



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:47 PM UTC

PDB ID : 5OUQ / pdb_00005ouq
Title : Structure of TgPLP1 MACPF domain
Authors : Ni, T.; Gilbert, R.J.C.
Deposited on : 2017-08-24
Resolution : 5.11 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

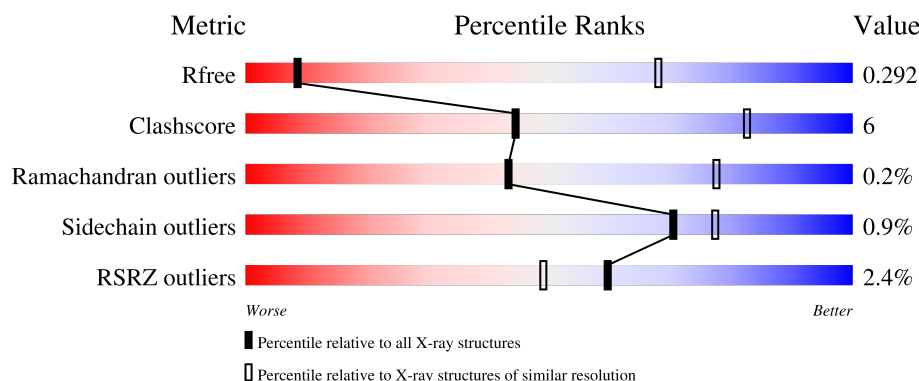
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.11 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	1002 (6.22-4.00)
Clashscore	190562	1057 (6.22-4.00)
Ramachandran outliers	187476	1026 (6.32-3.92)
Sidechain outliers	187428	1003 (6.32-3.92)
RSRZ outliers	180081	1019 (6.22-3.98)

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	356	3% 65% 12% 22%
1	C	356	3% 65% 12% 22%
1	D	356	2% 65% 12% 22%
1	E	356	3% 65% 13% 22%
1	F	356	0% 65% 13% 22%

