



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2026 – 04:31 pm BST

PDB ID : 9TP7 / pdb_00009tp7
Title : Crystal structure of the C-terminal Ser/Thr phosphatase domain of the Kelch phosphatase BSU1 from Arabidopsis thaliana
Authors : Moretti, A.; Hothorn, M.
Deposited on : 2025-12-17
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:

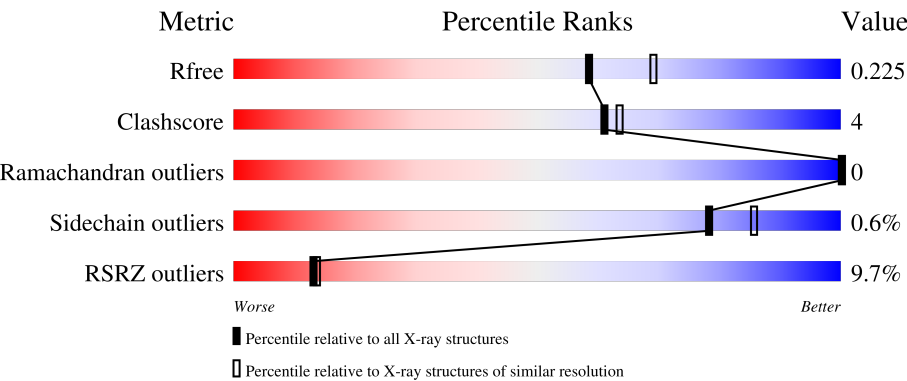
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.10 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	383	<div><div>5%</div><div><div></div><div>86%</div><div>6%</div><div>8%</div></div></div>
1	B	383	<div><div>4%</div><div><div></div><div>81%</div><div>7%</div><div>11%</div></div></div>
1	C	383	<div><div>2%</div><div><div></div><div>82%</div><div>7%</div><div>11%</div></div></div>
1	D	383	<div><div>10%</div><div><div></div><div>76%</div><div>11%</div><div>12%</div></div></div>
1	E	383	<div><div>3%</div><div><div></div><div>81%</div><div>7%</div><div>11%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	383	<div><div></div><div>28%</div><div>71%</div><div>16%</div><div>13%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33159 atoms, of which 16021 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 Serine/threonine-protein phosphatase BSU1.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	353	Total	C	H	N	O	P	S		0	1	0
			5539	1800	2741	471	510	1	16				
1	B	339	Total	C	H	N	O	P	S		0	0	0
			5390	1747	2680	453	493	1	16				
1	C	339	Total	C	H	N	O	P	S		0	1	0
			5376	1744	2669	455	492	1	15				
1	D	337	Total	C	H	N	O	P	S		0	1	0
			5317	1725	2638	453	484	1	16				
1	E	339	Total	C	H	N	O	P	S		0	1	0
			5405	1751	2691	456	490	1	16				
1	F	334	Total	C	H	N	O	S			0	0	0
			5194	1691	2570	446	471	16					

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	MET	-	initiating methionine	UNP Q9LR78
A	794	ALA	-	expression tag	UNP Q9LR78
A	795	ALA	-	expression tag	UNP Q9LR78
A	796	ALA	-	expression tag	UNP Q9LR78
A	797	GLU	-	expression tag	UNP Q9LR78
A	798	ASN	-	expression tag	UNP Q9LR78
A	799	LEU	-	expression tag	UNP Q9LR78
A	800	TYR	-	expression tag	UNP Q9LR78
A	801	PHE	-	expression tag	UNP Q9LR78
A	802	GLN	-	expression tag	UNP Q9LR78
B	420	MET	-	initiating methionine	UNP Q9LR78
B	794	ALA	-	expression tag	UNP Q9LR78
B	795	ALA	-	expression tag	UNP Q9LR78
B	796	ALA	-	expression tag	UNP Q9LR78
B	797	GLU	-	expression tag	UNP Q9LR78
B	798	ASN	-	expression tag	UNP Q9LR78
B	799	LEU	-	expression tag	UNP Q9LR78

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Chain	Residue	Modelled	Actual	Comment	Reference
B	800	TYR	-	expression tag	UNP Q9LR78
B	801	PHE	-	expression tag	UNP Q9LR78
B	802	GLN	-	expression tag	UNP Q9LR78
C	420	MET	-	initiating methionine	UNP Q9LR78
C	794	ALA	-	expression tag	UNP Q9LR78
C	795	ALA	-	expression tag	UNP Q9LR78
C	796	ALA	-	expression tag	UNP Q9LR78
C	797	GLU	-	expression tag	UNP Q9LR78
C	798	ASN	-	expression tag	UNP Q9LR78
C	799	LEU	-	expression tag	UNP Q9LR78
C	800	TYR	-	expression tag	UNP Q9LR78
C	801	PHE	-	expression tag	UNP Q9LR78
C	802	GLN	-	expression tag	UNP Q9LR78
D	420	MET	-	initiating methionine	UNP Q9LR78
D	794	ALA	-	expression tag	UNP Q9LR78
D	795	ALA	-	expression tag	UNP Q9LR78
D	796	ALA	-	expression tag	UNP Q9LR78
D	797	GLU	-	expression tag	UNP Q9LR78
D	798	ASN	-	expression tag	UNP Q9LR78
D	799	LEU	-	expression tag	UNP Q9LR78
D	800	TYR	-	expression tag	UNP Q9LR78
D	801	PHE	-	expression tag	UNP Q9LR78
D	802	GLN	-	expression tag	UNP Q9LR78
E	420	MET	-	initiating methionine	UNP Q9LR78
E	794	ALA	-	expression tag	UNP Q9LR78
E	795	ALA	-	expression tag	UNP Q9LR78
E	796	ALA	-	expression tag	UNP Q9LR78
E	797	GLU	-	expression tag	UNP Q9LR78
E	798	ASN	-	expression tag	UNP Q9LR78
E	799	LEU	-	expression tag	UNP Q9LR78
E	800	TYR	-	expression tag	UNP Q9LR78
E	801	PHE	-	expression tag	UNP Q9LR78
E	802	GLN	-	expression tag	UNP Q9LR78
F	420	MET	-	initiating methionine	UNP Q9LR78
F	794	ALA	-	expression tag	UNP Q9LR78
F	795	ALA	-	expression tag	UNP Q9LR78
F	796	ALA	-	expression tag	UNP Q9LR78
F	797	GLU	-	expression tag	UNP Q9LR78
F	798	ASN	-	expression tag	UNP Q9LR78
F	799	LEU	-	expression tag	UNP Q9LR78
F	800	TYR	-	expression tag	UNP Q9LR78
F	801	PHE	-	expression tag	UNP Q9LR78

