



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:34 AM GMT

PDB ID : 2ANU
Title : Crystal structure of Predicted metal-dependent phosphoesterase (PHP family)
(tm0559) from THERMOTOGA MARITIMA at 2.40 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2005-08-11
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

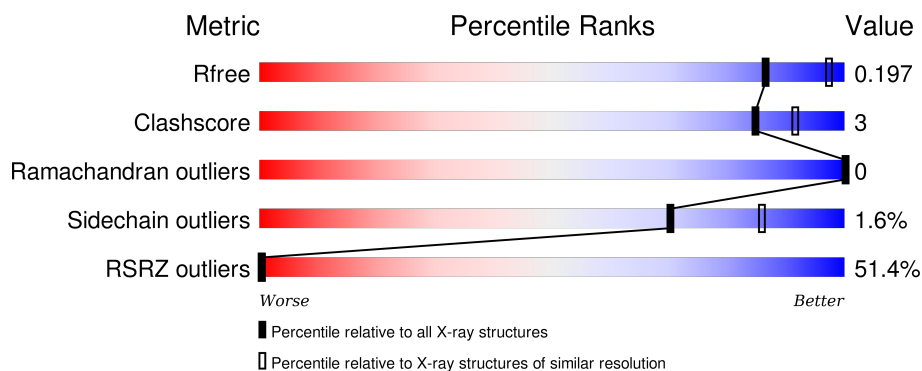
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	255	<div> <div>25%</div> <div>82%</div> <div>6%</div> <div>12%</div> </div>
1	B	255	<div> <div>27%</div> <div>76%</div> <div>10%</div> <div>13%</div> </div>
1	C	255	<div> <div>76%</div> <div>80%</div> <div>7%</div> <div>13%</div> </div>
1	D	255	<div> <div>76%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div>
1	E	255	<div> <div>28%</div> <div>80%</div> <div>7%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	255	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (31%), green (83%), yellow (5%), and grey (12%). The percentages are labeled above or below the corresponding segments.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11171 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 hypothetical protein TM0559.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	Se	0	0	0
			1835	1183	314	333	1	4			
1	B	221	Total	C	N	O	S	Se	0	0	0
			1816	1172	308	331	1	4			
1	C	222	Total	C	N	O	S	Se	0	0	0
			1810	1170	305	330	1	4			
1	D	220	Total	C	N	O	S	Se	0	0	0
			1813	1169	309	330	1	4			
1	E	223	Total	C	N	O	S	Se	0	0	0
			1819	1177	309	328	1	4			
1	F	224	Total	C	N	O	S	Se	0	0	0
			1827	1182	310	330	1	4			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	MODIFIED RESIDUE	UNP Q9WZ29
A	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZ29
A	-9	SER	-	LEADER SEQUENCE	UNP Q9WZ29
A	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZ29
A	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZ29
A	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZ29
A	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
A	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
A	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
A	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
A	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
A	0	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
A	18	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
A	90	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
A	159	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
A	231	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MSE	-	MODIFIED RESIDUE	UNP Q9WZ29
B	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZ29
B	-9	SER	-	LEADER SEQUENCE	UNP Q9WZ29
B	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZ29
B	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZ29
B	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZ29
B	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
B	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
B	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
B	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
B	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
B	0	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
B	18	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
B	90	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
B	159	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
B	231	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
C	-11	MSE	-	MODIFIED RESIDUE	UNP Q9WZ29
C	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZ29
C	-9	SER	-	LEADER SEQUENCE	UNP Q9WZ29
C	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZ29
C	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZ29
C	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZ29
C	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
C	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
C	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
C	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
C	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
C	0	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
C	18	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
C	90	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
C	159	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
C	231	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
D	-11	MSE	-	MODIFIED RESIDUE	UNP Q9WZ29
D	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZ29
D	-9	SER	-	LEADER SEQUENCE	UNP Q9WZ29
D	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZ29
D	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZ29
D	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZ29
D	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
D	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZ29

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
D	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
D	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
D	0	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
D	18	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
D	90	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
D	159	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
D	231	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
E	-11	MSE	-	MODIFIED RESIDUE	UNP Q9WZ29
E	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZ29
E	-9	SER	-	LEADER SEQUENCE	UNP Q9WZ29
E	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZ29
E	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZ29
E	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZ29
E	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
E	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
E	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
E	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
E	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
E	0	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
E	18	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
E	90	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
E	159	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
E	231	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
F	-11	MSE	-	MODIFIED RESIDUE	UNP Q9WZ29
F	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZ29
F	-9	SER	-	LEADER SEQUENCE	UNP Q9WZ29
F	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZ29
F	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZ29
F	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZ29
F	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
F	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
F	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
F	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
F	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
F	0	HIS	-	LEADER SEQUENCE	UNP Q9WZ29
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
F	18	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
F	90	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29
F	159	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29

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Chain	Residue	Modelled	Actual	Comment	Reference
F	231	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ29

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	4	Total 4	Zn 4	0	0
2	E	4	Total 4	Zn 4	0	0
2	B	4	Total 4	Zn 4	0	0
2	C	4	Total 4	Zn 4	0	0
2	A	4	Total 4	Zn 4	0	0
2	F	4	Total 4	Zn 4	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total 2	Cl 2	0	0
3	E	3	Total 3	Cl 3	0	0
3	B	2	Total 2	Cl 2	0	0
3	C	3	Total 3	Cl 3	0	0
3	A	3	Total 3	Cl 3	0	0
3	F	2	Total 2	Cl 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total 44	O 44	0	0
4	B	31	Total 31	O 31	0	0

