



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:22 AM UTC

PDB ID : 4KTY / pdb_00004kty
Title : Fibrin-stabilizing factor with a bound ligand
Authors : Stieler, M.; Heine, A.; Klebe, G.
Deposited on : 2013-05-21
Resolution : 1.98 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

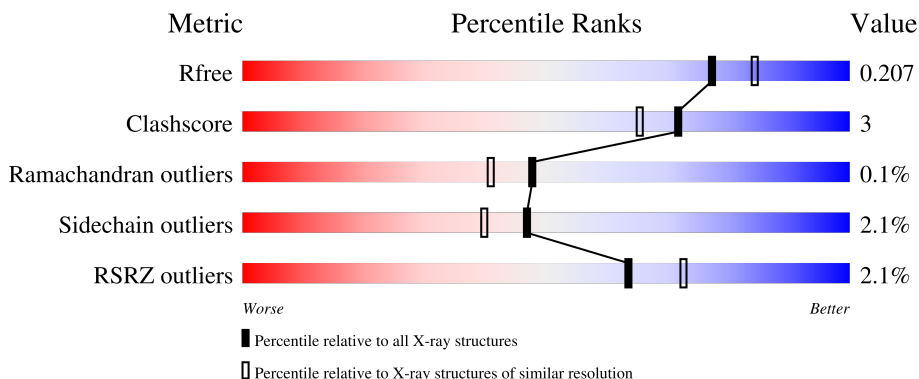
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	738	2% 86% 7% 6%
1	B	738	2% 86% 8% 5%
2	C	9	78% 11% 11%
2	D	9	67% 22% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12087 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 Coagulation factor XIII A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	695	Total	C	N	O	S	0	12	0
			5458	3476	919	1037	26			
1	B	698	Total	C	N	O	S	0	10	0
			5496	3501	925	1043	27			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP P00488
A	-5	HIS	-	expression tag	UNP P00488
A	-4	HIS	-	expression tag	UNP P00488
A	-3	HIS	-	expression tag	UNP P00488
A	-2	HIS	-	expression tag	UNP P00488
A	-1	HIS	-	expression tag	UNP P00488
A	0	HIS	-	expression tag	UNP P00488
A	649	ILE	THR	engineered mutation	UNP P00488
A	651	GLU	GLN	engineered mutation	UNP P00488
B	-6	MET	-	expression tag	UNP P00488
B	-5	HIS	-	expression tag	UNP P00488
B	-4	HIS	-	expression tag	UNP P00488
B	-3	HIS	-	expression tag	UNP P00488
B	-2	HIS	-	expression tag	UNP P00488
B	-1	HIS	-	expression tag	UNP P00488
B	0	HIS	-	expression tag	UNP P00488
B	649	ILE	THR	engineered mutation	UNP P00488
B	651	GLU	GLN	engineered mutation	UNP P00488

- Molecule 2 is a protein called Peptide-like ligand.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			74	51	9	14			

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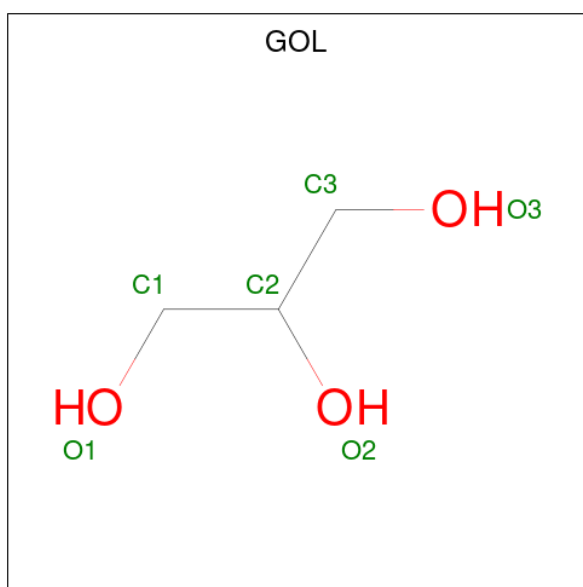
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	9	Total	C	N	O	0	0	0
			74	51	9	14			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		
3	B	3	Total	Ca	0	0
			3	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	435	Total	O	0	0
			435	435		
6	B	474	Total	O	0	0
			474	474		
6	C	4	Total	O	0	0
			4	4		
6	D	7	Total	O	0	0
			7	7		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.76Å 80.51Å 102.84Å 88.14° 76.70° 82.01°	Depositor
Resolution (Å)	20.80 – 1.98 20.80 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.9 (20.80-1.98) 97.0 (20.80-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 1.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.169 , 0.206 0.170 , 0.207	Depositor DCC
R_{free} test set	5985 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12087	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 38.20 % 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 3.8237e-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: DAS, NLE, ABA, GOL, SO4, ACY, CA, 1TX