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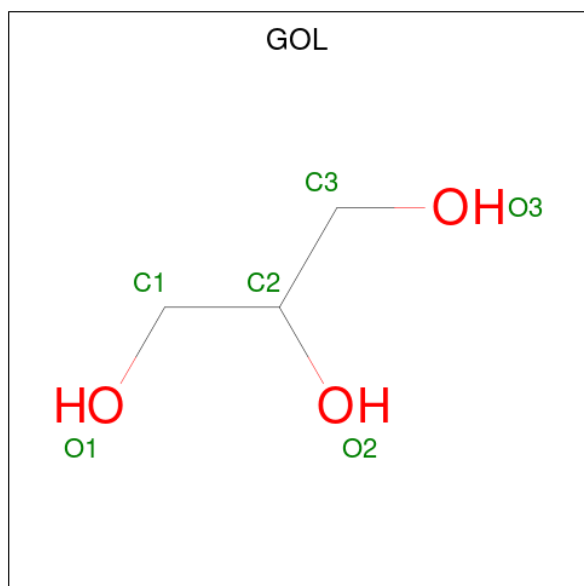
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Chain	Residue	Modelled	Actual	Comment	Reference
F	802	GLN	-	expression tag	UNP Q9LR78

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	H	O	0	0
			14	3	8	3		

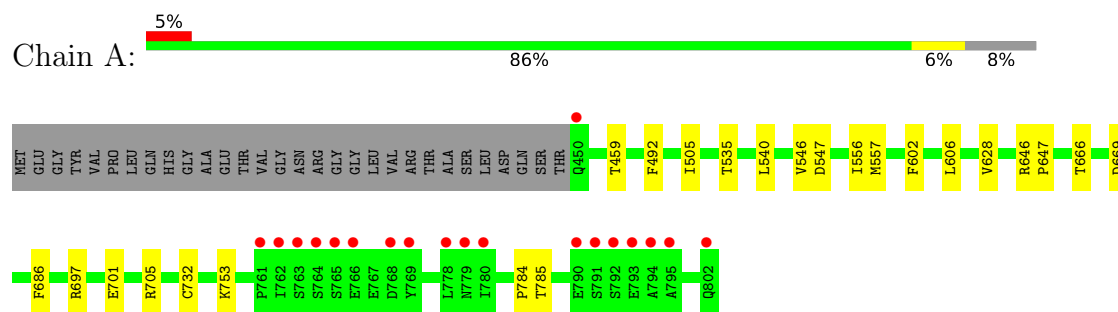
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	168	Total	O	0	0
			168	168		
4	B	185	Total	O	0	0
			185	185		
4	C	189	Total	O	0	0
			189	189		
4	D	104	Total	O	0	0
			104	104		
4	E	163	Total	O	0	0
			163	163		
4	F	61	Total	O	0	0
			61	61		

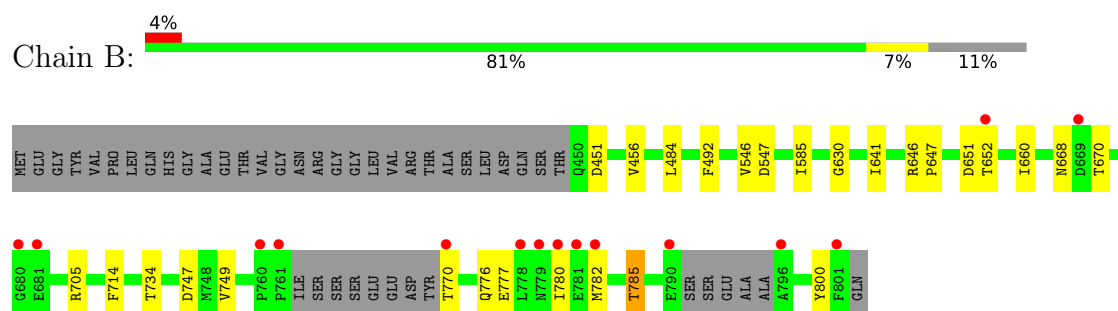
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

