



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:07 AM UTC

PDB ID : 7DJL / pdb_00007djl
Title : Structure of four truncated and mutated forms of quenching protein
Authors : Yu, G.M.; Pan, X.W.; Li, M.
Deposited on : 2020-11-20
Resolution : 2.96 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

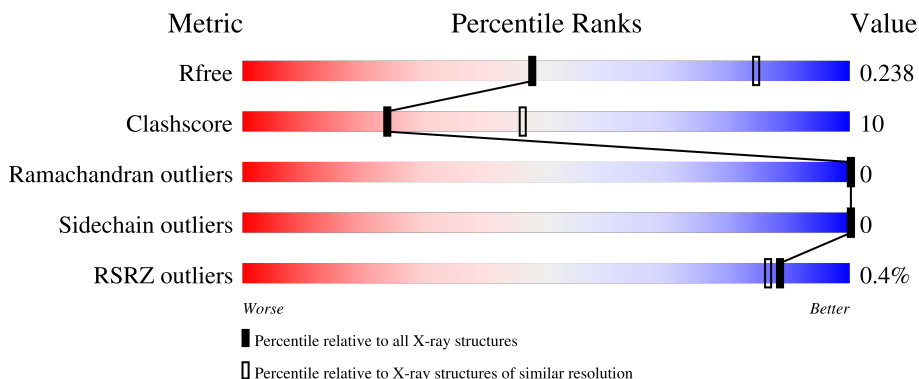
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

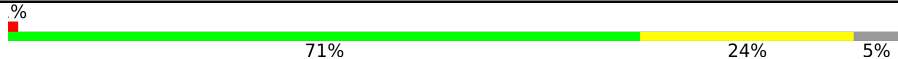
The reported resolution of this entry is 2.96 Å.

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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	498	 71% 24% 5%
1	B	498	 76% 18% 6%
1	C	498	 75% 20% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10958 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 Protein SUPPRESSOR OF QUENCHING 1, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	473	Total	C	N	O	S	0	4	0
			3644	2291	620	725	8			
1	A	473	Total	C	N	O	S	0	3	0
			3644	2288	621	727	8			
1	B	470	Total	C	N	O	S	0	3	0
			3614	2271	614	721	8			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	558	MET	-	initiating methionine	UNP Q8VZ10
C	559	GLY	-	expression tag	UNP Q8VZ10
C	859	LYS	GLU	engineered mutation	UNP Q8VZ10
A	558	MET	-	initiating methionine	UNP Q8VZ10
A	559	GLY	-	expression tag	UNP Q8VZ10
A	859	LYS	GLU	engineered mutation	UNP Q8VZ10
B	558	MET	-	initiating methionine	UNP Q8VZ10
B	559	GLY	-	expression tag	UNP Q8VZ10
B	859	LYS	GLU	engineered mutation	UNP Q8VZ10

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

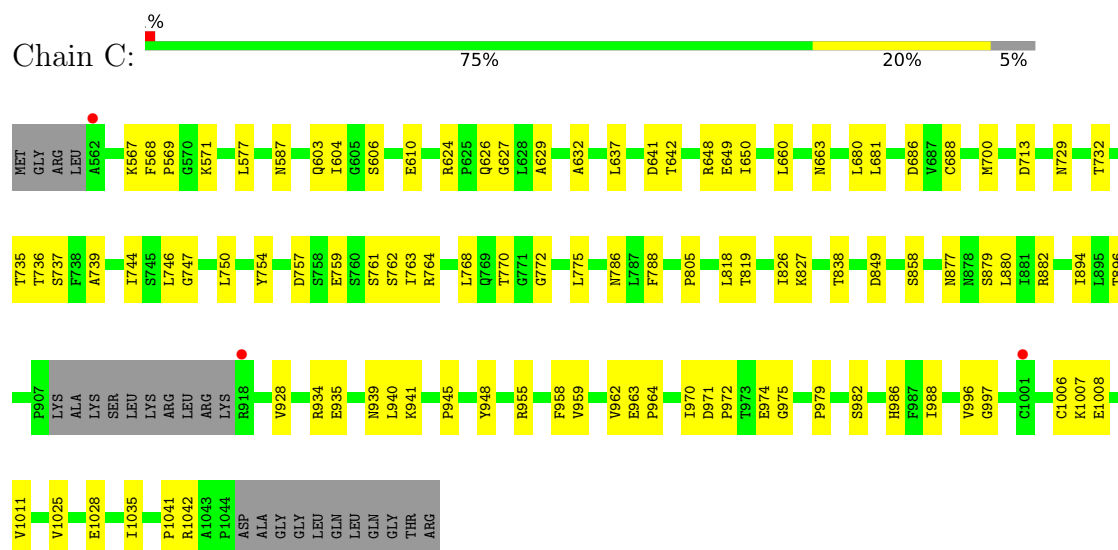
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	26	Total 26	O 26	0	0
4	A	12	Total 12	O 12	0	0
4	B	15	Total 15	O 15	0	0

