



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 10:32 AM UTC

PDB ID : 9NPF / pdb_00009npf
Title : Crystal structure of the inactive conformation of a glycoside hydrolase (CapGH2b) from the GH2 family in the space group P1 at 2.15 Å
Authors : Martins, M.P.; Spadeto, J.P.M.; Miyamoto, R.Y.; Morais, M.A.B.; Murakami, M.T.
Deposited on : 2025-03-11
Resolution : 2.15 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

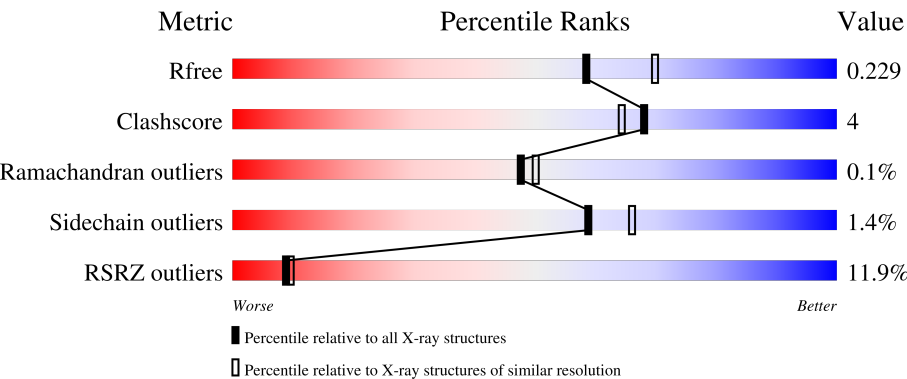
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	798	7% 83%9%8%
1	B	798	6% 83%9%8%
1	C	798	16% 83%8%8%
1	D	798	5% 84%7%8%
1	E	798	8% 84%8%8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	798	22% 78% 12% 9%

2 Entry composition [i](#)

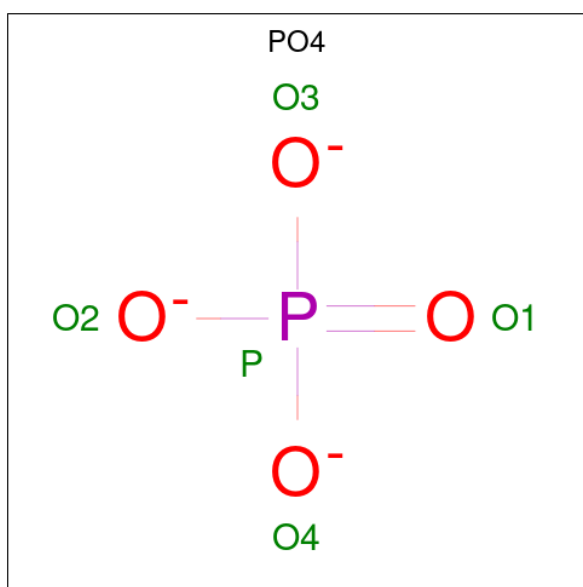
There are 5 unique types of molecules in this entry. The entry contains 37135 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	736	Total	C	N	O	S	Se	0	0	0
			5917	3782	1011	1094	8	22			
1	B	736	Total	C	N	O	S	Se	0	0	0
			5917	3786	1008	1093	8	22			
1	C	731	Total	C	N	O	S	Se	0	0	0
			5879	3755	1005	1089	8	22			
1	D	733	Total	C	N	O	S	Se	0	0	0
			5891	3766	1007	1089	8	21			
1	E	733	Total	C	N	O	S	Se	0	0	0
			5898	3773	1007	1088	8	22			
1	F	728	Total	C	N	O	S	Se	0	0	0
			5859	3742	1001	1086	8	22			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



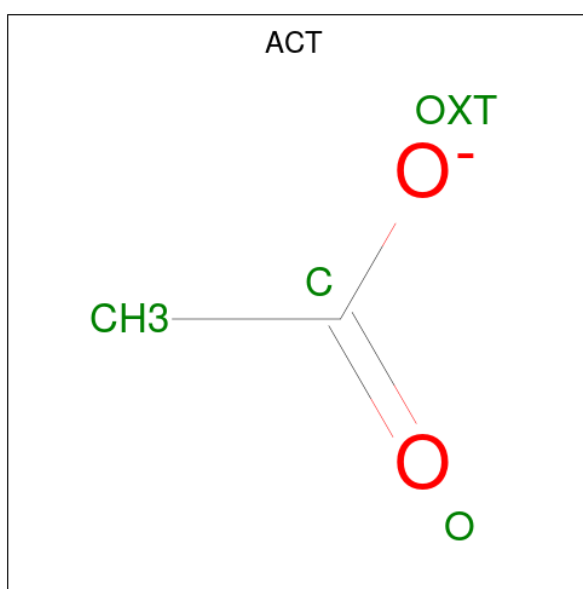
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	357	Total	O	0	0
			357	357		
5	B	331	Total	O	0	0
			331	331		
5	C	194	Total	O	0	0
			194	194		

Continued on next page...

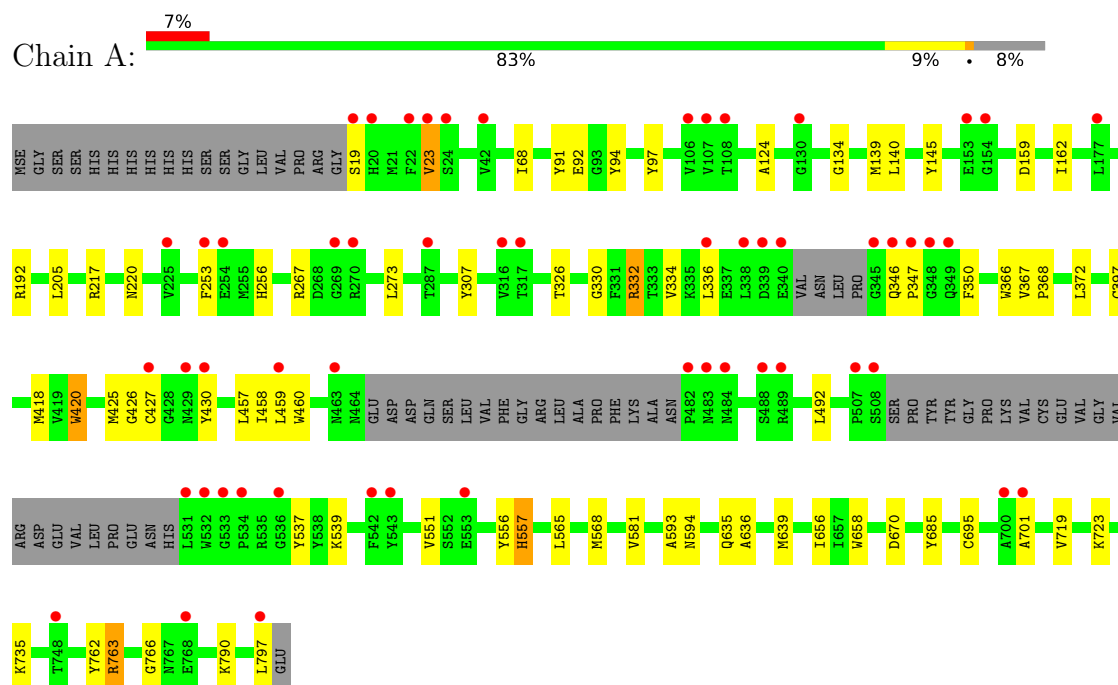
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	305	Total 305	O 305	0	0
5	E	288	Total 288	O 288	0	0
5	F	113	Total 113	O 113	0	0

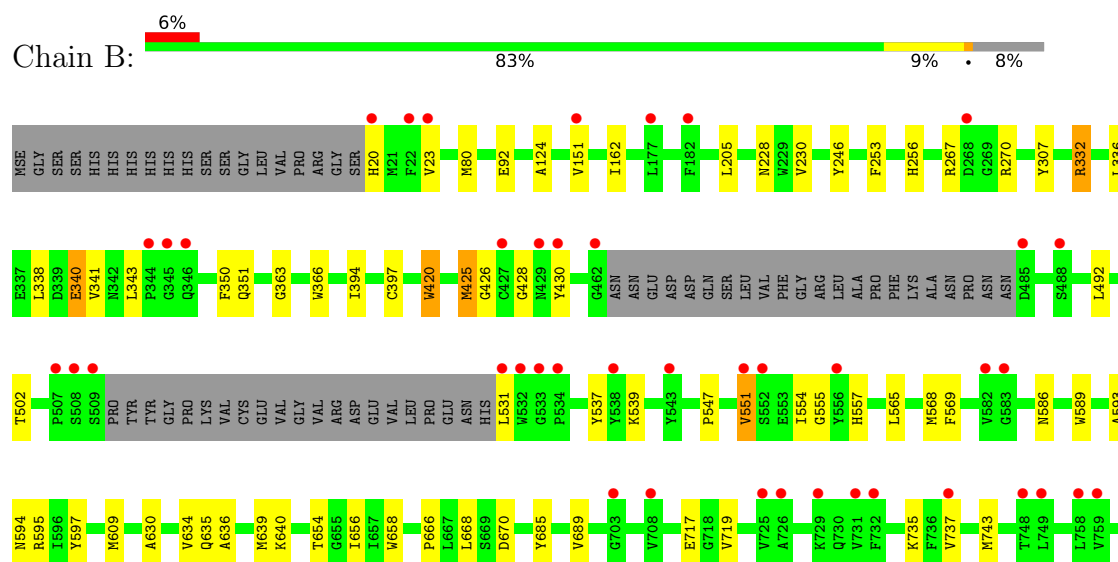
3 Residue-property plots

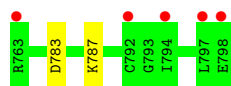
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 2

