



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:56 AM UTC

PDB ID : 5MHL / pdb_00005mhl
Title : FXIIIa in complex with the inhibitor Mi0621
Authors : Stieler, M.; Heine, A.; Klebe, G.
Deposited on : 2016-11-24
Resolution : 2.40 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

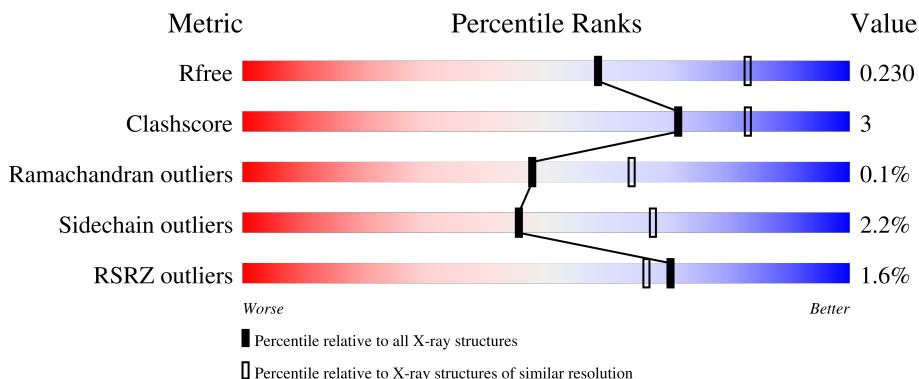
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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% 84% 9% 6%
1	B	738	% 86% 8% 6%
2	K	9	56% 22% 22%
2	O	9	44% 56%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11313 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	692	Total	C	N	O	S	0	1	0
			5338	3412	898	1003	25			
1	B	697	Total	C	N	O	S	0	0	0
			5437	3481	910	1021	25			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	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	-	initiating methionine	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 inhibitor Mi0621.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	9	Total	C	N	O	0	0	1
			51	33	8	10			

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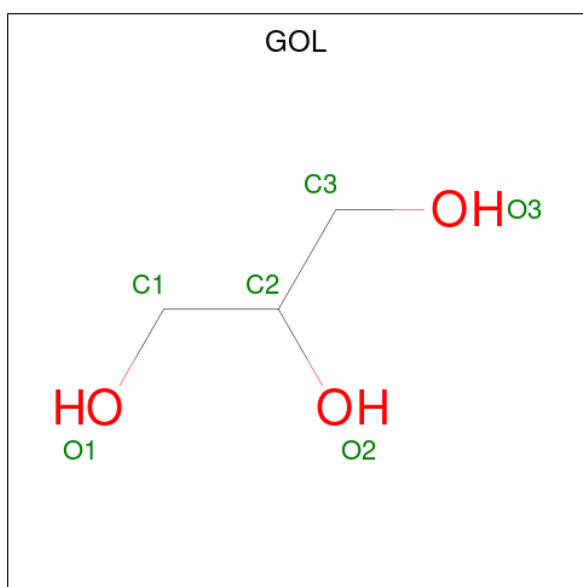
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	9	Total	C	N	O	0	0	1
			59	40	9	10			

- 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	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