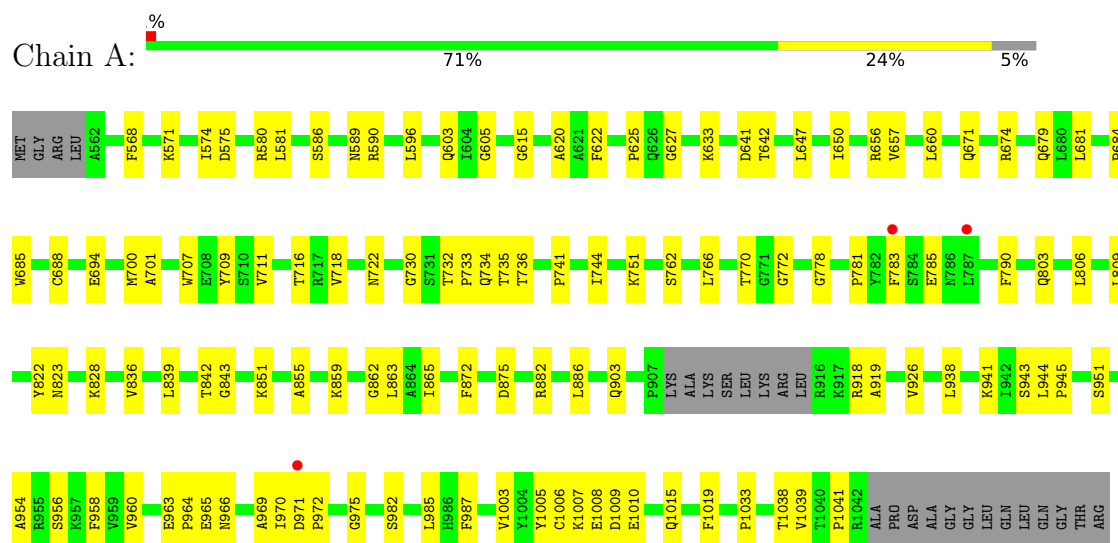
3 Residue-property plots

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

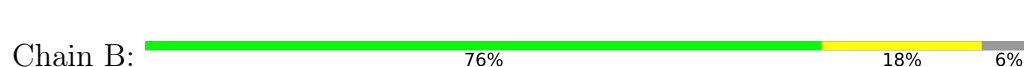
- Molecule 1: Protein SUPPRESSOR OF QUENCHING 1, chloroplastic



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V1025		LYS	H704	MET
I1035		ARG	W707	GLY
A1043		LEU	E708	LEU
PRO		LYS	Y709	A562
ASP		R918	T716	P565
ALA		V928	R717	F568
GLY		D929	V718	K371
LEU		S930	E725	L572
GLN		S933	P733	L581
GLN		R934	F738	S586
THR		L938	P741	R590
ARG		N939	L750	I591
		L940	S758	I592
		K941	Q769	D595
		F958	T770	L596
		V959	F783	S607
		V960	SER	G608
		E963	GLU	E609
		P964	N786	E618
		I970	V796	F622
		D971	E799	Q626
		P972	V800	G627
		S982	L801	L628
		T983	H804	D641
		N984	D849	R648
		L985	G850	D651
		H986	K851	N654
		Q989	V852	T659
		A994	K853	N663
		S995	N868	G664
		V996	D875	T665
		C1000	R882	Y670
		C1001	S892	T677
		Y1005	P904	L680
		C1006	P907	E690
		K1007	LYS	V696
		E1008	ALA	
		D1009	LYS	
		E1010	SER	
		V1011	LEU	
		C1012		
		L1013		
		V1017		
		P1022		
		F1023		
		V1024		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.93Å 166.30Å 95.74Å 90.00° 116.82° 90.00°	Depositor
Resolution (Å)	44.60 – 2.96 44.60 – 2.96	Depositor EDS
% Data completeness (in resolution range)	98.0 (44.60-2.96) 98.0 (44.60-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.168 , 0.226 (Not available) , 0.238	Depositor DCC
R_{free} test set	2133 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10958	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: NA, 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	0.49	0/3711	0.77	0/5025
1	B	0.48	0/3680	0.74	0/4984
1	C	0.50	0/3718	0.75	0/5036
All	All	0.49	0/11109	0.75	0/15045

There are no bond length outliers.