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	0.56	0/5619	0.80	3/7657 (0.0%)
1	B	0.59	0/5656	0.79	3/7705 (0.0%)
2	C	0.79	0/40	1.13	0/55
2	D	0.76	0/40	1.35	0/55
All	All	0.58	0/11355	0.80	6/15472 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	669	GLY	CA-C-N	6.65	128.15	119.84
1	A	669	GLY	C-N-CA	6.65	128.15	119.84
1	B	274	VAL	N-CA-C	6.43	117.18	110.62
1	B	329	GLY	CA-C-N	-5.78	118.67	122.60
1	B	329	GLY	C-N-CA	-5.78	118.67	122.60
1	A	674	ARG	N-CA-C	-5.08	103.76	109.60

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	5458	0	5163	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5496	0	5220	34	0
2	C	74	0	67	2	0
2	D	74	0	67	4	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	36	0	48	5	0
4	B	18	0	24	0	0
5	B	5	0	0	0	0
6	A	435	0	0	3	0
6	B	474	0	0	3	0
6	C	4	0	0	1	0
6	D	7	0	0	1	0
All	All	12087	0	10589	72	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 (72) 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:565:LYS:HD2	1:A:599:LEU:HD11	1.74	0.70
1:A:637:ARG:NH2	1:A:692:GLU:OE2	2.29	0.66
1:B:43[A]:GLU:OE2	6:B:1374:HOH:O	2.13	0.65
1:B:651:GLU:OE1	1:B:690:GLN:NE2	2.30	0.65
1:B:549:ILE:HB	1:B:575:VAL:HG12	1.80	0.64
1:B:245:ALA:HB2	1:B:265:MET:HG3	1.80	0.62
1:B:93:ASP:HB3	1:B:96:ARG:HG2	1.83	0.60
1:A:231:GLU:HG3	1:A:296:VAL:HG21	1.83	0.60
1:A:445:LYS:HB2	1:A:449:THR:HG23	1.84	0.59
1:B:489:GLU:OE2	1:B:489:GLU:N	2.36	0.58
1:B:136[B]:MET:HB2	1:B:143:ARG:HB3	1.87	0.56
1:B:529:LEU:HD13	1:B:629:ILE:HG23	1.87	0.56
1:A:92:TYR:O	1:A:137:ARG:NH2	2.29	0.56
1:A:673:THR:OG1	1:A:674:ARG:O	2.22	0.55
1:A:18:ASN:HD22	1:A:18:ASN:C	2.15	0.55
1:B:314:CYS:HB3	2:D:3:1TX:C25	2.37	0.54
1:B:539:PHE:HB3	1:B:577:LEU:HD11	1.90	0.54
1:B:245:ALA:HB2	1:B:265:MET:CG	2.38	0.53
1:B:697:PRO:HB2	1:B:725:ILE:HD13	1.90	0.52
1:A:524:VAL:HG11	1:A:625:THR:HG21	1.91	0.52
1:A:245:ALA:HB2	1:A:265:MET:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PHE:CD1	4:A:805:GOL:H11	2.47	0.49
1:B:439:LEU:HD11	1:B:459:HIS:CD2	2.48	0.49
1:B:669:GLY:HA3	1:B:705:LEU:HD23	1.95	0.49
1:B:189:GLU:HA	1:B:194:TYR:CG	2.48	0.48
