



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:11 PM GMT

PDB ID : 4KTY  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

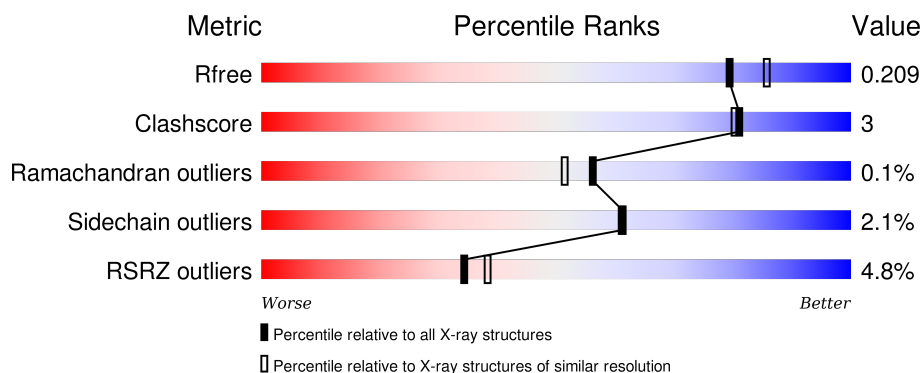
# 1 Overall quality at a glance

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))
$R_{free}$	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div>86%</div> <div>8% • 6%</div> </div>
1	B	738	<div> <div>5%</div> <div>86%</div> <div>8% • 5%</div> </div>
2	C	9	<div> <div>11%</div> <div>78%</div> <div>22%</div> </div>
2	D	9	<div> <div>67%</div> <div>33%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CA	A	801	-	-	-	X
4	GOL	A	805	-	-	-	X
4	GOL	A	807	-	-	-	X
4	GOL	A	808	-	-	-	X
4	GOL	A	809	-	-	-	X
4	GOL	B	805	-	-	-	X
4	GOL	B	806	-	-	-	X
5	SO4	B	807	-	-	-	X

## 2 Entry composition [i](#)

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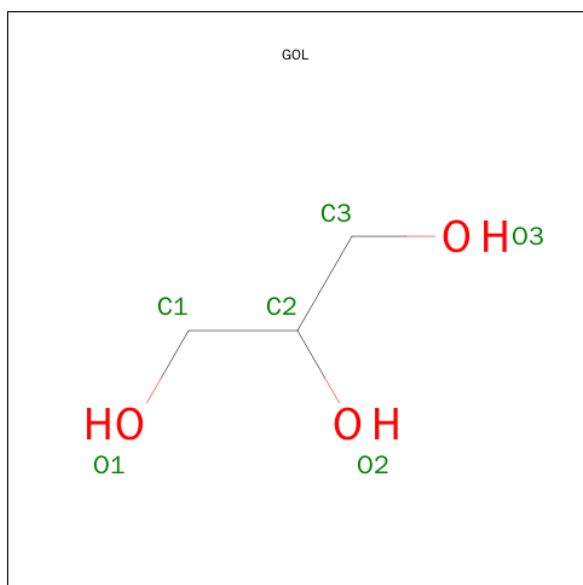
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	9	Total	C	N	O	0	0	0
			74	51	9	14			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

