



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:38 AM UTC

PDB ID : 5X3I / pdb_00005x3i
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 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

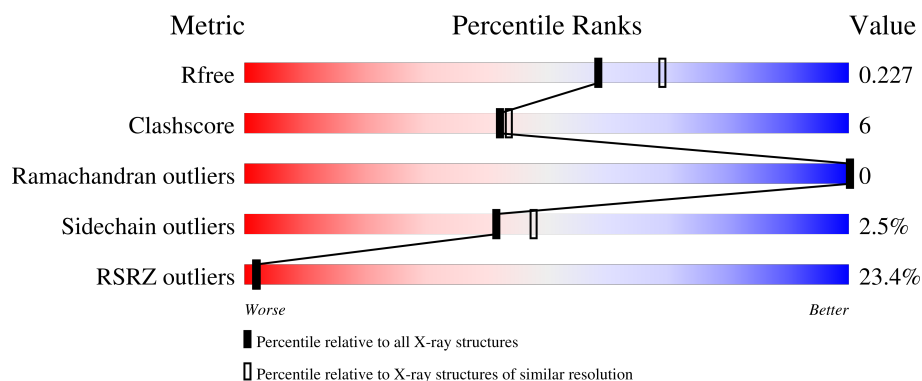
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	743	9% 86% 8% 5%
1	B	743	36% 81% 13% 5%

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

Continued on next page...

Continued from previous page...

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 (CCD ID: 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		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

Continued on next page...

Continued from previous page...

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

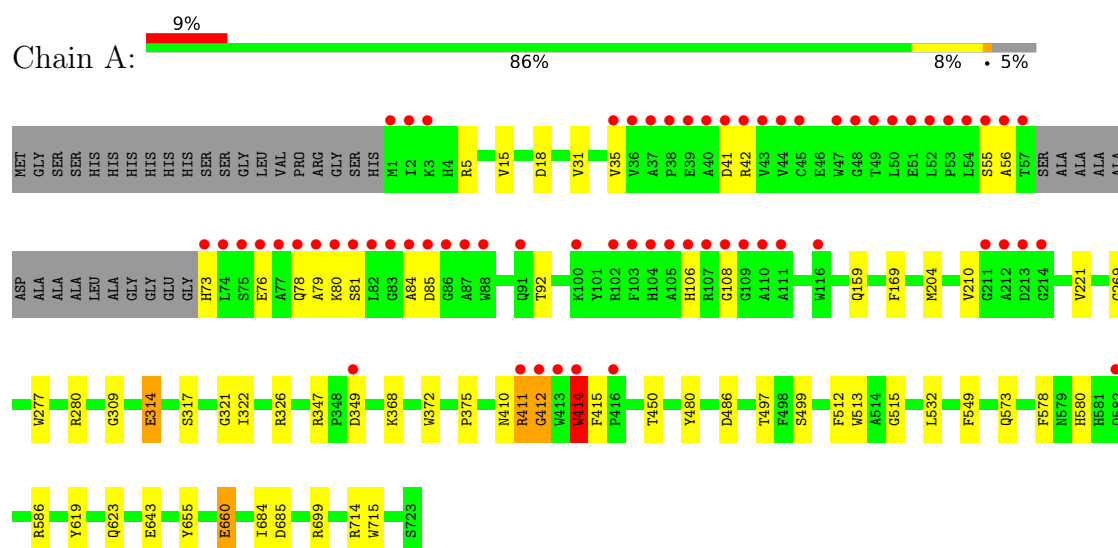
- Molecule 4 is water.