There are no bond angle outliers.

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	3644	0	3587	88	0
1	B	3614	0	3553	62	0
1	C	3644	0	3595	71	0
2	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	12	0	0	2	0
4	B	15	0	0	1	0
4	C	26	0	0	3	0
All	All	10958	0	10735	218	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 10.

All (218) 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:A:918:ARG:HG2	1:A:919:ALA:H	1.31	0.95
1:A:803:GLN:HG3	1:A:822:TYR:HB2	1.46	0.94
1:C:603:GLN:HE21	1:C:606:SER:HB2	1.34	0.89
1:A:1006:CYS:SG	4:A:1210:HOH:O	2.34	0.84
1:C:971:ASP:HB3	1:C:972:PRO:HD3	1.59	0.83
1:C:1006:CYS:SG	4:C:1123:HOH:O	2.39	0.79
1:C:688[B]:CYS:SG	4:C:1114:HOH:O	2.41	0.79
1:B:963:GLU:HB3	1:B:964:PRO:HD3	1.65	0.78
1:C:963:GLU:HB3	1:C:964:PRO:HD3	1.69	0.74
1:A:625:PRO:HA	1:A:641:ASP:HA	1.71	0.71
1:A:971:ASP:HB3	1:A:972:PRO:HD3	1.72	0.70
1:A:694:GLU:HB3	1:A:711:VAL:HG12	1.72	0.69
1:C:603:GLN:NE2	1:C:606:SER:HB2	2.06	0.69
1:B:690:GLU:HG2	1:B:750:LEU:HD22	1.74	0.68
1:C:849:ASP:HB3	1:C:882:ARG:HH21	1.59	0.68
1:C:849:ASP:HB2	1:C:894:ILE:O	1.94	0.67
1:C:604:ILE:HD12	1:C:650:ILE:HD13	1.77	0.66
1:A:709:TYR:HB2	1:A:716:THR:HG22	1.79	0.65
1:A:963:GLU:HB3	1:A:964:PRO:HD3	1.78	0.65
1:A:1007:LYS:HG2	1:A:1008:GLU:H	1.63	0.64
1:C:786:ASN:O	1:C:788:PHE:N	2.29	0.63
1:A:751:LYS:HE3	1:B:1008:GLU:OE2	1.98	0.63
1:C:935:GLU:HG3	1:C:988:ILE:HG12	1.81	0.63
1:A:965:GLU:HG3	1:A:966:ASN:OD1	1.99	0.62
1:B:1006:CYS:SG	4:B:1213:HOH:O	2.56	0.61
1:B:707:TRP:HE3	1:B:716:THR:HG22	1.64	0.61
1:A:903:GLN:N	1:A:903:GLN:OE1	2.34	0.60
1:B:591:ILE:HD12	1:B:628:LEU:HD21	1.83	0.60
1:B:663:ASN:OD1	1:B:665:THR:HG22	2.01	0.60
1:B:940:LEU:HB3	1:B:983:THR:HG22	1.84	0.60
1:B:690:GLU:OE1	1:B:750:LEU:HD13	2.02	0.59
1:C:577:LEU:HD13	1:C:1011:VAL:HG11	1.84	0.59
1:A:701:ALA:HA	1:A:741:PRO:HD2	1.85	0.58
1:B:933:SER:O	1:B:989:GLN:NE2	2.36	0.58
1:B:971:ASP:HB3	1:B:986:HIS:HB3	1.86	0.57
1:C:713:ASP:OD1	1:C:713:ASP:N	2.37	0.57
1:A:918:ARG:HG2	1:A:919:ALA:N	2.12	0.57
1:A:958:PHE:CZ	1:A:975:GLY:HA3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:969:ALA:O	1:A:987:PHE:HA	2.06	0.56
1:B:696:VAL:CG2	1:B:709:TYR:HB3	2.36	0.56
1:A:707:TRP:CZ2	1:A:718:VAL:HG12	2.41	0.55
1:A:575:ASP:HB3	1:A:580:ARG:HB2	1.89	0.55
1:A:941:LYS:HD3	1:A:982:SER:HB3	1.89	0.55
1:A:875:ASP:OD2	1:A:882:ARG:NH1	2.39	0.54
1:A:674:ARG:NE	1:A:674:ARG:HA	2.22	0.54
1:B:618:GLU:H	1:B:618:GLU:CD	2.16	0.54
1:A:671:GLN:O	1:A:718:VAL:HG13	2.07	0.54
1:A:633:LYS:HE3	1:A:1010:GLU:HB3	1.90	0.54