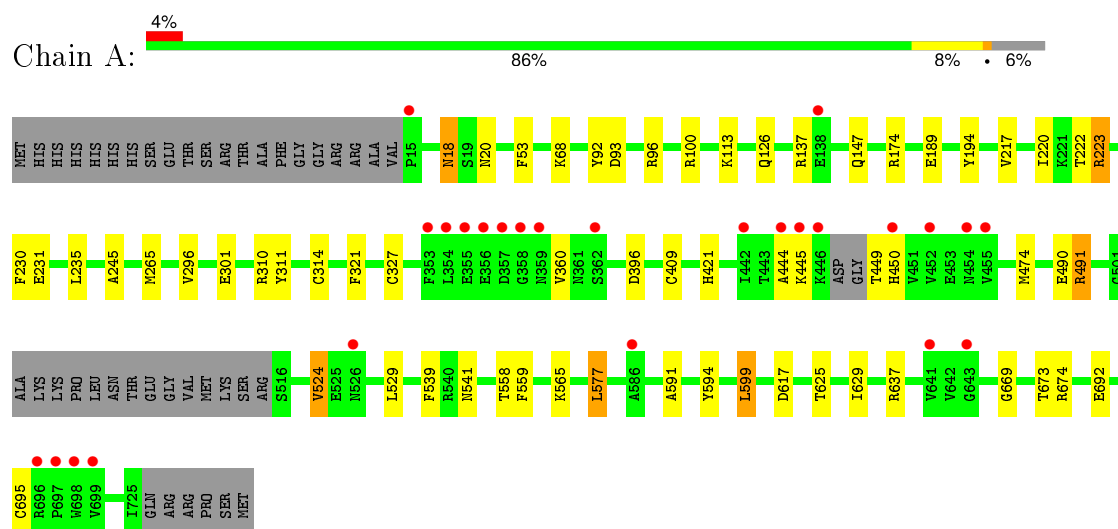
- Molecule 6 is water.

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		

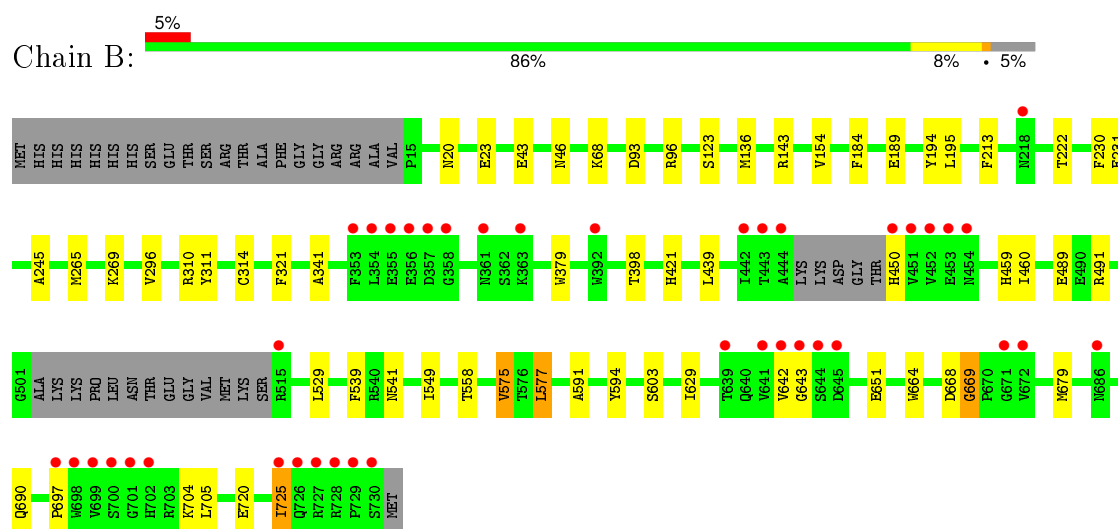
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

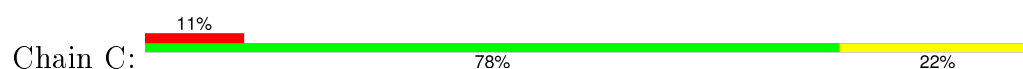
#### • Molecule 1: Coagulation factor XIII A chain

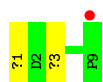


#### • Molecule 1: Coagulation factor XIII A chain



#### • Molecule 2: Peptide-like ligand





- Molecule 2: Peptide-like ligand

Chain D:  67% 33%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.76Å 80.51Å 102.84Å 88.14° 76.70° 82.01°	Depositor
Resolution (Å)	20.80 – 1.98 48.27 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.9 (20.80-1.98) 96.9 (48.27-1.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 1.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.169 , 0.206 0.174 , 0.209	Depositor DCC
$R_{free}$ test set	5957 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 55.6	EDS
Estimated twinning fraction	0.000 for -h,-k,-h+l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 119128 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ABA, GOL, CA, 1TX, NLE, SO4, DAS, ACY