1:A:565:LYS:HE3	1:A:599:LEU:HD21	1.96	0.48
1:A:673:THR:HB	1:A:695:CYS:SG	2.54	0.48
1:A:314:CYS:HB3	2:C:3:1TX:C25	2.44	0.47
1:A:529:LEU:HD23	1:A:629[A]:ILE:HG23	1.95	0.47
1:A:421:HIS:HD2	6:A:1273:HOH:O	1.96	0.47
1:A:396:ASP:HB3	1:A:409:CYS:HB3	1.97	0.47
1:A:68:LYS:HE3	1:A:230:PHE:CE2	2.50	0.47
1:A:126:GLN:O	1:A:147:GLN:NE2	2.48	0.47
1:B:341:ALA:HB2	1:B:460:ILE:HD12	1.97	0.46
1:B:459:HIS:CE1	2:D:9:PRO:HG3	2.50	0.46
1:A:220:ILE:HD13	1:A:474:MET:SD	2.56	0.46
1:B:222:THR:HG21	6:B:1184:HOH:O	2.16	0.46
1:A:174:ARG:NH2	4:A:807:GOL:H12	2.30	0.45
1:B:398:THR:HG21	2:D:3:1TX:H13	1.98	0.45
1:A:223[A]:ARG:NH1	6:A:1087:HOH:O	2.50	0.45
1:A:444:ALA:HA	1:A:450:HIS:HD2	1.82	0.45
1:A:301:GLU:OE1	4:A:806:GOL:H31	2.17	0.45
1:A:222:THR:HG21	6:A:1309:HOH:O	2.17	0.44
1:B:704:LYS:NZ	1:B:720:GLU:HB2	2.32	0.44
2:C:1:ACY:O	6:C:104:HOH:O	2.20	0.44
1:B:664:TRP:CE2	1:B:679:MET:HG3	2.53	0.44
1:A:591:ALA:HA	1:A:594:TYR:CE1	2.53	0.43
1:B:195:LEU:HD13	1:B:379:TRP:CE2	2.53	0.43
1:A:310:ARG:H	4:A:806:GOL:C3	2.31	0.43
1:B:231:GLU:HG3	1:B:296:VAL:HG21	2.01	0.43
1:A:189:GLU:HA	1:A:194:TYR:CG	2.54	0.43
1:A:541:ASN:HB2	1:A:577:LEU:HD13	2.01	0.42
1:B:489:GLU:H	1:B:489:GLU:CD	2.26	0.42
1:B:342:HIS:CD2	1:B:342:HIS:C	2.98	0.42
1:A:245:ALA:HB2	1:A:265:MET:CG	2.49	0.42
1:A:310:ARG:H	4:A:806:GOL:H32	1.85	0.42
1:B:558[B]:THR:HG23	1:B:603:SER:HB2	2.01	0.41
2:D:2:DAS:HB2	6:D:107:HOH:O	2.19	0.41
1:A:539:PHE:HB3	1:A:577:LEU:HD11	2.01	0.41
1:B:68:LYS:HE3	1:B:230:PHE:CE2	2.55	0.41
1:B:154:VAL:HG21	1:B:184:PHE:CD2	2.55	0.41
1:B:213:PHE:CD1	1:B:222:THR:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ARG:HA	1:A:311:TYR:HA	1.93	0.41
1:A:558:THR:HG22	1:A:559:PHE:O	2.20	0.41
1:B:541:ASN:HB2	1:B:577:LEU:HD13	2.02	0.41
1:B:310:ARG:HA	1:B:311:TYR:HA	1.84	0.41
1:B:642:VAL:HA	1:B:643:GLY:HA2	1.79	0.41
1:A:235:LEU:HA	1:A:327:CYS:SG	2.61	0.40
1:A:93:ASP:HB3	1:A:96:ARG:HG2	2.04	0.40
1:A:490:GLU:OE1	1:A:491[B]:ARG:HD2	2.21	0.40
1:B:421:HIS:HE1	6:B:1310:HOH:O	2.04	0.40
1:B:591:ALA:HA	1:B:594:TYR:CE1	2.55	0.40

There are no symmetry-related clashes.