1:C:955:ARG:HH12	1:C:979:PRO:HD3	1.72	0.54
1:A:730:GLY:CA	1:A:736:THR:HG22	2.37	0.54
1:C:732:THR:OG1	1:C:735:THR:HG23	2.08	0.53
1:C:963:GLU:CB	1:C:996:VAL:H	2.21	0.53
1:C:963:GLU:N	1:C:996:VAL:O	2.41	0.53
1:A:732:THR:O	1:A:736:THR:HG23	2.08	0.53
1:B:696:VAL:HG22	1:B:709:TYR:HB3	1.90	0.53
1:C:971:ASP:CB	1:C:972:PRO:HD3	2.36	0.53
1:C:649:GLU:HB2	1:C:660:LEU:HD11	1.90	0.53
1:A:694:GLU:HB3	1:A:711:VAL:CG1	2.39	0.53
1:C:959:VAL:HG22	1:C:974:GLU:HG3	1.90	0.53
1:A:642:THR:HG22	1:A:684:PRO:O	2.09	0.53
1:C:763:ILE:HG13	1:C:818:LEU:HD22	1.90	0.53
1:C:1042:ARG:HD2	4:C:1122:HOH:O	2.08	0.52
1:B:852:VAL:HG13	1:B:892:SER:O	2.09	0.52
1:A:944:LEU:HD23	1:A:1039:VAL:HG11	1.91	0.52
1:B:663:ASN:ND2	1:B:680:LEU:HD11	2.25	0.52
1:A:960:VAL:HG11	1:A:970:ILE:HG13	1.91	0.52
1:A:732:THR:HG22	1:A:735:THR:OG1	2.09	0.52
1:A:839:LEU:HD21	1:A:886:LEU:HD21	1.92	0.52
1:C:739:ALA:HB1	1:C:759:GLU:HB3	1.92	0.52
1:A:972:PRO:HD2	1:A:985:LEU:HA	1.92	0.52
1:B:565:PRO:HB3	1:B:904:PRO:HD3	1.91	0.51
1:C:948:TYR:CE1	1:C:1007:LYS:HG3	2.45	0.51
1:A:642:THR:HG21	1:A:685:TRP:CE3	2.46	0.51
1:B:938:LEU:N	1:B:985:LEU:O	2.44	0.51
1:C:737:SER:O	1:C:764:ARG:NH2	2.42	0.51
1:C:770:THR:HG22	1:C:772:GLY:H	1.76	0.51
1:A:943:SER:O	1:A:1038:THR:HA	2.11	0.51
1:A:945:PRO:HD3	1:A:1039:VAL:HG12	1.93	0.51
1:C:732:THR:O	1:C:736:THR:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:THR:HG23	1:A:855:ALA:O	2.10	0.50
1:B:704:HIS:CD2	1:B:725:GLU:HB3	2.46	0.50
1:B:595:ASP:OD1	1:B:596:LEU:N	2.45	0.50
1:A:650:ILE:HG12	1:A:657:VAL:HG12	1.93	0.50
1:C:770:THR:HG22	1:C:772:GLY:N	2.26	0.50
1:A:605:GLY:HA2	1:A:620:ALA:O	2.11	0.50
1:A:944:LEU:HA	1:A:1039:VAL:HG12	1.92	0.50
1:C:939:ASN:HB3	1:C:941[A]:LYS:HZ3	1.77	0.50
1:B:707:TRP:CE3	1:B:716:THR:HG22	2.47	0.50
1:A:679:GLN:HG2	1:A:716:THR:OG1	2.12	0.50
1:B:851:LYS:HE2	1:B:851:LYS:H	1.77	0.50
1:A:783:PHE:CD1	1:A:785:GLU:HA	2.46	0.49
1:B:572:LEU:HD22	1:B:581:LEU:HD11	1.94	0.49
1:C:686:ASP:HB3	1:C:744:ILE:HG22	1.94	0.49
1:C:849:ASP:OD2	1:C:896:THR:OG1	2.25	0.49
1:C:963:GLU:HB2	1:C:996:VAL:HB	1.95	0.49
1:A:590:ARG:NH1	1:A:603:GLN:OE1	2.41	0.49
1:A:1007:LYS:HG2	1:A:1008:GLU:N	2.25	0.49
1:C:681:LEU:HD22	1:C:700:MET:HE1	1.95	0.49
1:A:707:TRP:CE2	1:A:718:VAL:HG12	2.48	0.49
1:A:647:LEU:HD23	1:A:660:LEU:HB2	1.95	0.49
1:B:934:ARG:HE	1:B:1025:VAL:HG21	1.77	0.49
1:C:934[A]:ARG:HH21	1:C:1025:VAL:HG11	1.78	0.49
1:C:945:PRO:HG2	1:C:1041:PRO:HD3	1.94	0.48
1:A:783:PHE:C	1:A:785:GLU:H	2.21	0.48