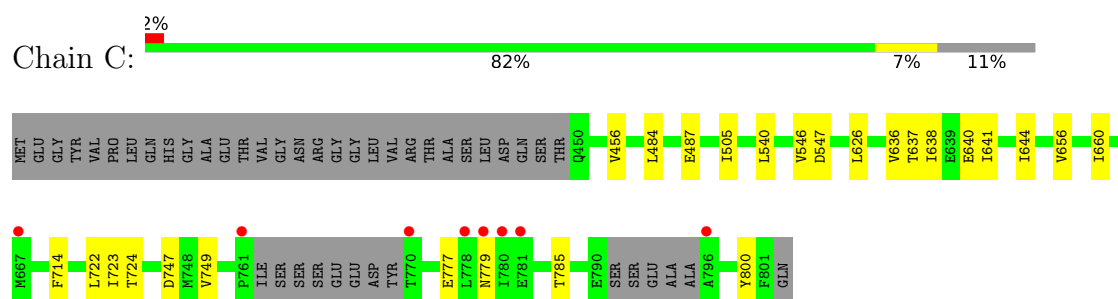
- Molecule 1: Serine/threonine-protein phosphatase BSU1



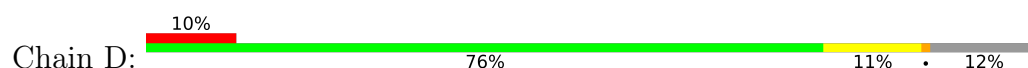
- Molecule 1: Serine/threonine-protein phosphatase BSU1

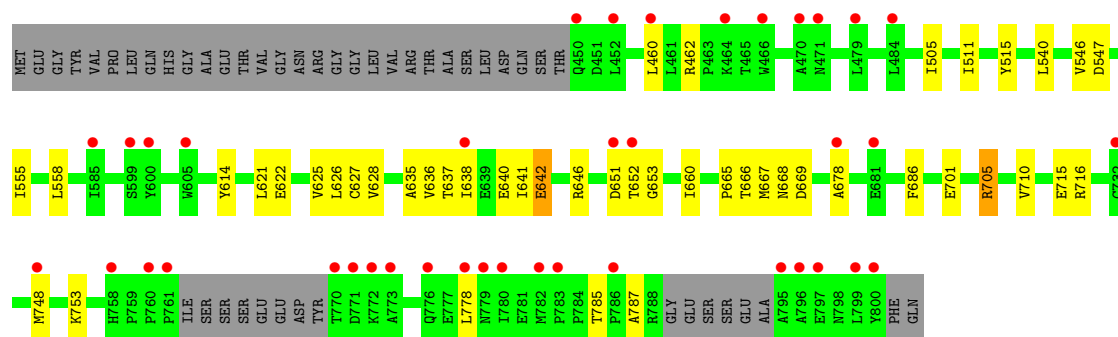


- Molecule 1: Serine/threonine-protein phosphatase BSU1

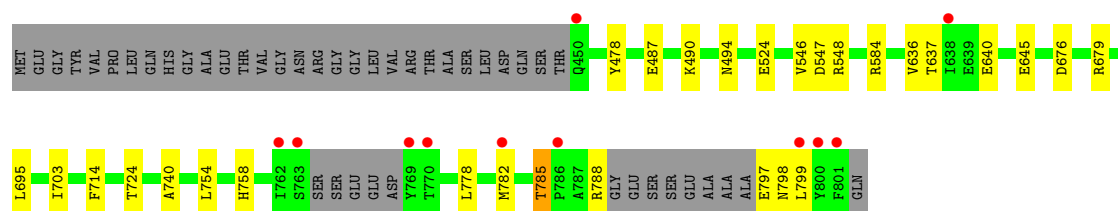
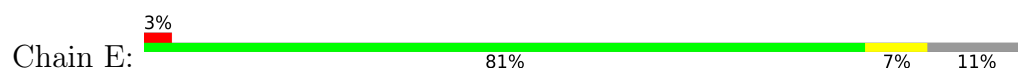