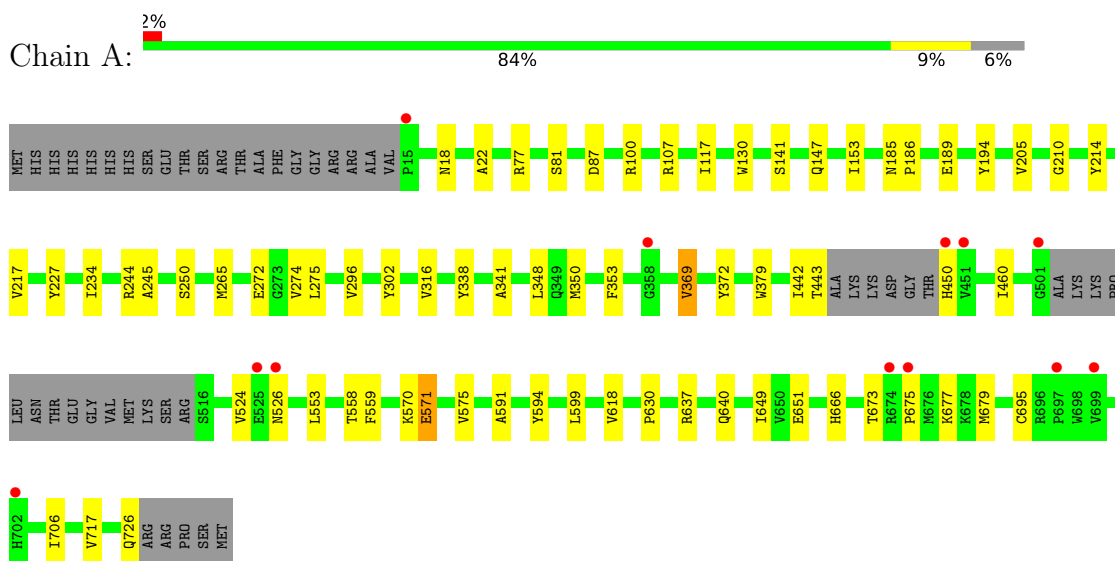
- Molecule 7 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	164	Total	O		0	0
			164	164			
7	B	203	Total	O		0	0
			203	203			
7	O	1	Total	O		0	0
			1	1			

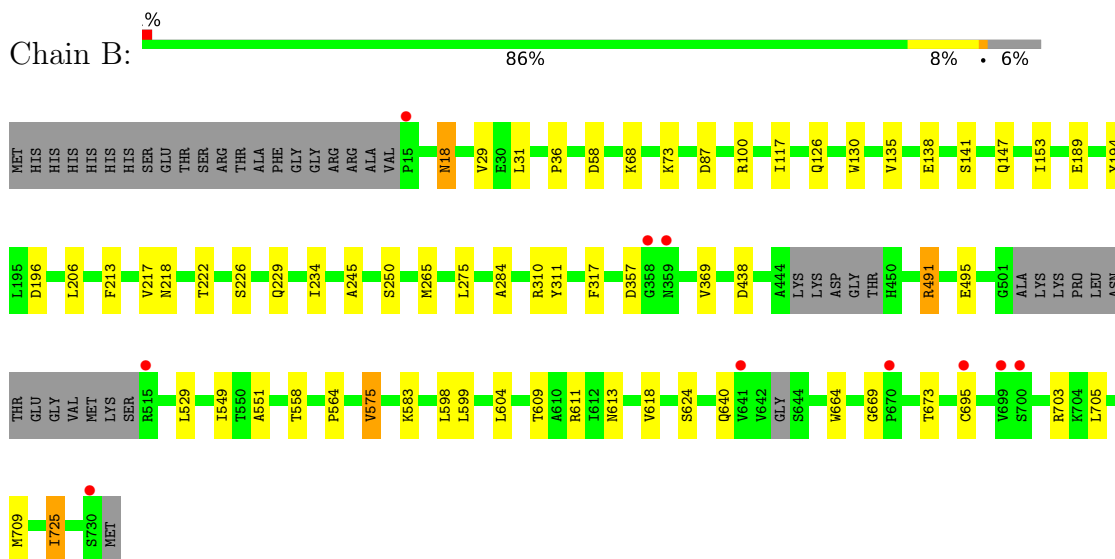
3 Residue-property plots [i](#)

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: Coagulation factor XIII A chain