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	0.47	0/5619	0.58	0/7657
1	B	0.49	0/5656	0.59	2/7705 (0.0%)
2	C	0.64	0/40	0.97	0/55
2	D	0.62	0/40	1.11	0/55
All	All	0.48	0/11355	0.59	2/15472 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	491	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	491	ARG	NE-CZ-NH1	5.20	122.90	120.30

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
1	B	5496	0	5220	32	0
2	C	74	0	70	2	0
2	D	74	0	70	5	0
3	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	10595	71	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 (71) 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: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
1:A:18:ASN:HD22	1:A:18:ASN:C	2.15	0.50
1:A:53:PHE:CD1	4:A:805:GOL:H11	2.47	0.49
1:B:669:GLY:HA3	1:B:705:LEU:HD23	1.95	0.49
1:B:439:LEU:HD11	1:B:459:HIS:CD2	2.48	0.49
1:B:189:GLU:HA	1:B:194:TYR:CG	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:398:THR:HG21	2:D:3:1TX:H13	1.98	0.45
1:A:174:ARG:NH2	4:A:807:GOL:H12	2.30	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
2:C:1:ACY:O	6:C:104:HOH:O	2.20	0.44
1:B:704:LYS:NZ	1:B:720:GLU:HB2	2.32	0.44
2:D:3:1TX:H6	2:D:3:1TX:H10	1.89	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: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
2:D:2:DAS:HB2	6:D:107:HOH:O	2.19	0.41
1:B:558[B]:THR:HG23	1:B:603:SER:HB2	2.01	0.41
1:B:213:PHE:CD1	1:B:222:THR:HG22	2.55	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:A:310:ARG:HA	1:A:311:TYR:HA	1.93	0.41
1:B:541:ASN:HB2	1:B:577:LEU:HD13	2.02	0.41
1:A:558:THR:HG22	1:A:559:PHE:O	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:591:ALA:HA	1:B:594:TYR:CE1	2.55	0.40
1:B:421:HIS:HE1	6:B:1310:HOH:O	2.04	0.40
1:A:490:GLU:OE1	1:A:491[B]:ARG:HD2	2.21	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%)	56	51
1	B	702/738 (95%)	682 (97%)	19 (3%)	1 (0%)	56	51
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%)	56	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	669	GLY
1	B	669	GLY

### 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	578/651 (89%)	563 (97%)	15 (3%)	54	51
1	B	587/651 (90%)	576 (98%)	11 (2%)	65	65
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%)	61	59

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

Mol	Chain	Res	Type
1	A	18	ASN
1	A	20	ASN
1	A	100	ARG
1	A	113	LYS
1	A	217	VAL
1	A	223[A]	ARG
1	A	223[B]	ARG
1	A	321	PHE
1	A	360	VAL
1	A	491[A]	ARG
1	A	491[B]	ARG
1	A	524	VAL
1	A	577	LEU
1	A	599	LEU
1	A	617	ASP
1	B	20	ASN
1	B	23	GLU
1	B	46	ASN
1	B	123	SER
1	B	269	LYS
1	B	321	PHE
1	B	450	HIS
1	B	575	VAL
1	B	577	LEU
1	B	668	ASP
1	B	725	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	421	HIS
1	A	450	HIS
1	A	640	GLN
1	A	724	GLN
1	B	421	HIS
1	B	459	HIS
1	B	640	GLN
1	B	690	GLN

### 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	DAS	C	2	2	3,7,8	0.72	0	1,8,10	2.29	1 (100%)
2	1TX	C	3	1,2	10,11,12	1.19	1 (10%)	10,12,14	1.28	1 (10%)
2	ABA	C	4	2	4,5,6	0.54	0	3,5,7	1.02	0
2	NLE	C	5	2	6,7,8	0.66	0	5,7,9	1.68	2 (40%)
2	DAS	D	2	2	3,7,8	0.74	0	1,8,10	2.47	1 (100%)
2	1TX	D	3	1,2	10,11,12	1.25	1 (10%)	10,12,14	1.33	1 (10%)
2	ABA	D	4	2	4,5,6	0.61	0	3,5,7	1.07	0
2	NLE	D	5	2	6,7,8	0.56	0	5,7,9	1.33	1 (20%)