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

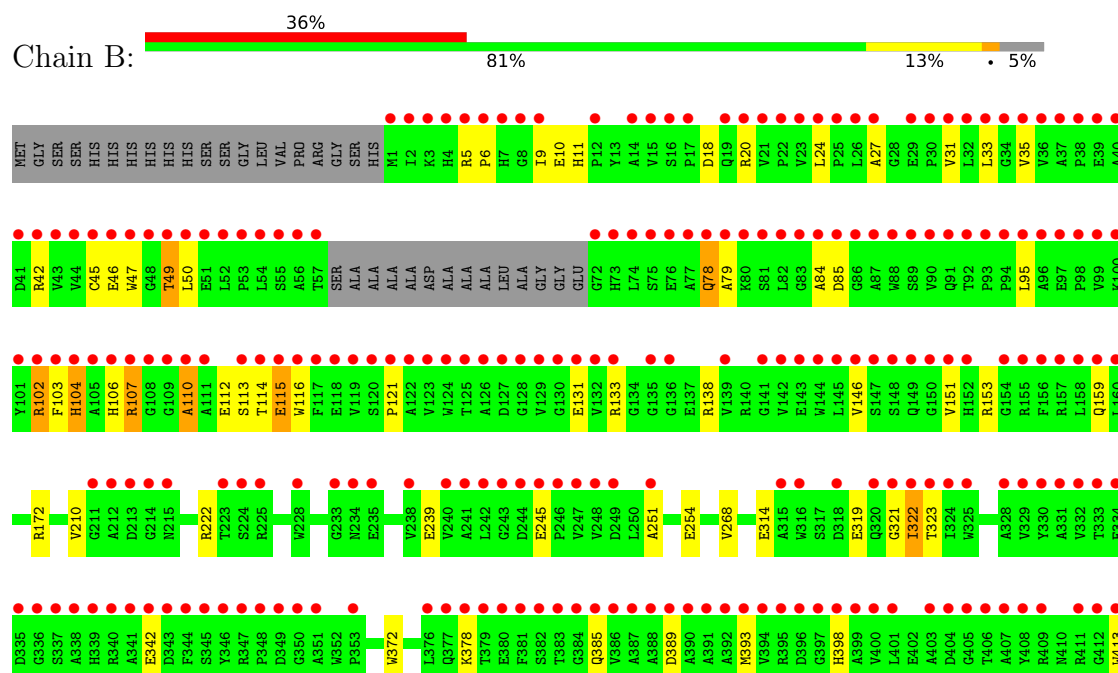
3 Residue-property plots

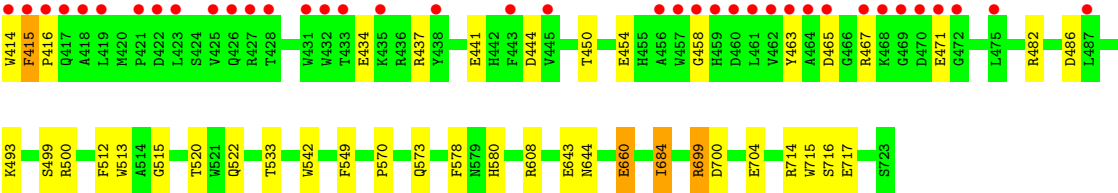
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 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 0.205 , 0.227	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)	0.36 , 41.5	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: SO4, GOL

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	0.62	3/5764 (0.1%)	0.84	10/7877 (0.1%)
1	B	0.56	6/5768 (0.1%)	0.80	6/7882 (0.1%)
All	All	0.59	9/11532 (0.1%)	0.82	16/15759 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	414	TRP	C-O	-6.68	1.15	1.23
1	B	716	SER	C-O	-6.35	1.16	1.24
1	B	416	PRO	N-CD	5.71	1.55	1.47
1	A	321	GLY	C-O	-5.46	1.17	1.24
1	B	415	PHE	C-N	5.31	1.40	1.33
1	A	414	TRP	N-CA	5.17	1.52	1.45
1	B	323	THR	CA-C	-5.09	1.46	1.52
1	B	717	GLU	C-O	-5.04	1.18	1.24
1	B	643	GLU	C-O	-5.02	1.17	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	ARG	N-CA-C	-10.79	100.42	112.72
1	B	110	ALA	N-CA-C	-6.61	101.80	110.53
1	A	414	TRP	CA-CB-CG	6.60	126.14	113.60
1	A	314	GLU	CA-C-N	-6.37	113.34	122.77
1	A	314	GLU	C-N-CA	-6.37	113.34	122.77
1	B	415	PHE	CA-C-N	-6.34	113.15	119.99
1	B	415	PHE	C-N-CA	-6.34	113.15	119.99
1	A	660	GLU	N-CA-C	6.32	120.99	113.28
1	B	717	GLU	N-CA-C	6.27	118.20	111.36
1	A	221	VAL	CA-C-N	-5.90	113.74	122.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	VAL	C-N-CA	-5.90	113.74	122.41
1	A	412	GLY	N-CA-C	-5.59	104.04	112.60
1	B	268	VAL	N-CA-C	5.35	116.83	111.00
1	A	269	GLY	N-CA-C	5.15	116.84	111.95
1	B	660	GLU	N-CA-C	5.14	119.82	113.50
1	A	497	THR	N-CA-C	-5.11	101.83	109.95