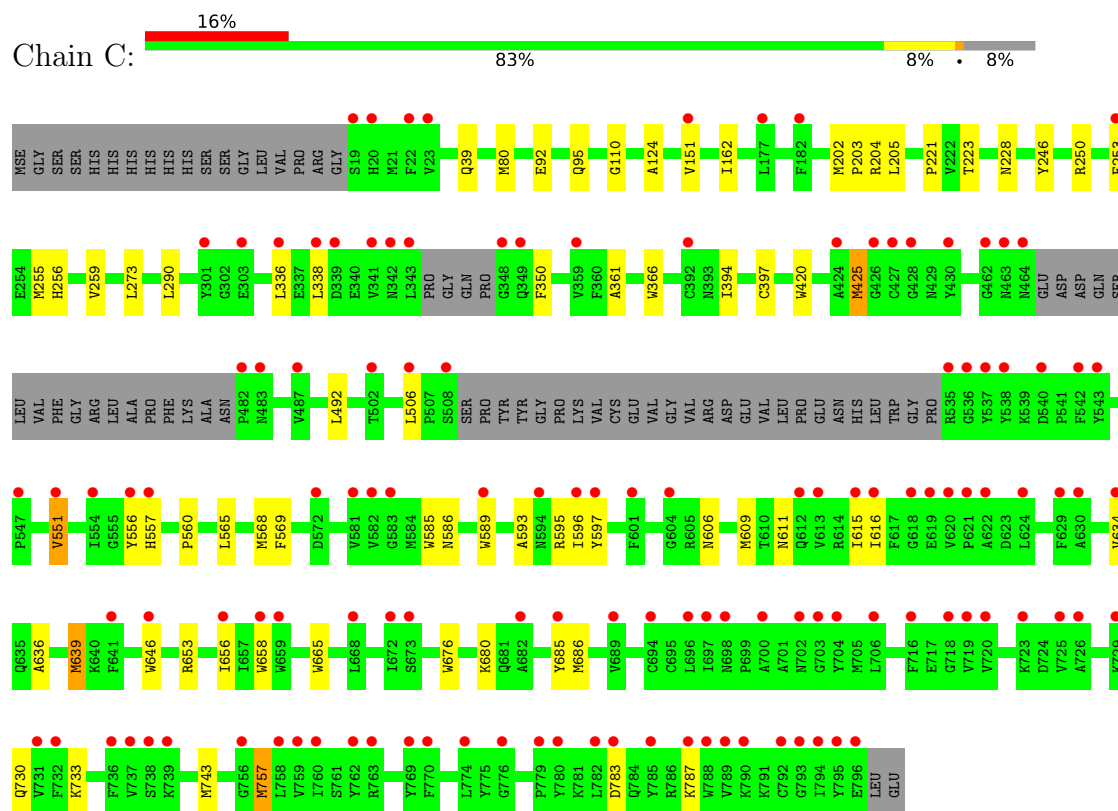


• Molecule 1: Glycoside hydrolase family 2

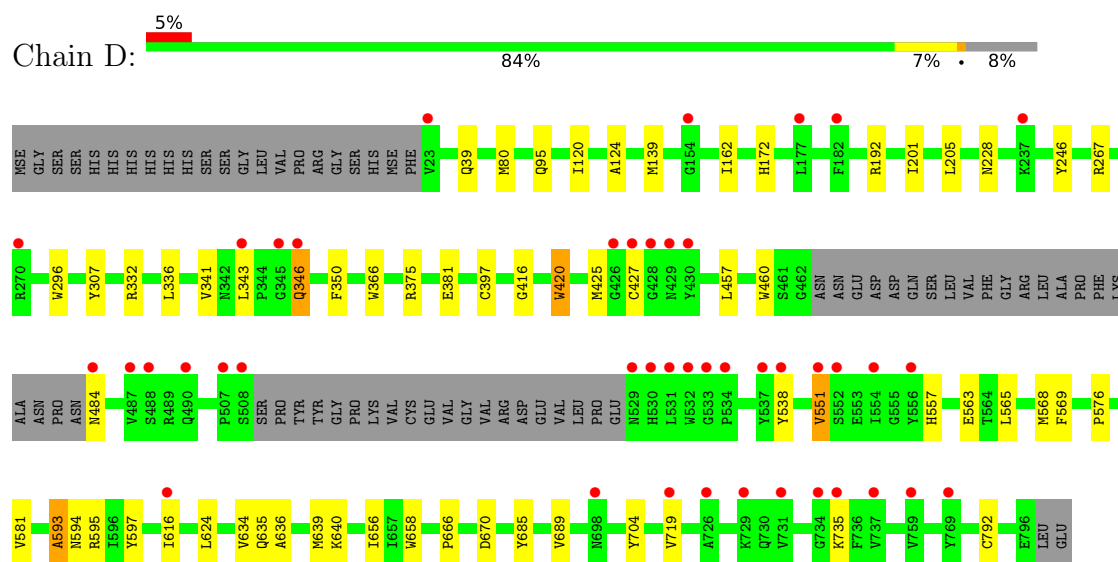




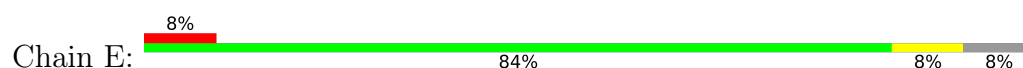
• Molecule 1: Glycoside hydrolase family 2