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Mol	Chain	Length	Quality of chain
1	G	356	 A horizontal bar chart showing the quality of chain G. The bar is divided into three segments: a green segment representing 64%, a yellow segment representing 13%, and a grey segment representing 22%. The percentages are labeled below the corresponding segments.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12948 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 Perforin-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2144	1360	367	406	11			
1	C	276	Total	C	N	O	S	0	0	0
			2144	1360	367	406	11			
1	D	276	Total	C	N	O	S	0	0	0
			2144	1360	367	406	11			
1	E	276	Total	C	N	O	S	0	0	0
			2144	1360	367	406	11			
1	F	276	Total	C	N	O	S	0	0	0
			2144	1360	367	406	11			
1	G	276	Total	C	N	O	S	0	0	0
			2144	1360	367	406	11			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	459	GLU	-	expression tag	UNP G3G7T1
A	460	THR	-	expression tag	UNP G3G7T1
A	461	GLY	-	expression tag	UNP G3G7T1
A	720	GLN	ASN	conflict	UNP G3G7T1
A	744	GLN	ASN	conflict	UNP G3G7T1
A	806	GLY	-	expression tag	UNP G3G7T1
A	807	THR	-	expression tag	UNP G3G7T1
A	808	LYS	-	expression tag	UNP G3G7T1
A	809	HIS	-	expression tag	UNP G3G7T1
A	810	HIS	-	expression tag	UNP G3G7T1
A	811	HIS	-	expression tag	UNP G3G7T1
A	812	HIS	-	expression tag	UNP G3G7T1
A	813	HIS	-	expression tag	UNP G3G7T1
A	814	HIS	-	expression tag	UNP G3G7T1
C	459	GLU	-	expression tag	UNP G3G7T1
C	460	THR	-	expression tag	UNP G3G7T1
C	461	GLY	-	expression tag	UNP G3G7T1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	720	GLN	ASN	conflict	UNP G3G7T1
C	744	GLN	ASN	conflict	UNP G3G7T1
C	806	GLY	-	expression tag	UNP G3G7T1
C	807	THR	-	expression tag	UNP G3G7T1
C	808	LYS	-	expression tag	UNP G3G7T1
C	809	HIS	-	expression tag	UNP G3G7T1
C	810	HIS	-	expression tag	UNP G3G7T1
C	811	HIS	-	expression tag	UNP G3G7T1
C	812	HIS	-	expression tag	UNP G3G7T1
C	813	HIS	-	expression tag	UNP G3G7T1
C	814	HIS	-	expression tag	UNP G3G7T1
D	459	GLU	-	expression tag	UNP G3G7T1
D	460	THR	-	expression tag	UNP G3G7T1
D	461	GLY	-	expression tag	UNP G3G7T1
D	720	GLN	ASN	conflict	UNP G3G7T1
D	744	GLN	ASN	conflict	UNP G3G7T1
D	806	GLY	-	expression tag	UNP G3G7T1
D	807	THR	-	expression tag	UNP G3G7T1
D	808	LYS	-	expression tag	UNP G3G7T1
D	809	HIS	-	expression tag	UNP G3G7T1
D	810	HIS	-	expression tag	UNP G3G7T1
D	811	HIS	-	expression tag	UNP G3G7T1
D	812	HIS	-	expression tag	UNP G3G7T1
D	813	HIS	-	expression tag	UNP G3G7T1
D	814	HIS	-	expression tag	UNP G3G7T1
E	459	GLU	-	expression tag	UNP G3G7T1
E	460	THR	-	expression tag	UNP G3G7T1
E	461	GLY	-	expression tag	UNP G3G7T1
E	720	GLN	ASN	conflict	UNP G3G7T1
E	744	GLN	ASN	conflict	UNP G3G7T1
E	806	GLY	-	expression tag	UNP G3G7T1
E	807	THR	-	expression tag	UNP G3G7T1
E	808	LYS	-	expression tag	UNP G3G7T1
E	809	HIS	-	expression tag	UNP G3G7T1
E	810	HIS	-	expression tag	UNP G3G7T1
E	811	HIS	-	expression tag	UNP G3G7T1
E	812	HIS	-	expression tag	UNP G3G7T1
E	813	HIS	-	expression tag	UNP G3G7T1
E	814	HIS	-	expression tag	UNP G3G7T1
F	459	GLU	-	expression tag	UNP G3G7T1
F	460	THR	-	expression tag	UNP G3G7T1
F	461	GLY	-	expression tag	UNP G3G7T1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	720	GLN	ASN	conflict	UNP G3G7T1
F	744	GLN	ASN	conflict	UNP G3G7T1
F	806	GLY	-	expression tag	UNP G3G7T1
F	807	THR	-	expression tag	UNP G3G7T1
F	808	LYS	-	expression tag	UNP G3G7T1
F	809	HIS	-	expression tag	UNP G3G7T1
F	810	HIS	-	expression tag	UNP G3G7T1
F	811	HIS	-	expression tag	UNP G3G7T1
F	812	HIS	-	expression tag	UNP G3G7T1
F	813	HIS	-	expression tag	UNP G3G7T1
F	814	HIS	-	expression tag	UNP G3G7T1
G	459	GLU	-	expression tag	UNP G3G7T1
G	460	THR	-	expression tag	UNP G3G7T1
G	461	GLY	-	expression tag	UNP G3G7T1
G	720	GLN	ASN	conflict	UNP G3G7T1
G	744	GLN	ASN	conflict	UNP G3G7T1
G	806	GLY	-	expression tag	UNP G3G7T1
G	807	THR	-	expression tag	UNP G3G7T1
G	808	LYS	-	expression tag	UNP G3G7T1
G	809	HIS	-	expression tag	UNP G3G7T1
G	810	HIS	-	expression tag	UNP G3G7T1
G	811	HIS	-	expression tag	UNP G3G7T1
G	812	HIS	-	expression tag	UNP G3G7T1
G	813	HIS	-	expression tag	UNP G3G7T1
G	814	HIS	-	expression tag	UNP G3G7T1