- Molecule 1: Serine/threonine-protein phosphatase BSU1

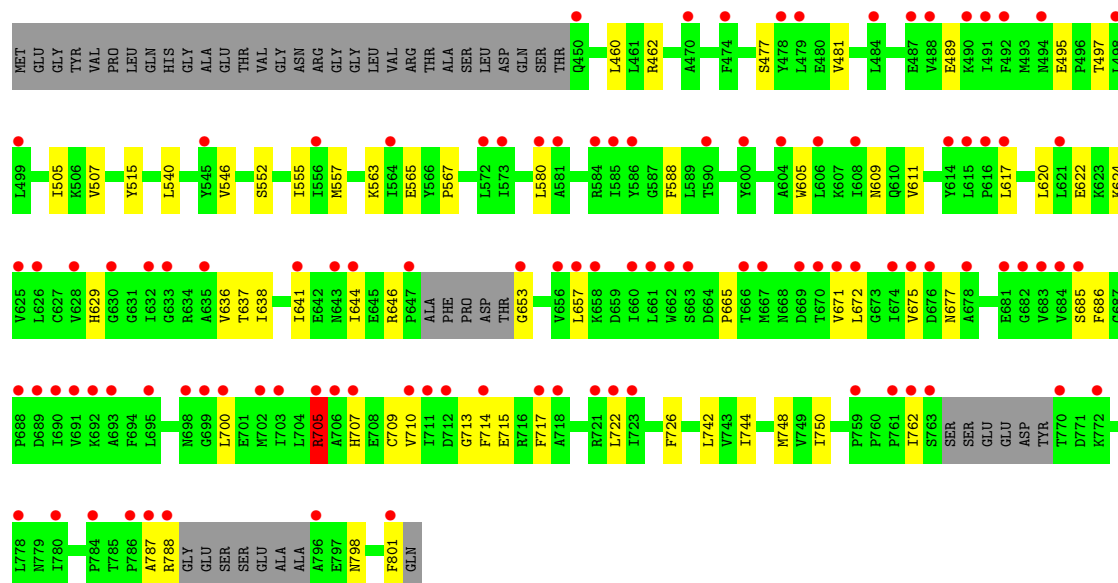




• Molecule 1: Serine/threonine-protein phosphatase BSU1



• Molecule 1: Serine/threonine-protein phosphatase BSU1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.41Å 97.78Å 157.80Å 90.00° 129.41° 90.00°	Depositor
Resolution (Å)	45.38 – 2.10 45.38 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.38-2.10) 88.9 (45.38-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.196 , 0.227 0.195 , 0.225	Depositor DCC
R_{free} test set	7764 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 54.7	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	0.96	EDS
Total number of atoms	33159	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 68.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5686e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GOL, TPO

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	0.09	0/2859	0.28	0/3878
1	B	0.10	0/2765	0.28	0/3745
1	C	0.10	0/2765	0.29	0/3746
1	D	0.09	0/2736	0.27	0/3708
1	E	0.10	0/2772	0.27	0/3755
1	F	0.10	0/2681	0.30	0/3632
All	All	0.10	0/16578	0.28	0/22464

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	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	705	ARG	Sidechain

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	2798	2741	2741	13	1
1	B	2710	2680	2680	19	0
1	C	2707	2669	2669	17	1
1	D	2679	2638	2638	28	0
1	E	2714	2691	2691	23	0
1	F	2624	2570	2569	39	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	B	6	8	8	0	0
3	C	6	8	8	0	0
3	D	6	8	8	0	0
3	F	6	8	8	0	0
4	A	168	0	0	4	0
4	B	185	0	0	4	0
4	C	189	0	0	3	0
4	D	104	0	0	9	0
4	E	163	0	0	10	0
4	F	61	0	0	3	0
All	All	17138	16021	16020	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 4.