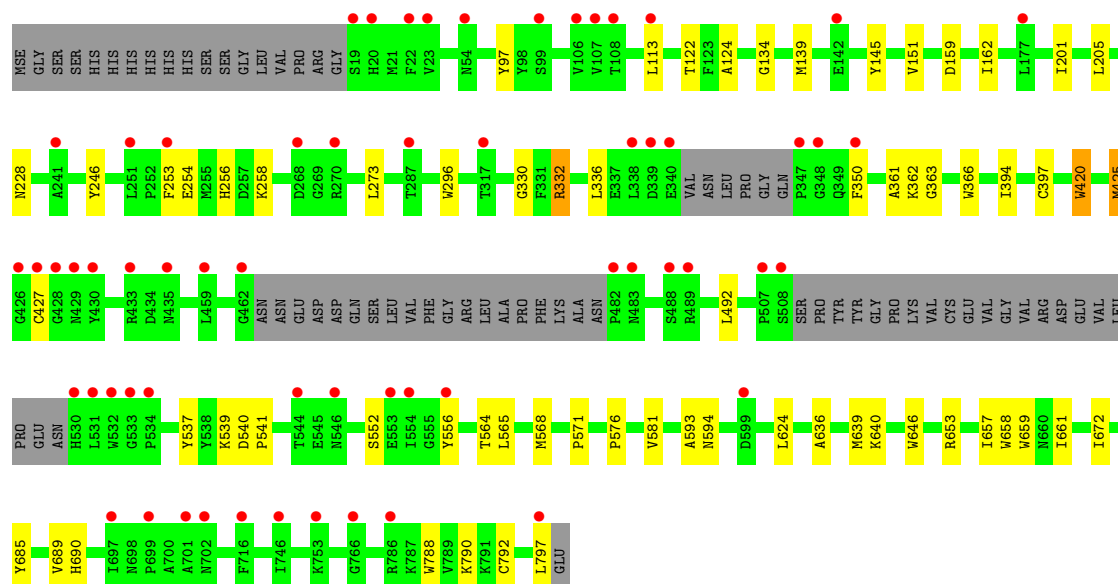


• Molecule 1: Glycoside hydrolase family 2

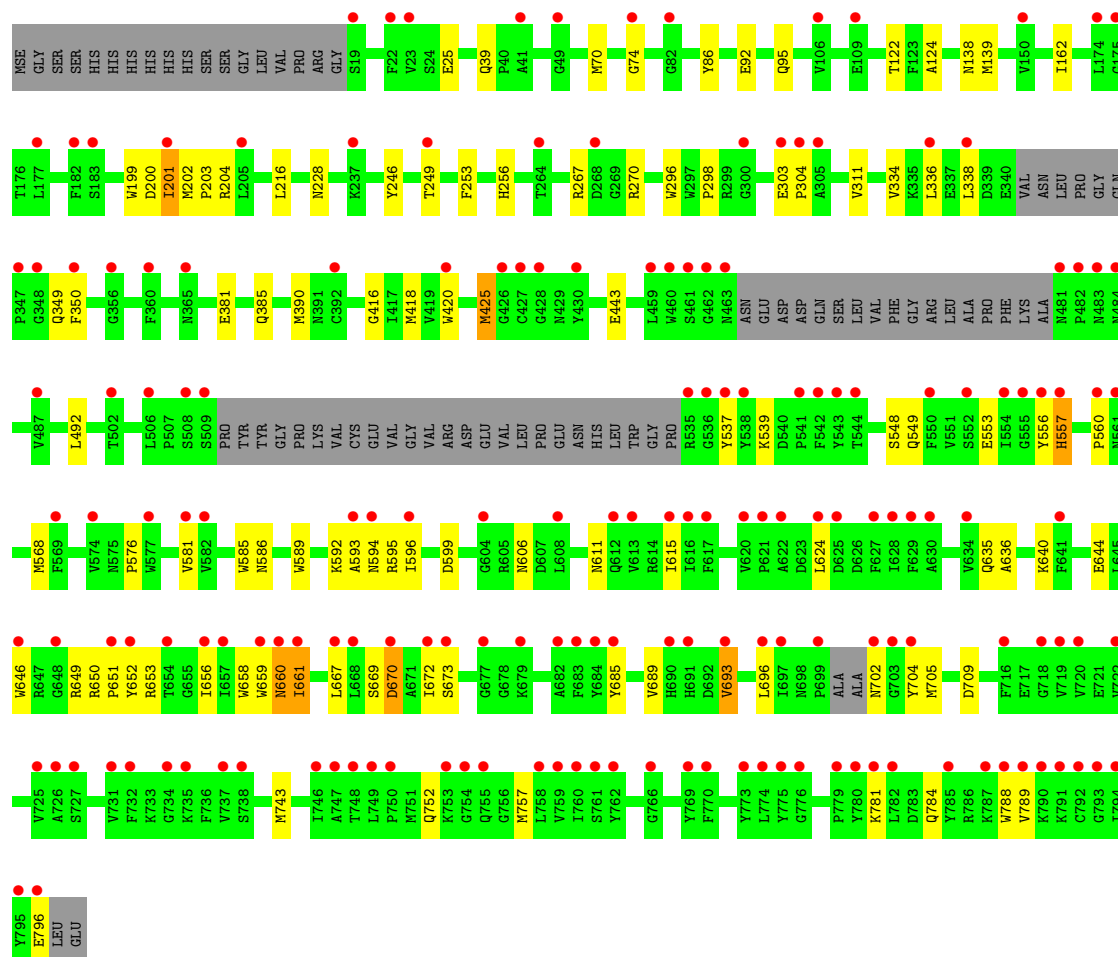
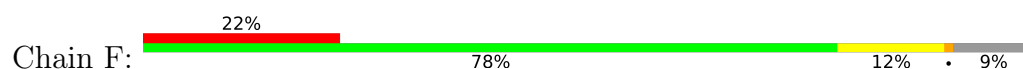


• Molecule 1: Glycoside hydrolase family 2





• Molecule 1: Glycoside hydrolase family 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	121.70Å 123.57Å 133.24Å 89.44° 117.29° 103.20°	Depositor
Resolution (Å)	49.00 – 2.15 49.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	90.1 (49.00-2.15) 90.1 (49.00-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.207 , 0.228 0.208 , 0.229	Depositor DCC
R_{free} test set	16398 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	37135	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.57% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ACT, 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	0.28	0/6050	0.47	2/8176 (0.0%)
1	B	0.25	0/6051	0.43	0/8180
1	C	0.31	5/6008 (0.1%)	0.43	0/8117
1	D	0.26	0/6025	0.45	0/8148
1	E	0.26	0/6032	0.47	2/8151 (0.0%)
1	F	0.30	3/5988 (0.1%)	0.47	4/8088 (0.0%)
All	All	0.28	8/36154 (0.0%)	0.45	8/48860 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
1	D	0	1
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	743	MSE	C-N	9.12	1.45	1.33
1	F	70	MSE	C-N	7.26	1.43	1.33
1	C	757	MSE	C-N	7.14	1.43	1.33
1	C	639	MSE	C-N	-6.80	1.25	1.33
1	F	425	MSE	C-N	-5.59	1.26	1.33
1	C	425	MSE	C-N	-5.44	1.26	1.33
1	F	705	MSE	C-N	5.27	1.41	1.33
1	C	609	MSE	C-N	5.21	1.40	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	VAL	N-CA-C	-8.76	104.76	112.12
1	E	425	MSE	CA-C-N	8.08	127.15	121.65
1	E	425	MSE	C-N-CA	8.08	127.15	121.65
1	F	661	ILE	N-CA-C	-7.17	104.40	113.22
1	F	670	ASP	N-CA-C	-5.38	106.59	112.72
1	F	425	MSE	CA-C-N	5.35	127.57	122.27
1	F	425	MSE	C-N-CA	5.35	127.57	122.27
1	A	140	LEU	N-CA-CB	-5.24	102.23	110.46

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	ARG	Sidechain
1	A	763	ARG	Sidechain
1	C	593	ALA	Peptide
1	D	593	ALA	Peptide

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	5917	0	5733	41	0
1	B	5917	0	5741	43	0
1	C	5879	0	5699	39	0
1	D	5891	0	5713	35	0
1	E	5898	0	5718	36	0
1	F	5859	0	5674	64	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	15	0	0	0	0
2	D	10	0	0	0	0
2	E	15	0	0	0	0
2	F	10	0	0	0	0
3	A	30	0	40	1	0
3	B	18	0	24	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	6	0	8	0	0
3	D	24	0	32	2	0
3	E	24	0	32	1	0
3	F	6	0	8	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	357	0	0	0	0
5	B	331	0	0	0	0
5	C	194	0	0	0	0
5	D	305	0	0	0	0
5	E	288	0	0	0	0
5	F	113	0	0	0	0
All	All	37135	0	34428	251	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 4.