1:C:928:VAL:HG11	1:C:1035:ILE:HG12	1.95	0.48
1:A:733:PRO:HD3	1:A:770:THR:O	2.14	0.48
1:B:960:VAL:HG11	1:B:970:ILE:HG13	1.94	0.48
1:C:624:ARG:O	1:C:642:THR:HG22	2.12	0.48
1:B:849:ASP:OD1	1:B:882:ARG:NH2	2.43	0.48
1:B:941:LYS:HD3	1:B:982:SER:HB3	1.96	0.47
1:B:641:ASP:OD2	1:B:648:ARG:NH1	2.45	0.47
1:C:939:ASN:HB3	1:C:941[A]:LYS:NZ	2.29	0.47
1:B:704:HIS:HA	1:B:741:PRO:HD2	1.96	0.47
1:C:568:PHE:HD2	1:C:587:ASN:OD1	1.98	0.47
1:B:670:TYR:O	1:B:718:VAL:HG21	2.15	0.47
1:A:918:ARG:CG	1:A:919:ALA:H	2.12	0.46
1:C:567:LYS:O	1:C:587:ASN:HB2	2.16	0.46
1:A:971:ASP:CB	1:A:972:PRO:HD3	2.43	0.46
1:C:858:SER:O	1:C:877:ASN:HB2	2.15	0.46
1:A:762:SER:HB3	1:A:778:GLY:HA3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:963:GLU:HB3	1:C:996:VAL:H	1.79	0.46
1:B:930:SER:HA	1:B:1022:PRO:HG2	1.98	0.46
1:C:948:TYR:CE2	1:C:1041:PRO:HG2	2.51	0.46
1:B:958:PHE:HA	1:B:1000:SER:O	2.16	0.46
1:B:1005:TYR:O	1:B:1013:LEU:HB2	2.16	0.46
1:A:688[A]:CYS:SG	1:A:744:ILE:HG12	2.56	0.45
1:B:851:LYS:H	1:B:851:LYS:CE	2.29	0.45
1:B:1001:CYS:HB2	1:B:1017:VAL:HG12	1.98	0.45
1:A:790:PHE:C	1:A:790:PHE:CD1	2.94	0.45
1:C:729:ASN:OD1	1:C:764:ARG:NE	2.49	0.45
1:A:926:VAL:HG21	1:A:1019:PHE:CD2	2.51	0.45
1:A:945:PRO:HD3	1:A:1039:VAL:CG1	2.47	0.45
1:B:928:VAL:HG11	1:B:1035:ILE:HG12	1.97	0.45
1:A:956:SER:HB3	1:A:1003:VAL:HA	1.99	0.45
1:A:1010:GLU:O	1:A:1010:GLU:HG3	2.16	0.45
1:A:736:THR:HG21	1:A:772:GLY:HA2	1.99	0.45
1:C:819:THR:HG22	1:C:826:ILE:HD13	1.98	0.45
1:A:859:LYS:O	1:A:859:LYS:HG2	2.17	0.45
1:C:761:SER:HA	1:C:805:PRO:HD2	1.98	0.45
1:A:781:PRO:CG	1:B:868:ASN:HB3	2.47	0.45
1:A:823:ASN:O	1:A:843:GLY:HA2	2.16	0.44
1:B:596:LEU:HD23	1:B:596:LEU:HA	1.75	0.44
1:C:663:ASN:ND2	1:C:680:LEU:HG	2.31	0.44
1:C:762:SER:HB2	1:C:775:LEU:HD11	1.99	0.44
1:B:971:ASP:CB	1:B:972:PRO:HD3	2.46	0.44
1:A:809:LEU:HD21	1:A:865:ILE:HB	1.99	0.44
1:B:994:ALA:HA	1:B:1024:LYS:HB2	1.99	0.44
1:A:766:LEU:HD12	1:A:772:GLY:O	2.17	0.44
1:B:972:PRO:HG2	1:B:984:MET:O	2.18	0.44
1:B:971:ASP:OD2	1:B:972:PRO:HD3	2.17	0.44
1:C:641:ASP:HB2	1:C:648:ARG:HG2	1.98	0.44
1:C:963:GLU:HB2	1:C:996:VAL:H	1.83	0.44
1:B:875:ASP:OD2	1:B:882:ARG:NH1	2.47	0.44
1:C:571:LYS:HG3	1:C:627:GLY:HA2	2.00	0.43
1:C:879:SER:O	1:C:880:LEU:HD23	2.19	0.43
1:C:746:LEU:HD22	1:C:768:LEU:HD11	1.99	0.43
1:C:568:PHE:CD2	1:C:587:ASN:OD1	2.72	0.43
1:B:568:PHE:O	1:B:586[A]:SER:HB2	2.18	0.43
1:A:783:PHE:CE1	1:A:785:GLU:HA	2.54	0.43
1:B:607:SER:HB3	1:B:609:GLU:HG3	1.99	0.43