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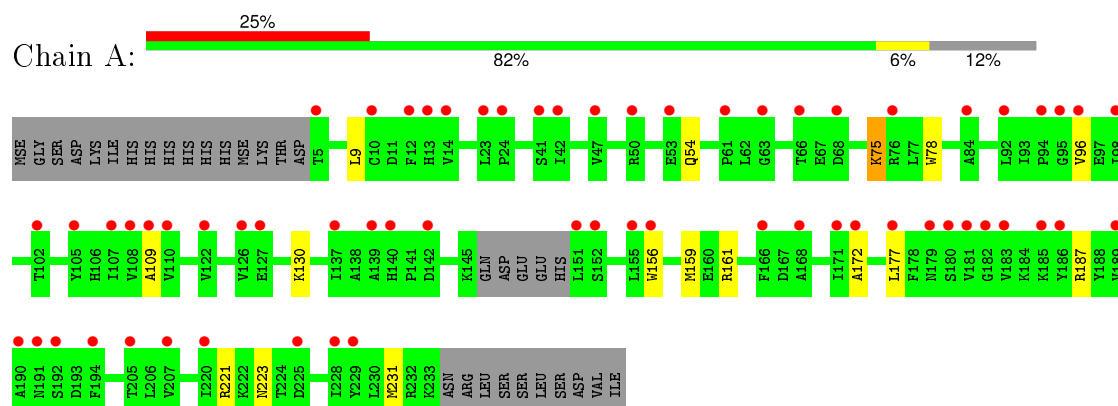
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	22	Total 22	O 22	0	0
4	D	30	Total 30	O 30	0	0
4	E	46	Total 46	O 46	0	0
4	F	39	Total 39	O 39	0	0

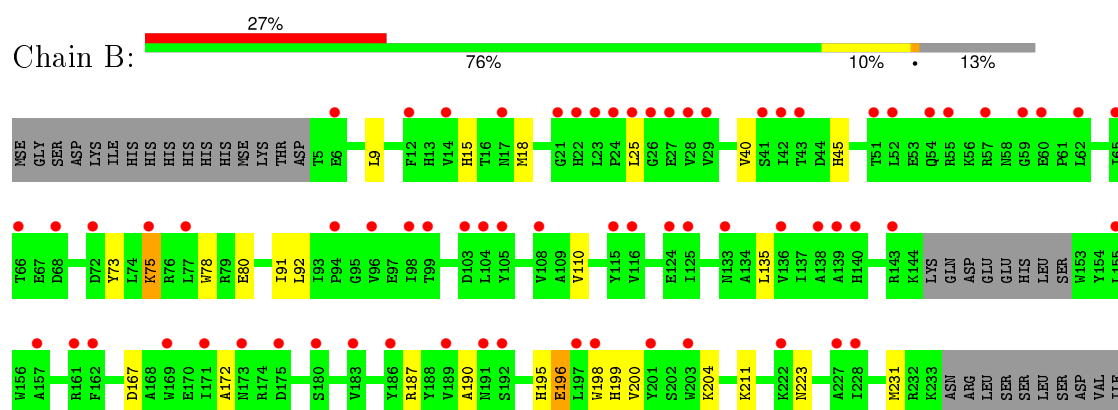
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

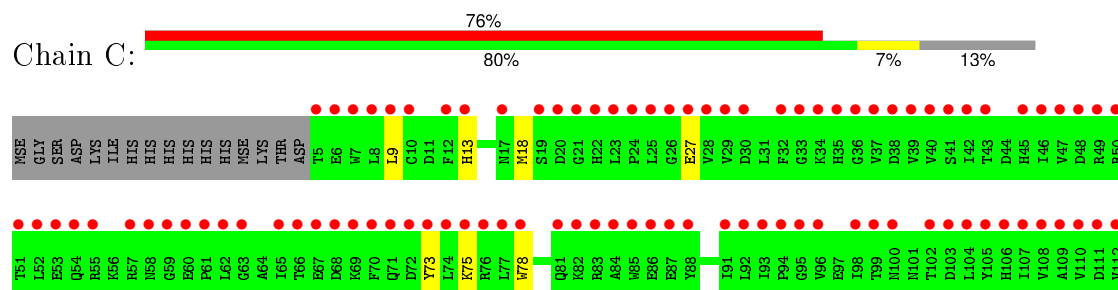
- Molecule 1: hypothetical protein TM0559

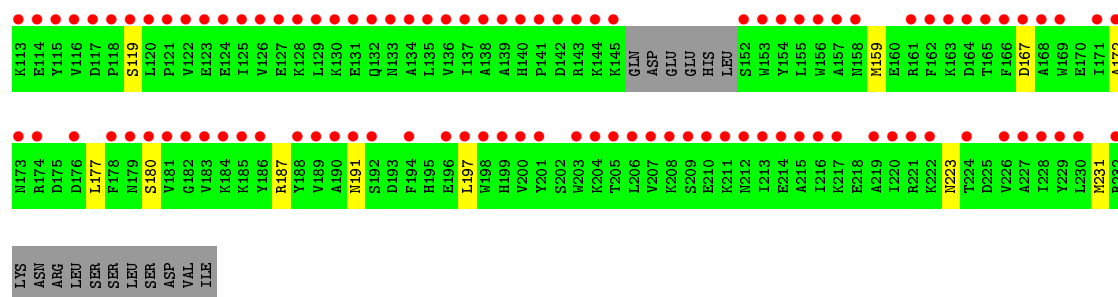


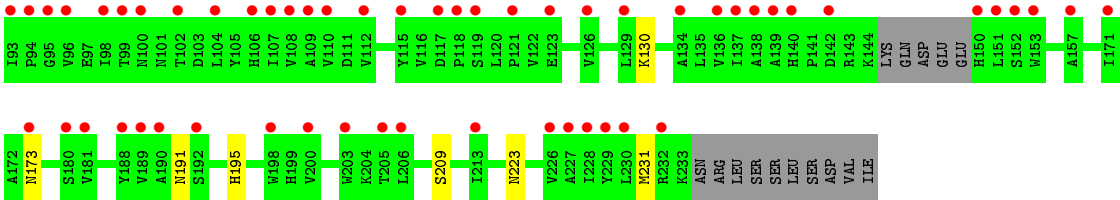
- Molecule 1: hypothetical protein TM0559