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:C:779:ASN:OD1	4:C:1101:HOH:O	1.95	0.83
1:E:636:VAL:HG23	1:E:637:THR:HG23	1.62	0.80
1:C:487:GLU:OE1	4:C:1102:HOH:O	2.00	0.79
1:E:478:TYR:OH	4:E:1101:HOH:O	2.01	0.78
1:E:548[B]:ARG:NH1	4:E:1106:HOH:O	2.16	0.78
1:D:642:GLU:OE1	4:D:1101:HOH:O	2.02	0.77
1:E:797:GLU:N	4:E:1105:HOH:O	2.16	0.77
1:E:788:ARG:O	4:E:1102:HOH:O	2.03	0.76
1:D:653:GLY:O	4:D:1102:HOH:O	2.05	0.75
1:E:487:GLU:OE1	4:E:1103:HOH:O	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:ILE:HG12	1:C:660:ILE:HD11	1.71	0.72
1:E:758:HIS:ND1	4:E:1109:HOH:O	2.22	0.72
1:B:641:ILE:HG12	1:B:660:ILE:HD11	1.71	0.72
1:B:785:TPO:O1P	4:B:1101:HOH:O	2.07	0.72
1:B:770:THR:N	4:B:1104:HOH:O	2.23	0.72
1:F:489:GLU:HB2	1:F:611:VAL:HG22	1.72	0.72
1:B:451:ASP:OD2	4:B:1102:HOH:O	2.08	0.71
1:F:495:GLU:O	1:F:646:ARG:NH2	2.23	0.71
1:F:565:GLU:O	4:F:1101:HOH:O	2.06	0.71
1:C:636:VAL:HG23	1:C:637:THR:HG23	1.71	0.70
1:F:546:VAL:HG23	1:F:552:SER:HB3	1.74	0.69
1:F:801:PHE:O	4:F:1102:HOH:O	2.11	0.69
1:A:697:ARG:NH2	4:A:1103:HOH:O	2.26	0.68
1:E:584:ARG:NH2	4:E:1111:HOH:O	2.27	0.67
1:B:651:ASP:OD1	4:B:1103:HOH:O	2.11	0.67
1:F:677:ASN:OD1	1:F:685:SER:OG	2.14	0.66
1:C:636:VAL:HG22	1:C:640:GLU:OE2	1.95	0.65
1:E:676:ASP:OD1	4:E:1104:HOH:O	2.14	0.64
1:F:715:GLU:OE1	1:F:788:ARG:NE	2.30	0.64
1:E:636:VAL:HG22	1:E:640:GLU:OE2	1.97	0.64
1:D:641:ILE:HG12	1:D:660:ILE:HD11	1.81	0.63
1:F:557:MET:HA	1:F:557:MET:HE2	1.79	0.62
1:A:753:LYS:NZ	4:A:1105:HOH:O	2.33	0.61
1:D:787:ALA:N	4:D:1107:HOH:O	2.33	0.61
1:C:777:GLU:OE1	1:C:777:GLU:N	2.32	0.58
1:D:511:ILE:HG21	1:D:555:ILE:HD12	1.87	0.56
1:D:515:TYR:OH	1:D:558:LEU:HD22	2.07	0.55
1:F:705:ARG:NH2	1:F:707:HIS:HB2	2.22	0.55
1:D:716:ARG:NH1	4:D:1111:HOH:O	2.40	0.54
1:F:515:TYR:HA	1:F:555:ILE:HD11	1.89	0.54
1:E:645:GLU:OE2	4:E:1107:HOH:O	2.18	0.53
1:F:744:ILE:HD13	1:F:750:ILE:HG12	1.90	0.53
1:D:651:ASP:OD1	1:D:652:THR:N	2.42	0.53
1:D:710:VAL:HG21	1:D:715:GLU:HB2	1.91	0.53
1:B:714:PHE:CE1	1:E:799:LEU:HD11	2.44	0.52
1:D:621:LEU:HD13	1:D:627:CYS:SG	2.50	0.52
1:F:636:VAL:HG23	1:F:637:THR:HG23	1.89	0.52
1:F:713:GLY:O	1:F:726:PHE:N	2.36	0.52
1:A:556:ILE:HG23	1:A:557:MET:HE2	1.92	0.52
1:F:497:THR:HG23	1:F:617:LEU:HD12	1.92	0.52
1:B:456:VAL:HG21	1:B:484:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:GLN:O	1:B:780:ILE:HD12	2.11	0.51
1:A:459:THR:O	4:A:1101:HOH:O	2.19	0.51
1:F:638:ILE:HD11	1:F:700:LEU:HD11	1.92	0.51
1:B:749:VAL:HG23	1:E:798:ASN:CG	2.36	0.51
1:E:679:ARG:NH1	1:E:785:TPO:O3P	2.43	0.51
1:A:505:ILE:HD11	1:A:540:LEU:HB2	1.91	0.50
1:D:665:PRO:O	4:D:1103:HOH:O	2.18	0.50
1:D:753:LYS:NZ	4:D:1114:HOH:O	2.45	0.50
1:B:585:ILE:HB	1:B:782:MET:HE1	1.93	0.50
1:D:635:ALA:O	4:D:1104:HOH:O	2.19	0.50
1:F:675:VAL:HG22	1:F:685:SER:HB2	1.92	0.50
1:D:710:VAL:HG21	1:D:715:GLU:CB	2.42	0.49
1:E:524:GLU:OE2	4:E:1108:HOH:O	2.19	0.49
1:C:747:ASP:OD1	1:C:747:ASP:N	2.37	0.49
1:C:626:LEU:HD13	1:C:638:ILE:HD11	1.94	0.49
1:B:800:TYR:OH	1:D:701:GLU:OE1	2.27	0.49
1:A:535:THR:OG1	4:A:1102:HOH:O	2.20	0.48
1:C:722:LEU:HD23	1:C:723:ILE:N	2.28	0.48
1:C:505:ILE:HD11	1:C:540:LEU:HB2	1.96	0.47
1:F:705:ARG:HD3	1:F:705:ARG:C	2.38	0.47
1:B:668:ASN:OD1	1:B:670:THR:HG23	2.14	0.47
1:D:666:THR:HG23	1:D:686:PHE:C	2.39	0.47
1:F:710:VAL:HG11	1:F:714:PHE:O	2.14	0.47
1:F:620:LEU:O	4:F:1103:HOH:O	2.20	0.46
1:D:622:GLU:HG3	1:D:748:MET:HE1	1.97	0.46
1:A:666:THR:HG23	1:A:686:PHE:C	2.41	0.46
1:F:622:GLU:HB2	1:F:748:MET:HE1	1.97	0.46
1:F:477:SER:O	1:F:481:VAL:HG23	2.15	0.46
1:F:762:ILE:HD12	1:F:762:ILE:N	2.31	0.46
1:F:665:PRO:HA	1:F:686:PHE:O	2.16	0.45
1:E:785:TPO:O1P	1:E:785:TPO:N	2.44	0.45
1:F:620:LEU:HD11	1:F:700:LEU:HD22	1.98	0.45
1:D:462:ARG:NE	4:D:1115:HOH:O	2.50	0.45
1:F:717:PHE:CB	1:F:722:LEU:HD22	2.47	0.45
1:B:646:ARG:HA	1:B:647:PRO:C	2.42	0.45
1:C:546:VAL:O	1:C:547:ASP:HB2	2.15	0.45
1:F:624:LYS:HD2	1:F:748:MET:HE3	1.99	0.45
1:F:653:GLY:HA3	1:F:657:LEU:HD23	1.99	0.45
1:D:626:LEU:HD13	1:D:638:ILE:HD11	1.98	0.44
1:D:628:VAL:O	1:D:705:ARG:HA	2.17	0.44
1:E:798:ASN:OD1	1:E:799:LEU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:VAL:O	1:A:547:ASP:HB2	2.17	0.44
1:B:630:GLY:O	1:B:705:ARG:NE	2.41	0.44
1:B:777:GLU:OE1	1:B:777:GLU:N	2.43	0.44
1:D:505:ILE:HD11	1:D:540:LEU:HB2	2.00	0.44
1:D:636:VAL:HG23	1:D:637:THR:HG23	2.00	0.44
1:E:490:LYS:O	1:E:494:ASN:ND2	2.48	0.44
1:C:456:VAL:HG21	1:C:484:LEU:HD11	2.00	0.43
1:F:641:ILE:HA	1:F:644:ILE:HD12	1.99	0.43
1:A:732:CYS:SG	1:A:784:PRO:HB3	2.58	0.43
1:E:546:VAL:O	1:E:547:ASP:HB2	2.17	0.43
1:C:722:LEU:HD23	1:C:722:LEU:C	2.43	0.43
1:D:460:LEU:HB3	1:D:515:TYR:OH	2.19	0.43
1:F:546:VAL:HG21	1:F:588:PHE:CG	2.53	0.43
1:C:749:VAL:HG23	1:F:798:ASN:CG	2.44	0.43
1:D:614:TYR:O	1:D:646:ARG:NH1	2.45	0.43
1:F:580:LEU:HD22	1:F:605:TRP:CH2	2.53	0.43
1:F:671:VAL:C	1:F:672:LEU:HD12	2.44	0.43
1:A:492:PHE:O	1:A:646:ARG:NH2	2.52	0.42
1:E:740:ALA:HB2	1:E:754:LEU:HD22	2.01	0.42
1:B:546:VAL:O	1:B:547:ASP:HB2	2.19	0.42
1:B:747:ASP:OD1	1:B:749:VAL:HG12	2.19	0.42
1:C:656:VAL:HG23	4:C:1252:HOH:O	2.20	0.42
1:B:652:THR:HG23	1:B:652:THR:O	2.19	0.41
1:A:628:VAL:O	1:A:705:ARG:HA	2.19	0.41
1:F:507:VAL:CG2	1:F:742:LEU:HB2	2.51	0.41
1:D:636:VAL:HG22	1:D:640:GLU:OE2	2.20	0.41
1:D:621:LEU:HB2	1:D:625:VAL:HB	2.02	0.41
1:D:678:ALA:N	4:D:1108:HOH:O	2.36	0.41
1:E:778:LEU:C	1:E:778:LEU:HD23	2.45	0.41
1:B:492:PHE:O	1:B:646:ARG:NH2	2.54	0.41
1:C:644:ILE:HD11	1:C:656:VAL:HG12	2.03	0.41
1:F:460:LEU:O	1:F:462:ARG:N	2.52	0.41
1:A:602:PHE:CE2	1:A:606:LEU:HD11	2.56	0.41
1:F:665:PRO:HD2	1:F:705:ARG:NH1	2.36	0.41
1:F:709:CYS:O	1:F:787:ALA:HB1	2.20	0.41
1:D:546:VAL:O	1:D:547:ASP:HB2	2.22	0.40
1:F:505:ILE:HD11	1:F:540:LEU:HB2	2.03	0.40
1:F:629:HIS:CD2	1:F:707:HIS:CE1	3.09	0.40
1:A:646:ARG:HA	1:A:647:PRO:C	2.46	0.40
1:C:714:PHE:HA	1:C:724:THR:O	2.21	0.40
1:E:714:PHE:HA	1:E:724:THR:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:563:LYS:NZ	1:F:567:PRO:O	2.53	0.40
1:E:695:LEU:HD21	1:E:703:ILE:HG13	2.02	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:701:GLU:OE1	1:C:800:TYR:HH[3_555]	1.59	0.01