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

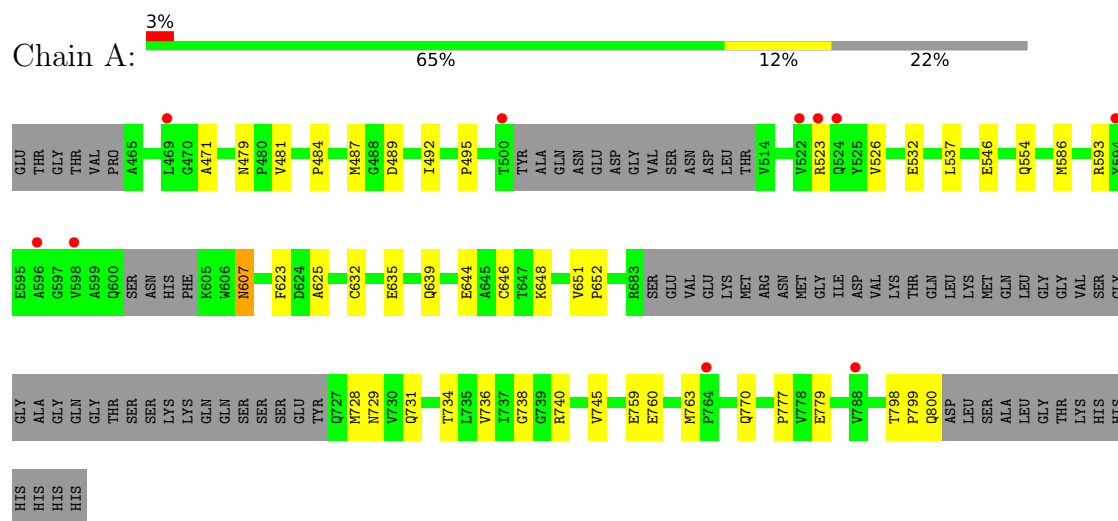


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	14	0
			14	8	1	5		
2	C	1	Total	C	N	O	14	0
			14	8	1	5		
2	D	1	Total	C	N	O	14	0
			14	8	1	5		
2	E	1	Total	C	N	O	14	0
			14	8	1	5		
2	F	1	Total	C	N	O	14	0
			14	8	1	5		
2	G	1	Total	C	N	O	14	0
			14	8	1	5		