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	DAS	C	2	2	-	0/2/6/8	0/0/0/0
2	1TX	C	3	1,2	-	0/9/11/13	0/0/0/0
2	ABA	C	4	2	-	0/2/4/6	0/0/0/0
2	NLE	C	5	2	-	0/4/6/8	0/0/0/0
2	DAS	D	2	2	-	0/2/6/8	0/0/0/0
2	1TX	D	3	1,2	-	0/9/11/13	0/0/0/0
2	ABA	D	4	2	-	0/2/4/6	0/0/0/0
2	NLE	D	5	2	-	0/4/6/8	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	1TX	O14-C25	3.41	1.44	1.32
2	D	3	1TX	O14-C25	3.50	1.44	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	NLE	O-C-CA	-2.79	118.23	125.49
2	D	5	NLE	O-C-CA	-2.55	118.85	125.49
2	C	5	NLE	CB-CA-N	-2.48	103.47	110.52
2	D	2	DAS	O-C-CA	-2.47	119.07	125.49
2	C	3	1TX	C22-C23-C24	-2.35	104.67	113.29
2	D	3	1TX	C22-C23-C24	-2.34	104.72	113.29
2	C	2	DAS	O-C-CA	-2.29	119.52	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

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	804	-	5,5,5	0.55	0	5,5,5	0.68	0
4	GOL	A	805	-	5,5,5	0.43	0	5,5,5	0.45	0
4	GOL	A	806	-	5,5,5	0.31	0	5,5,5	0.58	0
4	GOL	A	807	-	5,5,5	0.33	0	5,5,5	0.38	0
4	GOL	A	808	-	5,5,5	0.36	0	5,5,5	0.26	0
4	GOL	A	809	-	5,5,5	0.31	0	5,5,5	0.25	0
4	GOL	B	804	-	5,5,5	0.21	0	5,5,5	0.55	0
4	GOL	B	805	-	5,5,5	0.39	0	5,5,5	0.45	0
4	GOL	B	806	-	5,5,5	0.26	0	5,5,5	0.77	0
5	SO4	B	807	-	4,4,4	0.26	0	6,6,6	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
4	GOL	A	804	-	-	0/4/4/4	0/0/0/0
4	GOL	A	805	-	-	0/4/4/4	0/0/0/0
4	GOL	A	806	-	-	0/4/4/4	0/0/0/0
4	GOL	A	807	-	-	0/4/4/4	0/0/0/0
4	GOL	A	808	-	-	0/4/4/4	0/0/0/0
4	GOL	A	809	-	-	0/4/4/4	0/0/0/0
4	GOL	B	804	-	-	0/4/4/4	0/0/0/0
4	GOL	B	805	-	-	0/4/4/4	0/0/0/0
4	GOL	B	806	-	-	0/4/4/4	0/0/0/0
5	SO4	B	807	-	-	0/0/0/0	0/0/0/0