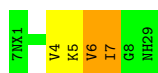


- Molecule 1: Coagulation factor XIII A chain

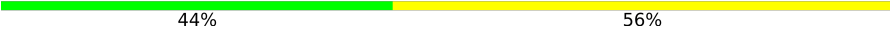


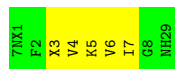
- Molecule 2: inhibitor Mi0621

Chain K:  56% 22% 22%



● Molecule 2: inhibitor Mi0621

Chain O:  44% 56%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.21Å 80.99Å 103.33Å 88.12° 76.87° 81.47°	Depositor
Resolution (Å)	48.83 – 2.40 48.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.5 (48.83-2.40) 93.1 (48.83-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.172 , 0.231 0.172 , 0.230	Depositor DCC
R_{free} test set	3255 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.735	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11313	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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 43.44 % 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 1.7622e-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: NH2, ONL, CA, SO4, 7NX, GOL, EDO

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	0.33	0/5471	0.53	0/7457
1	B	0.34	0/5568	0.54	0/7581
2	K	4.42	5/36 (13.9%)	2.08	2/46 (4.3%)
2	O	4.04	5/45 (11.1%)	2.10	2/57 (3.5%)
All	All	0.49	10/11120 (0.1%)	0.56	4/15141 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	5	LYS	C-N	14.67	1.50	1.33
2	K	5	LYS	C-N	13.78	1.49	1.33
2	K	4	VAL	C-N	12.22	1.50	1.33
2	O	6	VAL	C-N	11.99	1.48	1.33
2	K	7	ILE	C-N	11.42	1.49	1.33
2	O	7	ILE	C-N	11.10	1.48	1.33
2	K	6	VAL	C-N	11.08	1.48	1.33
2	O	4	VAL	C-N	10.68	1.48	1.33
2	O	7	ILE	C-O	-5.18	1.18	1.23
2	K	7	ILE	C-O	-5.12	1.18	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	6	VAL	N-CA-C	-7.82	105.39	112.90
2	K	6	VAL	N-CA-C	-7.28	105.92	112.90
2	O	5	LYS	N-CA-C	-5.19	101.51	109.76
2	K	5	LYS	N-CA-C	-5.08	102.33	109.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5338	0	5001	36	0
1	B	5437	0	5137	34	0
2	K	51	0	45	1	0
2	O	59	0	59	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	18	0	24	1	0
4	B	12	0	16	2	0
5	A	4	0	6	0	0
6	A	10	0	0	0	0
6	B	10	0	0	0	0
7	A	164	0	0	0	0
7	B	203	0	0	2	0
7	O	1	0	0	0	0
All	All	11313	0	10288	69	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 (69) 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:703:ARG:HG3	1:B:725:ILE:HD11	1.66	0.76
1:B:640:GLN:HB3	1:B:725:ILE:HG22	1.73	0.71
1:B:549:ILE:HB	1:B:575:VAL:HG12	1.78	0.66
1:B:189:GLU:HA	1:B:194:TYR:CG	2.38	0.58
1:A:341:ALA:HB2	1:A:460:ILE:HD12	1.86	0.57
1:A:153:ILE:HD11	1:A:250:SER:HA	1.88	0.56
1:A:234:ILE:HD11	1:A:296:VAL:HG13	1.87	0.56
1:A:275:LEU:HD11	1:A:316:VAL:HG12	1.87	0.56
1:B:575:VAL:HG22	1:B:583:LYS:HE2	1.90	0.54
1:B:18:ASN:HD22	1:B:18:ASN:C	2.14	0.54
1:A:189:GLU:HA	1:A:194:TYR:CG	2.43	0.53
1:A:673:THR:HB	1:A:695:CYS:SG	2.49	0.52