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	5590	0	5311	42	1
1	B	5594	0	5314	94	0
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	138	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 (138) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:78:GLN:HA	1:B:413:TRP:HZ2	1.44	0.79
1:B:102:ARG:NH2	1:B:116:TRP:NE1	2.30	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
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:HD12	1:B:50:LEU:N	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:VAL:HG22	1:A:73:HIS:CE1	2.34	0.62
1:B:321:GLY:C	1:B:322:ILE:HG12	2.25	0.61
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:513:TRP:CD1	1:B:515:GLY:H	2.21	0.58
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: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:660:GLU:CD	1:B:714:ARG:HG3	2.32	0.54
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:245:GLU:H	1:B:245:GLU:CD	2.15	0.54
1:B:10:GLU:CD	1:B:458:GLY:HA2	2.33	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
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:A:410:ASN:C	1:A:412:GLY:H	2.16	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:500:ARG:NH1	3:B:804:GOL:H31	2.27	0.49
1:B:684:ILE:HD12	1:B:715:TRP:CG	2.47	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:342:GLU:H	1:B:342:GLU:CD	2.23	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:513:TRP:CD1	1:A:515:GLY:H	2.33	0.46
1:A:169:PHE:HA	1:A:204:MET:O	2.16	0.45
1:A:78:GLN:O	1:A:81:SER:OG	2.27	0.45
1:A:660:GLU:CD	1:A:714:ARG:HG3	2.42	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:B:49:THR:C	1:B:50:LEU:HD12	2.41	0.44
1:A:79:ALA:HB1	1:A:84:ALA:HB2	2.00	0.44
1:B:319:GLU:O	1:B:378:LYS:NZ	2.39	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
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:HD3	1:A:347:ARG:HA	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:444:ASP:OD1	1:B:493:LYS:NZ	2.47	0.41
1:B:104:HIS:HA	1:B:112:GLU:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:HD13	1:B:103:PHE:CZ	2.53	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: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 [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	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 [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	567/588 (96%)	557 (98%)	10 (2%)	51	60
1	B	567/588 (96%)	549 (97%)	18 (3%)	34	38
All	All	1134/1176 (96%)	1106 (98%)	28 (2%)	42	48