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	701/738 (95%)	683 (97%)	17 (2%)	1 (0%)	48	41
1	B	702/738 (95%)	682 (97%)	19 (3%)	1 (0%)	48	41
2	C	3/9 (33%)	3 (100%)	0	0	100	100
2	D	3/9 (33%)	3 (100%)	0	0	100	100
All	All	1409/1494 (94%)	1371 (97%)	36 (3%)	2 (0%)	48	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	669	GLY
1	B	669	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	578/651 (89%)	563 (97%)	15 (3%)	40	32
1	B	587/651 (90%)	576 (98%)	11 (2%)	50	44
2	C	4/4 (100%)	4 (100%)	0	100	100
2	D	4/4 (100%)	4 (100%)	0	100	100
All	All	1173/1310 (90%)	1147 (98%)	26 (2%)	47	38

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	100	ARG
1	A	216	GLU
1	A	217	VAL
1	A	223[A]	ARG
1	A	223[B]	ARG
1	A	231	GLU
1	A	348	LEU
1	A	360	VAL
1	A	491[A]	ARG
1	A	491[B]	ARG
1	A	499	MET
1	A	524	VAL
1	A	599	LEU
1	A	617	ASP
1	B	23	GLU
1	B	46	ASN
1	B	123	SER
1	B	269	LYS
1	B	387	VAL
1	B	450	HIS
1	B	575	VAL
1	B	577	LEU
1	B	599	LEU

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Mol	Chain	Res	Type
1	B	668	ASP
1	B	725	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	246	GLN
1	A	344	ASN
1	A	421	HIS
1	A	450	HIS
1	A	545	ASN
1	A	640	GLN
1	A	662	ASN
1	A	724	GLN
1	B	313	GLN
1	B	344	ASN
1	B	421	HIS
1	B	459	HIS
1	B	545	ASN
1	B	640	GLN
1	B	666	HIS
1	B	716	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	NLE	D	5	2	6,7,8	0.48	0	2,7,9	0.56	0
2	1TX	C	3	1,2	10,11,12	1.29	1 (10%)	7,12,14	1.40	1 (14%)
2	ABA	C	4	2	4,5,6	0.64	0	1,5,7	0.87	0
2	1TX	D	3	1,2	10,11,12	1.35	1 (10%)	7,12,14	1.46	1 (14%)
2	ABA	D	4	2	4,5,6	0.72	0	1,5,7	0.33	0
2	NLE	C	5	2	6,7,8	0.54	0	2,7,9	0.32	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
2	NLE	D	5	2	-	0/5/6/8	-
2	1TX	C	3	1,2	-	1/10/11/13	-
2	ABA	C	4	2	-	1/3/4/6	-
2	1TX	D	3	1,2	-	1/10/11/13	-
2	ABA	D	4	2	-	0/3/4/6	-
2	NLE	C	5	2	-	3/5/6/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	1TX	O14-C25	3.80	1.44	1.33
2	C	3	1TX	O14-C25	3.71	1.44	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	1TX	C22-C23-C24	-2.30	104.67	113.13
2	D	3	1TX	C22-C23-C24	-2.29	104.72	113.13