1:B:68:LYS:NZ	1:B:206:LEU:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:GLU:HB3	1:B:618:VAL:HG21	1.93	0.51
1:A:245:ALA:HB2	1:A:265:MET:HG3	1.93	0.50
1:A:443:THR:O	1:A:450:HIS:HA	2.12	0.50
1:B:87:ASP:OD1	1:B:141:SER:HB3	2.12	0.50
1:B:213:PHE:CD1	1:B:222:THR:HG22	2.47	0.50
1:A:379:TRP:HZ2	4:A:804:GOL:H12	1.78	0.49
1:B:245:ALA:HB2	1:B:265:MET:HG2	1.94	0.49
1:B:669:GLY:HA3	1:B:705:LEU:HD23	1.94	0.49
1:B:153:ILE:HD11	1:B:250:SER:HA	1.95	0.49
1:B:29:VAL:HG12	1:B:31:LEU:HG	1.94	0.48
1:B:275:LEU:HD23	1:B:317:PHE:CD1	2.49	0.48
1:A:244:ARG:HH21	1:A:272:GLU:HB3	1.80	0.47
1:B:196:ASP:H	4:B:803:GOL:C1	2.28	0.47
1:A:369:VAL:HG13	2:K:7:ILE:HB	1.97	0.47
1:A:341:ALA:HB1	1:A:350:MET:HE3	1.96	0.47
1:B:558:THR:HG22	1:B:564:PRO:HA	1.98	0.46
1:A:637:ARG:NH2	1:A:649:ILE:HD11	2.31	0.46
1:B:58:ASP:OD1	4:B:804:GOL:O2	2.30	0.46
1:A:630:PRO:HB2	1:A:717:VAL:HG11	1.98	0.45
1:A:77:ARG:HB3	1:A:185:ASN:HB2	1.99	0.45
1:A:353:PHE:HA	1:A:442:ILE:O	2.17	0.45
1:B:73:LYS:NZ	7:B:911:HOH:O	2.50	0.45
1:A:274:VAL:HA	1:A:302:TYR:CD1	2.52	0.45
1:A:245:ALA:HB2	1:A:265:MET:CG	2.46	0.44
1:B:310:ARG:HB3	1:B:311:TYR:CD2	2.53	0.44
1:A:186:PRO:HG2	1:A:205:VAL:HG21	2.00	0.44
1:B:529:LEU:HD12	1:B:598:LEU:HD13	1.99	0.44
1:A:553:LEU:O	1:A:570:LYS:HA	2.18	0.44
1:B:229:GLN:HA	1:B:234:ILE:HG21	2.00	0.44
1:A:666[A]:HIS:CE1	1:A:675:PRO:HB3	2.52	0.44
1:A:591:ALA:HA	1:A:594:TYR:CE1	2.53	0.43
1:A:341:ALA:HB1	1:A:350:MET:SD	2.59	0.43
1:A:214:TYR:HB2	1:A:372:TYR:CE2	2.54	0.43
1:B:100:ARG:HD2	7:B:1047:HOH:O	2.19	0.43
1:B:664:TRP:O	1:B:709:MET:HA	2.19	0.42
1:A:87:ASP:OD1	1:A:141:SER:HB3	2.19	0.42
1:A:214:TYR:HB2	1:A:372:TYR:CZ	2.54	0.42
1:A:217:VAL:HG22	1:A:338:TYR:HB3	2.00	0.42
1:B:673:THR:HB	1:B:695:CYS:SG	2.59	0.42
1:A:22:ALA:HB1	1:A:107:ARG:HB2	2.00	0.42
1:A:558:THR:HG22	1:A:559:PHE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TRP:HA	1:A:147:GLN:O	2.19	0.42
1:A:640:GLN:O	1:A:726:GLN:HG3	2.19	0.42
1:B:438:ASP:OD2	1:B:491:ARG:NH2	2.52	0.42
1:A:210:GLY:HA3	1:A:227:TYR:CE2	2.55	0.42
1:B:117:ILE:HG21	1:B:130:TRP:CE2	2.55	0.42
1:B:611:ARG:HD2	1:B:613:ASN:OD1	2.19	0.42
1:B:284:ALA:O	1:B:311:TYR:OH	2.35	0.42
1:A:553:LEU:N	1:A:571:GLU:O	2.52	0.41
1:B:126:GLN:O	1:B:147:GLN:NE2	2.51	0.41
1:B:725:ILE:H	1:B:725:ILE:HG12	1.82	0.41
1:A:117:ILE:HG21	1:A:130:TRP:CE2	2.55	0.40
1:B:604:LEU:O	1:B:624:SER:HA	2.20	0.40
1:A:706:ILE:HG23	1:B:36:PRO:HG2	2.03	0.40
1:A:679:MET:HE2	1:A:679:MET:HB3	1.81	0.40
1:B:551:ALA:HA	1:B:609:THR:O	2.22	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	687/738 (93%)	667 (97%)	19 (3%)	1 (0%)	48	64
1	B	689/738 (93%)	671 (97%)	18 (3%)	0	100	100
2	K	5/9 (56%)	4 (80%)	1 (20%)	0	100	100
2	O	5/9 (56%)	5 (100%)	0	0	100	100
All	All	1386/1494 (93%)	1347 (97%)	38 (3%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	526	ASN