1:C:827:LYS:HG2	1:C:838:THR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:747:GLY:O	1:C:750:LEU:HD23	2.19	0.43
1:A:1005:TYR:OH	1:A:1041:PRO:HB3	2.19	0.43
1:C:632:ALA:HB1	1:C:1011:VAL:HG13	2.00	0.43
1:C:786:ASN:OD1	1:C:788:PHE:HB2	2.19	0.43
1:C:934[B]:ARG:HD3	1:C:1028:GLU:OE2	2.18	0.42
1:A:615:GLY:HA2	1:A:656:ARG:HH11	1.84	0.42
1:A:730:GLY:HA3	1:A:736:THR:HG22	2.00	0.42
1:B:725:GLU:HA	1:B:738:PHE:O	2.19	0.42
1:A:734:GLN:CD	1:A:734:GLN:H	2.26	0.42
1:A:803:GLN:HG3	1:A:822:TYR:CB	2.33	0.42
1:C:571:LYS:HB2	1:C:626:GLN:O	2.20	0.42
1:C:610:GLU:OE1	1:C:610:GLU:N	2.46	0.42
1:A:568:PHE:O	1:A:586[A]:SER:HB2	2.20	0.42
1:B:796:VAL:O	1:B:799:GLU:HG3	2.19	0.42
1:A:574:ILE:HD11	1:A:872:PHE:CD2	2.54	0.42
1:A:828:LYS:O	1:A:836:VAL:HA	2.19	0.42
1:A:851:LYS:HB2	1:A:851:LYS:HE2	1.92	0.42
1:C:744:ILE:HA	1:C:754:TYR:O	2.19	0.42
1:A:571:LYS:HB2	1:A:627:GLY:H	1.85	0.41
1:A:722:ASN:HB3	1:A:734:GLN:O	2.20	0.41
1:C:757:ASP:OD2	1:C:764:ARG:NH1	2.51	0.41
1:B:571:LYS:HB2	1:B:626:GLN:O	2.20	0.41
1:C:962:VAL:HA	1:C:997:GLY:HA2	2.03	0.41
1:B:853:LYS:HA	1:B:853:LYS:HD2	1.78	0.41
1:C:940:LEU:O	1:C:982:SER:HA	2.20	0.41
1:A:862:GLY:C	1:A:863:LEU:HG	2.44	0.41
1:B:651:ASP:OD2	1:B:654:ASN:ND2	2.53	0.41
1:B:972:PRO:HD2	1:B:985:LEU:HA	2.03	0.41
1:C:569:PRO:HD2	1:C:879:SER:HA	2.02	0.41
1:C:1008:GLU:OE2	1:B:769:GLN:NE2	2.53	0.41
1:A:926:VAL:HG22	1:A:1019:PHE:HA	2.02	0.41
1:B:622:PHE:HD1	1:B:641:ASP:OD2	2.03	0.41
1:B:659:THR:HG22	1:B:677:THR:HG22	2.02	0.41
1:C:627:GLY:HA3	1:C:686:ASP:HA	2.02	0.41
1:C:629:ALA:O	1:C:637:LEU:HD12	2.21	0.41
1:C:958:PHE:CE1	1:C:975:GLY:HA3	2.56	0.41
1:C:970:ILE:HA	1:C:986:HIS:O	2.21	0.41
1:A:965:GLU:OE2	1:A:966:ASN:N	2.48	0.41
1:B:663:ASN:OD1	1:B:663:ASN:C	2.64	0.41
1:B:851:LYS:H	1:B:851:LYS:CD	2.34	0.41
1:B:1009:ASP:HB3	1:B:1011:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:ASP:O	1:A:1010:GLU:HB3	2.21	0.41
1:A:806:LEU:HD23	1:A:806:LEU:HA	1.87	0.40
1:B:733:PRO:HD3	1:B:770:THR:O	2.20	0.40
1:A:951:SER:OG	1:A:954:ALA:HB3	2.20	0.40
1:A:1003:VAL:CG1	1:A:1015:GLN:HB3	2.52	0.40
1:B:590:ARG:CZ	1:B:592[B]:ILE:HD11	2.51	0.40
1:A:581:LEU:HB2	1:A:596:LEU:HD23	2.03	0.40
1:A:943:SER:O	1:A:1038:THR:HG23	2.22	0.40
1:B:801:LEU:HD23	1:B:801:LEU:HA	1.78	0.40
1:B:963:GLU:HB2	1:B:996:VAL:HB	2.02	0.40
1:A:589:ASN:HB3	1:A:622:PHE:O	2.21	0.40
1:A:938:LEU:HD13	1:A:1033:PRO:HG2	2.03	0.40
1:B:758:SER:O	1:B:804:HIS:HA	2.21	0.40
1:A:681:LEU:HD22	1:A:700:MET:HE1	2.03	0.40
1:A:709:TYR:CB	1:A:716:THR:HG22	2.50	0.40
1:A:809:LEU:HD12	4:A:1204:HOH:O	2.21	0.40

