



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 03:53 pm BST

PDB ID : 5X3I
Title : Kfla1895 D451A mutant
Authors : Tanaka, Y.; Chen, M.; Tagami, T.; Yao, M.; Kimura, A.
Deposited on : 2017-02-06
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

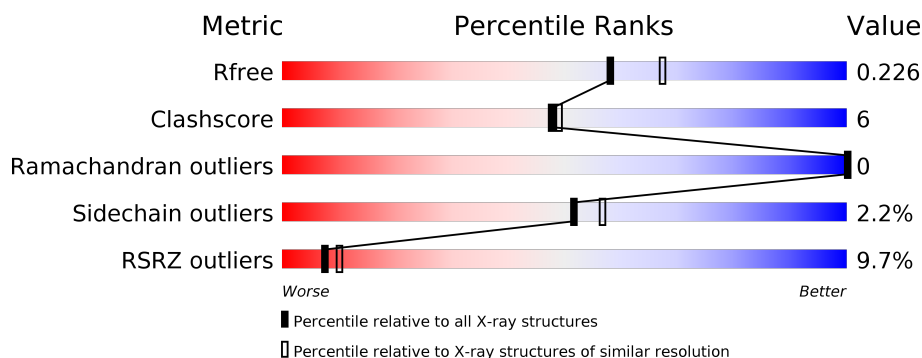
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 ≥ 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	743	<div> <div>7%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
1	B	743	<div> <div>11%</div> <div>82%</div> <div>12%</div> <div>5%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12040 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 Glycoside hydrolase family 31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	708	Total	C	N	O	S	0	0	0
			5590	3556	992	1030	12			
1	B	709	Total	C	N	O	S	0	0	0
			5594	3558	993	1031	12			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP D2PPM7
A	-18	GLY	-	expression tag	UNP D2PPM7
A	-17	SER	-	expression tag	UNP D2PPM7
A	-16	SER	-	expression tag	UNP D2PPM7
A	-15	HIS	-	expression tag	UNP D2PPM7
A	-14	HIS	-	expression tag	UNP D2PPM7
A	-13	HIS	-	expression tag	UNP D2PPM7
A	-12	HIS	-	expression tag	UNP D2PPM7
A	-11	HIS	-	expression tag	UNP D2PPM7
A	-10	HIS	-	expression tag	UNP D2PPM7
A	-9	SER	-	expression tag	UNP D2PPM7
A	-8	SER	-	expression tag	UNP D2PPM7
A	-7	GLY	-	expression tag	UNP D2PPM7
A	-6	LEU	-	expression tag	UNP D2PPM7
A	-5	VAL	-	expression tag	UNP D2PPM7
A	-4	PRO	-	expression tag	UNP D2PPM7
A	-3	ARG	-	expression tag	UNP D2PPM7
A	-2	GLY	-	expression tag	UNP D2PPM7
A	-1	SER	-	expression tag	UNP D2PPM7
A	0	HIS	-	expression tag	UNP D2PPM7
A	451	ALA	ASP	engineered mutation	UNP D2PPM7
B	-19	MET	-	expression tag	UNP D2PPM7
B	-18	GLY	-	expression tag	UNP D2PPM7
B	-17	SER	-	expression tag	UNP D2PPM7
B	-16	SER	-	expression tag	UNP D2PPM7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP D2PPM7
B	-14	HIS	-	expression tag	UNP D2PPM7
B	-13	HIS	-	expression tag	UNP D2PPM7
B	-12	HIS	-	expression tag	UNP D2PPM7
B	-11	HIS	-	expression tag	UNP D2PPM7
B	-10	HIS	-	expression tag	UNP D2PPM7
B	-9	SER	-	expression tag	UNP D2PPM7
B	-8	SER	-	expression tag	UNP D2PPM7
B	-7	GLY	-	expression tag	UNP D2PPM7
B	-6	LEU	-	expression tag	UNP D2PPM7
B	-5	VAL	-	expression tag	UNP D2PPM7
B	-4	PRO	-	expression tag	UNP D2PPM7
B	-3	ARG	-	expression tag	UNP D2PPM7
B	-2	GLY	-	expression tag	UNP D2PPM7
B	-1	SER	-	expression tag	UNP D2PPM7
B	0	HIS	-	expression tag	UNP D2PPM7
B	451	ALA	ASP	engineered mutation	UNP D2PPM7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