- Molecule 1: hypothetical protein TM0559







4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	111.31Å 111.31Å 383.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.00 – 2.40 29.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.00-2.40) 99.3 (29.00-2.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.169 , 0.220 0.181 , 0.197	Depositor DCC
R_{free} test set	3506 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.2	EDS
Estimated twinning fraction	0.148 for -h-k,k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 83420 reflections	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	11171	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, CL

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	0.66	0/1876	0.72	0/2536
1	B	0.67	0/1856	0.68	0/2511
1	C	0.62	0/1851	0.66	0/2503
1	D	0.63	0/1854	0.70	0/2506
1	E	0.66	0/1860	0.72	0/2515
1	F	0.61	0/1869	0.66	0/2526
All	All	0.64	0/11166	0.69	0/15097

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	B	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	B	45	HIS	Peptide

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	1835	0	1786	8	0
1	B	1816	0	1760	18	0
1	C	1810	0	1750	10	0
1	D	1813	0	1764	10	0
1	E	1819	0	1769	12	0
1	F	1827	0	1764	5	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
3	A	3	0	0	1	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
3	E	3	0	0	0	0
3	F	2	0	0	0	0
4	A	44	0	0	1	0
4	B	31	0	0	0	0
4	C	22	0	0	0	0
4	D	30	0	0	1	0
4	E	46	0	0	0	0
4	F	39	0	0	0	0
All	All	11171	0	10593	63	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (63) 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)
3:A:1001:CL:CL	4:A:1055:HOH:O	2.24	0.92
1:C:9:LEU:HD21	1:C:231:MSE:CE	2.06	0.86
1:E:9:LEU:HD21	1:E:231:MSE:CE	2.14	0.77
1:B:9:LEU:HD21	1:B:231:MSE:HE3	1.65	0.77
1:C:9:LEU:HD21	1:C:231:MSE:HE3	1.67	0.76
1:A:9:LEU:HD21	1:A:231:MSE:HE3	1.69	0.74
1:E:40:VAL:HG13	1:E:92:LEU:HD12	1.71	0.70
1:B:196:GLU:OE2	1:B:198:TRP:CZ2	2.49	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ARG:HA	1:C:27:GLU:HG3	1.79	0.63
1:A:9:LEU:HD21	1:A:231:MSE:CE	2.28	0.61
1:E:75:LYS:HA	1:E:78:TRP:CE3	2.35	0.61
1:B:40:VAL:HG13	1:B:92:LEU:HD12	1.83	0.60
1:E:40:VAL:HG13	1:E:92:LEU:CD1	2.33	0.59
1:B:9:LEU:HD21	1:B:231:MSE:CE	2.33	0.58
1:E:9:LEU:HD21	1:E:231:MSE:HE3	1.86	0.58
1:E:167:ASP:O	1:E:187:ARG:HD2	2.05	0.56
1:F:9:LEU:HD21	1:F:231:MSE:HE3	1.87	0.55
1:F:75:LYS:HA	1:F:78:TRP:CE3	2.42	0.55
1:D:75:LYS:HA	1:D:78:TRP:CE3	2.43	0.54
1:D:187:ARG:NH2	4:D:1033:HOH:O	2.41	0.54
1:F:15:HIS:CD2	1:F:195:HIS:CE1	2.96	0.53
1:B:196:GLU:OE2	1:B:198:TRP:HZ2	1.91	0.53
1:A:75:LYS:HA	1:A:78:TRP:CE3	2.44	0.52
1:E:91:ILE:HD11	1:E:211:LYS:HG2	1.91	0.52
1:C:18:MSE:HE1	1:C:73:TYR:HA	1.91	0.52
1:D:202:SER:OG	1:D:204:LYS:HE2	2.10	0.51
1:D:159:MSE:HB2	1:D:184:LYS:HZ2	1.76	0.50
1:B:167:ASP:O	1:B:187:ARG:HD2	2.12	0.50
1:F:173:ASN:HA	1:F:191:ASN:O	2.12	0.49
1:E:9:LEU:HD21	1:E:231:MSE:HE1	1.92	0.49
1:A:187:ARG:HD3	1:A:221:ARG:O	2.13	0.48
1:B:75:LYS:HG2	1:B:78:TRP:CZ3	2.49	0.48
1:A:172:ALA:HB2	1:A:177:LEU:HD23	1.96	0.48
1:A:156:TRP:HE3	1:A:159:MSE:HE2	1.78	0.47
1:B:18:MSE:HE1	1:B:73:TYR:HA	1.96	0.47
1:D:173:ASN:HB2	1:D:178:PHE:HE2	1.81	0.46
1:E:154:TYR:OH	1:E:161:ARG:NH1	2.49	0.46
1:B:25:LEU:HG	1:B:80:GLU:HG3	1.97	0.45
1:C:197:LEU:HD23	1:C:197:LEU:O	2.16	0.45
1:B:75:LYS:HA	1:B:78:TRP:CE3	2.51	0.45
1:B:91:ILE:HD11	1:B:211:LYS:HG2	2.00	0.44
1:B:196:GLU:HG2	1:B:199:HIS:CE1	2.53	0.44
1:E:44:ASP:HB3	1:E:65:ILE:HD11	2.00	0.43
1:A:96:VAL:HG12	1:A:109:ALA:HB3	2.01	0.43
1:B:15:HIS:CD2	1:B:195:HIS:CE1	3.07	0.43
1:D:15:HIS:CD2	1:D:195:HIS:CE1	3.07	0.42
1:D:10:CYS:HA	1:D:39:VAL:O	2.18	0.42
1:B:9:LEU:CD2	1:B:231:MSE:CE	2.97	0.42
1:C:75:LYS:HA	1:C:78:TRP:CE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ALA:HB2	1:C:177:LEU:HD23	2.02	0.42
1:E:44:ASP:CB	1:E:65:ILE:HD11	2.50	0.42
1:F:9:LEU:HD21	1:F:231:MSE:CE	2.50	0.42
1:B:110:VAL:HB	1:B:135:LEU:HB3	2.01	0.42
1:B:25:LEU:CD2	1:B:80:GLU:HG3	2.49	0.42
1:D:140:HIS:HB2	1:D:156:TRP:CZ2	2.56	0.41
1:C:159:MSE:HE1	1:C:180:SER:HB2	2.03	0.41
1:D:52:LEU:HA	1:D:52:LEU:HD23	1.96	0.41
1:C:167:ASP:O	1:C:187:ARG:HD2	2.21	0.41
1:C:13:HIS:HB3	1:C:191:ASN:HB3	2.03	0.41
1:E:173:ASN:O	1:E:174:ARG:C	2.59	0.41
1:B:172:ALA:HB3	1:B:190:ALA:HB1	2.01	0.41
1:D:7:TRP:HB3	1:D:206:LEU:HG	2.03	0.40
1:B:200:VAL:O	1:B:204:LYS:NZ	2.52	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	220/255 (86%)	210 (96%)	10 (4%)	0	100	100
1	B	217/255 (85%)	209 (96%)	8 (4%)	0	100	100
1	C	218/255 (86%)	207 (95%)	11 (5%)	0	100	100
1	D	216/255 (85%)	207 (96%)	9 (4%)	0	100	100
1	E	219/255 (86%)	211 (96%)	8 (4%)	0	100	100
1	F	220/255 (86%)	210 (96%)	10 (4%)	0	100	100
All	All	1310/1530 (86%)	1254 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/226 (85%)	188 (98%)	4 (2%)	61	80
1	B	189/226 (84%)	186 (98%)	3 (2%)	70	86
1	C	190/226 (84%)	188 (99%)	2 (1%)	80	92
1	D	190/226 (84%)	188 (99%)	2 (1%)	80	92
1	E	188/226 (83%)	186 (99%)	2 (1%)	80	92
1	F	188/226 (83%)	183 (97%)	5 (3%)	52	73
All	All	1137/1356 (84%)	1119 (98%)	18 (2%)	70	86

