VAL:HB	1.98	0.45
1:A:595:ARG:HG3	1:A:599:MET:HE2	1.99	0.44
1:B:736:LEU:O	1:B:740:ILE:HG12	2.17	0.44
1:B:829:PRO:HB3	1:B:835:MET:HG2	1.99	0.44
1:A:74:GLY:HA3	1:A:184:MET:HE2	1.98	0.44
1:B:932:GLN:HG3	1:B:933:PRO:HD2	1.98	0.44
1:A:695:GLU:OE2	1:A:771:ARG:NH2	2.50	0.44
1:A:829:PRO:HB3	1:A:835:MET:HG2	2.00	0.43
1:A:759:VAL:HG13	1:A:791:GLN:HG3	2.01	0.43
1:B:437:ASP:OD1	1:B:437:ASP:N	2.50	0.43
1:B:600:LEU:HD21	1:B:618:PRO:HB3	2.01	0.43
1:A:944:GLN:HG3	1:A:950:PRO:HB3	2.00	0.43
1:A:854:HIS:NE2	1:A:890:LYS:HG2	2.33	0.42
1:A:501:ARG:NH1	1:A:687:ARG:HH11	2.17	0.42
1:B:773:ILE:HG13	1:B:795:VAL:HG21	2.00	0.42
1:B:501:ARG:NH2	1:B:687:ARG:HH11	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:802:GLY:HA3	1:B:809:ASP:HA	2.01	0.42
1:B:944:GLN:OE1	1:B:950:PRO:HB3	2.19	0.42
1:B:964:PRO:HB2	1:B:969:LEU:HD11	2.02	0.42
1:B:556:PRO:HB3	1:B:654:HIS:CE1	2.55	0.42
1:A:300:ALA:CB	1:A:470:MET:HE1	2.50	0.42
1:B:267:GLY:HA3	1:B:424:ALA:HB2	2.01	0.41
1:A:802:GLY:HA3	1:A:809:ASP:HA	2.02	0.41
1:B:343:ILE:HD12	1:B:358:VAL:HG22	2.01	0.41
1:A:610:ARG:NH1	1:A:624:VAL:HG21	2.35	0.41
1:B:869:GLU:HB2	3:B:1105:FLC:CAC	2.51	0.41
1:A:752:PRO:HD2	1:A:778:GLU:HB2	2.03	0.41
1:B:96:GLN:O	1:B:102:ARG:NH1	2.54	0.41
1:B:945:ASP:HB3	1:B:946:ARG:H	1.62	0.41
1:A:896:ARG:HD3	1:A:906:LEU:HD11	2.03	0.41
1:A:674:GLU:OE2	1:A:862:ARG:HD3	2.21	0.40
1:B:380:LEU:HB3	1:B:382:PRO:HD2	2.02	0.40
1:A:97:ARG:NE	1:A:190:GLU:OE2	2.53	0.40
1:A:587:LEU:HD22	1:A:599:MET:HE3	2.03	0.40
1:B:286:SER:HB3	1:B:291:THR:O	2.20	0.40
1:A:509:VAL:HG22	1:A:675:HIS:ND1	2.36	0.40
1:A:509:VAL:HG23	1:A:578:LEU:HD13	2.04	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	955/964 (99%)	927 (97%)	27 (3%)	1 (0%)	48	72
1	B	955/964 (99%)	924 (97%)	25 (3%)	6 (1%)	21	45
All	All	1910/1928 (99%)	1851 (97%)	52 (3%)	7 (0%)	30	53

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	884	PRO
1	B	807	THR
1	B	808	VAL
1	B	884	PRO
1	B	119	PRO
1	B	945	ASP
1	B	947	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	755/762 (99%)	749 (99%)	6 (1%)	73	85
1	B	758/762 (100%)	744 (98%)	14 (2%)	51	72
All	All	1513/1524 (99%)	1493 (99%)	20 (1%)	61	78

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	662	SER
1	A	700	LYS
1	A	703	PHE
1	A	799	ASN
1	A	932	GLN
1	A	944	GLN
1	B	55	ARG
1	B	61	GLN
1	B	136	LEU
1	B	202	LYS
1	B	381	LYS
1	B	414	ASP
1	B	454	GLU
1	B	595	ARG
1	B	610	ARG
1	B	645	ARG

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Mol	Chain	Res	Type
1	B	703	PHE
1	B	944	GLN
1	B	946	ARG
1	B	949	ASP

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	53	GLN
1	A	98	HIS
1	A	164	ASN
1	A	490	HIS
1	A	680	ASN
1	A	699	GLN
1	A	791	GLN
1	A	859	GLN
1	B	53	GLN
1	B	369	GLN
1	B	490	HIS
1	B	633	GLN
1	B	680	ASN
1	B	699	GLN
1	B	832	ASN
1	B	859	GLN

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

Of 34 ligands modelled in this entry, 19 are monoatomic - leaving 15 for Mogul analysis.