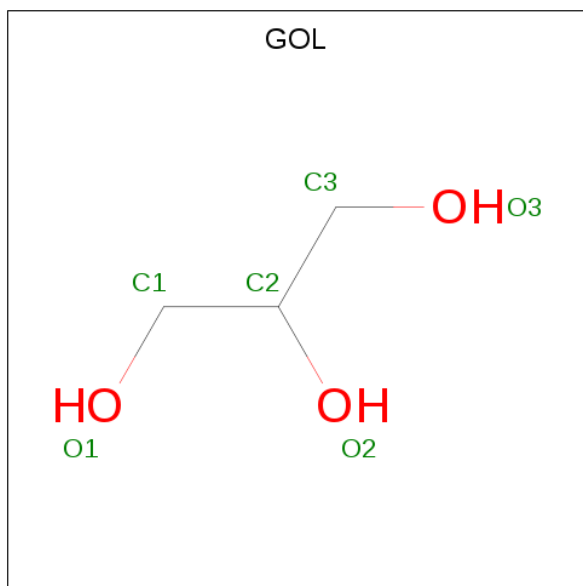
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

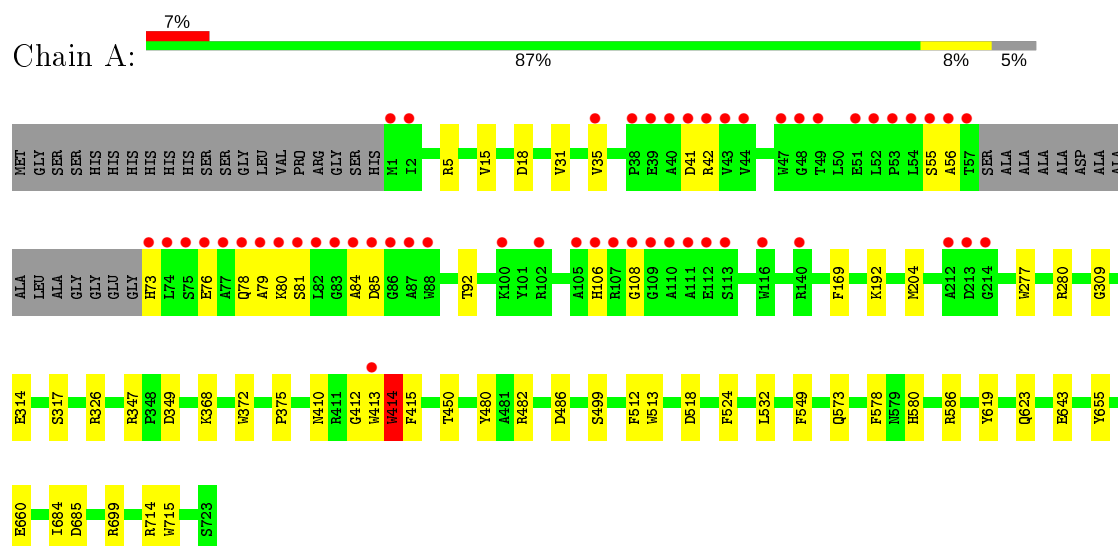
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	467	Total	O	0	0
			467	467		
4	B	275	Total	O	0	0
			275	275		