All (251) 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:F:425:MSE:HE1	1:F:492:LEU:HD11	1.79	0.63
1:B:593:ALA:N	1:B:594:ASN:HA	2.12	0.63
1:B:425:MSE:HE1	1:B:492:LEU:HD11	1.80	0.62
1:F:640:LYS:HG3	1:F:689:VAL:HG21	1.80	0.62
1:F:649:ARG:HE	1:F:653:ARG:HE	1.48	0.62
1:D:616:ILE:HD12	1:D:634:VAL:HG13	1.82	0.62
1:E:639:MSE:HE1	1:E:658:TRP:HB2	1.83	0.60
1:C:338:LEU:HD23	1:C:350:PHE:HB3	1.84	0.59
1:E:790:LYS:HB2	1:E:797:LEU:HD11	1.84	0.59
1:B:425:MSE:HG3	1:B:430:TYR:CE1	2.37	0.59
1:C:228:ASN:HB3	1:C:246:TYR:HB2	1.84	0.59
1:C:204:ARG:HB2	1:C:596:ILE:HG23	1.85	0.58
1:E:564:THR:HG22	1:E:568:MSE:HE2	1.86	0.58
1:A:593:ALA:N	1:A:594:ASN:HA	2.18	0.58
1:E:593:ALA:N	1:E:594:ASN:HA	2.19	0.58
1:A:346:GLN:HG3	1:A:347:PRO:HD2	1.86	0.57
1:E:425:MSE:HE1	1:E:492:LEU:HD11	1.87	0.57
1:C:560:PRO:HA	1:C:680:LYS:HE2	1.87	0.56
1:C:595:ARG:HG2	1:C:597:TYR:O	2.05	0.56
1:D:139:MSE:HG2	1:D:192:ARG:HA	1.87	0.56
1:B:565:LEU:HD12	1:B:568:MSE:HE2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:ALA:HB3	1:F:74:GLY:O	2.06	0.56
1:D:593:ALA:N	1:D:594:ASN:HA	2.20	0.56
1:B:92:GLU:HB2	1:C:253:PHE:CZ	2.40	0.56
1:F:661:ILE:O	1:F:673:SER:HB3	2.06	0.56
1:F:693:VAL:HA	1:F:709:ASP:O	2.06	0.55
1:A:418:MSE:HB3	1:A:458:ILE:HG12	1.88	0.55
1:C:565:LEU:HD23	1:C:568:MSE:HE2	1.89	0.55
1:C:730:GLN:HG3	1:C:733:LYS:HG3	1.89	0.55
1:D:565:LEU:HD23	1:D:568:MSE:CE	2.36	0.55
1:D:563:GLU:HB2	3:D:803:GOL:H11	1.88	0.55
1:A:253:PHE:CZ	1:C:92:GLU:HB2	2.42	0.54
1:A:639:MSE:HE1	1:A:658:TRP:HB2	1.90	0.54
1:D:565:LEU:HD23	1:D:568:MSE:HE2	1.89	0.53
1:E:113:LEU:HD23	1:E:151:VAL:HG11	1.91	0.53
1:C:565:LEU:HD23	1:C:568:MSE:CE	2.39	0.53
1:F:349:GLN:NE2	1:F:548:SER:HA	2.23	0.53
1:B:551:VAL:HG23	1:B:656:ILE:HA	1.89	0.53
1:D:343:LEU:HB3	1:D:346:GLN:HB3	1.90	0.53
1:C:425:MSE:HE1	1:C:492:LEU:HD11	1.91	0.52
1:A:92:GLU:HB2	1:B:253:PHE:CZ	2.44	0.52
1:E:253:PHE:CZ	1:F:92:GLU:HB2	2.45	0.52
1:D:640:LYS:HG3	1:D:689:VAL:HG11	1.91	0.52
1:A:425:MSE:HE1	1:A:492:LEU:HD11	1.92	0.52
1:A:719:VAL:HG12	1:A:735:LYS:HG2	1.91	0.51
1:F:586:ASN:HD21	1:F:589:TRP:CD1	2.28	0.51
1:E:565:LEU:HA	1:E:568:MSE:HE3	1.92	0.51
1:B:568:MSE:HE3	1:B:569:PHE:CE2	2.45	0.51
1:A:330:GLY:O	3:A:804:GOL:H32	2.11	0.51
1:C:568:MSE:HE3	1:C:569:PHE:CE2	2.46	0.51
1:B:719:VAL:HG12	1:B:735:LYS:HG3	1.92	0.51
1:A:124:ALA:HB2	1:A:162:ILE:HG12	1.93	0.50
1:E:124:ALA:HB2	1:E:162:ILE:HG12	1.94	0.50
1:E:330:GLY:O	3:E:807:GOL:H12	2.10	0.50
1:F:743:MSE:SE	1:F:743:MSE:C	3.04	0.50
1:A:763:ARG:HE	1:A:766:GLY:HA2	1.77	0.50
1:B:332:ARG:C	1:B:332:ARG:HD3	2.36	0.50
1:C:636:ALA:HB1	1:C:685:TYR:CG	2.46	0.49
1:B:640:LYS:HG3	1:B:689:VAL:HG11	1.93	0.49
1:C:551:VAL:HG13	1:C:656:ILE:HA	1.94	0.49
1:E:636:ALA:HB1	1:E:685:TYR:CG	2.47	0.49
1:F:560:PRO:HG3	1:F:568:MSE:HE1	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:595:ARG:HD2	1:F:599:ASP:O	2.12	0.49
1:A:426:GLY:O	1:A:427:CYS:C	2.56	0.49
1:F:646:TRP:CD1	1:F:653:ARG:HB3	2.48	0.49
1:C:639:MSE:HE1	1:C:658:TRP:HB2	1.95	0.49
1:D:228:ASN:HB3	1:D:246:TYR:HB2	1.95	0.49
1:A:425:MSE:HG2	1:A:430:TYR:CZ	2.48	0.48
1:A:273:LEU:HA	1:D:341:VAL:O	2.14	0.48
1:A:636:ALA:HB1	1:A:685:TYR:CG	2.48	0.48
1:D:551:VAL:HG13	1:D:656:ILE:HA	1.96	0.48
1:E:336:LEU:HD11	1:E:350:PHE:CD1	2.48	0.48
1:F:784:GLN:HB3	1:F:788:TRP:CZ2	2.49	0.48
1:D:595:ARG:HG2	1:D:597:TYR:O	2.13	0.48
1:C:616:ILE:HG13	1:C:634:VAL:HG23	1.96	0.47
1:D:636:ALA:HB1	1:D:685:TYR:CG	2.49	0.47
1:A:790:LYS:HB2	1:A:797:LEU:HD11	1.95	0.47
1:F:336:LEU:HD11	1:F:350:PHE:CD1	2.50	0.47
1:F:644:GLU:HG3	1:F:689:VAL:HG11	1.95	0.47
1:F:303:GLU:HG2	1:F:304:PRO:HD2	1.97	0.47
1:F:650:ARG:N	1:F:651:PRO:HD2	2.30	0.47
1:B:338:LEU:HD23	1:B:350:PHE:HB3	1.96	0.47
1:C:273:LEU:HD13	1:C:290:LEU:HD23	1.95	0.47
1:A:336:LEU:HD11	1:A:350:PHE:CD1	2.50	0.47
1:B:531:LEU:HD12	1:B:554:ILE:HD12	1.97	0.47
1:B:636:ALA:HB1	1:B:685:TYR:CG	2.50	0.47
1:D:124:ALA:HB2	1:D:162:ILE:HG12	1.97	0.46
1:F:202:MSE:HE3	1:F:203:PRO:HD2	1.98	0.46
1:F:138:ASN:HD21	1:F:443:GLU:HB2	1.81	0.46
1:F:636:ALA:HB1	1:F:685:TYR:CG	2.49	0.46
1:C:80:MSE:HE2	1:C:676:TRP:CZ2	2.50	0.46
1:B:343:LEU:HD11	1:B:547:PRO:HB2	1.98	0.46
1:B:426:GLY:C	1:B:428:GLY:H	2.23	0.46
1:F:122:THR:OG1	1:F:139:MSE:HB2	2.16	0.46
1:F:228:ASN:HB3	1:F:246:TYR:HB2	1.97	0.46
1:A:139:MSE:HG2	1:A:192:ARG:HA	1.98	0.46
1:C:783:ASP:O	1:C:787:LYS:HG2	2.16	0.46
1:D:538:TYR:HE2	1:D:616:ILE:HD11	1.80	0.46
1:A:557:HIS:O	1:A:635:GLN:HB2	2.16	0.45
1:B:332:ARG:HD3	1:B:332:ARG:O	2.15	0.45
1:D:366:TRP:HB3	1:D:397:CYS:HA	1.98	0.45
1:E:362:LYS:HD2	1:E:690:HIS:CD2	2.51	0.45
1:D:172:HIS:HA	3:D:806:GOL:H32	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:GLN:HE22	1:F:548:SER:HA	1.81	0.45
1:F:390:MSE:HE2	1:F:390:MSE:HB2	1.86	0.45
1:C:646:TRP:CD1	1:C:653:ARG:HB3	2.52	0.45
1:A:551:VAL:HG23	1:A:656:ILE:HA	1.98	0.45
1:B:717:GLU:HG2	1:B:737:VAL:HG22	1.97	0.45
1:D:568:MSE:HE3	1:D:569:PHE:CE2	2.51	0.45
1:F:124:ALA:HB2	1:F:162:ILE:HG12	1.97	0.45
1:B:609:MSE:HE1	1:B:668:LEU:HB3	1.97	0.45
1:F:25:GLU:HA	1:F:216:LEU:O	2.17	0.45
1:F:203:PRO:HD3	1:F:667:LEU:HD11	1.98	0.45
1:F:644:GLU:HB3	1:F:696:LEU:HD13	1.99	0.45
1:F:689:VAL:HG12	1:F:689:VAL:O	2.16	0.45
1:A:420:TRP:CD1	1:A:420:TRP:C	2.95	0.45
1:E:420:TRP:CD1	1:E:420:TRP:C	2.95	0.45
1:B:228:ASN:HB3	1:B:246:TYR:HB2	1.99	0.44
1:B:366:TRP:HB3	1:B:397:CYS:HA	1.99	0.44
1:F:611:ASN:O	1:F:615:ILE:HG12	2.17	0.44
1:D:420:TRP:CD1	1:D:420:TRP:C	2.94	0.44
1:A:537:TYR:CE2	1:A:539:LYS:HB2	2.52	0.44
1:B:639:MSE:HE1	1:B:658:TRP:HB2	1.98	0.44
1:E:228:ASN:HB3	1:E:246:TYR:HB2	1.99	0.44
1:F:585:TRP:CE2	1:F:606:ASN:HB3	2.51	0.44
1:A:68:ILE:HG13	1:A:372:LEU:HD13	1.99	0.44
1:A:420:TRP:CD2	1:A:459:LEU:HD23	2.53	0.44
1:F:200:ASP:OD1	1:F:201:ILE:HG23	2.18	0.44
1:F:253:PHE:HA	1:F:256:HIS:ND1	2.33	0.44
1:A:565:LEU:HD23	1:A:568:MSE:HE2	2.00	0.44