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	5	NLE	N-CA-CB-CG
2	C	5	NLE	C-CA-CB-CG
2	D	3	1TX	C22-C23-C24-C25
2	C	3	1TX	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
2	C	5	NLE	CA-CB-CG-CD
2	C	4	ABA	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	1TX	1	0
2	D	3	1TX	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	$\# Z > 2$
4	GOL	A	807	-	5,5,5	0.35	0	5,5,5	0.42	0
4	GOL	A	804	-	5,5,5	0.58	0	5,5,5	0.65	0
4	GOL	B	805	-	5,5,5	0.41	0	5,5,5	0.48	0
4	GOL	A	809	-	5,5,5	0.35	0	5,5,5	0.31	0
4	GOL	B	806	-	5,5,5	0.28	0	5,5,5	0.91	0
4	GOL	A	808	-	5,5,5	0.39	0	5,5,5	0.31	0
4	GOL	A	805	-	5,5,5	0.45	0	5,5,5	0.47	0
4	GOL	B	804	-	5,5,5	0.25	0	5,5,5	0.53	0
5	SO4	B	807	-	4,4,4	0.22	0	6,6,6	0.29	0
4	GOL	A	806	-	5,5,5	0.34	0	5,5,5	0.64	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
4	GOL	A	807	-	-	2/4/4/4	-
4	GOL	A	804	-	-	2/4/4/4	-
4	GOL	B	805	-	-	2/4/4/4	-
4	GOL	A	809	-	-	4/4/4/4	-
4	GOL	B	806	-	-	0/4/4/4	-
4	GOL	A	808	-	-	0/4/4/4	-
4	GOL	A	805	-	-	2/4/4/4	-
4	GOL	B	804	-	-	2/4/4/4	-
4	GOL	A	806	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	805	GOL	C1-C2-C3-O3
4	A	807	GOL	C1-C2-C3-O3
4	A	809	GOL	O1-C1-C2-O2
4	A	809	GOL	C1-C2-C3-O3
4	B	804	GOL	O1-C1-C2-C3
4	B	805	GOL	O1-C1-C2-C3
4	A	804	GOL	O1-C1-C2-C3
4	A	806	GOL	O1-C1-C2-C3
4	A	809	GOL	O1-C1-C2-C3
4	B	804	GOL	O1-C1-C2-O2
4	A	805	GOL	O2-C2-C3-O3
4	A	807	GOL	O2-C2-C3-O3
4	B	805	GOL	O1-C1-C2-O2
4	A	809	GOL	O2-C2-C3-O3
4	A	804	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	807	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	805	GOL	1	0
4	A	806	GOL	3	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	695/738 (94%)	-0.30	16 (2%) 61 70	9, 25, 54, 80	12 (1%)
1	B	698/738 (94%)	-0.28	14 (2%) 65 74	11, 25, 53, 86	10 (1%)
2	C	4/9 (44%)	-0.19	0 100 100	34, 40, 40, 47	0
2	D	4/9 (44%)	0.12	0 100 100	36, 40, 46, 51	0
All	All	1401/1494 (93%)	-0.29	30 (2%) 63 72	9, 25, 54, 86	22 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	446	LYS	3.5
1	B	515	ARG	3.3
1	A	354	LEU	3.1
1	B	644	SER	3.1
1	B	642	VAL	3.0
1	B	357	ASP	2.9
1	A	359	ASN	2.7
1	A	449	THR	2.6
1	B	501	GLY	2.5
1	A	642	VAL	2.5
1	B	702	HIS	2.5
1	B	699	VAL	2.4
1	B	729	PRO	2.4
1	B	694	VAL	2.3
1	A	560	TYR	2.3
1	A	445	LYS	2.3
1	B	730	SER	2.2
1	B	641	VAL	2.2
1	A	698	TRP	2.2
1	A	641	VAL	2.2
1	A	526	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	725	ILE	2.1
1	A	725	ILE	2.1
1	A	644	SER	2.1
1	A	444	ALA	2.1
1	B	582	PHE	2.0
1	B	639	THR	2.0
1	A	599	LEU	2.0
1	A	362	SER	2.0
1	A	700	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	DAS	D	2	8/9	0.92	0.09	31,36,40,46	0
2	NLE	D	5	8/9	0.93	0.09	32,34,37,39	0
2	ABA	C	4	6/7	0.93	0.10	26,29,32,35	0
2	ABA	D	4	6/7	0.94	0.10	32,32,37,41	0
2	1TX	D	3	12/13	0.94	0.07	29,30,32,34	0
2	NLE	C	5	8/9	0.95	0.07	30,33,35,36	0
2	DAS	C	2	8/9	0.95	0.07	25,29,39,40	0
2	1TX	C	3	12/13	0.96	0.06	21,24,32,37	0

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
4	GOL	A	809	6/6	0.72	0.15	52,54,56,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	B	806	6/6	0.87	0.10	38,44,45,45	0
4	GOL	A	806	6/6	0.89	0.10	33,37,40,41	6
4	GOL	A	808	6/6	0.91	0.11	27,32,33,34	6
4	GOL	A	805	6/6	0.92	0.08	33,34,37,37	0
4	GOL	B	805	6/6	0.93	0.07	31,34,35,36	0
4	GOL	B	804	6/6	0.94	0.07	23,26,27,27	0
5	SO4	B	807	5/5	0.95	0.08	32,34,36,38	5
4	GOL	A	804	6/6	0.96	0.06	18,27,27,27	0
4	GOL	A	807	6/6	0.96	0.07	16,22,24,26	6
3	CA	B	802	1/1	0.97	0.05	26,26,26,26	0
3	CA	A	803	1/1	0.98	0.04	20,20,20,20	0
3	CA	A	802	1/1	0.99	0.03	29,29,29,29	0
3	CA	B	803	1/1	0.99	0.03	22,22,22,22	0
3	CA	B	801	1/1	0.99	0.03	15,15,15,15	0
3	CA	A	801	1/1	1.00	0.03	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.