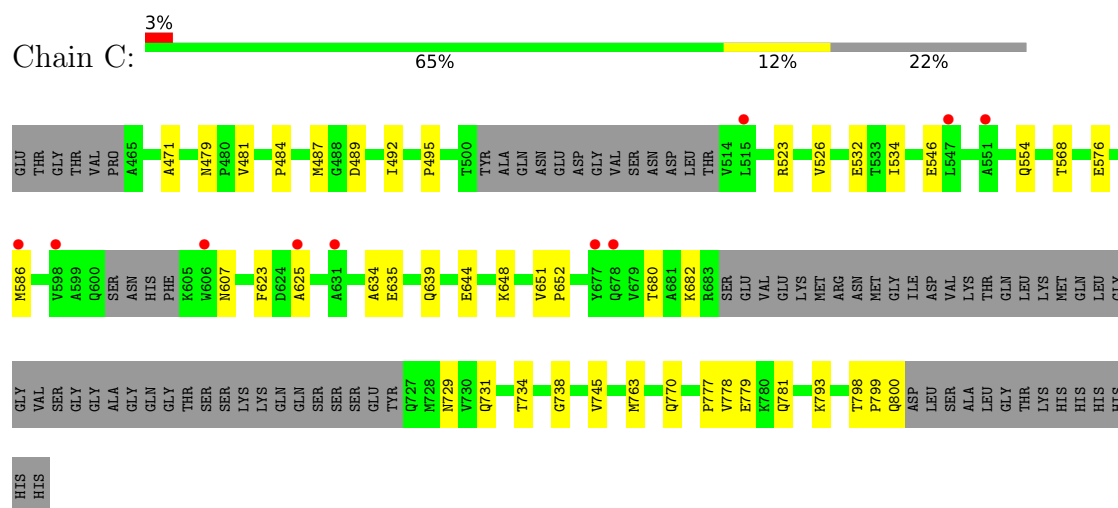
3 Residue-property plots

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: Perforin-like protein 1



• Molecule 1: Perforin-like protein 1

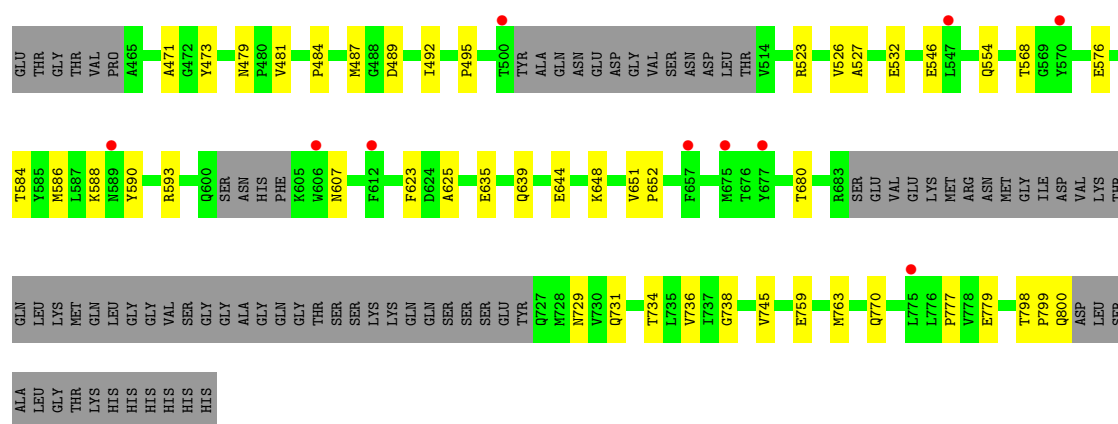


• Molecule 1: Perforin-like protein 1

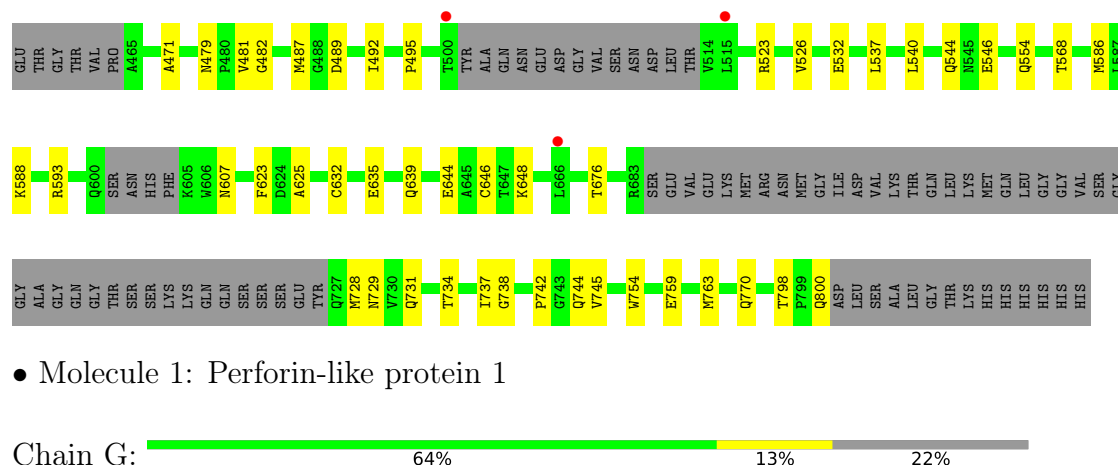




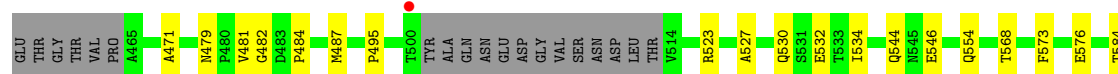
Chain E:

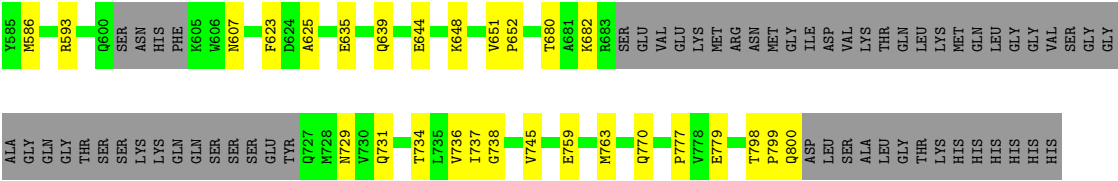


Chain F: %



Chain G: 64% 13% 22%





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	159.49Å 185.74Å 104.19Å 90.00° 121.48° 90.00°	Depositor
Resolution (Å)	56.35 – 5.11 56.35 – 5.11	Depositor EDS
% Data completeness (in resolution range)	99.5 (56.35-5.11) 99.4 (56.35-5.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 5.12Å)	Xtriage
Refinement program	PHENIX (dev_2283: ???)	Depositor
R, R_{free}	0.287 , 0.298 0.286 , 0.292	Depositor DCC
R_{free} test set	499 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	241.3	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 459.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	12948	wwPDB-VP
Average B, all atoms (Å ²)	330.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.16	0/2194	0.41	0/2979
1	C	0.17	0/2194	0.41	0/2979
1	D	0.17	0/2194	0.40	1/2979 (0.0%)
1	E	0.18	0/2194	0.41	1/2979 (0.0%)
1	F	0.16	0/2194	0.40	0/2979
1	G	0.15	0/2194	0.38	0/2979
All	All	0.16	0/13164	0.40	2/17874 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	527	ALA	CB-CA-C	-5.28	110.04	117.23
1	E	527	ALA	CB-CA-C	-5.19	110.17	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2144	0	2085	32	0
1	C	2144	0	2085	28	1
1	D	2144	0	2085	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2144	0	2085	28	1
1	F	2144	0	2085	32	0
1	G	2144	0	2085	31	0
2	A	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
2	G	14	0	13	0	0
All	All	12948	0	12588	153	1