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	351/383 (92%)	337 (96%)	14 (4%)	0	100	100
1	B	332/383 (87%)	322 (97%)	10 (3%)	0	100	100
1	C	333/383 (87%)	322 (97%)	11 (3%)	0	100	100
1	D	331/383 (86%)	315 (95%)	16 (5%)	0	100	100
1	E	333/383 (87%)	319 (96%)	14 (4%)	0	100	100
1	F	325/383 (85%)	301 (93%)	24 (7%)	0	100	100
All	All	2005/2298 (87%)	1916 (96%)	89 (4%)	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	295/328 (90%)	294 (100%)	1 (0%)	86	91
1	B	291/328 (89%)	290 (100%)	1 (0%)	86	91
1	C	289/328 (88%)	289 (100%)	0	100	100
1	D	284/328 (87%)	278 (98%)	6 (2%)	47	54
1	E	292/328 (89%)	291 (100%)	1 (0%)	86	91
1	F	276/328 (84%)	274 (99%)	2 (1%)	76	83
All	All	1727/1968 (88%)	1716 (99%)	11 (1%)	78	86

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	669	ASP
1	B	734	THR
1	D	642	GLU
1	D	667	MET
1	D	668	ASN
1	D	669	ASP
1	D	705	ARG
1	D	778	LEU
1	E	782	MET
1	F	609	ASN
1	F	705	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	776	GLN
1	C	471	ASN
1	C	758	HIS
1	D	527	HIS
1	D	668	ASN
1	E	571	HIS
1	F	629	HIS
1	F	707	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	D	785	1	8,10,11	2.50	1 (12%)	10,14,16	1.20	1 (10%)
1	TPO	A	785	1	8,10,11	2.50	1 (12%)	10,14,16	1.27	1 (10%)
1	TPO	E	785	1	8,10,11	2.54	1 (12%)	10,14,16	1.20	1 (10%)
1	TPO	C	785	1	8,10,11	2.52	1 (12%)	10,14,16	1.24	1 (10%)
1	TPO	B	785	1	8,10,11	2.51	1 (12%)	10,14,16	1.26	1 (10%)
1	TPO	F	785	1	3,4,11	0.72	0	2,4,16	1.05	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
1	TPO	D	785	1	-	0/9/11/13	-
1	TPO	A	785	1	-	0/9/11/13	-
1	TPO	E	785	1	-	3/9/11/13	-
1	TPO	C	785	1	-	0/9/11/13	-
1	TPO	B	785	1	-	0/9/11/13	-
1	TPO	F	785	1	-	0/0/2/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	785	TPO	P-OG1	7.01	1.72	1.59
1	C	785	TPO	P-OG1	6.96	1.72	1.59
1	B	785	TPO	P-OG1	6.92	1.72	1.59
1	A	785	TPO	P-OG1	6.89	1.72	1.59
1	D	785	TPO	P-OG1	6.89	1.72	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	785	TPO	OG1-P-O1P	-2.30	100.51	109.39
1	A	785	TPO	OG1-P-O1P	-2.29	100.56	109.39
1	B	785	TPO	OG1-P-O1P	-2.29	100.56	109.39
1	C	785	TPO	OG1-P-O1P	-2.23	100.80	109.39
1	E	785	TPO	OG1-P-O1P	-2.18	100.97	109.39