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	546/651 (84%)	534 (98%)	12 (2%)	45	67
1	B	562/651 (86%)	550 (98%)	12 (2%)	47	69
2	K	3/5 (60%)	2 (67%)	1 (33%)	0	0
2	O	5/5 (100%)	5 (100%)	0	100	100
All	All	1116/1312 (85%)	1091 (98%)	25 (2%)	45	67

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	81	SER
1	A	100	ARG
1	A	348	LEU
1	A	369	VAL
1	A	524	VAL
1	A	571	GLU
1	A	575	VAL
1	A	599	LEU
1	A	618	VAL
1	A	651	GLU
1	A	677	LYS
1	B	18	ASN
1	B	135	VAL
1	B	138	GLU
1	B	217	VAL
1	B	218	ASN
1	B	226	SER
1	B	357	ASP
1	B	369	VAL
1	B	491	ARG

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Mol	Chain	Res	Type
1	B	575	VAL
1	B	599	LEU
1	B	725	ILE
2	K	6	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	402	ASN
1	A	542	ASN
1	A	556	ASN
1	A	726	GLN
1	B	18	ASN
1	B	459	HIS
1	B	484	GLN
1	B	544	HIS
1	B	640	GLN
1	B	666	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	ONL	K	3	1,2	7,8,9	0.69	0	4,9,11	0.84	0
2	ONL	O	3	1,2	7,8,9	0.69	0	4,9,11	1.17	1 (25%)

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	ONL	K	3	1,2	-	3/6/7/9	-
2	ONL	O	3	1,2	-	2/6/7/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	3	ONL	CB-CG-CD	-2.09	111.51	114.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	3	ONL	O-C-CA-CB
2	O	3	ONL	CE-CD-CG-CB
2	O	3	ONL	OD-CD-CG-CB
2	K	3	ONL	CE-CD-CG-CB
2	K	3	ONL	OD-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