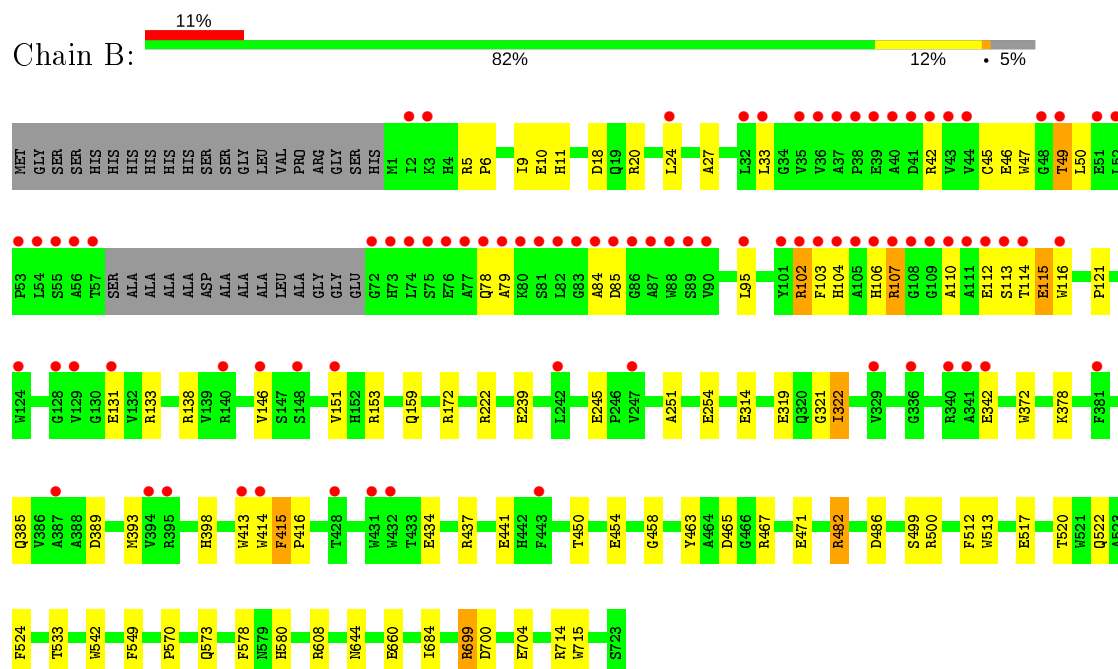
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Glycoside hydrolase family 31



• Molecule 1: Glycoside hydrolase family 31



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	181.15Å 181.15Å 391.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.55 – 2.10 48.55 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.55-2.10) 100.0 (48.55-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.204 , 0.226 0.204 , 0.226	Depositor DCC
R_{free} test set	2641 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12040	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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: GOL, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	1/5764 (0.0%)	0.57	1/7877 (0.0%)
1	B	0.40	1/5768 (0.0%)	0.52	1/7882 (0.0%)
All	All	0.43	2/11532 (0.0%)	0.54	2/15759 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	413	TRP	CB-CG	-6.46	1.38	1.50
1	B	416	PRO	N-CD	5.64	1.55	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	TRP	CA-CB-CG	6.55	126.14	113.70
1	B	415	PHE	C-N-CD	5.10	139.10	128.40