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

All (153) 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:484:PRO:HB2	1:D:525:TYR:HA	1.71	0.72
1:E:798:THR:O	1:E:800:GLN:N	2.23	0.71
1:C:798:THR:O	1:C:800:GLN:N	2.25	0.70
1:E:729:ASN:OD1	1:E:731:GLN:NE2	2.24	0.69
1:C:734:THR:HG21	1:C:745:VAL:HG11	1.74	0.69
1:F:554:GLN:NE2	1:F:770:GLN:OE1	2.24	0.69
1:G:554:GLN:NE2	1:G:770:GLN:OE1	2.26	0.69
1:C:568:THR:HG21	1:D:523:ARG:NH2	2.06	0.69
1:C:729:ASN:OD1	1:C:731:GLN:NE2	2.26	0.68
1:E:554:GLN:NE2	1:E:770:GLN:OE1	2.27	0.68
1:G:729:ASN:OD1	1:G:731:GLN:NE2	2.30	0.65
1:G:798:THR:O	1:G:800:GLN:N	2.28	0.65
1:F:744:GLN:NE2	1:G:530:GLN:OE1	2.30	0.65
1:D:554:GLN:NE2	1:D:770:GLN:OE1	2.29	0.64
1:C:644:GLU:HB3	1:C:648:LYS:HE3	1.80	0.64
1:A:729:ASN:OD1	1:A:731:GLN:NE2	2.32	0.63
1:F:729:ASN:OD1	1:F:731:GLN:NE2	2.32	0.62
1:D:729:ASN:OD1	1:D:731:GLN:NE2	2.33	0.62
1:G:471:ALA:HA	1:G:495:PRO:HA	1.82	0.61
1:F:742:PRO:O	1:G:527:ALA:HB2	1.99	0.61
1:C:778:VAL:HA	1:C:781:GLN:HG3	1.83	0.61
1:E:738:GLY:HA2	1:E:763:MET:HE3	1.84	0.60
1:D:487:MET:HB3	1:D:763:MET:HE1	1.84	0.60
1:E:484:PRO:HA	1:F:526:VAL:HG23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:736:VAL:CG1	1:E:526:VAL:HG11	2.32	0.59
1:C:554:GLN:NE2	1:C:770:GLN:OE1	2.35	0.59
1:A:471:ALA:HA	1:A:495:PRO:HA	1.85	0.58
1:A:487:MET:HB3	1:A:763:MET:HE1	1.85	0.58
1:A:736:VAL:CG1	1:C:526:VAL:HG11	2.34	0.57
1:F:734:THR:HG21	1:F:745:VAL:HG11	1.85	0.57
1:F:728:MET:HG3	1:G:534:ILE:HG21	1.87	0.57
1:D:644:GLU:HB3	1:D:648:LYS:HE3	1.87	0.57
1:D:738:GLY:HA2	1:D:763:MET:HE3	1.88	0.55
1:F:471:ALA:HA	1:F:495:PRO:HA	1.88	0.55
1:G:738:GLY:HA2	1:G:763:MET:HE3	1.89	0.55
1:A:593:ARG:HD2	1:A:759:GLU:HG3	1.89	0.55
1:E:623:PHE:CE2	1:E:625:ALA:HB3	2.42	0.55
1:F:798:THR:O	1:F:800:GLN:N	2.36	0.55
1:A:546:GLU:HB3	1:A:586:MET:HE1	1.88	0.54
1:F:568:THR:HG21	1:G:523:ARG:NH2	2.22	0.54
1:F:738:GLY:HA2	1:F:763:MET:HE3	1.89	0.54
1:D:798:THR:O	1:D:800:GLN:N	2.37	0.54
1:A:484:PRO:HG3	1:C:523:ARG:NH2	2.23	0.54
1:F:635:GLU:O	1:F:639:GLN:HG2	2.08	0.54
1:G:734:THR:HG21	1:G:745:VAL:HG11	1.90	0.54
1:A:734:THR:HG21	1:A:745:VAL:HG11	1.90	0.53
1:A:798:THR:O	1:A:800:GLN:N	2.34	0.53
1:A:644:GLU:HB3	1:A:648:LYS:HE3	1.90	0.53
1:A:738:GLY:HA2	1:A:763:MET:HE3	1.91	0.53
1:F:487:MET:HB3	1:F:763:MET:HE1	1.90	0.53
1:D:635:GLU:N	1:D:635:GLU:OE1	2.40	0.53
1:E:644:GLU:HB3	1:E:648:LYS:HE3	1.91	0.52
1:D:734:THR:HG21	1:D:745:VAL:HG11	1.91	0.52
1:A:736:VAL:HG12	1:C:526:VAL:HG11	1.92	0.51
1:E:635:GLU:H	1:E:635:GLU:CD	2.19	0.51
1:A:623:PHE:CE2	1:A:625:ALA:HB3	2.46	0.51
1:E:736:VAL:CG1	1:F:526:VAL:HG11	2.41	0.51
1:G:635:GLU:N	1:G:635:GLU:OE1	2.41	0.51
1:C:634:ALA:HB3	1:C:793:LYS:HE3	1.93	0.51
1:C:738:GLY:HA2	1:C:763:MET:HE3	1.92	0.51
1:G:479:ASN:OD1	1:G:481:VAL:HG22	2.11	0.51
1:C:777:PRO:HB2	1:C:779:GLU:CD	2.36	0.51
1:C:484:PRO:O	1:D:526:VAL:HG23	2.11	0.51
1:G:546:GLU:HB3	1:G:586:MET:HE1	1.94	0.50
1:A:728:MET:HG2	1:C:534:ILE:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:479:ASN:OD1	1:F:481:VAL:HG22	2.12	0.50
1:G:635:GLU:O	1:G:639:GLN:HG2	2.12	0.50
1:C:479:ASN:OD1	1:C:481:VAL:HG22	2.12	0.50
1:A:489:ASP:HB3	1:A:492:ILE:HG12	1.94	0.49
1:A:479:ASN:OD1	1:A:481:VAL:HG22	2.12	0.49
1:D:623:PHE:CE2	1:D:625:ALA:HB3	2.47	0.49
1:E:471:ALA:HA	1:E:495:PRO:HA	1.95	0.49
1:G:623:PHE:CE2	1:G:625:ALA:HB3	2.47	0.49
1:C:682:LYS:HB2	1:C:729:ASN:HB3	1.94	0.49
1:F:635:GLU:OE1	1:F:635:GLU:N	2.44	0.49
1:D:479:ASN:OD1	1:D:481:VAL:HG22	2.12	0.48