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	85	ASP
1	A	159	GLN
1	A	210	VAL
1	A	322	ILE
1	A	411	ARG
1	A	414	TRP
1	A	450	THR
1	A	549	PHE
1	A	573	GLN
1	B	24	LEU
1	B	31	VAL
1	B	35	VAL
1	B	49	THR
1	B	78	GLN
1	B	85	ASP
1	B	102	ARG
1	B	104	HIS
1	B	107	ARG
1	B	115	GLU
1	B	159	GLN
1	B	210	VAL
1	B	322	ILE
1	B	450	THR
1	B	549	PHE
1	B	573	GLN
1	B	684	ILE
1	B	699	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	106	HIS
1	B	580	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	GOL	A	814	-	5,5,5	0.38	0	5,5,5	0.98	0
2	SO4	A	803	-	4,4,4	0.25	0	6,6,6	0.27	0
3	GOL	B	805	-	5,5,5	0.88	0	5,5,5	0.61	0
3	GOL	B	803	-	5,5,5	0.68	0	5,5,5	1.10	1 (20%)
3	GOL	A	815	-	5,5,5	0.39	0	5,5,5	0.15	0
3	GOL	A	812	-	5,5,5	1.02	0	5,5,5	0.97	0
3	GOL	A	813	-	5,5,5	0.41	0	5,5,5	0.49	0
2	SO4	A	808	-	4,4,4	0.22	0	6,6,6	0.08	0
3	GOL	A	816	-	5,5,5	0.40	0	5,5,5	0.27	0
2	SO4	B	802	-	4,4,4	0.25	0	6,6,6	0.18	0
2	SO4	A	805	-	4,4,4	0.21	0	6,6,6	0.18	0
2	SO4	B	801	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	806	-	4,4,4	0.26	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	801	-	4,4,4	0.24	0	6,6,6	0.18	0
3	GOL	B	804	-	5,5,5	0.43	0	5,5,5	0.78	0
2	SO4	A	802	-	4,4,4	0.22	0	6,6,6	0.09	0
2	SO4	A	807	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	A	809	-	4,4,4	0.21	0	6,6,6	0.09	0
2	SO4	A	804	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	A	810	-	4,4,4	0.23	0	6,6,6	0.14	0
3	GOL	A	811	-	5,5,5	1.21	1 (20%)	5,5,5	1.28	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	815	-	-	2/4/4/4	-
3	GOL	A	814	-	-	0/4/4/4	-
3	GOL	A	812	-	-	1/4/4/4	-
3	GOL	A	811	-	-	3/4/4/4	-
3	GOL	A	813	-	-	1/4/4/4	-
3	GOL	B	804	-	-	2/4/4/4	-
3	GOL	A	816	-	-	1/4/4/4	-
3	GOL	B	805	-	-	2/4/4/4	-
3	GOL	B	803	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	811	GOL	O2-C2	-2.53	1.36	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	803	GOL	O2-C2-C1	2.05	117.66	109.18

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	811	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

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

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	814	GOL	1	0
3	B	803	GOL	3	0
3	A	812	GOL	1	0
2	A	808	SO4	1	0
2	B	802	SO4	1	0
2	A	806	SO4	1	0
3	B	804	GOL	2	0
2	A	807	SO4	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	708/743 (95%)	0.17	65 (9%) 14 15	11, 20, 70, 112	0
1	B	709/743 (95%)	1.51	267 (37%) 1 1	12, 33, 99, 122	0
All	All	1417/1486 (95%)	0.84	332 (23%) 2 2	11, 25, 88, 122	0