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	5590	0	5311	42	1
1	B	5594	0	5314	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	50	0	0	3	0
2	B	10	0	0	1	0
3	A	36	0	47	2	0
3	B	18	0	24	5	0
4	A	467	0	0	3	0
4	B	275	0	0	3	0
All	All	12040	0	10696	135	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (135) 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:102:ARG:HD2	1:B:116:TRP:CE2	1.76	1.21
1:B:102:ARG:CD	1:B:116:TRP:CZ2	2.33	1.11
1:B:465:ASP:OD2	1:B:467:ARG:NH1	1.81	1.11
1:A:15:VAL:H	1:A:73:HIS:CE1	1.73	1.07
1:B:103:PHE:H	1:B:114:THR:HG22	1.24	1.03
1:B:5:ARG:NH1	1:B:18:ASP:OD2	1.97	0.96
1:B:102:ARG:CD	1:B:116:TRP:CE2	2.52	0.92
1:B:103:PHE:H	1:B:114:THR:CG2	1.81	0.91
1:A:15:VAL:HG22	1:A:73:HIS:NE2	1.86	0.91
1:B:102:ARG:HD3	1:B:116:TRP:CZ2	2.09	0.87
1:B:42:ARG:CZ	1:B:106:HIS:CD2	2.58	0.86
1:B:102:ARG:HD2	1:B:116:TRP:CZ2	2.04	0.85
1:A:41:ASP:OD2	1:A:108:GLY:N	2.10	0.84
1:B:78:GLN:HA	1:B:413:TRP:CZ2	2.13	0.83
1:B:42:ARG:CZ	1:B:106:HIS:HD2	1.91	0.83
1:B:520:THR:HB	3:B:803:GOL:H31	1.62	0.82
1:B:414:TRP:CZ2	1:B:415:PHE:CE2	2.67	0.81
1:B:78:GLN:HG3	1:B:413:TRP:CZ2	2.17	0.80
1:B:102:ARG:NH2	1:B:116:TRP:NE1	2.30	0.79
1:B:78:GLN:HA	1:B:413:TRP:HZ2	1.44	0.79
1:B:414:TRP:CH2	1:B:415:PHE:CD2	2.72	0.77
1:A:15:VAL:HG22	1:A:73:HIS:HE2	1.49	0.77
1:A:15:VAL:H	1:A:73:HIS:HE2	1.32	0.76
1:A:15:VAL:N	1:A:73:HIS:NE2	2.32	0.76
1:B:414:TRP:CZ2	1:B:415:PHE:CD2	2.75	0.74
1:B:414:TRP:CH2	1:B:415:PHE:CE2	2.75	0.74
1:B:520:THR:HB	3:B:803:GOL:C3	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:VAL:N	1:A:73:HIS:CE1	2.56	0.72
2:A:807:SO4:O4	4:A:901:HOH:O	2.08	0.71
1:B:138:ARG:NH1	1:B:254:GLU:OE1	2.24	0.69
1:B:467:ARG:HD3	1:B:471:GLU:HG2	1.74	0.68
1:B:454:GLU:O	4:B:901:HOH:O	2.10	0.67
1:A:685:ASP:OD2	1:A:699:ARG:NH2	2.28	0.67
1:A:15:VAL:N	1:A:73:HIS:HE2	1.90	0.67
1:B:50:LEU:N	1:B:50:LEU:HD12	2.10	0.67
1:A:586:ARG:NH2	2:A:806:SO4:O3	2.27	0.66
1:B:314:GLU:HA	1:B:372:TRP:HB2	1.77	0.66
1:B:45:CYS:HB2	1:B:103:PHE:CE2	2.32	0.65
1:A:15:VAL:O	1:A:73:HIS:HE1	1.80	0.65
1:B:434:GLU:O	4:B:902:HOH:O	2.14	0.64