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	75	LYS
1	A	130	LYS
1	A	223	ASN
1	B	75	LYS
1	B	196	GLU
1	B	223	ASN
1	C	119	SER
1	C	223	ASN
1	D	68	ASP
1	D	223	ASN
1	E	119	SER
1	E	223	ASN
1	F	68	ASP
1	F	83	ARG
1	F	130	LYS
1	F	209	SER
1	F	223	ASN

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

Mol	Chain	Res	Type
1	E	54	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 39 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	220/255 (86%)	1.54	63 (28%)  	25, 31, 42, 54	0
1	B	217/255 (85%)	1.65	69 (31%)  	24, 31, 42, 54	0
1	C	218/255 (85%)	4.52	194 (88%)  	24, 31, 40, 63	0
1	D	216/255 (84%)	4.90	195 (90%)  	25, 31, 41, 54	0
1	E	219/255 (85%)	1.69	72 (32%)  	24, 31, 42, 55	0
1	F	220/255 (86%)	1.80	80 (36%)  	23, 30, 40, 59	0
All	All	1310/1530 (85%)	2.67	673 (51%)  	23, 31, 41, 63	0

All (673) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	125	ILE	18.0
1	C	108	VAL	15.1
1	C	51	THR	14.7
1	D	209	SER	13.4
1	D	21	GLY	12.9
1	C	152	SER	12.8
1	D	62	LEU	11.9
1	C	72	ASP	11.5
1	D	157	ALA	11.5
1	D	59	GLY	11.2
1	C	25	LEU	10.7
1	D	102	THR	10.3
1	C	143	ARG	10.2
1	C	135	LEU	10.2
1	D	88	TYR	10.0
1	D	111	ASP	10.0
1	D	213	ILE	10.0
1	C	165	THR	9.6
1	C	112	VAL	9.5

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Mol	Chain	Res	Type	RSRZ
1	D	200	VAL	9.5
1	C	49	ARG	9.2
1	C	154	TYR	9.1
1	C	153	TRP	9.1
1	C	53	GLU	9.0
1	D	60	GLU	8.9
1	D	26	GLY	8.9
1	D	115	TYR	8.9
1	D	215	ALA	8.9
1	D	216	ILE	8.9
1	D	191	ASN	8.8
1	C	188	TYR	8.8
1	C	178	PHE	8.6
1	D	92	LEU	8.6
1	D	181	VAL	8.4
1	C	228	ILE	8.4
1	D	64	ALA	8.2
1	C	156	TRP	8.2
1	D	45	HIS	8.2
1	D	135	LEU	8.1
1	D	134	ALA	8.1
1	D	61	PRO	8.0
1	D	52	LEU	8.0
1	D	49	ARG	8.0
1	D	144	LYS	7.9
1	C	107	ILE	7.9
1	D	40	VAL	7.9
1	D	77	LEU	7.8
1	C	157	ALA	7.8
1	C	61	PRO	7.8
1	C	54	GLN	7.7
1	D	105	TYR	7.7
1	E	61	PRO	7.7
1	D	133	ASN	7.7
1	C	183	VAL	7.6
1	D	95	GLY	7.6
1	C	115	TYR	7.5
1	D	192	SER	7.5
1	C	203	TRP	7.5
1	C	62	LEU	7.5
1	C	106	HIS	7.5
1	A	152	SER	7.4