1:B:783:ASP:O	1:B:787:LYS:HG3	2.18	0.44
1:C:124:ALA:HB2	1:C:162:ILE:HG12	1.98	0.44
1:A:366:TRP:HB3	1:A:397:CYS:HA	1.99	0.44
1:D:616:ILE:HD12	1:D:634:VAL:HG22	1.99	0.44
1:F:649:ARG:NE	1:F:653:ARG:HE	2.13	0.44
1:C:202:MSE:HE3	1:C:203:PRO:HD2	2.00	0.44
1:F:39:GLN:HB2	1:F:95:GLN:HG3	2.00	0.44
1:F:537:TYR:CE2	1:F:539:LYS:HB2	2.53	0.44
1:A:253:PHE:HA	1:A:256:HIS:ND1	2.33	0.43
1:B:80:MSE:HB3	1:B:666:PRO:HG2	2.00	0.43
1:C:336:LEU:HD11	1:C:350:PHE:CD1	2.53	0.43
1:C:586:ASN:HD21	1:C:589:TRP:CD1	2.36	0.43
1:D:80:MSE:HE2	1:D:375:ARG:HH22	1.83	0.43
1:E:363:GLY:HA3	1:E:394:ILE:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:ARG:HB2	1:F:596:ILE:HG23	2.00	0.43
1:A:723:LYS:HB3	1:A:723:LYS:HE2	1.85	0.43
1:F:650:ARG:HD3	1:F:709:ASP:OD1	2.19	0.43
1:F:781:LYS:HB2	1:F:784:GLN:HG3	2.00	0.43
1:C:110:GLY:HA3	1:C:221:PRO:HG3	2.00	0.43
1:F:267:ARG:O	1:F:270:ARG:HG3	2.19	0.43
1:F:593:ALA:HB2	1:F:606:ASN:OD1	2.19	0.43
1:A:97:TYR:HE1	1:A:159:ASP:HB3	1.83	0.43
1:C:253:PHE:HA	1:C:256:HIS:ND1	2.34	0.43
1:D:120:ILE:O	1:D:139:MSE:HA	2.19	0.43
1:D:719:VAL:HG12	1:D:735:LYS:HG3	2.01	0.43
1:F:670:ASP:OD1	1:F:670:ASP:N	2.52	0.43
1:A:19:SER:HB3	1:A:326:THR:HB	2.01	0.43
1:B:420:TRP:CD1	1:B:420:TRP:C	2.96	0.43
1:B:537:TYR:CE2	1:B:539:LYS:HB2	2.54	0.43
1:E:97:TYR:HE1	1:E:159:ASP:HB3	1.84	0.43
1:B:341:VAL:O	1:E:273:LEU:HA	2.19	0.43
1:E:253:PHE:HA	1:E:256:HIS:ND1	2.34	0.43
1:E:366:TRP:HB3	1:E:397:CYS:HA	2.00	0.43
1:F:86:TYR:OH	1:F:595:ARG:HB3	2.18	0.43
1:F:659:TRP:CG	1:F:660:ASN:H	2.36	0.43
1:E:254:GLU:O	1:E:258:LYS:HD2	2.19	0.43
1:F:661:ILE:HG13	1:F:672:ILE:HD11	2.01	0.43
1:A:332:ARG:NH2	1:A:334:VAL:HG12	2.34	0.43
1:B:340:GLU:H	1:B:340:GLU:HG2	1.63	0.43
1:C:255:MSE:HE3	1:C:259:VAL:CG2	2.48	0.43
1:C:420:TRP:C	1:C:420:TRP:CD1	2.97	0.43
1:B:267:ARG:HD2	1:B:307:TYR:CE2	2.54	0.42
1:B:426:GLY:C	1:B:428:GLY:N	2.77	0.42
1:C:757:MSE:HE3	1:C:757:MSE:HB2	1.92	0.42
1:D:639:MSE:HE1	1:D:658:TRP:HB2	2.00	0.42
1:C:585:TRP:CE2	1:C:606:ASN:HB3	2.54	0.42
1:C:639:MSE:HE3	1:C:686:MSE:HE2	2.00	0.42
1:C:223:THR:HG22	1:C:250:ARG:HB2	2.02	0.42
1:D:735:LYS:H	1:D:735:LYS:HD2	1.83	0.42
1:F:381:GLU:O	1:F:385:GLN:HG2	2.19	0.42
1:E:565:LEU:HD23	1:E:568:MSE:CE	2.50	0.42
1:B:555:GLY:HA2	1:B:639:MSE:SE	2.70	0.42
1:E:576:PRO:HD3	1:E:624:LEU:HD13	2.01	0.42
1:F:557:HIS:HA	1:F:670:ASP:HA	2.00	0.42
1:A:695:CYS:HB2	1:A:762:TYR:CD1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:ALA:HB1	1:C:394:ILE:HG21	2.01	0.42
1:C:425:MSE:HE3	1:C:425:MSE:HB2	1.93	0.42
1:D:425:MSE:HB2	1:D:425:MSE:HE3	1.75	0.42
1:D:457:LEU:HD21	1:D:460:TRP:CZ2	2.54	0.42
1:E:296:TRP:HB3	1:E:332:ARG:HG2	2.01	0.42
1:A:23:VAL:HG22	1:A:220:ASN:ND2	2.34	0.42
1:C:611:ASN:O	1:C:615:ILE:HG13	2.20	0.42
1:B:595:ARG:HG2	1:B:597:TYR:O	2.20	0.42
1:F:420:TRP:CD1	1:F:420:TRP:C	2.98	0.42
1:F:593:ALA:HB2	1:F:606:ASN:CG	2.45	0.42
1:C:39:GLN:HB2	1:C:95:GLN:HG3	2.02	0.42
1:F:658:TRP:CD1	1:F:658:TRP:H	2.37	0.42
1:E:361:ALA:HB1	1:E:394:ILE:HG21	2.03	0.41
1:F:199:TRP:HD1	1:F:200:ASP:OD1	2.02	0.41
1:F:592:LYS:C	1:F:594:ASN:H	2.28	0.41
1:E:540:ASP:CG	1:E:541:PRO:HD2	2.45	0.41
1:F:296:TRP:CZ2	1:F:416:GLY:HA2	2.55	0.41
1:F:557:HIS:O	1:F:635:GLN:HB2	2.20	0.41
1:A:636:ALA:HB1	1:A:685:TYR:CD2	2.55	0.41
1:B:363:GLY:HA3	1:B:394:ILE:O	2.20	0.41
1:D:80:MSE:HE2	1:D:375:ARG:NH2	2.36	0.41
1:D:267:ARG:HD2	1:D:307:TYR:CE2	2.56	0.41
1:E:134:GLY:HA3	1:E:145:TYR:CE1	2.55	0.41
1:E:201:ILE:HD13	1:E:659:TRP:HZ2	1.86	0.41
1:F:549:GLN:HG2	1:F:652:TYR:CZ	2.55	0.41
1:F:704:TYR:HE2	1:F:752:GLN:HG2	1.86	0.41
1:F:660:ASN:OD1	1:F:660:ASN:N	2.52	0.41
1:C:80:MSE:HG2	1:C:665:TRP:CH2	2.55	0.41
1:D:296:TRP:CZ2	1:D:416:GLY:HA2	2.55	0.41
1:D:576:PRO:HD3	1:D:624:LEU:HD13	2.03	0.41
1:E:661:ILE:HA	1:E:672:ILE:HG12	2.03	0.41
1:A:267:ARG:HD2	1:A:307:TYR:CE2	2.56	0.41
1:E:122:THR:OG1	1:E:139:MSE:HB2	2.20	0.41
1:E:565:LEU:HD23	1:E:568:MSE:HE1	2.03	0.41
1:B:230:VAL:HG13	1:B:502:THR:HG21	2.02	0.41
1:C:636:ALA:HB1	1:C:685:TYR:CD2	2.56	0.41
1:D:39:GLN:HB2	1:D:95:GLN:HG3	2.02	0.41
1:D:336:LEU:HD11	1:D:350:PHE:CD1	2.56	0.41
1:E:788:TRP:O	1:E:792:CYS:HB2	2.20	0.41
1:A:425:MSE:HE3	1:A:425:MSE:HB2	2.03	0.41
1:B:270:ARG:HE	1:B:270:ARG:HB2	1.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:537:TYR:CE2	1:E:539:LYS:HB2	2.55	0.41
1:A:134:GLY:HA3	1:A:145:TYR:CE1	2.56	0.41
1:B:124:ALA:HB2	1:B:162:ILE:HG12	2.03	0.41
1:B:336:LEU:HD11	1:B:350:PHE:CD1	2.55	0.41
1:B:351:GLN:HB2	1:B:654:THR:HG21	2.03	0.41
1:D:80:MSE:HB3	1:D:666:PRO:HG2	2.03	0.41
1:E:640:LYS:HG3	1:E:689:VAL:HG11	2.03	0.41
1:F:549:GLN:H	1:F:549:GLN:HG3	1.69	0.41
1:B:253:PHE:HA	1:B:256:HIS:ND1	2.36	0.40
1:B:630:ALA:O	1:B:634:VAL:HG23	2.21	0.40
1:C:366:TRP:HB3	1:C:397:CYS:HA	2.02	0.40
1:E:552:SER:HA	1:E:657:ILE:HB	2.02	0.40
1:F:338:LEU:HD23	1:F:350:PHE:HB3	2.02	0.40
1:F:576:PRO:HD3	1:F:624:LEU:HD13	2.02	0.40
1:B:586:ASN:HD21	1:B:589:TRP:CD1	2.39	0.40
1:A:91:TYR:HA	1:A:94:TYR:CD1	2.56	0.40
1:A:457:LEU:HD21	1:A:460:TRP:CZ2	2.56	0.40
1:D:557:HIS:O	1:D:635:GLN:HB2	2.21	0.40
1:F:298:PRO:HB3	1:F:418:MSE:HG3	2.04	0.40
1:F:781:LYS:HE2	1:F:784:GLN:HG3	2.02	0.40
1:A:367:VAL:HB	1:A:368:PRO:HD2	2.03	0.40
1:E:646:TRP:CD1	1:E:653:ARG:HB3	2.56	0.40
1:B:557:HIS:O	1:B:635:GLN:HB2	2.21	0.40
1:B:743:MSE:SE	1:B:743:MSE:C	3.14	0.40
1:F:757:MSE:HE1	1:F:789:VAL:HB	2.02	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	728/798 (91%)	708 (97%)	20 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	730/798 (92%)	712 (98%)	18 (2%)	0	100	100
1	C	723/798 (91%)	701 (97%)	22 (3%)	0	100	100
1	D	727/798 (91%)	709 (98%)	17 (2%)	1 (0%)	48	50
1	E	725/798 (91%)	706 (97%)	18 (2%)	1 (0%)	48	50
1	F	718/798 (90%)	691 (96%)	26 (4%)	1 (0%)	48	50
All	All	4351/4788 (91%)	4227 (97%)	121 (3%)	3 (0%)	48	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	427	CYS
1	F	660	ASN
1	E	427	CYS