1:B:103:PHE:N	1:B:114:THR:HG22	2.06	0.64
1:B:102:ARG:HD3	1:B:116:TRP:CH2	2.31	0.64
1:B:102:ARG:CZ	1:B:116:TRP:NE1	2.62	0.63
1:B:393:MET:HA	1:B:398:HIS:HB2	1.81	0.63
1:B:42:ARG:NH1	1:B:106:HIS:CD2	2.66	0.63
1:B:102:ARG:NE	1:B:116:TRP:CZ2	2.67	0.62
1:B:102:ARG:HD2	1:B:116:TRP:CD2	2.33	0.62
1:A:15:VAL:HG22	1:A:73:HIS:CE1	2.34	0.62
1:A:314:GLU:HA	1:A:372:TRP:HB2	1.83	0.61
1:B:153:ARG:NH1	1:B:239:GLU:OE2	2.34	0.61
1:B:102:ARG:CZ	1:B:116:TRP:HE1	2.15	0.60
1:B:608:ARG:NH1	1:B:704:GLU:O	2.22	0.60
1:B:437:ARG:NH1	1:B:441:GLU:OE2	2.28	0.60
1:B:385:GLN:NE2	1:B:389:ASP:OD1	2.32	0.58
1:B:45:CYS:HB2	1:B:103:PHE:HE2	1.68	0.57
1:B:321:GLY:C	1:B:322:ILE:HG12	2.25	0.57
1:B:42:ARG:NE	1:B:106:HIS:HD2	2.02	0.57
1:B:114:THR:HG23	1:B:115:GLU:O	2.05	0.56
1:B:9:ILE:HG23	1:B:11:HIS:H	1.70	0.56
1:A:76:GLU:O	1:A:80:LYS:HG2	2.05	0.56
3:A:812:GOL:H32	4:A:927:HOH:O	2.06	0.56
1:B:49:THR:OG1	1:B:50:LEU:CD1	2.54	0.55
1:A:578:PHE:CZ	1:A:580:HIS:HA	2.42	0.55
1:B:102:ARG:NH2	1:B:116:TRP:CD1	2.76	0.54
1:B:78:GLN:CA	1:B:413:TRP:CZ2	2.88	0.54
1:B:49:THR:OG1	1:B:50:LEU:HD12	2.07	0.54
1:A:643:GLU:OE2	4:A:902:HOH:O	2.19	0.53
1:B:78:GLN:HG3	1:B:413:TRP:CH2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:HD13	1:B:103:PHE:HZ	1.73	0.52
1:B:146:VAL:HG12	1:B:151:VAL:HG22	1.92	0.51
1:B:50:LEU:N	1:B:50:LEU:CD1	2.72	0.51
1:B:319:GLU:OE2	4:B:903:HOH:O	2.19	0.51
1:B:131:GLU:OE1	1:B:133:ARG:NE	2.37	0.51
1:B:46:GLU:HB3	1:B:102:ARG:HG2	1.92	0.50
1:B:319:GLU:O	1:B:378:LYS:NZ	2.39	0.50
1:B:47:TRP:CZ2	1:B:95:LEU:HD13	2.46	0.50
1:B:47:TRP:HZ2	1:B:95:LEU:HD13	1.77	0.50
1:B:660:GLU:CD	1:B:714:ARG:HG3	2.32	0.50
1:B:684:ILE:HD12	1:B:715:TRP:CG	2.47	0.49
1:B:500:ARG:NH1	3:B:804:GOL:H31	2.27	0.49
1:B:79:ALA:HB1	1:B:84:ALA:HB2	1.95	0.49
1:A:499:SER:O	1:A:512:PHE:HA	2.13	0.49
1:B:10:GLU:CD	1:B:458:GLY:HA2	2.33	0.49
1:B:245:GLU:CD	1:B:245:GLU:H	2.15	0.49
1:B:414:TRP:CE2	1:B:415:PHE:CD2	3.00	0.49
1:A:486:ASP:HB3	3:A:814:GOL:H32	1.94	0.48
1:A:42:ARG:NH1	1:A:106:HIS:NE2	2.61	0.48
1:B:222:ARG:HE	1:B:251:ALA:HB2	1.78	0.48