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Mol	Chain	Res	Type	RSRZ
1	D	110	VAL	7.3
1	C	162	PHE	7.3
1	D	136	VAL	7.3
1	D	182	GLY	7.3
1	D	54	GLN	7.2
1	D	118	PRO	7.2
1	C	120	LEU	7.2
1	C	213	ILE	7.2
1	C	224	THR	7.1
1	D	104	LEU	7.0
1	D	56	LYS	7.0
1	D	55	ARG	7.0
1	D	125	ILE	7.0
1	D	44	ASP	7.0
1	D	63	GLY	7.0
1	D	126	VAL	6.9
1	D	117	ASP	6.9
1	D	206	LEU	6.8
1	C	163	LYS	6.8
1	D	185	LYS	6.8
1	D	87	GLU	6.8
1	D	101	ASN	6.7
1	D	141	PRO	6.7
1	C	201	TYR	6.7
1	C	129	LEU	6.7
1	C	117	ASP	6.6
1	D	129	LEU	6.6
1	C	179	ASN	6.6
1	D	197	LEU	6.6
1	C	57	ARG	6.6
1	C	99	THR	6.6
1	D	76	ARG	6.6
1	C	52	LEU	6.6
1	C	94	PRO	6.5
1	C	161	ARG	6.4
1	D	46	ILE	6.4
1	D	228	ILE	6.4
1	C	134	ALA	6.4
1	D	13	HIS	6.4
1	D	230	LEU	6.3
1	C	119	SER	6.3
1	C	185	LYS	6.3