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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	805	GOL	1	0
4	A	806	GOL	3	0
4	A	807	GOL	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	695/738 (94%)	0.06	26 (3%) 45 49	11, 25, 54, 80	0
1	B	698/738 (94%)	0.14	40 (5%) 27 31	11, 26, 53, 86	0
2	C	4/9 (44%)	0.84	1 (25%) 1 1	34, 40, 40, 47	0
2	D	4/9 (44%)	0.97	0 100 100	36, 40, 46, 51	0
All	All	1401/1494 (93%)	0.11	67 (4%) 34 38	11, 25, 54, 86	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	729	PRO	7.0
1	B	358	GLY	6.8
1	B	730	SER	6.3
1	A	358	GLY	5.4
1	A	444	ALA	5.3
1	B	699	VAL	5.2
1	B	354	LEU	5.1
1	B	698	TRP	4.4
1	B	357	ASP	4.4
1	B	444	ALA	4.4
1	B	725	ILE	4.3
1	B	454	ASN	4.1
1	B	642	VAL	4.0
1	B	644	SER	3.9
1	B	645	ASP	3.9
1	B	443	THR	3.9
1	A	643	GLY	3.8
1	B	641	VAL	3.7
1	A	359	ASN	3.7
1	B	643	GLY	3.6
1	B	361	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	451	VAL	3.4
1	B	450	HIS	3.4
1	B	356	GLU	3.3
1	B	442	ILE	3.3
1	B	515	ARG	3.2
1	A	442	ILE	3.2
1	A	353	PHE	3.2
1	A	699	VAL	3.1
1	A	355	GLU	3.1
1	A	698	TRP	3.1
1	B	697	PRO	3.1
1	A	445	LYS	3.0
1	B	453	GLU	3.0
1	B	639	THR	3.0
1	B	355	GLU	3.0
1	B	452	VAL	3.0
1	B	726	GLN	2.9
1	A	446	LYS	2.8
1	A	357	ASP	2.8
1	B	728	ARG	2.7
1	B	353	PHE	2.7
1	B	700	SER	2.7
1	A	356	GLU	2.7
1	A	354	LEU	2.7
1	A	696	ARG	2.6
1	A	450	HIS	2.5
1	B	363	LYS	2.5
1	A	526	ASN	2.5
1	B	686	ASN	2.5
1	B	671	GLY	2.4
1	B	727	ARG	2.4
2	C	9	PRO	2.4
1	B	672	VAL	2.3
1	A	586	ALA	2.3
1	A	138	GLU	2.3
1	A	362	SER	2.2
1	A	697	PRO	2.2
1	A	15	PRO	2.2
1	B	701	GLY	2.2
1	B	702	HIS	2.1
1	A	454	ASN	2.1
1	A	452	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	641	VAL	2.1
1	B	392	TRP	2.1
1	B	218	ASN	2.0
1	A	455	VAL	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	DAS	C	2	8/9	0.96	0.10	-	25,29,39,40	0
2	1TX	C	3	12/13	0.97	0.10	-	21,24,32,37	0
2	NLE	C	5	8/9	0.97	0.10	-	30,33,35,36	0
2	ABA	D	4	6/7	0.97	0.10	-	32,32,37,41	0
2	1TX	D	3	12/13	0.96	0.10	-	29,30,32,34	0
2	ABA	C	4	6/7	0.95	0.10	-	26,29,32,35	0
2	NLE	D	5	8/9	0.96	0.12	-	32,34,37,39	0
2	DAS	D	2	8/9	0.95	0.13	-	31,36,40,46	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	A	807	6/6	0.94	0.17	16.00	16,22,24,26	6
4	GOL	A	809	6/6	0.81	0.27	11.13	52,54,56,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	B	806	6/6	0.88	0.14	4.00	38,44,45,45	0
4	GOL	A	808	6/6	0.86	0.20	3.59	27,32,33,34	6
4	GOL	A	805	6/6	0.94	0.17	2.17	33,34,37,37	0
5	SO4	B	807	5/5	0.96	0.14	2.16	32,34,36,38	5
4	GOL	B	805	6/6	0.95	0.13	2.03	31,34,35,36	0
3	CA	A	801	1/1	1.00	0.13	2.03	15,15,15,15	0
4	GOL	A	806	6/6	0.90	0.14	1.66	33,37,40,41	6
3	CA	B	801	1/1	0.99	0.13	0.78	15,15,15,15	0
4	GOL	B	804	6/6	0.95	0.14	0.28	23,26,27,27	0
4	GOL	A	804	6/6	0.96	0.13	-0.08	18,27,27,27	0
3	CA	A	802	1/1	1.00	0.10	-0.10	29,29,29,29	0
3	CA	A	803	1/1	0.98	0.04	-2.45	20,20,20,20	0
3	CA	B	803	1/1	0.99	0.04	-3.81	22,22,22,22	0
3	CA	B	802	1/1	0.97	0.04	-4.42	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.