1:A:5:ARG:NE	1:A:18:ASP:OD2	2.37	0.48
1:A:76:GLU:HG2	1:A:80:LYS:HE3	1.96	0.47
1:B:644:ASN:ND2	2:B:802:SO4:O3	2.46	0.47
1:B:414:TRP:CZ3	1:B:415:PHE:CD2	3.01	0.47
1:A:42:ARG:HB2	1:A:106:HIS:CE1	2.50	0.47
1:A:15:VAL:CG2	1:A:73:HIS:CE1	2.99	0.46
1:A:169:PHE:HA	1:A:204:MET:O	2.16	0.45
1:A:410:ASN:C	1:A:412:GLY:H	2.16	0.45
1:A:78:GLN:O	1:A:81:SER:OG	2.27	0.45
1:B:245:GLU:N	1:B:245:GLU:OE1	2.49	0.45
1:B:608:ARG:NH1	1:B:704:GLU:HB2	2.31	0.45
1:A:42:ARG:NH1	1:A:106:HIS:CE1	2.85	0.45
1:B:578:PHE:CZ	1:B:580:HIS:HA	2.52	0.45
1:A:714:ARG:HD3	2:A:808:SO4:O4	2.17	0.45
1:A:79:ALA:HB1	1:A:84:ALA:HB2	2.00	0.44
1:B:414:TRP:CE2	1:B:415:PHE:HD2	2.35	0.44
1:B:27:ALA:HB2	1:B:121:PRO:HB2	2.00	0.44
1:A:277:TRP:CD2	1:A:368:LYS:HG3	2.53	0.44
1:B:542:TRP:O	1:B:570:PRO:HB2	2.19	0.43
1:A:317:SER:O	1:A:326:ARG:HB2	2.18	0.43
1:B:112:GLU:HG3	1:B:113:SER:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:GLN:H	3:B:803:GOL:H31	1.84	0.43
1:B:6:PRO:HB3	1:B:20:ARG:NH1	2.33	0.42
1:B:500:ARG:HH11	3:B:804:GOL:C3	2.32	0.42
1:A:55:SER:OG	1:A:56:ALA:N	2.52	0.42
1:B:699:ARG:HD3	1:B:700:ASP:O	2.20	0.42
1:B:103:PHE:H	1:B:114:THR:HG21	1.78	0.42
1:A:347:ARG:HA	1:A:347:ARG:HD3	1.81	0.42
1:A:532:LEU:HD21	1:A:655:TYR:HB3	2.02	0.42
1:B:463:TYR:HB2	1:B:465:ASP:OD1	2.19	0.42
1:A:31:VAL:HG12	1:A:92:THR:OG1	2.20	0.41
1:B:499:SER:O	1:B:512:PHE:HA	2.20	0.41
1:A:414:TRP:CZ2	1:A:415:PHE:CE1	3.08	0.41
1:B:102:ARG:CD	1:B:116:TRP:CH2	2.92	0.41
1:B:104:HIS:HA	1:B:112:GLU:O	2.21	0.41
1:A:192:LYS:NZ	1:A:518:ASP:OD1	2.40	0.41
1:B:33:LEU:HD13	1:B:103:PHE:CZ	2.53	0.41
1:B:342:GLU:CD	1:B:342:GLU:H	2.23	0.41
1:B:378:LYS:HE3	1:B:415:PHE:CZ	2.56	0.41
1:A:280:ARG:HB2	1:A:309:GLY:HA3	2.02	0.41
1:A:684:ILE:HD13	1:A:715:TRP:CD1	2.56	0.41
1:A:660:GLU:CD	1:A:714:ARG:HG3	2.42	0.41
1:B:107:ARG:O	1:B:110:ALA:HB3	2.21	0.41
1:A:375:PRO:HD3	1:A:480:TYR:CZ	2.56	0.40
1:A:619:TYR:CZ	1:A:623:GLN:HG3	2.57	0.40
1:B:172:ARG:HB2	1:B:533:THR:HG21	2.02	0.40
1:B:482:ARG:NE	1:B:486:ASP:OD2	2.49	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ARG:NH1	1:A:349:ASP:OD2[3_465]	1.84	0.36