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	B	804	-	5,5,5	0.47	0	5,5,5	0.31	0
4	GOL	B	803	-	5,5,5	0.32	0	5,5,5	0.19	0
4	GOL	A	804	-	5,5,5	0.44	0	5,5,5	0.46	0
6	SO4	A	809	-	4,4,4	0.26	0	6,6,6	0.10	0
6	SO4	B	805	-	4,4,4	0.32	0	6,6,6	0.15	0
6	SO4	B	806	-	4,4,4	0.29	0	6,6,6	0.09	0
4	GOL	A	806	-	5,5,5	0.41	0	5,5,5	0.26	0
5	EDO	A	807	-	3,3,3	0.44	0	2,2,2	0.39	0
6	SO4	A	808	-	4,4,4	0.29	0	6,6,6	0.23	0
4	GOL	A	805	-	5,5,5	0.41	0	5,5,5	0.31	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	B	804	-	-	4/4/4/4	-
4	GOL	B	803	-	-	4/4/4/4	-
4	GOL	A	804	-	-	4/4/4/4	-
4	GOL	A	806	-	-	0/4/4/4	-
5	EDO	A	807	-	-	0/1/1/1	-
4	GOL	A	805	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	804	GOL	O1-C1-C2-C3
4	A	804	GOL	C1-C2-C3-O3
4	A	805	GOL	O1-C1-C2-C3
4	B	803	GOL	O1-C1-C2-O2
4	B	803	GOL	O1-C1-C2-C3
4	B	803	GOL	C1-C2-C3-O3
4	B	804	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	804	GOL	O1-C1-C2-O2
4	A	805	GOL	C1-C2-C3-O3
4	B	804	GOL	C1-C2-C3-O3
4	A	804	GOL	O2-C2-C3-O3
4	A	805	GOL	O1-C1-C2-O2
4	A	805	GOL	O2-C2-C3-O3
4	B	803	GOL	O2-C2-C3-O3
4	B	804	GOL	O1-C1-C2-O2
4	B	804	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	804	GOL	1	0
4	B	803	GOL	1	0
4	A	804	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, 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	692/738 (93%)	-0.16	12 (1%) 69 65	18, 38, 72, 94	1 (0%)
1	B	697/738 (94%)	-0.27	10 (1%) 73 69	19, 35, 65, 92	0
2	K	6/9 (66%)	0.11	0 100 100	32, 38, 53, 54	0
2	O	6/9 (66%)	-0.09	0 100 100	25, 40, 45, 51	0
All	All	1401/1494 (93%)	-0.21	22 (1%) 70 66	18, 36, 69, 94	1 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	PRO	3.2
1	A	525	GLU	2.9
1	A	526	ASN	2.9
1	B	730	SER	2.7
1	A	675	PRO	2.4
1	A	451	VAL	2.3
1	A	358	GLY	2.3
1	B	695	CYS	2.3
1	B	515	ARG	2.3
1	B	641	VAL	2.3
1	A	702	HIS	2.2
1	B	670	PRO	2.2
1	A	699	VAL	2.2
1	B	699	VAL	2.2
1	B	700	SER	2.1
1	A	450	HIS	2.1
1	A	501	GLY	2.1
1	B	359	ASN	2.1
1	B	358	GLY	2.0
1	A	697	PRO	2.0
1	B	15	PRO	2.0
1	A	674	ARG	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	ONL	K	3	9/10	0.93	0.10	29,32,38,41	0
2	ONL	O	3	9/10	0.96	0.07	24,30,35,36	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	806	6/6	0.82	0.15	56,61,66,66	0
4	GOL	A	805	6/6	0.93	0.09	47,50,53,55	0
4	GOL	B	804	6/6	0.93	0.11	36,51,56,60	0
5	EDO	A	807	4/4	0.93	0.10	49,51,51,52	0
6	SO4	A	808	5/5	0.93	0.10	50,51,56,57	5
6	SO4	B	805	5/5	0.93	0.09	35,36,47,54	5
6	SO4	B	806	5/5	0.94	0.11	48,54,60,61	5
4	GOL	B	803	6/6	0.95	0.08	27,28,30,37	0
4	GOL	A	804	6/6	0.96	0.07	29,33,36,39	0
6	SO4	A	809	5/5	0.96	0.09	29,34,44,45	5
3	CA	A	803	1/1	0.99	0.02	46,46,46,46	0
3	CA	B	807	1/1	0.99	0.01	26,26,26,26	0
3	CA	A	801	1/1	0.99	0.04	37,37,37,37	0
3	CA	A	802	1/1	0.99	0.04	38,38,38,38	0
3	CA	B	802	1/1	1.00	0.01	32,32,32,32	0
3	CA	B	801	1/1	1.00	0.02	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.