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	635/666 (95%)	628 (99%)	7 (1%)	65	72
1	B	635/666 (95%)	625 (98%)	10 (2%)	55	61
1	C	632/666 (95%)	626 (99%)	6 (1%)	70	77
1	D	632/666 (95%)	620 (98%)	12 (2%)	50	56
1	E	633/666 (95%)	627 (99%)	6 (1%)	70	77
1	F	631/666 (95%)	618 (98%)	13 (2%)	47	52
All	All	3798/3996 (95%)	3744 (99%)	54 (1%)	59	66

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	LEU
1	A	332	ARG
1	A	420	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	556	TYR
1	A	557	HIS
1	A	581	VAL
1	A	670	ASP
1	B	20	HIS
1	B	23	VAL
1	B	151	VAL
1	B	205	LEU
1	B	332	ARG
1	B	340	GLU
1	B	420	TRP
1	B	425	MSE
1	B	551	VAL
1	B	670	ASP
1	C	151	VAL
1	C	205	LEU
1	C	506	LEU
1	C	551	VAL
1	C	556	TYR
1	C	557	HIS
1	D	201	ILE
1	D	205	LEU
1	D	332	ARG
1	D	346	GLN
1	D	381	GLU
1	D	420	TRP
1	D	484	ASN
1	D	551	VAL
1	D	581	VAL
1	D	670	ASP
1	D	704	TYR
1	D	792	CYS
1	E	205	LEU
1	E	332	ARG
1	E	420	TRP
1	E	556	TYR
1	E	571	PRO
1	E	581	VAL
1	F	201	ILE
1	F	249	THR
1	F	311	VAL
1	F	334	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	553	GLU
1	F	556	TYR
1	F	557	HIS
1	F	581	VAL
1	F	656	ILE
1	F	669	SER
1	F	693	VAL
1	F	702	ASN
1	F	796	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	742	GLN
1	B	181	ASN
1	B	575	ASN
1	C	464	ASN
1	D	575	ASN
1	E	435	ASN
1	F	681	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

34 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	B	803	-	5,5,5	0.36	0	5,5,5	0.61	0
3	GOL	A	806	-	5,5,5	0.37	0	5,5,5	0.52	0
2	PO4	A	801	-	4,4,4	1.52	1 (25%)	6,6,6	0.49	0
2	PO4	D	802	-	4,4,4	0.77	0	6,6,6	0.46	0
3	GOL	A	805	-	5,5,5	0.35	0	5,5,5	0.48	0
3	GOL	C	804	-	5,5,5	0.31	0	5,5,5	0.39	0
3	GOL	F	803	-	5,5,5	0.32	0	5,5,5	0.42	0
4	ACT	A	808	-	3,3,3	1.16	0	3,3,3	1.21	0
2	PO4	F	801	-	4,4,4	1.56	1 (25%)	6,6,6	0.51	0
2	PO4	F	802	-	4,4,4	1.58	1 (25%)	6,6,6	0.52	0
3	GOL	D	804	-	5,5,5	0.36	0	5,5,5	0.56	0
3	GOL	E	804	-	5,5,5	0.34	0	5,5,5	0.51	0
3	GOL	E	807	-	5,5,5	0.39	0	5,5,5	0.57	0
2	PO4	E	802	-	4,4,4	0.78	0	6,6,6	0.46	0
3	GOL	B	805	-	5,5,5	0.34	0	5,5,5	0.51	0
3	GOL	D	803	-	5,5,5	0.35	0	5,5,5	0.43	0
3	GOL	E	805	-	5,5,5	0.33	0	5,5,5	0.42	0
2	PO4	C	801	-	4,4,4	1.59	1 (25%)	6,6,6	0.55	0
3	GOL	D	806	-	5,5,5	0.34	0	5,5,5	0.44	0
3	GOL	E	806	-	5,5,5	0.34	0	5,5,5	0.42	0
2	PO4	B	802	-	4,4,4	0.79	0	6,6,6	0.45	0
3	GOL	A	807	-	5,5,5	0.33	0	5,5,5	0.46	0
3	GOL	B	804	-	5,5,5	0.34	0	5,5,5	0.35	0
2	PO4	C	802	-	4,4,4	0.85	0	6,6,6	0.43	0
2	PO4	D	801	-	4,4,4	1.49	1 (25%)	6,6,6	0.55	0
3	GOL	D	805	-	5,5,5	0.32	0	5,5,5	0.41	0
3	GOL	A	803	-	5,5,5	0.34	0	5,5,5	0.43	0
2	PO4	C	803	-	4,4,4	0.80	0	6,6,6	0.49	0
3	GOL	A	804	-	5,5,5	0.34	0	5,5,5	0.47	0
2	PO4	B	801	-	4,4,4	1.55	1 (25%)	6,6,6	0.50	0
4	ACT	B	806	-	3,3,3	1.16	0	3,3,3	1.18	0
2	PO4	E	803	-	4,4,4	0.79	0	6,6,6	0.45	0
2	PO4	E	801	-	4,4,4	1.54	1 (25%)	6,6,6	0.54	0
2	PO4	A	802	-	4,4,4	0.80	0	6,6,6	0.44	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	B	803	-	-	0/4/4/4	-
3	GOL	D	805	-	-	0/4/4/4	-
3	GOL	D	806	-	-	0/4/4/4	-
3	GOL	E	806	-	-	0/4/4/4	-
3	GOL	A	803	-	-	1/4/4/4	-
3	GOL	D	804	-	-	0/4/4/4	-
3	GOL	E	804	-	-	3/4/4/4	-
3	GOL	E	807	-	-	0/4/4/4	-
3	GOL	A	806	-	-	0/4/4/4	-
3	GOL	A	804	-	-	0/4/4/4	-
3	GOL	A	807	-	-	2/4/4/4	-
3	GOL	A	805	-	-	2/4/4/4	-
3	GOL	B	804	-	-	0/4/4/4	-
3	GOL	B	805	-	-	3/4/4/4	-
3	GOL	D	803	-	-	0/4/4/4	-
3	GOL	C	804	-	-	0/4/4/4	-
3	GOL	F	803	-	-	1/4/4/4	-
3	GOL	E	805	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	802	PO4	P-O1	2.81	1.57	1.50
2	C	801	PO4	P-O1	2.78	1.57	1.50
2	F	801	PO4	P-O1	2.71	1.56	1.50
2	A	801	PO4	P-O1	2.69	1.56	1.50
2	B	801	PO4	P-O1	2.68	1.56	1.50
2	E	801	PO4	P-O1	2.66	1.56	1.50
2	D	801	PO4	P-O1	2.57	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	807	GOL	O1-C1-C2-O2
3	A	807	GOL	O1-C1-C2-C3
3	E	804	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

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

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	807	GOL	1	0
3	D	803	GOL	1	0
3	D	806	GOL	1	0
3	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	714/798 (89%)	0.62	55 (7%)	19 22	36, 53, 75, 90	0
1	B	714/798 (89%)	0.57	47 (6%)	24 27	35, 53, 83, 98	0
1	C	709/798 (88%)	1.06	127 (17%)	3 4	39, 65, 117, 147	0
1	D	712/798 (89%)	0.60	43 (6%)	27 31	35, 54, 85, 100	0
1	E	711/798 (89%)	0.76	61 (8%)	16 17	37, 57, 80, 89	0
1	F	706/798 (88%)	1.34	174 (24%)	2 2	41, 76, 138, 172	0
All	All	4266/4788 (89%)	0.83	507 (11%)	9 9	35, 58, 107, 172	0