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	704/743 (95%)	695 (99%)	9 (1%)	0	100	100
1	B	705/743 (95%)	695 (99%)	10 (1%)	0	100	100
All	All	1409/1486 (95%)	1390 (99%)	19 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	567/588 (96%)	558 (98%)	9 (2%)	62	69
1	B	567/588 (96%)	551 (97%)	16 (3%)	43	47
All	All	1134/1176 (96%)	1109 (98%)	25 (2%)	52	57

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

Mol	Chain	Res	Type
1	A	35	VAL
1	A	85	ASP
1	A	414	TRP
1	A	450	THR
1	A	482	ARG
1	A	513	TRP
1	A	524	PHE
1	A	549	PHE
1	A	573	GLN
1	B	24	LEU
1	B	49	THR
1	B	85	ASP
1	B	102	ARG
1	B	107	ARG
1	B	115	GLU

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Mol	Chain	Res	Type
1	B	159	GLN
1	B	322	ILE
1	B	450	THR
1	B	482	ARG
1	B	513	TRP
1	B	517	GLU
1	B	524	PHE
1	B	549	PHE
1	B	573	GLN
1	B	699	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	106	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	801	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	A	806	-	4,4,4	0.17	0	6,6,6	0.14	0
3	GOL	A	814	-	5,5,5	0.36	0	5,5,5	0.93	0
3	GOL	B	805	-	5,5,5	0.85	0	5,5,5	0.55	0
2	SO4	A	804	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	A	809	-	4,4,4	0.14	0	6,6,6	0.13	0
3	GOL	A	811	-	5,5,5	1.18	1 (20%)	5,5,5	1.20	0
3	GOL	A	812	-	5,5,5	0.99	0	5,5,5	0.92	0
2	SO4	B	801	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	A	807	-	4,4,4	0.16	0	6,6,6	0.08	0
3	GOL	B	803	-	5,5,5	0.66	0	5,5,5	1.05	0
3	GOL	A	816	-	5,5,5	0.40	0	5,5,5	0.24	0
2	SO4	A	803	-	4,4,4	0.17	0	6,6,6	0.24	0
2	SO4	A	808	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	A	802	-	4,4,4	0.13	0	6,6,6	0.13	0
3	GOL	A	813	-	5,5,5	0.40	0	5,5,5	0.44	0
2	SO4	B	802	-	4,4,4	0.17	0	6,6,6	0.15	0
3	GOL	A	815	-	5,5,5	0.38	0	5,5,5	0.13	0
3	GOL	B	804	-	5,5,5	0.42	0	5,5,5	0.72	0
2	SO4	A	810	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	A	805	-	4,4,4	0.14	0	6,6,6	0.13	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
3	GOL	A	814	-	-	0/4/4/4	-
3	GOL	B	805	-	-	2/4/4/4	-
3	GOL	A	811	-	-	3/4/4/4	-
3	GOL	A	812	-	-	1/4/4/4	-
3	GOL	A	815	-	-	2/4/4/4	-
3	GOL	B	803	-	-	2/4/4/4	-
3	GOL	A	816	-	-	2/4/4/4	-
3	GOL	A	813	-	-	2/4/4/4	-
3	GOL	B	804	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	811	GOL	O2-C2	-2.47	1.36	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	805	GOL	O1-C1-C2-C3
3	A	811	GOL	O1-C1-C2-C3
3	A	815	GOL	O1-C1-C2-C3
3	B	804	GOL	O1-C1-C2-C3
3	A	815	GOL	O1-C1-C2-O2
3	A	811	GOL	C1-C2-C3-O3
3	A	812	GOL	O1-C1-C2-C3
3	B	805	GOL	O1-C1-C2-O2
3	A	811	GOL	O2-C2-C3-O3
3	B	803	GOL	O1-C1-C2-O2
3	B	804	GOL	O1-C1-C2-O2
3	A	813	GOL	O1-C1-C2-O2
3	A	816	GOL	O1-C1-C2-O2
3	A	813	GOL	O1-C1-C2-C3
3	B	803	GOL	O1-C1-C2-C3
3	A	816	GOL	O1-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	806	SO4	1	0
3	A	814	GOL	1	0
3	A	812	GOL	1	0
2	A	807	SO4	1	0
3	B	803	GOL	3	0
2	A	808	SO4	1	0
2	B	802	SO4	1	0
3	B	804	GOL	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	708/743 (95%)	0.12	53 (7%) 14 18	11, 20, 70, 112	0
1	B	709/743 (95%)	0.61	84 (11%) 4 5	12, 33, 99, 122	0
All	All	1417/1486 (95%)	0.36	137 (9%) 7 10	11, 25, 88, 122	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	LEU	11.6
1	B	40	ALA	9.1
1	A	107	ARG	8.6
1	A	83	GLY	8.1