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	785	TPO	CB-OG1-P-O3P
1	E	785	TPO	CA-CB-OG1-P
1	E	785	TPO	CB-OG1-P-O2P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	785	TPO	2	0
1	B	785	TPO	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	D	1003	-	5,5,5	0.34	0	5,5,5	0.36	0
3	GOL	B	1003	-	5,5,5	0.34	0	5,5,5	0.37	0
3	GOL	F	1003	-	5,5,5	0.34	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	C	1003	-	5,5,5	0.34	0	5,5,5	0.38	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	D	1003	-	-	3/4/4/4	-
3	GOL	B	1003	-	-	2/4/4/4	-
3	GOL	F	1003	-	-	2/4/4/4	-
3	GOL	C	1003	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1003	GOL	O1-C1-C2-C3
3	F	1003	GOL	C1-C2-C3-O3
3	D	1003	GOL	O1-C1-C2-O2
3	C	1003	GOL	O1-C1-C2-C3
3	D	1003	GOL	O1-C1-C2-C3
3	B	1003	GOL	O1-C1-C2-O2
3	C	1003	GOL	O1-C1-C2-O2
3	F	1003	GOL	O2-C2-C3-O3
3	D	1003	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	352/383 (91%)	0.23	19 (5%)	31 33	28, 50, 93, 131	1 (0%)
1	B	338/383 (88%)	-0.04	15 (4%)	39 41	27, 42, 84, 124	0
1	C	338/383 (88%)	-0.12	8 (2%)	59 62	21, 41, 77, 116	1 (0%)
1	D	336/383 (87%)	0.68	39 (11%)	9 10	29, 60, 106, 127	1 (0%)
1	E	338/383 (88%)	0.07	11 (3%)	49 51	27, 49, 82, 108	1 (0%)
1	F	333/383 (86%)	1.66	106 (31%)	1 1	41, 92, 135, 163	0
All	All	2035/2298 (88%)	0.41	198 (9%)	13 14	21, 51, 111, 163	4 (0%)