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$
6	GOL	A	1114	-	5,5,5	0.93	0	5,5,5	1.09	0
2	FMT	B	1103	-	2,2,2	0.74	0	1,1,1	0.23	0
6	GOL	A	1112	-	5,5,5	0.93	0	5,5,5	1.08	0
4	ACT	A	1103	-	3,3,3	1.39	1 (33%)	3,3,3	1.35	0
3	FLC	A	1102	-	12,12,12	1.13	0	17,17,17	1.38	1 (5%)
7	SO4	A	1116	-	4,4,4	0.23	0	6,6,6	0.06	0
3	FLC	B	1105	-	12,12,12	1.14	0	17,17,17	1.38	1 (5%)
2	FMT	A	1101	-	2,2,2	0.74	0	1,1,1	0.23	0
6	GOL	A	1111	-	5,5,5	0.96	0	5,5,5	1.06	0
2	FMT	B	1102	-	2,2,2	0.74	0	1,1,1	0.24	0
6	GOL	A	1110	-	5,5,5	0.92	0	5,5,5	1.09	0
2	FMT	B	1104	-	2,2,2	0.75	0	1,1,1	0.24	0
6	GOL	A	1113	-	5,5,5	0.94	0	5,5,5	1.06	0
7	SO4	A	1115	-	4,4,4	0.23	0	6,6,6	0.07	0
2	FMT	B	1101	-	2,2,2	0.73	0	1,1,1	0.23	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
6	GOL	A	1114	-	-	2/4/4/4	-
6	GOL	A	1112	-	-	0/4/4/4	-
3	FLC	A	1102	-	-	7/16/16/16	-
3	FLC	B	1105	-	-	11/16/16/16	-
6	GOL	A	1111	-	-	0/4/4/4	-
6	GOL	A	1110	-	-	0/4/4/4	-
6	GOL	A	1113	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1103	ACT	CH3-C	2.01	1.57	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1102	FLC	OB2-CBC-CB	3.54	119.93	113.14
3	B	1105	FLC	OB2-CBC-CB	3.49	119.83	113.14

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1114	GOL	C1-C2-C3-O3
3	B	1105	FLC	CA-CB-CG-CGC
6	A	1114	GOL	O2-C2-C3-O3
3	B	1105	FLC	CBC-CB-CG-CGC
3	A	1102	FLC	CA-CB-CG-CGC
3	B	1105	FLC	OHB-CB-CBC-OB1
3	B	1105	FLC	CB-CA-CAC-OA1
3	A	1102	FLC	CBC-CB-CG-CGC
3	B	1105	FLC	CB-CA-CAC-OA2
3	B	1105	FLC	CA-CB-CBC-OB1
3	B	1105	FLC	CA-CB-CBC-OB2
3	B	1105	FLC	CG-CB-CBC-OB2
3	B	1105	FLC	OHB-CB-CBC-OB2
3	B	1105	FLC	CG-CB-CBC-OB1
3	B	1105	FLC	OHB-CB-CG-CGC
3	A	1102	FLC	CG-CB-CBC-OB1
3	A	1102	FLC	CG-CB-CBC-OB2
3	A	1102	FLC	CA-CB-CBC-OB1
3	A	1102	FLC	CB-CA-CAC-OA1
3	A	1102	FLC	OHB-CB-CG-CGC