1:E:489:ASP:HB3	1:E:492:ILE:HG12	1.95	0.48
1:E:487:MET:HB3	1:E:763:MET:HE1	1.95	0.48
1:G:593:ARG:HD2	1:G:759:GLU:HG3	1.95	0.48
1:C:489:ASP:HB3	1:C:492:ILE:HG12	1.95	0.48
1:A:484:PRO:HA	1:C:526:VAL:HG23	1.95	0.48
1:D:484:PRO:HG3	1:E:523:ARG:NH2	2.29	0.48
1:A:607:ASN:N	1:A:607:ASN:OD1	2.46	0.48
1:F:644:GLU:HB3	1:F:648:LYS:HE3	1.96	0.48
1:F:742:PRO:HB3	1:F:754:TRP:HB2	1.96	0.48
1:G:487:MET:HB3	1:G:763:MET:HE1	1.94	0.48
1:F:489:ASP:HB3	1:F:492:ILE:HG12	1.96	0.48
1:D:471:ALA:HA	1:D:495:PRO:HA	1.96	0.47
1:A:554:GLN:NE2	1:A:770:GLN:OE1	2.47	0.47
1:G:586:MET:HE2	1:G:586:MET:HB3	1.76	0.47
1:D:635:GLU:O	1:D:639:GLN:HG2	2.14	0.47
1:E:593:ARG:HD2	1:E:759:GLU:HG3	1.96	0.47
1:E:479:ASN:OD1	1:E:481:VAL:HG22	2.14	0.47
1:A:777:PRO:HB2	1:A:779:GLU:CD	2.40	0.47
1:D:534:ILE:HA	1:D:586:MET:O	2.15	0.46
1:A:635:GLU:O	1:A:639:GLN:HG2	2.15	0.46
1:E:734:THR:HG21	1:E:745:VAL:HG11	1.98	0.46
1:F:586:MET:HE2	1:F:586:MET:HB3	1.74	0.46
1:A:635:GLU:OE1	1:A:635:GLU:N	2.46	0.46
1:F:623:PHE:CE2	1:F:625:ALA:HB3	2.51	0.45
1:F:593:ARG:HD2	1:F:759:GLU:HG3	1.98	0.45
1:C:546:GLU:HB3	1:C:586:MET:HE1	1.99	0.45
1:E:777:PRO:HB2	1:E:779:GLU:CD	2.41	0.45
1:D:593:ARG:HD2	1:D:759:GLU:HG3	1.99	0.45
1:C:623:PHE:CE2	1:C:625:ALA:HB3	2.52	0.44
1:E:576:GLU:OE2	1:E:680:THR:HG21	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:ALA:HA	1:C:495:PRO:HA	2.00	0.44
1:G:573:PHE:HE1	1:G:584:THR:OG1	2.00	0.44
1:E:736:VAL:HG12	1:F:526:VAL:HG11	1.99	0.44
1:A:523:ARG:NH2	1:G:484:PRO:HG3	2.33	0.43
1:D:777:PRO:HB2	1:D:779:GLU:CD	2.43	0.43
1:C:576:GLU:OE2	1:C:680:THR:HG21	2.18	0.43
1:C:635:GLU:O	1:C:639:GLN:HG2	2.18	0.43
1:E:635:GLU:O	1:E:639:GLN:HG2	2.19	0.43
1:A:523:ARG:NH2	1:G:568:THR:HG21	2.33	0.43
1:G:576:GLU:OE2	1:G:680:THR:HG21	2.19	0.42
1:G:777:PRO:HB2	1:G:779:GLU:CD	2.44	0.42
1:A:526:VAL:HG23	1:G:484:PRO:O	2.19	0.42
1:E:584:THR:HG22	1:E:680:THR:HG23	2.02	0.42
1:A:526:VAL:HG11	1:G:736:VAL:CG1	2.50	0.42
1:G:651:VAL:N	1:G:652:PRO:HD2	2.35	0.42
1:D:487:MET:CB	1:D:763:MET:HE1	2.49	0.42
1:F:537:LEU:HD21	1:F:546:GLU:HG3	2.02	0.42
1:F:546:GLU:HB3	1:F:586:MET:HE1	2.01	0.42
1:A:586:MET:HE2	1:A:586:MET:HB3	1.74	0.42
1:G:482:GLY:HA2	1:G:737:ILE:HD11	2.01	0.42
1:F:632:CYS:HB2	1:F:646:CYS:HA	2.02	0.42
1:C:487:MET:HB3	1:C:763:MET:HE1	2.02	0.41
1:D:568:THR:HG21	1:E:523:ARG:NH2	2.36	0.41
1:D:778:VAL:HA	1:D:781:GLN:HG3	2.02	0.41
1:E:568:THR:HG21	1:F:523:ARG:HH21	1.85	0.41
1:A:740:ARG:HH12	1:A:760:GLU:CD	2.26	0.41
1:D:473:TYR:HD1	1:D:492:ILE:HD13	1.85	0.41
1:A:651:VAL:N	1:A:652:PRO:HD2	2.36	0.41
1:A:487:MET:CB	1:A:763:MET:HE1	2.50	0.41
1:C:651:VAL:N	1:C:652:PRO:HD2	2.36	0.41
1:E:651:VAL:N	1:E:652:PRO:HD2	2.36	0.41
1:E:473:TYR:HD1	1:E:492:ILE:HD13	1.85	0.41
1:F:482:GLY:HA2	1:F:737:ILE:HD11	2.03	0.41
1:F:544:GLN:HE21	1:F:544:GLN:HB2	1.74	0.41
1:F:588:LYS:HG2	1:F:676:THR:HG22	2.03	0.41
1:F:728:MET:CG	1:G:534:ILE:HG21	2.49	0.41
1:G:644:GLU:HB3	1:G:648:LYS:HE3	2.02	0.41
1:G:682:LYS:HB2	1:G:729:ASN:HB3	2.02	0.41
1:D:651:VAL:N	1:D:652:PRO:HD2	2.36	0.41
1:F:540:LEU:HD23	1:F:540:LEU:HA	1.95	0.41
1:A:537:LEU:HD21	1:A:546:GLU:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:778:VAL:HA	1:C:781:GLN:CG	2.51	0.40
1:G:544:GLN:HE21	1:G:544:GLN:HB2	1.77	0.40
1:E:546:GLU:HB3	1:E:586:MET:HE1	2.03	0.40
1:A:632:CYS:HB2	1:A:646:CYS:HA	2.03	0.40
1:E:588:LYS:HD3	1:E:590:TYR:OH	2.21	0.40
1:D:518:LEU:HD22	1:D:518:LEU:HA	1.83	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:C:793:LYS:NZ	1:E:635:GLU:OE1[4_455]	2.17	0.03