All (332) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	LEU	11.1
1	B	413	TRP	8.0
1	A	57	THR	7.9
1	B	79	ALA	7.5
1	B	86	GLY	7.4
1	B	464	ALA	7.4
1	B	116	TRP	7.2
1	A	413	TRP	7.2
1	B	84	ALA	7.0
1	A	83	GLY	6.9
1	A	84	ALA	6.5
1	B	332	VAL	6.5
1	B	44	VAL	6.4
1	B	110	ALA	6.3
1	B	146	VAL	6.3
1	B	83	GLY	6.3
1	A	56	ALA	6.3
1	B	104	HIS	6.1
1	B	2	ILE	6.1
1	B	74	LEU	6.1
1	B	50	LEU	6.1
1	B	72	GLY	6.0
1	B	1	MET	6.0
1	B	77	ALA	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	44	VAL	5.8
1	A	79	ALA	5.8
1	B	38	PRO	5.8
1	B	432	TRP	5.6
1	B	462	VAL	5.6
1	B	3	LYS	5.6
1	B	129	VAL	5.6
1	A	73	HIS	5.5
1	B	56	ALA	5.5
1	A	107	ARG	5.4
1	A	106	HIS	5.4
1	B	414	TRP	5.3
1	B	43	VAL	5.3
1	A	77	ALA	5.3
1	B	96	ALA	5.3
1	B	117	PHE	5.2
1	A	86	GLY	5.2
1	B	128	GLY	5.2
1	A	110	ALA	5.2
1	B	101	TYR	5.2
1	A	1	MET	5.2
1	B	99	VAL	5.2
1	A	82	LEU	5.1
1	B	75	SER	5.1
1	B	431	TRP	5.1
1	B	88	TRP	5.0
1	B	386	VAL	5.0
1	B	33	LEU	5.0
1	B	49	THR	5.0
1	A	55	SER	4.9
1	B	150	GLY	4.9
1	B	24	LEU	4.9
1	B	48	GLY	4.9
1	B	40	ALA	4.9
1	B	119	VAL	4.9
1	B	47	TRP	4.8
1	B	111	ALA	4.8
1	B	415	PHE	4.8
1	B	247	VAL	4.8
1	B	52	LEU	4.8
1	B	36	VAL	4.8
1	A	40	ALA	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	338	ALA	4.7
1	B	145	LEU	4.7
1	B	124	TRP	4.7
1	B	35	VAL	4.7
1	B	54	LEU	4.7
1	B	95	LEU	4.7
1	B	98	PRO	4.7
1	B	103	PHE	4.7
1	B	94	PRO	4.7
1	B	57	THR	4.6
1	A	74	LEU	4.6
1	B	125	THR	4.6
1	A	111	ALA	4.6
1	B	123	VAL	4.5
1	B	80	LYS	4.5
1	B	34	GLY	4.5
1	B	102	ARG	4.5
1	B	394	VAL	4.5
1	A	212	ALA	4.5
1	B	113	SER	4.4
1	B	90	VAL	4.4
1	B	425	VAL	4.4
1	B	73	HIS	4.4
1	A	38	PRO	4.4
1	B	53	PRO	4.4
1	B	37	ALA	4.4
1	B	388	ALA	4.4
1	B	105	ALA	4.3
1	B	465	ASP	4.3
1	B	32	LEU	4.3
1	B	87	ALA	4.3
1	B	151	VAL	4.3
1	A	37	ALA	4.2
1	B	381	PHE	4.2
1	B	412	GLY	4.2
1	B	139	VAL	4.2
1	B	457	TRP	4.2
1	B	107	ARG	4.2
1	A	88	TRP	4.1
1	B	333	THR	4.1
1	A	214	GLY	4.1
1	B	109	GLY	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	100	LYS	4.1
1	B	407	ALA	4.0
1	A	52	LEU	4.0
1	B	331	ALA	4.0
1	A	39	GLU	4.0
1	B	242	LEU	4.0
1	B	122	ALA	4.0
1	B	387	ALA	4.0
1	B	330	TYR	4.0
1	B	468	LYS	4.0
1	B	397	GLY	4.0
1	B	463	TYR	3.9
1	A	75	SER	3.9
1	B	114	THR	3.9
1	B	344	PHE	3.9
1	B	384	GLY	3.9
1	B	148	SER	3.9
1	B	241	ALA	3.9
1	B	428	THR	3.9
1	B	325	TRP	3.8
1	B	85	ASP	3.8