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	632	ILE	7.5
1	D	770	THR	6.0
1	F	615	LEU	5.9
1	F	660	ILE	5.9
1	F	675	VAL	5.4
1	F	484	LEU	5.2
1	A	765	SER	5.1
1	F	479	LEU	5.1
1	F	671	VAL	5.0
1	F	689	ASP	5.0
1	F	657	LEU	5.0
1	F	695	LEU	4.9
1	F	717	PHE	4.8
1	F	653	GLY	4.7
1	F	762	ILE	4.6
1	D	761	PRO	4.6
1	F	707	HIS	4.5
1	F	718	ALA	4.4
1	F	691	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	656	VAL	4.3
1	A	791	SER	4.3
1	A	793	GLU	4.3
1	D	771	ASP	4.3
1	A	764	SER	4.2
1	D	795	ALA	4.2
1	F	635	ALA	4.2
1	F	670	THR	4.1
1	D	800	TYR	4.1
1	F	661	LEU	4.1
1	F	630	GLY	4.1
1	F	450	GLN	4.0
1	E	769	TYR	3.9
1	F	662	TRP	3.9
1	B	801	PHE	3.9
1	A	794	ALA	3.8
1	A	450	GLN	3.7
1	D	772	LYS	3.7
1	D	780	ILE	3.6
1	F	581	ALA	3.6
1	D	799	LEU	3.6
1	A	795	ALA	3.6
1	A	766	GLU	3.6
1	F	700	LEU	3.5
1	F	683	VAL	3.5
1	F	604	ALA	3.4
1	F	617	LEU	3.4
1	D	797	GLU	3.4
1	F	763	SER	3.3
1	F	672	LEU	3.3
1	E	450	GLN	3.3
1	F	667	MET	3.3
1	F	658	LYS	3.3
1	B	761	PRO	3.3
1	F	684	VAL	3.3
1	F	699	GLY	3.2
1	F	606	LEU	3.2
1	F	688	PRO	3.2
1	A	780	ILE	3.2
1	D	681	GLU	3.2
1	F	681	GLU	3.1
1	A	790	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	770	THR	3.1
1	A	769	TYR	3.1
1	F	678	ALA	3.0
1	A	778	LEU	3.0
1	C	780	ILE	3.0
1	D	779	ASN	3.0
1	F	572	LEU	3.0
1	F	556	ILE	3.0
1	D	773	ALA	3.0
1	F	706	ALA	2.9
1	A	762	ILE	2.9
1	F	492	PHE	2.9
1	A	763	SER	2.9
1	D	652	THR	2.9
1	C	761	PRO	2.9
1	F	580	LEU	2.9
1	A	792	SER	2.9
1	F	470	ALA	2.9
1	F	703	ILE	2.8
1	E	800	TYR	2.8
1	F	614	TYR	2.8
1	F	641	ILE	2.8
1	F	600	TYR	2.8
1	F	693	ALA	2.8
1	F	643	ASN	2.7
1	F	633	GLY	2.7
1	D	678	ALA	2.7
1	F	626	LEU	2.7
1	F	770	THR	2.7
1	A	779	ASN	2.7
1	F	721	ARG	2.7
1	D	452	LEU	2.7
1	F	666	THR	2.7
1	F	786	PRO	2.7
1	F	644	ILE	2.7
1	D	460	LEU	2.6
1	E	763	SER	2.6
1	F	478	TYR	2.6
1	F	669	ASP	2.6
1	C	779	ASN	2.6
1	F	796	ALA	2.6
1	F	722	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	768	ASP	2.6
1	F	788	ARG	2.6
1	F	625	VAL	2.6
1	D	782	MET	2.6
1	D	484	LEU	2.6
1	F	761	PRO	2.6
1	F	487	GLU	2.6
1	F	787	ALA	2.6
1	F	499	LEU	2.6
1	B	779	ASN	2.5
1	F	685	SER	2.5
1	C	778	LEU	2.5
1	F	590	THR	2.5
1	F	616	PRO	2.5
1	F	474	PHE	2.5
1	B	780	ILE	2.5
1	B	669	ASP	2.4
1	D	776	GLN	2.4
1	D	638	ILE	2.4
1	F	585	ILE	2.4
1	D	466	TRP	2.4
1	F	628	VAL	2.4
1	F	714	PHE	2.4
1	F	674	ILE	2.4
1	E	782	MET	2.4
1	D	600	TYR	2.4
1	D	651	ASP	2.4
1	F	712	ASP	2.4
1	F	608	ILE	2.4
1	F	584	ARG	2.4
1	F	710	VAL	2.4
1	B	781	GLU	2.3
1	F	498	LEU	2.3
1	D	585	ILE	2.3
1	E	638	ILE	2.3
1	F	690	ILE	2.3
1	B	760	PRO	2.3
1	F	647	PRO	2.3
1	F	676	ASP	2.3
1	F	772	LYS	2.3
1	F	573	ILE	2.3
1	F	784	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	796	ALA	2.3
1	E	762	ILE	2.3
1	D	786	PRO	2.3
1	D	778	LEU	2.3
1	F	702	MET	2.3
1	F	778	LEU	2.3
1	F	586	TYR	2.3
1	D	605	TRP	2.3
1	D	758	HIS	2.2
1	A	802	GLN	2.2
1	F	663	SER	2.2
1	F	564	ILE	2.2
1	F	692	LYS	2.2
1	F	711	ILE	2.2
1	E	799	LEU	2.2
1	D	450	GLN	2.2
1	F	705	ARG	2.2
1	D	748	MET	2.2
1	C	781	GLU	2.2
1	C	796	ALA	2.2
1	D	470	ALA	2.2
1	D	796	ALA	2.2
1	F	545	TYR	2.2
1	E	786	PRO	2.1
1	F	759	PRO	2.1
1	B	681	GLU	2.1
1	B	778	LEU	2.1
1	D	479	LEU	2.1
1	B	782	MET	2.1
1	C	667	MET	2.1
1	F	494	ASN	2.1
1	F	723	ILE	2.1
1	F	488	VAL	2.1
1	F	490	LYS	2.1
1	B	790	GLU	2.1
1	D	471	ASN	2.1
1	B	652	THR	2.1
1	F	780	ILE	2.1
1	D	599	SER	2.1
1	D	760	PRO	2.1
1	E	770	THR	2.1
1	B	680	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	491	ILE	2.1
1	E	801	PHE	2.1
1	F	801	PHE	2.1
1	F	698	ASN	2.0
1	A	761	PRO	2.0
1	B	770	THR	2.0
1	D	783	PRO	2.0
1	D	464	LYS	2.0
1	F	621	LEU	2.0
1	D	732	CYS	2.0
1	F	682	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	F	785	5/12	0.49	0.23	115,121,138,145	0
1	TPO	E	785	11/12	0.66	0.20	88,103,128,132	0
1	TPO	D	785	11/12	0.76	0.15	92,108,129,130	0
1	TPO	C	785	11/12	0.79	0.16	65,74,91,93	0
1	TPO	A	785	11/12	0.83	0.15	76,91,112,120	0
1	TPO	B	785	11/12	0.83	0.15	73,81,98,99	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	D	1003	6/6	0.68	0.26	70,84,101,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	F	1003	6/6	0.71	0.26	77,104,125,125	0
2	ZN	F	1002	1/1	0.82	0.15	139,139,139,139	0
3	GOL	C	1003	6/6	0.86	0.14	33,55,70,83	0
3	GOL	B	1003	6/6	0.88	0.16	42,68,90,108	0
2	ZN	F	1001	1/1	0.95	0.07	78,78,78,78	0
2	ZN	E	1001	1/1	0.95	0.18	65,65,65,65	0
2	ZN	A	1002	1/1	0.97	0.10	57,57,57,57	0
2	ZN	D	1001	1/1	0.97	0.04	36,36,36,36	0
2	ZN	A	1001	1/1	0.97	0.04	26,26,26,26	0
2	ZN	D	1002	1/1	0.98	0.12	69,69,69,69	0
2	ZN	B	1001	1/1	0.98	0.05	31,31,31,31	0
2	ZN	C	1002	1/1	0.99	0.03	26,26,26,26	0
2	ZN	E	1002	1/1	0.99	0.03	31,31,31,31	0
2	ZN	B	1002	1/1	0.99	0.12	55,55,55,55	0
2	ZN	C	1001	1/1	0.99	0.06	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.