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1105	FLC	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	958/964 (99%)	0.30	32 (3%)	49 42	26, 68, 116, 166	1 (0%)
1	B	957/964 (99%)	0.30	33 (3%)	48 41	28, 68, 115, 168	2 (0%)
All	All	1915/1928 (99%)	0.30	65 (3%)	48 41	26, 68, 116, 168	3 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	ALA	4.6
1	A	131	ALA	4.3
1	B	418	ALA	4.2
1	A	404	PRO	4.1
1	B	405	GLY	4.1
1	A	946	ARG	3.6
1	A	409	GLY	3.6
1	B	419	GLY	3.5
1	B	946	ARG	3.5
1	A	553	GLY	3.4
1	A	961	ALA	3.3
1	A	44	ALA	3.2
1	A	911	HIS	3.2
1	B	402	PRO	3.2
1	B	417	PRO	3.2
1	A	403	GLN	3.1
1	A	807	THR	3.1
1	B	884	PRO	3.1
1	B	553	GLY	3.1
1	B	404	PRO	3.1
1	B	963	ALA	3.1
1	B	662	SER	3.0
1	B	65	ALA	3.0
1	A	418	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	882	GLY	2.9
1	A	402	PRO	2.9
1	B	962	ALA	2.9
1	A	125	PHE	2.8
1	B	207	ILE	2.8
1	B	948	GLY	2.8
1	A	916	ARG	2.7
1	A	987	VAL	2.7
1	A	947	PRO	2.6
1	A	434	ASP	2.6
1	B	520	SER	2.5
1	A	530	GLY	2.5
1	A	777	GLY	2.5
1	B	131	ALA	2.5
1	B	961	ALA	2.5
1	A	130	GLY	2.4
1	A	325	ARG	2.3
1	B	165	GLU	2.3
1	B	67	SER	2.3
1	A	979	GLU	2.3
1	B	44	ALA	2.3
1	A	113	VAL	2.3
1	A	152	THR	2.2
1	B	58	PHE	2.2
1	B	643	LEU	2.2
1	B	624	VAL	2.2
1	B	665	THR	2.2
1	A	948	GLY	2.2
1	B	505	ARG	2.1
1	A	58	PHE	2.1
1	B	916	ARG	2.1
1	A	206	GLU	2.1
1	A	399	GLN	2.1
1	B	287	GLN	2.1
1	B	763	GLY	2.1
1	B	77	THR	2.0
1	A	382	PRO	2.0
1	A	210	LEU	2.0
1	B	411	LEU	2.0
1	B	123	ALA	2.0
1	B	62	MET	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	FMT	B	1102	3/3	0.61	0.18	74,74,76,79	0
6	GOL	A	1114	6/6	0.73	0.23	46,76,85,95	0
5	CL	B	1113	1/1	0.75	0.35	89,89,89,89	0
7	SO4	A	1116	5/5	0.75	0.23	109,111,115,117	5
2	FMT	A	1101	3/3	0.76	0.17	75,75,82,82	0
4	ACT	A	1103	4/4	0.77	0.20	51,57,57,62	0
6	GOL	A	1112	6/6	0.78	0.18	62,75,81,85	0
5	CL	B	1106	1/1	0.80	0.16	77,77,77,77	0
7	SO4	A	1115	5/5	0.81	0.19	121,124,128,132	0
2	FMT	B	1104	3/3	0.81	0.22	64,64,72,73	0
6	GOL	A	1113	6/6	0.82	0.19	55,62,76,77	0
6	GOL	A	1111	6/6	0.82	0.19	47,77,89,90	0
5	CL	B	1107	1/1	0.83	0.21	75,75,75,75	0
5	CL	B	1108	1/1	0.86	0.17	91,91,91,91	0
2	FMT	B	1103	3/3	0.86	0.14	51,51,55,56	0
6	GOL	A	1110	6/6	0.86	0.14	41,58,68,70	0
5	CL	A	1109	1/1	0.87	0.10	53,53,53,53	0
5	CL	A	1106	1/1	0.87	0.24	99,99,99,99	0
5	CL	A	1107	1/1	0.87	0.13	83,83,83,83	0
5	CL	B	1114	1/1	0.88	0.09	83,83,83,83	0
5	CL	B	1117	1/1	0.89	0.12	74,74,74,74	0
5	CL	A	1108	1/1	0.89	0.27	105,105,105,105	0
2	FMT	B	1101	3/3	0.90	0.15	51,51,60,63	0
5	CL	A	1105	1/1	0.91	0.09	76,76,76,76	0
5	CL	B	1118	1/1	0.91	0.15	85,85,85,85	0
3	FLC	A	1102	13/13	0.91	0.09	44,52,71,75	0
5	CL	B	1112	1/1	0.92	0.17	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FLC	B	1105	13/13	0.92	0.08	46,53,70,73	0
5	CL	B	1109	1/1	0.93	0.08	64,64,64,64	0
5	CL	B	1110	1/1	0.94	0.19	91,91,91,91	0
5	CL	A	1104	1/1	0.94	0.06	69,69,69,69	0
5	CL	B	1116	1/1	0.94	0.06	72,72,72,72	0
5	CL	B	1111	1/1	0.95	0.08	70,70,70,70	1
5	CL	B	1115	1/1	0.96	0.13	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.