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Mol	Chain	Res	Type	RSRZ
1	E	143	ARG	6.3
1	D	93	ILE	6.2
1	D	119	SER	6.2
1	D	6	GLU	6.2
1	C	181	VAL	6.2
1	D	122	VAL	6.2
1	C	180	SER	6.1
1	C	59	GLY	6.1
1	D	57	ARG	6.1
1	C	65	ILE	6.1
1	D	223	ASN	6.1
1	D	108	VAL	6.0
1	D	99	THR	6.0
1	D	202	SER	6.0
1	D	100	ASN	6.0
1	C	136	VAL	6.0
1	C	126	VAL	6.0
1	C	166	PHE	6.0
1	D	155	LEU	6.0
1	C	222	LYS	6.0
1	C	122	VAL	6.0
1	D	131	GLU	5.9
1	E	151	LEU	5.9
1	D	205	THR	5.9
1	C	69	LYS	5.8
1	C	184	LYS	5.8
1	D	156	TRP	5.8
1	D	154	TYR	5.7
1	D	68	ASP	5.7
1	C	104	LEU	5.6
1	F	157	ALA	5.6
1	D	137	ILE	5.6
1	C	124	GLU	5.6
1	D	161	ARG	5.6
1	D	163	LYS	5.6
1	D	32	PHE	5.6
1	C	24	PRO	5.5
1	C	93	ILE	5.5
1	C	145	LYS	5.5
1	C	196	GLU	5.5
1	C	76	ARG	5.4
1	D	97	GLU	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	22	HIS	5.4
1	F	150	HIS	5.4
1	D	153	TRP	5.3
1	D	178	PHE	5.3
1	C	46	ILE	5.3
1	C	103	ASP	5.3
1	D	14	VAL	5.3
1	D	221	ARG	5.3
1	D	86	GLU	5.3
1	C	5	THR	5.2
1	D	142	ASP	5.2
1	C	186	TYR	5.2
1	D	167	ASP	5.1
1	C	131	GLU	5.1
1	D	7	TRP	5.1
1	D	37	VAL	5.1
1	D	9	LEU	5.1
1	D	17	ASN	5.1
1	C	37	VAL	5.0
1	D	23	LEU	5.0
1	C	77	LEU	5.0
1	D	183	VAL	5.0
1	C	85	TRP	5.0
1	D	28	VAL	4.9
1	D	189	VAL	4.9
1	C	220	ILE	4.9
1	C	212	ASN	4.9
1	C	96	VAL	4.9
1	D	219	ALA	4.9
1	C	133	ASN	4.9
1	D	120	LEU	4.9
1	C	142	ASP	4.9
1	F	108	VAL	4.8
1	D	124	GLU	4.8
1	D	158	ASN	4.8
1	C	113	LYS	4.8
1	D	15	HIS	4.8
1	D	160	GLU	4.8
1	C	84	ALA	4.8
1	C	227	ALA	4.8
1	C	67	GLU	4.8
1	C	33	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	116	VAL	4.7
1	C	7	TRP	4.7
1	C	128	LYS	4.7
1	C	8	LEU	4.7
1	D	58	ASN	4.7
1	D	224	THR	4.7
1	D	24	PRO	4.6
1	C	100	ASN	4.6
1	C	167	ASP	4.6
1	C	30	ASP	4.6
1	E	162	PHE	4.6
1	C	58	ASN	4.6
1	D	98	ILE	4.5
1	D	66	THR	4.5
1	C	87	GLU	4.5
1	D	180	SER	4.5
1	C	169	TRP	4.5
1	D	132	GLN	4.5
1	C	123	GLU	4.5
1	D	130	LYS	4.5
1	C	158	ASN	4.4
1	C	10	CYS	4.4
1	B	62	LEU	4.4
1	C	121	PRO	4.4
1	D	53	GLU	4.4
1	C	110	VAL	4.3
1	D	16	THR	4.3
1	C	70	PHE	4.3
1	D	78	TRP	4.3
1	D	225	ASP	4.3
1	C	171	ILE	4.3
1	D	198	TRP	4.3
1	E	150	HIS	4.3
1	B	197	LEU	4.3
1	C	168	ALA	4.3
1	F	102	THR	4.3
1	C	17	ASN	4.3
1	C	127	GLU	4.3
1	C	140	HIS	4.3
1	D	12	PHE	4.3
1	D	187	ARG	4.3
1	C	92	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	116	VAL	4.3
1	A	155	LEU	4.2
1	C	68	ASP	4.2
1	F	62	LEU	4.2
1	D	51	THR	4.2
1	E	42	ILE	4.2
1	D	113	LYS	4.2
1	C	47	VAL	4.2
1	B	42	ILE	4.2
1	C	111	ASP	4.2
1	C	60	GLU	4.2
1	A	151	LEU	4.2
1	D	73	TYR	4.2
1	D	107	ILE	4.2
1	E	98	ILE	4.2
1	D	196	GLU	4.2
1	D	112	VAL	4.1
1	F	12	PHE	4.1
1	D	208	LYS	4.1
1	F	58	ASN	4.1
1	D	186	TYR	4.1
1	D	31	LEU	4.1
1	C	43	THR	4.1
1	C	50	ARG	4.1
1	C	216	ILE	4.1
1	D	94	PRO	4.1
1	C	95	GLY	4.1
1	D	11	ASP	4.1
1	C	9	LEU	4.0
1	D	25	LEU	4.0
1	C	105	TYR	4.0
1	C	21	GLY	4.0
1	D	109	ALA	4.0
1	D	139	ALA	4.0
1	D	176	ASP	4.0
1	F	40	VAL	4.0
1	C	66	THR	4.0
1	E	152	SER	4.0
1	A	181	VAL	3.9
1	C	114	GLU	3.9
1	D	121	PRO	3.9
1	F	43	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	77	LEU	3.9
1	D	81	GLN	3.9
1	B	157	ALA	3.9
1	D	41	SER	3.9
1	B	66	THR	3.8
1	F	181	VAL	3.8
1	D	96	VAL	3.8
1	C	29	VAL	3.8
1	E	68	ASP	3.8
1	B	180	SER	3.8
1	C	20	ASP	3.8
1	E	189	VAL	3.7
1	C	88	TYR	3.7
1	A	108	VAL	3.7
1	D	114	GLU	3.7
1	C	164	ASP	3.7
1	E	40	VAL	3.7
1	B	136	VAL	3.7
1	D	204	LYS	3.7
1	C	211	LYS	3.7
1	B	22	HIS	3.7
1	C	42	ILE	3.7
1	D	43	THR	3.6
1	C	74	LEU	3.6
1	D	70	PHE	3.6
1	F	41	SER	3.6
1	B	138	ALA	3.6
1	C	63	GLY	3.6
1	C	209	SER	3.6
1	D	29	VAL	3.6
1	D	201	TYR	3.6
1	D	20	ASP	3.6
1	C	190	ALA	3.6
1	F	110	VAL	3.6
1	D	195	HIS	3.6
1	B	125	ILE	3.6
1	D	226	VAL	3.5
1	C	208	LYS	3.5
1	C	141	PRO	3.5
1	D	74	LEU	3.5
1	F	189	VAL	3.5
1	B	43	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	230	LEU	3.5
1	A	137	ILE	3.5
1	F	47	VAL	3.5
1	A	53	GLU	3.5
1	D	128	LYS	3.5
1	D	106	HIS	3.4
1	F	190	ALA	3.4
1	D	174	ARG	3.4
1	E	102	THR	3.4
1	D	217	LYS	3.4
1	C	198	TRP	3.4
1	C	200	VAL	3.4
1	F	96	VAL	3.4
1	D	162	PHE	3.4