1	A	111	ALA	7.8
1	B	413	TRP	7.2
1	B	57	THR	7.2
1	A	57	THR	7.2
1	A	106	HIS	7.0
1	B	108	GLY	7.0
1	A	56	ALA	7.0
1	B	79	ALA	6.9
1	B	84	ALA	6.8
1	B	54	LEU	6.6
1	B	2	ILE	6.4
1	A	73	HIS	6.4
1	B	41	ASP	6.3
1	A	110	ALA	6.3
1	B	83	GLY	6.2
1	B	111	ALA	6.1
1	B	86	GLY	6.1
1	B	43	VAL	5.9
1	B	116	TRP	5.9
1	B	110	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	108	GLY	5.8
1	B	88	TRP	5.8
1	A	79	ALA	5.5
1	A	109	GLY	5.4
1	A	76	GLU	5.3
1	A	2	ILE	5.3
1	A	52	LEU	5.3
1	B	37	ALA	5.1
1	B	73	HIS	5.0
1	B	39	GLU	5.0
1	B	107	ARG	4.9
1	A	86	GLY	4.9
1	A	44	VAL	4.8
1	A	40	ALA	4.8
1	A	82	LEU	4.7
1	A	88	TRP	4.7
1	A	75	SER	4.7
1	B	42	ARG	4.6
1	B	77	ALA	4.5
1	B	109	GLY	4.5
1	A	213	ASP	4.5
1	B	80	LYS	4.4
1	B	56	ALA	4.4
1	A	84	ALA	4.3
1	A	39	GLU	4.2
1	B	85	ASP	4.2
1	B	414	TRP	4.1
1	A	42	ARG	4.1
1	B	32	LEU	4.1
1	B	53	PRO	4.1
1	B	103	PHE	4.0
1	B	336	GLY	4.0
1	A	41	ASP	4.0
1	A	113	SER	4.0
1	B	81	SER	3.9
1	B	55	SER	3.9
1	B	431	TRP	3.8
1	A	55	SER	3.7
1	B	105	ALA	3.7
1	B	101	TYR	3.7
1	B	106	HIS	3.7
1	A	112	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	24	LEU	3.7
1	A	212	ALA	3.6
1	B	113	SER	3.6
1	B	33	LEU	3.6
1	B	44	VAL	3.5
1	B	432	TRP	3.5
1	B	95	LEU	3.5
1	B	340	ARG	3.5
1	A	116	TRP	3.5
1	A	77	ALA	3.4
1	A	81	SER	3.4
1	B	443	PHE	3.4
1	B	87	ALA	3.4
1	B	394	VAL	3.4
1	A	413	TRP	3.4
1	B	381	PHE	3.3
1	B	342	GLU	3.2
1	B	52	LEU	3.2
1	A	80	LYS	3.1
1	A	49	THR	3.0
1	B	72	GLY	3.0
1	A	105	ALA	3.0
1	B	247	VAL	3.0
1	B	49	THR	3.0
1	A	214	GLY	3.0
1	B	38	PRO	3.0
1	B	76	GLU	2.9
1	B	48	GLY	2.9
1	B	242	LEU	2.9
1	A	74	LEU	2.9
1	B	75	SER	2.9
1	A	87	ALA	2.9
1	A	43	VAL	2.8
1	A	53	PRO	2.8
1	B	124	TRP	2.8
1	B	151	VAL	2.7
1	A	48	GLY	2.7
1	B	3	LYS	2.7
1	B	428	THR	2.7
1	B	36	VAL	2.6
1	B	148	SER	2.6
1	B	102	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	38	PRO	2.6
1	B	89	SER	2.6
1	B	140	ARG	2.6
1	A	85	ASP	2.6
1	B	131	GLU	2.5
1	A	54	LEU	2.5
1	A	51	GLU	2.5
1	B	387	ALA	2.4
1	B	35	VAL	2.4
1	B	90	VAL	2.4
1	B	112	GLU	2.4
1	A	47	TRP	2.4
1	B	104	HIS	2.4
1	B	78	GLN	2.4
1	B	329	VAL	2.3
1	B	395	ARG	2.3
1	B	341	ALA	2.2
1	B	146	VAL	2.2
1	A	102	ARG	2.2
1	B	51	GLU	2.1
1	B	114	THR	2.1
1	A	1	MET	2.1
1	A	35	VAL	2.1
1	A	140	ARG	2.1
1	A	78	GLN	2.1
1	B	128	GLY	2.0
1	B	74	LEU	2.0
1	A	100	LYS	2.0
1	B	129	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
3	GOL	A	815	6/6	0.62	0.27	32,35,38,39	0
3	GOL	A	814	6/6	0.81	0.18	14,20,28,32	0
3	GOL	B	805	6/6	0.83	0.24	25,29,40,42	0
2	SO4	A	810	5/5	0.85	0.24	64,65,87,88	0
2	SO4	A	806	5/5	0.86	0.31	45,54,55,69	0
3	GOL	A	811	6/6	0.87	0.16	14,23,32,32	0
3	GOL	B	803	6/6	0.88	0.18	20,22,29,32	0
2	SO4	A	801	5/5	0.89	0.24	44,47,64,68	0
2	SO4	B	802	5/5	0.90	0.30	46,56,62,70	0
3	GOL	B	804	6/6	0.91	0.16	27,29,31,39	0
2	SO4	A	808	5/5	0.92	0.19	57,67,73,77	0
2	SO4	A	807	5/5	0.93	0.17	40,43,62,67	0
2	SO4	A	802	5/5	0.93	0.22	46,50,64,70	0
2	SO4	B	801	5/5	0.93	0.18	44,49,67,67	0
3	GOL	A	812	6/6	0.94	0.14	15,18,24,29	0
2	SO4	A	809	5/5	0.94	0.24	49,49,64,67	0
2	SO4	A	805	5/5	0.94	0.23	47,47,62,64	0
3	GOL	A	813	6/6	0.95	0.18	21,22,29,32	0
2	SO4	A	804	5/5	0.95	0.16	38,40,58,61	0
2	SO4	A	803	5/5	0.97	0.11	23,30,33,34	0
3	GOL	A	816	6/6	0.97	0.14	29,32,42,43	6

6.5 Other polymers ⓘ

There are no such residues in this entry.