1	B	81	SER	3.8
1	B	144	TRP	3.8
1	A	43	VAL	3.8
1	B	132	VAL	3.8
1	B	245	GLU	3.8
1	B	340	ARG	3.8
1	A	80	LYS	3.8
1	B	45	CYS	3.7
1	B	248	VAL	3.7
1	B	89	SER	3.7
1	B	406	THR	3.7
1	B	416	PRO	3.6
1	A	104	HIS	3.6
1	B	31	VAL	3.6
1	B	405	GLY	3.6
1	A	81	SER	3.6
1	B	27	ALA	3.6
1	B	346	TYR	3.6
1	B	106	HIS	3.6
1	B	130	GLY	3.6
1	B	336	GLY	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	49	THR	3.6
1	B	126	ALA	3.6
1	B	419	LEU	3.6
1	A	211	GLY	3.6
1	B	55	SER	3.6
1	A	213	ASP	3.5
1	B	323	THR	3.5
1	B	403	ALA	3.5
1	B	383	THR	3.5
1	B	16	SER	3.5
1	B	142	VAL	3.5
1	B	418	ALA	3.5
1	B	4	HIS	3.5
1	B	15	VAL	3.5
1	A	414	TRP	3.4
1	A	87	ALA	3.4
1	B	341	ALA	3.4
1	B	141	GLY	3.4
1	B	78	GLN	3.4
1	B	21	VAL	3.4
1	B	392	ALA	3.4
1	B	399	ALA	3.4
1	A	42	ARG	3.4
1	B	22	PRO	3.4
1	B	120	SER	3.4
1	A	105	ALA	3.4
1	B	97	GLU	3.4
1	B	212	ALA	3.4
1	B	7	HIS	3.4
1	B	157	ARG	3.4
1	B	6	PRO	3.4
1	B	458	GLY	3.4
1	B	401	LEU	3.4
1	B	329	VAL	3.3
1	B	443	PHE	3.3
1	B	393	MET	3.3
1	B	380	GLU	3.3
1	B	41	ASP	3.3
1	B	213	ASP	3.3
1	A	76	GLU	3.2
1	B	26	LEU	3.2
1	B	460	ASP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	382	SER	3.2
1	B	351	ALA	3.2
1	B	461	LEU	3.2
1	B	152	HIS	3.2
1	B	400	VAL	3.2
1	B	391	ALA	3.2
1	B	91	GLN	3.2
1	A	47	TRP	3.1
1	A	50	LEU	3.1
1	B	345	SER	3.1
1	B	246	PRO	3.1
1	B	127	ASP	3.1
1	B	25	PRO	3.1
1	B	390	ALA	3.1
1	A	100	LYS	3.1
1	A	109	GLY	3.1
1	B	233	GLY	3.1
1	B	251	ALA	3.1
1	B	324	ILE	3.1
1	B	92	THR	3.0
1	B	17	PRO	3.0
1	B	421	PRO	3.0
1	B	339	HIS	3.0
1	B	14	ALA	3.0
1	B	23	VAL	3.0
1	B	9	ILE	3.0
1	A	108	GLY	3.0
1	B	214	GLY	3.0
1	B	30	PRO	3.0
1	B	320	GLN	3.0
1	B	131	GLU	3.0
1	A	53	PRO	3.0
1	B	93	PRO	3.0
1	B	348	PRO	3.0
1	B	398	HIS	3.0
1	B	411	ARG	3.0
1	A	2	ILE	3.0
1	A	412	GLY	3.0
1	B	20	ARG	2.9
1	B	118	GLU	2.9
1	B	334	GLU	2.9
1	B	335	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	379	THR	2.9
1	B	149	GLN	2.9
1	B	385	GLN	2.9
1	B	243	GLY	2.9
1	B	342	GLU	2.9
1	B	423	LEU	2.9
1	B	445	VAL	2.9
1	B	417	GLN	2.9
1	B	459	HIS	2.9
1	A	36	VAL	2.8
1	A	45	CYS	2.8
1	B	121	PRO	2.8
1	B	147	SER	2.8
1	B	328	ALA	2.8
1	B	422	ASP	2.8
1	B	108	GLY	2.8
1	A	116	TRP	2.8
1	A	3	LYS	2.8
1	B	19	GLN	2.8
1	B	404	ASP	2.8
1	B	395	ARG	2.7
1	B	249	ASP	2.7
1	A	54	LEU	2.7
1	B	408	TYR	2.7
1	B	46	GLU	2.7
1	B	349	ASP	2.7