There are no symmetry-related clashes.

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	472/498 (95%)	445 (94%)	27 (6%)	0	100	100
1	B	467/498 (94%)	442 (95%)	25 (5%)	0	100	100
1	C	473/498 (95%)	446 (94%)	27 (6%)	0	100	100
All	All	1412/1494 (94%)	1333 (94%)	79 (6%)	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	402/417 (96%)	402 (100%)	0	100	100
1	B	398/417 (95%)	398 (100%)	0	100	100
1	C	402/417 (96%)	402 (100%)	0	100	100
All	All	1202/1251 (96%)	1202 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	671	GLN
1	C	703	GLN
1	C	986	HIS
1	A	578	ASN
1	A	587	ASN
1	A	786	ASN
1	A	804	HIS
1	B	729	ASN
1	B	740	GLN
1	B	989	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

Of 3 ligands modelled in this entry, 3 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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	473/498 (94%)	-0.22	3 (0%) 85 82	29, 71, 98, 119	3 (0%)
1	B	470/498 (94%)	-0.40	0 100 100	26, 65, 94, 116	3 (0%)
1	C	473/498 (94%)	-0.36	3 (0%) 85 82	26, 63, 91, 109	4 (0%)
All	All	1416/1494 (94%)	-0.32	6 (0%) 88 86	26, 66, 95, 119	10 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1001	CYS	3.0
1	C	562	ALA	3.0
1	A	787	LEU	2.6
1	A	783	PHE	2.5
1	A	971	ASP	2.4
1	C	918	ARG	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	A	1102	1/1	0.91	0.07	83,83,83,83	0
2	CL	A	1101	1/1	0.95	0.12	100,100,100,100	0
3	NA	B	1101	1/1	0.96	0.13	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.