All (507) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	347	PRO	5.7
1	F	726	ALA	5.5
1	F	651	PRO	5.3
1	B	427	CYS	5.2
1	C	343	LEU	5.1
1	C	789	VAL	5.1
1	F	789	VAL	5.1
1	E	23	VAL	5.0
1	A	482	PRO	4.9
1	C	341	VAL	4.9
1	A	22	PHE	4.8
1	F	699	PRO	4.8
1	B	345	GLY	4.8
1	E	22	PHE	4.7
1	D	427	CYS	4.6
1	A	347	PRO	4.6
1	F	201	ILE	4.6
1	F	22	PHE	4.5
1	D	430	TYR	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	532	TRP	4.3
1	F	347	PRO	4.3
1	B	430	TYR	4.2
1	C	726	ALA	4.2
1	B	22	PHE	4.2
1	A	533	GLY	4.2
1	B	797	LEU	4.2
1	F	693	VAL	4.2
1	C	793	GLY	4.1
1	F	780	TYR	4.1
1	F	659	TRP	4.0
1	E	508	SER	4.0
1	F	482	PRO	4.0
1	F	338	LEU	3.9
1	D	531	LEU	3.9
1	F	594	ASN	3.9
1	F	759	VAL	3.9
1	C	630	ALA	3.9
1	A	508	SER	3.9
1	D	534	PRO	3.9
1	F	581	VAL	3.9
1	E	177	LEU	3.9
1	E	531	LEU	3.9
1	A	430	TYR	3.8
1	B	429	ASN	3.8
1	F	593	ALA	3.8
1	F	793	GLY	3.8
1	E	797	LEU	3.8
1	F	749	LEU	3.8
1	B	534	PRO	3.7
1	F	794	ILE	3.7
1	B	531	LEU	3.7
1	E	427	CYS	3.7
1	C	464	ASN	3.7
1	E	429	ASN	3.7
1	A	531	LEU	3.7
1	A	23	VAL	3.7
1	F	785	TYR	3.7
1	C	427	CYS	3.6
1	F	660	ASN	3.6
1	F	509	SER	3.6
1	E	339	ASP	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	746	ILE	3.6
1	A	338	LEU	3.6
1	B	20	HIS	3.6
1	F	537	TYR	3.6
1	F	766	GLY	3.6
1	B	488	SER	3.6
1	A	463	ASN	3.5
1	F	556	TYR	3.5
1	C	572	ASP	3.5
1	A	534	PRO	3.5
1	A	701	ALA	3.5
1	C	622	ALA	3.5
1	A	345	GLY	3.5
1	B	508	SER	3.5
1	C	19	SER	3.5
1	F	737	VAL	3.5
1	F	615	ILE	3.5
1	F	350	PHE	3.5
1	F	535	ARG	3.5
1	C	177	LEU	3.4
1	E	533	GLY	3.4
1	F	74	GLY	3.4
1	C	22	PHE	3.4
1	E	534	PRO	3.4
1	F	667	LEU	3.4
1	F	770	PHE	3.4
1	C	538	TYR	3.3
1	B	509	SER	3.3
1	C	348	GLY	3.3
1	F	542	PHE	3.3
1	F	646	TRP	3.3
1	C	428	GLY	3.3
1	E	482	PRO	3.3
1	F	668	LEU	3.3
1	F	182	PHE	3.3
1	C	20	HIS	3.2
1	C	785	TYR	3.2
1	E	430	TYR	3.2
1	E	108	THR	3.2
1	F	508	SER	3.2
1	D	487	VAL	3.2
1	F	657	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	482	PRO	3.2
1	D	532	TRP	3.2
1	A	483	ASN	3.2
1	C	463	ASN	3.2
1	D	529	ASN	3.2
1	C	581	VAL	3.2
1	C	624	LEU	3.2
1	C	774	LEU	3.2
1	F	428	GLY	3.2
1	F	679	LYS	3.2
1	A	429	ASN	3.2
1	C	788	TRP	3.1
1	F	582	VAL	3.1
1	A	339	ASP	3.1
1	C	556	TYR	3.1
1	D	488	SER	3.1
1	F	627	PHE	3.1
1	C	551	VAL	3.1
1	B	177	LEU	3.1
1	C	182	PHE	3.1
1	C	732	PHE	3.1
1	F	348	GLY	3.1
1	E	483	ASN	3.1
1	C	620	VAL	3.1
1	D	343	LEU	3.1
1	D	616	ILE	3.1
1	F	795	TYR	3.1
1	F	750	PRO	3.1
1	A	427	CYS	3.1
1	D	726	ALA	3.1
1	C	725	VAL	3.1
1	F	673	SER	3.1
1	C	430	TYR	3.0
1	E	426	GLY	3.0
1	D	429	ASN	3.0
1	A	507	PRO	3.0
1	F	787	LYS	3.0
1	C	582	VAL	3.0
1	D	533	GLY	3.0
1	E	530	HIS	3.0
1	A	797	LEU	3.0
1	B	23	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	336	LEU	3.0
1	F	23	VAL	3.0
1	F	552	SER	3.0
1	F	782	LEU	3.0
1	C	583	GLY	3.0
1	F	682	ALA	3.0
1	F	747	ALA	3.0
1	B	792	CYS	3.0
1	F	481	ASN	3.0
1	C	673	SER	2.9
1	F	776	GLY	2.9
1	A	270	ARG	2.9
1	F	796	GLU	2.9
1	C	682	ALA	2.9
1	C	694	CYS	2.9
1	F	612	GLN	2.9
1	F	702	ASN	2.9
1	F	788	TRP	2.9
1	B	726	ALA	2.9
1	B	794	ILE	2.9
1	C	729	LYS	2.9
1	E	19	SER	2.9
1	F	538	TYR	2.9
1	B	533	GLY	2.9
1	F	577	TRP	2.9
1	E	338	LEU	2.8
1	F	205	LEU	2.8
1	F	596	ILE	2.8
1	C	303	GLU	2.8
1	D	484	ASN	2.8
1	C	795	TYR	2.8
1	C	763	ARG	2.8
1	E	270	ARG	2.8
1	C	659	TRP	2.8
1	F	620	VAL	2.8
1	F	735	LYS	2.8
1	E	488	SER	2.8
1	D	530	HIS	2.8
1	F	629	PHE	2.8
1	D	345	GLY	2.8
1	E	317	THR	2.8
1	B	344	PRO	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	151	VAL	2.8
1	D	237	LYS	2.8
1	F	781	LYS	2.8
1	C	535	ARG	2.8
1	C	770	PHE	2.8
1	E	428	GLY	2.8
1	F	774	LEU	2.8
1	C	596	ILE	2.8
1	F	656	ILE	2.8
1	D	508	SER	2.7
1	C	339	ASP	2.7
1	E	553	GLU	2.7
1	F	622	ALA	2.7
1	F	543	TYR	2.7
1	C	720	VAL	2.7
1	F	725	VAL	2.7
1	C	615	ILE	2.7
1	C	697	ILE	2.7
1	F	616	ILE	2.7
1	C	508	SER	2.7
1	E	20	HIS	2.7
1	F	630	ALA	2.7
1	F	641	PHE	2.7
1	A	459	LEU	2.7
1	C	685	TYR	2.7
1	F	430	TYR	2.7
1	F	487	VAL	2.7
1	F	672	ILE	2.7
1	C	787	LYS	2.7
1	C	426	GLY	2.7
1	F	360	PHE	2.7
1	A	543	TYR	2.7
1	A	488	SER	2.7
1	F	604	GLY	2.7
1	F	617	PHE	2.6
1	C	782	LEU	2.6
1	F	459	LEU	2.6
1	F	624	LEU	2.6
1	C	779	PRO	2.6
1	C	780	TYR	2.6
1	A	316	VAL	2.6
1	F	426	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	754	GLY	2.6
1	F	420	TRP	2.6
1	C	698	ASN	2.6
1	F	484	ASN	2.6
1	B	507	PRO	2.6
1	C	359	VAL	2.6
1	D	23	VAL	2.6
1	F	634	VAL	2.6
1	F	792	CYS	2.6
1	E	348	GLY	2.6
1	E	702	ASN	2.6
1	C	424	ALA	2.6
1	F	249	THR	2.6
1	F	654	THR	2.6
1	F	791	LYS	2.6
1	C	641	PHE	2.6
1	E	350	PHE	2.6
1	F	550	PHE	2.6
1	C	301	TYR	2.6
1	C	613	VAL	2.6
1	C	616	ILE	2.6
1	C	731	VAL	2.6
1	A	340	GLU	2.6
1	B	748	THR	2.6
1	B	758	LEU	2.6
1	A	346	GLN	2.5
1	F	628	ILE	2.5
1	F	731	VAL	2.5
1	B	556	TYR	2.5
1	C	769	TYR	2.5
1	F	49	GLY	2.5
1	F	536	GLY	2.5
1	F	483	ASN	2.5
1	F	753	LYS	2.5
1	C	547	PRO	2.5
1	C	612	GLN	2.5
1	F	336	LEU	2.5
1	F	732	PHE	2.5
1	C	487	VAL	2.5
1	C	718	GLY	2.5
1	F	150	VAL	2.5
1	F	661	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	729	LYS	2.5
1	F	762	TYR	2.5
1	C	738	SER	2.5
1	D	346	GLN	2.5
1	E	459	LEU	2.5
1	F	696	LEU	2.5
1	B	732	PHE	2.5
1	C	737	VAL	2.5
1	F	697	ILE	2.5
1	C	392	CYS	2.5
1	D	556	TYR	2.5
1	F	427	CYS	2.5
1	A	24	SER	2.5
1	F	264	THR	2.5
1	E	251	LEU	2.5
1	E	786	ARG	2.5
1	F	691	HIS	2.5
1	F	463	ASN	2.5
1	B	737	VAL	2.4
1	C	634	VAL	2.4
1	C	719	VAL	2.4
1	D	731	VAL	2.4
1	F	106	VAL	2.4
1	A	19	SER	2.4