1	B	435	LYS	2.7
1	B	409	ARG	2.7
1	B	143	GLU	2.7
1	B	39	GLU	2.6
1	B	51	GLU	2.6
1	B	347	ARG	2.6
1	B	234	ASN	2.6
1	B	156	PHE	2.6
1	B	487	LEU	2.6
1	B	42	ARG	2.6
1	B	76	GLU	2.6
1	A	41	ASP	2.6
1	A	35	VAL	2.6
1	B	215	ASN	2.6
1	B	8	GLY	2.5
1	B	438	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	322	ILE	2.5
1	A	78	GLN	2.5
1	B	244	ASP	2.4
1	B	377	GLN	2.4
1	B	350	GLY	2.4
1	B	225	ARG	2.4
1	A	582	GLN	2.4
1	A	102	ARG	2.4
1	B	5	ARG	2.4
1	B	315	ALA	2.4
1	B	158	LEU	2.4
1	B	376	LEU	2.4
1	B	115	GLU	2.4
1	B	159	GLN	2.4
1	B	343	ASP	2.4
1	B	396	ASP	2.4
1	B	378	LYS	2.4
1	A	51	GLU	2.3
1	B	337	SER	2.3
1	B	316	TRP	2.3
1	A	411	ARG	2.3
1	B	321	GLY	2.3
1	A	91	GLN	2.3
1	A	416	PRO	2.3
1	B	133	ARG	2.3
1	B	469	GLY	2.3
1	B	224	SER	2.2
1	A	103	PHE	2.2
1	B	238	VAL	2.2
1	B	467	ARG	2.2
1	A	85	ASP	2.2
1	B	318	ASP	2.2
1	B	135	GLY	2.2
1	B	211	GLY	2.2
1	B	472	GLY	2.2
1	B	160	LEU	2.2
1	B	29	GLU	2.2
1	B	12	PRO	2.2
1	B	389	ASP	2.2
1	A	48	GLY	2.2
1	B	228	TRP	2.2
1	B	353	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	223	THR	2.1
1	B	240	VAL	2.1
1	B	470	ASP	2.1
1	B	471	GLU	2.1
1	B	155	ARG	2.1
1	B	136	GLY	2.1
1	B	235	GLU	2.0
1	B	426	GLN	2.0
1	B	433	THR	2.0
1	B	456	ALA	2.0
1	B	475	LEU	2.0
1	A	349	ASP	2.0
1	B	427	ARG	2.0
1	B	154	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	808	5/5	0.64	0.12	57,67,73,77	0
3	GOL	A	815	6/6	0.70	0.25	32,35,38,39	0
3	GOL	B	805	6/6	0.73	0.24	25,29,40,42	0
2	SO4	A	806	5/5	0.74	0.27	45,54,55,69	0
2	SO4	B	802	5/5	0.74	0.13	46,56,62,70	0
3	GOL	A	814	6/6	0.78	0.18	14,20,28,32	0
2	SO4	A	802	5/5	0.79	0.12	46,50,64,70	0
2	SO4	A	801	5/5	0.80	0.21	44,47,64,68	0
2	SO4	A	810	5/5	0.81	0.12	64,65,87,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	803	6/6	0.84	0.14	20,22,29,32	0
2	SO4	B	801	5/5	0.85	0.30	44,49,67,67	0
3	GOL	B	804	6/6	0.85	0.16	27,29,31,39	0
2	SO4	A	809	5/5	0.85	0.26	49,49,64,67	0
3	GOL	A	811	6/6	0.87	0.15	14,23,32,32	0
2	SO4	A	807	5/5	0.87	0.20	40,43,62,67	0
2	SO4	A	805	5/5	0.89	0.18	47,47,62,64	0
3	GOL	A	813	6/6	0.90	0.14	21,22,29,32	0
3	GOL	A	816	6/6	0.91	0.13	29,32,42,43	6
2	SO4	A	804	5/5	0.91	0.18	38,40,58,61	0
3	GOL	A	812	6/6	0.92	0.12	15,18,24,29	0
2	SO4	A	803	5/5	0.96	0.12	23,30,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.