1	E	65	ILE	3.4
1	C	182	GLY	3.4
1	B	52	LEU	3.4
1	F	14	VAL	3.3
1	C	229	TYR	3.3
1	A	139	ALA	3.3
1	D	48	ASP	3.3
1	D	65	ILE	3.3
1	E	77	LEU	3.3
1	C	40	VAL	3.3
1	D	39	VAL	3.3
1	A	41	SER	3.3
1	D	138	ALA	3.3
1	C	199	HIS	3.3
1	C	83	ARG	3.3
1	A	192	SER	3.3
1	C	102	THR	3.3
1	F	203	TRP	3.3
1	E	136	VAL	3.3
1	C	19	SER	3.3
1	B	17	ASN	3.3
1	D	42	ILE	3.3
1	C	13	HIS	3.3
1	D	35	HIS	3.3
1	B	54	GLN	3.3
1	D	169	TRP	3.2
1	D	214	GLU	3.2
1	C	191	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	55	ARG	3.2
1	A	98	ILE	3.2
1	C	137	ILE	3.2
1	D	188	TYR	3.2
1	E	139	ALA	3.2
1	F	123	GLU	3.2
1	D	194	PHE	3.2
1	F	230	LEU	3.2
1	D	227	ALA	3.2
1	C	214	GLU	3.2
1	F	46	ILE	3.2
1	D	199	HIS	3.1
1	A	179	ASN	3.1
1	E	142	ASP	3.1
1	C	26	GLY	3.1
1	C	38	ASP	3.1
1	E	196	GLU	3.1
1	C	206	LEU	3.1
1	B	115	TYR	3.1
1	D	165	THR	3.1
1	F	39	VAL	3.1
1	F	29	VAL	3.1
1	C	155	LEU	3.1
1	A	228	ILE	3.1
1	B	41	SER	3.1
1	C	210	GLU	3.1
1	A	110	VAL	3.0
1	B	60	GLU	3.0
1	D	143	ARG	3.0
1	F	152	SER	3.0
1	F	173	ASN	3.0
1	D	71	GLN	3.0
1	D	5	THR	3.0
1	D	34	LYS	3.0
1	E	160	GLU	3.0
1	D	80	GLU	3.0
1	A	10	CYS	3.0
1	E	41	SER	3.0
1	D	193	ASP	3.0
1	E	107	ILE	3.0
1	C	173	ASN	3.0
1	A	183	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	119	SER	2.9
1	F	119	SER	2.9
1	F	66	THR	2.9
1	C	28	VAL	2.9
1	B	162	PHE	2.9
1	C	78	TRP	2.9
1	E	126	VAL	2.9
1	B	124	GLU	2.9
1	A	102	THR	2.9
1	C	138	ALA	2.9
1	B	143	ARG	2.9
1	B	161	ARG	2.9
1	A	182	GLY	2.9
1	C	48	ASP	2.9
1	A	5	THR	2.9
1	B	55	ARG	2.9
1	C	35	HIS	2.9
1	A	156	TRP	2.9
1	B	183	VAL	2.9
1	D	212	ASN	2.9
1	B	21	GLY	2.9
1	E	27	GLU	2.8
1	B	14	VAL	2.8
1	D	8	LEU	2.8
1	D	47	VAL	2.8
1	C	32	PHE	2.8
1	F	227	ALA	2.8
1	C	91	ILE	2.8
1	D	232	ARG	2.8
1	C	232	ARG	2.8
1	F	42	ILE	2.8
1	E	23	LEU	2.8
1	F	206	LEU	2.8
1	A	126	VAL	2.8
1	E	51	THR	2.8
1	E	157	ALA	2.8
1	A	107	ILE	2.8
1	E	228	ILE	2.8
1	D	229	TYR	2.8
1	A	14	VAL	2.8
1	E	226	VAL	2.8
1	C	144	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	174	ARG	2.8
1	B	24	PRO	2.8
1	E	227	ALA	2.8
1	C	41	SER	2.8
1	D	30	ASP	2.8
1	F	13	HIS	2.8
1	E	14	VAL	2.8
1	E	105	TYR	2.8
1	D	168	ALA	2.8
1	B	72	ASP	2.8
1	C	217	LYS	2.8
1	C	98	ILE	2.7
1	A	47	VAL	2.7
1	B	96	VAL	2.7
1	E	28	VAL	2.7
1	B	198	TRP	2.7
1	D	171	ILE	2.7
1	C	23	LEU	2.7
1	A	24	PRO	2.7
1	D	72	ASP	2.7
1	D	166	PHE	2.7
1	D	175	ASP	2.7
1	E	110	VAL	2.7
1	F	126	VAL	2.7
1	A	84	ALA	2.7
1	F	228	ILE	2.7
1	D	218	GLU	2.7
1	D	84	ALA	2.7
1	C	75	LYS	2.7
1	F	171	ILE	2.7
1	C	45	HIS	2.7
1	D	140	HIS	2.7
1	F	94	PRO	2.7
1	A	166	PHE	2.7
1	C	221	ARG	2.7
1	E	60	GLU	2.7
1	B	228	ILE	2.7
1	E	100	ASN	2.7
1	F	137	ILE	2.7
1	F	104	LEU	2.7
1	A	13	HIS	2.7
1	C	39	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	172	ALA	2.7
1	A	95	GLY	2.7
1	A	92	LEU	2.7
1	D	50	ARG	2.7
1	F	232	ARG	2.7
1	B	139	ALA	2.7
1	E	108	VAL	2.7
1	C	73	TYR	2.7
1	C	36	GLY	2.6
1	C	82	LYS	2.6
1	D	222	LYS	2.6
1	A	189	VAL	2.6
1	B	171	ILE	2.6
1	F	107	ILE	2.6
1	B	51	THR	2.6
1	D	85	TRP	2.6
1	C	34	LYS	2.6
1	C	205	THR	2.6
1	F	59	GLY	2.6
1	F	95	GLY	2.6
1	B	189	VAL	2.6
1	F	28	VAL	2.6
1	F	129	LEU	2.6
1	E	5	THR	2.6
1	C	12	PHE	2.6
1	F	139	ALA	2.6
1	E	180	SER	2.6
1	F	100	ASN	2.6
1	E	215	ALA	2.6
1	F	112	VAL	2.6
1	A	186	TYR	2.6
1	E	46	ILE	2.6
1	C	109	ALA	2.6
1	F	35	HIS	2.6
1	A	207	VAL	2.5
1	F	118	PRO	2.5
1	B	104	LEU	2.5
1	A	12	PHE	2.5
1	F	57	ARG	2.5
1	A	109	ALA	2.5
1	B	27	GLU	2.5
1	A	122	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	108	VAL	2.5
1	A	42	ILE	2.5
1	A	168	ALA	2.5
1	C	192	SER	2.5
1	B	29	VAL	2.5
1	C	189	VAL	2.5
1	C	197	LEU	2.5
1	F	92	LEU	2.5
1	B	105	TYR	2.5
1	F	213	ILE	2.5
1	F	229	TYR	2.5
1	A	191	ASN	2.5
1	D	173	ASN	2.5
1	F	136	VAL	2.5
1	F	68	ASP	2.5
1	E	16	THR	2.5
1	E	188	TYR	2.5
1	B	191	ASN	2.5
1	A	96	VAL	2.5
1	E	153	TRP	2.5
1	F	198	TRP	2.5
1	C	130	LYS	2.5
1	C	22	HIS	2.5
1	B	26	GLY	2.5
1	E	109	ALA	2.5
1	B	25	LEU	2.4
1	E	57	ARG	2.4
1	B	75	LYS	2.4
1	E	138	ALA	2.4
1	B	169	TRP	2.4
1	F	74	LEU	2.4
1	D	203	TRP	2.4