1	D	507	PRO	2.4
1	F	779	PRO	2.4
1	E	241	ALA	2.4
1	A	348	GLY	2.4
1	C	604	GLY	2.4
1	C	736	PHE	2.4
1	D	426	GLY	2.4
1	A	484	ASN	2.4
1	E	340	GLU	2.4
1	B	582	VAL	2.4
1	F	574	VAL	2.4
1	D	538	TYR	2.4
1	F	727	SER	2.4
1	F	738	SER	2.4
1	F	506	LEU	2.4
1	B	703	GLY	2.4
1	C	542	PHE	2.4
1	B	485	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	540	ASP	2.4
1	A	225	VAL	2.4
1	F	719	VAL	2.4
1	A	317	THR	2.4
1	D	537	TYR	2.4
1	F	621	PRO	2.4
1	C	338	LEU	2.4
1	A	553	GLU	2.4
1	F	109	GLU	2.4
1	C	462	GLY	2.4
1	C	536	GLY	2.4
1	C	703	GLY	2.4
1	C	756	GLY	2.4
1	C	776	GLY	2.4
1	D	428	GLY	2.4
1	E	766	GLY	2.4
1	F	625	ASP	2.4
1	A	106	VAL	2.4
1	B	759	VAL	2.4
1	C	554	ILE	2.4
1	C	689	VAL	2.4
1	E	697	ILE	2.4
1	F	720	VAL	2.4
1	A	20	HIS	2.4
1	C	543	TYR	2.3
1	F	684	TYR	2.3
1	F	773	TYR	2.3
1	A	349	GLN	2.3
1	D	177	LEU	2.3
1	E	113	LEU	2.3
1	B	583	GLY	2.3
1	E	462	GLY	2.3
1	F	175	GLY	2.3
1	F	703	GLY	2.3
1	A	253	PHE	2.3
1	B	552	SER	2.3
1	C	760	ILE	2.3
1	D	554	ILE	2.3
1	D	719	VAL	2.3
1	B	538	TYR	2.3
1	C	597	TYR	2.3
1	A	177	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	268	ASP	2.3
1	E	268	ASP	2.3
1	F	268	ASP	2.3
1	E	489	ARG	2.3
1	C	723	LYS	2.3
1	D	729	LYS	2.3
1	D	182	PHE	2.3
1	F	716	PHE	2.3
1	B	725	VAL	2.3
1	C	619	GLU	2.3
1	C	759	VAL	2.3
1	D	759	VAL	2.3
1	B	346	GLN	2.3
1	D	490	GLN	2.3
1	C	483	ASN	2.3
1	A	536	GLY	2.3
1	C	706	LEU	2.3
1	F	608	LEU	2.3
1	F	769	TYR	2.3
1	F	183	SER	2.3
1	A	542	PHE	2.3
1	C	716	PHE	2.3
1	F	683	PHE	2.3
1	C	349	GLN	2.3
1	A	700	ALA	2.3
1	D	734	GLY	2.3
1	F	356	GLY	2.3
1	F	555	GLY	2.3
1	C	696	LEU	2.3
1	B	543	TYR	2.3
1	C	762	TYR	2.3
1	E	532	TRP	2.3
1	F	690	HIS	2.2
1	D	552	SER	2.2
1	F	755	GLN	2.2
1	F	304	PRO	2.2
1	F	365	ASN	2.2
1	C	790	LYS	2.2
1	F	462	GLY	2.2
1	C	537	TYR	2.2
1	F	303	GLU	2.2
1	F	685	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	461	SER	2.2
1	C	601	PHE	2.2
1	E	435	ASN	2.2
1	F	554	ILE	2.2
1	A	107	VAL	2.2
1	B	151	VAL	2.2
1	F	82	GLY	2.2
1	F	652	TYR	2.2
1	F	19	SER	2.2
1	F	761	SER	2.2
1	C	646	TRP	2.2
1	C	656	ILE	2.2
1	E	746	ILE	2.2
1	F	541	PRO	2.2
1	F	670	ASP	2.2
1	B	551	VAL	2.2
1	B	731	VAL	2.2
1	A	254	GLU	2.2
1	B	798	GLU	2.2
1	F	300	GLY	2.2
1	F	677	GLY	2.2
1	C	700	ALA	2.2
1	F	758	LEU	2.2
1	C	704	TYR	2.2
1	E	753	LYS	2.2
1	D	698	ASN	2.2
1	A	108	THR	2.2
1	E	287	THR	2.2
1	E	599	ASP	2.2
1	B	182	PHE	2.1
1	D	551	VAL	2.1
1	F	722	VAL	2.1
1	A	130	GLY	2.1
1	C	618	GLY	2.1
1	D	154	GLY	2.1
1	F	557	HIS	2.1
1	A	489	ARG	2.1
1	F	790	LYS	2.1
1	C	342	ASN	2.1
1	D	769	TYR	2.1
1	A	153	GLU	2.1
1	A	768	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	142	GLU	2.1
1	A	748	THR	2.1
1	C	621	PRO	2.1
1	C	794	ILE	2.1
1	E	716	PHE	2.1
1	B	462	GLY	2.1
1	E	106	VAL	2.1
1	F	648	GLY	2.1
1	F	305	ALA	2.1
1	A	336	LEU	2.1
1	C	506	LEU	2.1
1	F	177	LEU	2.1
1	C	792	CYS	2.1
1	E	546	ASN	2.1
1	E	556	TYR	2.1
1	E	507	PRO	2.1
1	F	748	THR	2.1
1	A	269	GLY	2.1
1	D	270	ARG	2.1
1	E	554	ILE	2.1
1	F	760	ILE	2.1
1	C	658	TRP	2.1
1	C	23	VAL	2.1
1	E	107	VAL	2.1
1	F	613	VAL	2.1
1	C	796	GLU	2.1
1	C	594	ASN	2.1
1	C	702	ASN	2.1
1	A	287	THR	2.1
1	C	502	THR	2.1
1	F	502	THR	2.1
1	F	775	TYR	2.1
1	A	154	GLY	2.1
1	F	718	GLY	2.1
1	F	734	GLY	2.1
1	C	672	ILE	2.1
1	F	237	LYS	2.1
1	A	42	VAL	2.1
1	C	629	PHE	2.1
1	E	253	PHE	2.1
1	C	589	TRP	2.1
1	F	460	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	99	SER	2.1
1	F	41	ALA	2.1
1	B	749	LEU	2.0
1	E	54	ASN	2.0
1	B	763	ARG	2.0
1	E	433	ARG	2.0
1	C	557	HIS	2.0
1	E	544	THR	2.0
1	E	699	PRO	2.0
1	F	544	THR	2.0
1	C	739	LYS	2.0
1	D	735	LYS	2.0
1	B	708	VAL	2.0
1	C	253	PHE	2.0
1	D	737	VAL	2.0
1	F	569	PHE	2.0
1	A	532	TRP	2.0
1	E	701	ALA	2.0
1	F	561	ASN	2.0
1	C	668	LEU	2.0
1	C	758	LEU	2.0
1	F	174	LEU	2.0
1	C	783	ASP	2.0
1	F	392	CYS	2.0
1	F	560	PRO	2.0
1	F	704	TYR	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	PO4	E	803	5/5	0.49	0.20	112,135,145,296	0
3	GOL	B	804	6/6	0.74	0.17	57,64,66,68	0
4	ACT	B	806	4/4	0.76	0.23	58,62,67,71	0
2	PO4	C	803	5/5	0.77	0.20	53,56,56,68	5
3	GOL	D	806	6/6	0.79	0.17	59,68,70,74	0
3	GOL	D	805	6/6	0.79	0.17	60,71,75,76	0
4	ACT	A	808	4/4	0.83	0.20	48,52,55,62	0
3	GOL	E	807	6/6	0.83	0.16	49,55,59,61	0
3	GOL	A	807	6/6	0.84	0.17	64,66,68,72	0
2	PO4	B	802	5/5	0.86	0.18	58,61,66,66	5
2	PO4	C	802	5/5	0.86	0.18	48,52,54,61	5
3	GOL	E	806	6/6	0.86	0.13	51,55,57,62	0
3	GOL	F	803	6/6	0.87	0.14	62,65,67,69	0
2	PO4	F	802	5/5	0.87	0.17	59,61,64,71	5
3	GOL	A	803	6/6	0.87	0.12	46,57,63,65	0
3	GOL	B	805	6/6	0.89	0.13	56,58,63,68	0
3	GOL	C	804	6/6	0.89	0.12	56,58,62,64	0
3	GOL	D	803	6/6	0.89	0.12	59,60,64,64	0
3	GOL	B	803	6/6	0.89	0.14	39,45,48,53	0
2	PO4	D	802	5/5	0.89	0.24	77,80,103,262	0
3	GOL	A	806	6/6	0.90	0.13	53,55,56,61	0
3	GOL	D	804	6/6	0.90	0.13	42,47,49,50	0
2	PO4	A	802	5/5	0.90	0.17	60,60,65,71	5
2	PO4	E	802	5/5	0.91	0.12	65,67,70,72	5
3	GOL	A	804	6/6	0.92	0.14	47,51,56,60	0
3	GOL	E	805	6/6	0.93	0.11	53,57,62,73	0
2	PO4	C	801	5/5	0.93	0.14	52,56,58,65	0
3	GOL	A	805	6/6	0.93	0.11	51,52,54,57	0
2	PO4	E	801	5/5	0.94	0.08	61,62,64,65	0
3	GOL	E	804	6/6	0.94	0.10	52,59,60,60	0
2	PO4	F	801	5/5	0.94	0.10	64,64,65,66	0
2	PO4	A	801	5/5	0.94	0.12	58,58,60,61	0
2	PO4	B	801	5/5	0.97	0.10	49,53,58,59	0
2	PO4	D	801	5/5	0.97	0.09	53,54,57,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.