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	268/356 (75%)	260 (97%)	7 (3%)	1 (0%)	30	67
1	C	268/356 (75%)	259 (97%)	8 (3%)	1 (0%)	30	67
1	D	268/356 (75%)	260 (97%)	8 (3%)	0	100	100
1	E	268/356 (75%)	260 (97%)	7 (3%)	1 (0%)	30	67
1	F	268/356 (75%)	259 (97%)	9 (3%)	0	100	100
1	G	268/356 (75%)	260 (97%)	7 (3%)	1 (0%)	30	67
All	All	1608/2136 (75%)	1558 (97%)	46 (3%)	4 (0%)	43	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	799	PRO
1	C	799	PRO

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Mol	Chain	Res	Type
1	G	799	PRO
1	A	799	PRO

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	229/296 (77%)	227 (99%)	2 (1%)	70	77
1	C	229/296 (77%)	227 (99%)	2 (1%)	70	77
1	D	229/296 (77%)	226 (99%)	3 (1%)	61	73
1	E	229/296 (77%)	227 (99%)	2 (1%)	70	77
1	F	229/296 (77%)	227 (99%)	2 (1%)	70	77
1	G	229/296 (77%)	227 (99%)	2 (1%)	70	77
All	All	1374/1776 (77%)	1361 (99%)	13 (1%)	70	77