1	E	67	GLU	2.4
1	F	142	ASP	2.4
1	E	25	LEU	2.4
1	B	6	GLU	2.4
1	A	68	ASP	2.4
1	C	176	ASP	2.4
1	D	19	SER	2.4
1	E	10	CYS	2.4
1	E	125	ILE	2.4
1	B	222	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	109	ALA	2.4
1	F	138	ALA	2.4
1	F	115	TYR	2.4
1	A	23	LEU	2.4
1	E	92	LEU	2.4
1	E	203	TRP	2.4
1	C	6	GLU	2.4
1	E	12	PHE	2.4
1	D	211	LYS	2.4
1	F	226	VAL	2.4
1	B	99	THR	2.4
1	F	205	THR	2.4
1	A	171	ILE	2.4
1	A	172	ALA	2.4
1	F	153	TRP	2.3
1	C	86	GLU	2.3
1	D	75	LYS	2.3
1	A	63	GLY	2.3
1	A	205	THR	2.3
1	E	179	ASN	2.3
1	E	94	PRO	2.3
1	F	134	ALA	2.3
1	F	140	HIS	2.3
1	A	94	PRO	2.3
1	B	68	ASP	2.3
1	E	201	TYR	2.3
1	A	66	THR	2.3
1	E	13	HIS	2.3
1	F	99	THR	2.3
1	D	210	GLU	2.3
1	A	61	PRO	2.3
1	B	98	ILE	2.3
1	C	118	PRO	2.3
1	A	177	LEU	2.3
1	E	206	LEU	2.3
1	B	28	VAL	2.3
1	C	207	VAL	2.3
1	B	57	ARG	2.3
1	F	56	LYS	2.2
1	E	156	TRP	2.2
1	F	93	ILE	2.2
1	C	194	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	50	ARG	2.2
1	E	99	THR	2.2
1	B	155	LEU	2.2
1	E	129	LEU	2.2
1	B	94	PRO	2.2
1	A	190	ALA	2.2
1	E	213	ILE	2.2
1	F	106	HIS	2.2
1	F	180	SER	2.2
1	F	9	LEU	2.2
1	C	226	VAL	2.2
1	F	200	VAL	2.2
1	B	227	ALA	2.2
1	E	172	ALA	2.2
1	F	117	ASP	2.2
1	B	140	HIS	2.2
1	B	173	ASN	2.2
1	B	201	TYR	2.2
1	B	65	ILE	2.2
1	B	133	ASN	2.2
1	F	192	SER	2.1
1	E	137	ILE	2.1
1	A	185	LYS	2.1
1	A	194	PHE	2.1
1	B	23	LEU	2.1
1	B	175	ASP	2.1
1	F	151	LEU	2.1
1	C	139	ALA	2.1
1	C	204	LYS	2.1
1	C	219	ALA	2.1
1	A	76	ARG	2.1
1	D	220	ILE	2.1
1	E	190	ALA	2.1
1	F	60	GLU	2.1
1	C	71	GLN	2.1
1	E	118	PRO	2.1
1	E	29	VAL	2.1
1	E	207	VAL	2.1
1	B	12	PHE	2.1
1	D	33	GLY	2.1
1	D	36	GLY	2.1
1	A	127	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	225	ASP	2.1
1	C	215	ALA	2.1
1	C	81	GLN	2.1
1	A	220	ILE	2.1
1	F	188	TYR	2.1
1	F	121	PRO	2.1
1	F	98	ILE	2.1
1	E	205	THR	2.1
1	B	103	ASP	2.1
1	B	116	VAL	2.0
1	A	180	SER	2.0
1	A	140	HIS	2.0
1	B	203	TRP	2.0
1	A	105	TYR	2.0
1	A	229	TYR	2.0
1	B	186	TYR	2.0
1	B	192	SER	2.0
1	C	27	GLU	2.0
1	E	66	THR	2.0
1	B	59	GLY	2.0
1	A	142	ASP	2.0
1	C	132	GLN	2.0
1	E	124	GLU	2.0
1	B	77	LEU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	C	405	1/1	0.93	0.29	0.01	42,42,42,42	0
2	ZN	C	605	1/1	0.95	0.37	-0.13	54,54,54,54	0
3	CL	D	1008	1/1	0.75	0.31	-1.15	40,40,40,40	0
3	CL	C	1006	1/1	0.68	0.17	-1.81	44,44,44,44	0
3	CL	C	1005	1/1	0.89	0.08	-1.88	31,31,31,31	0
3	CL	E	1010	1/1	0.67	0.17	-1.96	32,32,32,32	0
2	ZN	D	405	1/1	0.97	0.22	-2.48	40,40,40,40	0
3	CL	E	1009	1/1	0.92	0.10	-2.51	25,25,25,25	0
3	CL	D	1007	1/1	0.79	0.16	-2.63	31,31,31,31	0
2	ZN	E	605	1/1	0.88	0.08	-2.89	47,47,47,47	0
3	CL	F	1012	1/1	0.93	0.19	-2.91	33,33,33,33	0
2	ZN	E	405	1/1	0.94	0.08	-3.48	37,37,37,37	0
3	CL	B	1004	1/1	0.76	0.16	-3.90	41,41,41,41	0
3	CL	B	1003	1/1	0.94	0.09	-3.92	27,27,27,27	0
2	ZN	B	405	1/1	0.86	0.07	-4.15	39,39,39,39	0
3	CL	F	1011	1/1	0.91	0.13	-4.27	24,24,24,24	0
2	ZN	A	405	1/1	0.90	0.09	-4.57	32,32,32,32	0
3	CL	A	1001	1/1	0.79	0.10	-4.74	25,25,25,25	0
3	CL	A	1002	1/1	0.87	0.10	-5.31	33,33,33,33	0
2	ZN	F	405	1/1	0.93	0.06	-5.47	34,34,34,34	0
2	ZN	D	605	1/1	0.89	0.22	-	53,53,53,53	0
2	ZN	D	505	1/1	0.95	0.24	-	35,35,35,35	0
2	ZN	A	605	1/1	0.93	0.07	-	46,46,46,46	0
2	ZN	C	705	1/1	0.53	0.38	-	73,73,73,73	0
2	ZN	E	705	1/1	0.92	0.15	-	65,65,65,65	0
2	ZN	E	505	1/1	0.87	0.07	-	30,30,30,30	0
2	ZN	B	605	1/1	0.84	0.14	-	62,62,62,62	0
3	CL	E	1015	1/1	0.88	0.09	-	19,19,19,19	0
2	ZN	F	505	1/1	0.87	0.07	-	31,31,31,31	0
2	ZN	A	505	1/1	0.96	0.06	-	29,29,29,29	0
2	ZN	B	505	1/1	0.95	0.06	-	30,30,30,30	0
2	ZN	D	705	1/1	0.83	0.16	-	73,73,73,73	0
2	ZN	A	705	1/1	0.60	0.17	-	67,67,67,67	0
2	ZN	F	705	1/1	0.91	0.15	-	61,61,61,61	0
3	CL	A	1013	1/1	0.95	0.07	-	24,24,24,24	0
2	ZN	F	605	1/1	0.89	0.09	-	41,41,41,41	0
3	CL	C	1014	1/1	0.94	0.13	-	24,24,24,24	0
2	ZN	C	505	1/1	0.96	0.19	-	33,33,33,33	0
2	ZN	B	705	1/1	0.67	0.27	-	79,79,79,79	0

6.5 Other polymers ⓘ

There are no such residues in this entry.