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	532	GLU
1	A	607	ASN
1	C	532	GLU
1	C	607	ASN
1	D	518	LEU
1	D	532	GLU
1	D	607	ASN
1	E	532	GLU
1	E	607	ASN
1	F	532	GLU
1	F	607	ASN
1	G	532	GLU
1	G	607	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	626	HIS
1	A	744	GLN
1	C	544	GLN
1	E	626	HIS
1	G	636	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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	G	901	1	14,14,15	0.54	0	17,19,21	0.50	0
2	NAG	C	901	1	14,14,15	0.20	0	17,19,21	0.41	0
2	NAG	D	901	1	14,14,15	0.36	0	17,19,21	0.45	0
2	NAG	E	901	1	14,14,15	0.59	0	17,19,21	0.52	0
2	NAG	A	901	1	14,14,15	1.38	1 (7%)	17,19,21	0.68	0
2	NAG	F	901	1	14,14,15	0.31	0	17,19,21	0.47	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
2	NAG	G	901	1	-	2/6/23/26	0/1/1/1
2	NAG	C	901	1	-	1/6/23/26	0/1/1/1
2	NAG	D	901	1	-	3/6/23/26	0/1/1/1
2	NAG	E	901	1	-	2/6/23/26	0/1/1/1
2	NAG	A	901	1	-	2/6/23/26	0/1/1/1
2	NAG	F	901	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	NAG	C1-C2	4.65	1.58	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	901	NAG	C4-C5-C6-O6
2	D	901	NAG	O5-C5-C6-O6
2	G	901	NAG	O5-C5-C6-O6
2	A	901	NAG	C1-C2-N2-C7
2	E	901	NAG	O5-C5-C6-O6
2	A	901	NAG	C3-C2-N2-C7
2	C	901	NAG	C3-C2-N2-C7
2	D	901	NAG	C3-C2-N2-C7
2	E	901	NAG	C3-C2-N2-C7
2	F	901	NAG	C3-C2-N2-C7
2	G	901	NAG	C3-C2-N2-C7

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	276/356 (77%)	0.06	10 (3%)	46 40	257, 334, 387, 423	0
1	C	276/356 (77%)	0.08	10 (3%)	46 40	229, 295, 349, 376	0
1	D	276/356 (77%)	0.00	6 (2%)	62 50	244, 323, 405, 442	0
1	E	276/356 (77%)	0.12	10 (3%)	46 40	226, 300, 361, 399	0
1	F	276/356 (77%)	-0.07	3 (1%)	78 63	253, 344, 416, 453	0
1	G	276/356 (77%)	-0.17	1 (0%)	88 77	291, 355, 424, 468	0
All	All	1656/2136 (77%)	0.00	40 (2%)	59 49	226, 326, 403, 468	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	594	TYR	4.7
1	A	764	PRO	4.5
1	C	677	TYR	4.3
1	A	469	LEU	4.0
1	A	522	VAL	3.6
1	D	594	TYR	3.6
1	E	612	PHE	3.5
1	E	500	THR	3.4
1	E	677	TYR	3.2
1	A	500	THR	3.1
1	C	515	LEU	3.0
1	C	606	TRP	2.9
1	A	524	GLN	2.9
1	D	667	VAL	2.8
1	C	678	GLN	2.8
1	C	586	MET	2.8
1	C	598	VAL	2.7
1	A	598	VAL	2.7
1	C	631	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	589	ASN	2.6
1	E	606	TRP	2.6
1	F	666	LEU	2.5
1	A	523	ARG	2.5
1	G	500	THR	2.5
1	A	596	ALA	2.4
1	E	775	LEU	2.4
1	D	764	PRO	2.4
1	A	788	VAL	2.4
1	E	675	MET	2.3
1	F	500	THR	2.3
1	C	625	ALA	2.3
1	D	500	THR	2.3
1	C	551	ALA	2.3
1	E	570	TYR	2.2
1	E	657	PHE	2.1
1	D	679	VAL	2.1
1	D	473	TYR	2.1
1	F	515	LEU	2.0
1	E	547	LEU	2.0
1	C	547	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	901	14/15	-	-	341,350,360,360	14
2	NAG	C	901	14/15	-	-	334,342,351,353	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	901	14/15	-	-	349,354,362,363	14
2	NAG	E	901	14/15	-	-	358,363,370,370	14
2	NAG	F	901	14/15	-	-	361,366,373,373	14
2	NAG	G	901	14/15	-	-	387,393,401,401	14

6.5 Other polymers [i](#)

There are no such residues in this entry.