



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 10:53 AM JST

PDB ID : 7DJL
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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

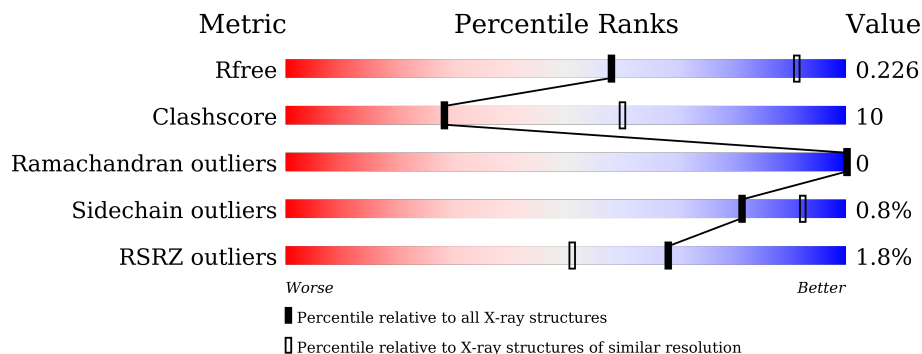
1 Overall quality at a glance

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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	 2% 72% 23% 5%
1	B	498	 3% 76% 18% 6%
1	C	498	 74% 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
			Total	C	N	O	S			
1	C	473	Total 3644	C 2291	N 620	O 725	S 8	0	4	0
1	A	473	Total 3644	C 2288	N 621	O 727	S 8	0	3	0
1	B	470	Total 3614	C 2271	N 614	O 721	S 8	0	3	0

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 (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is water.

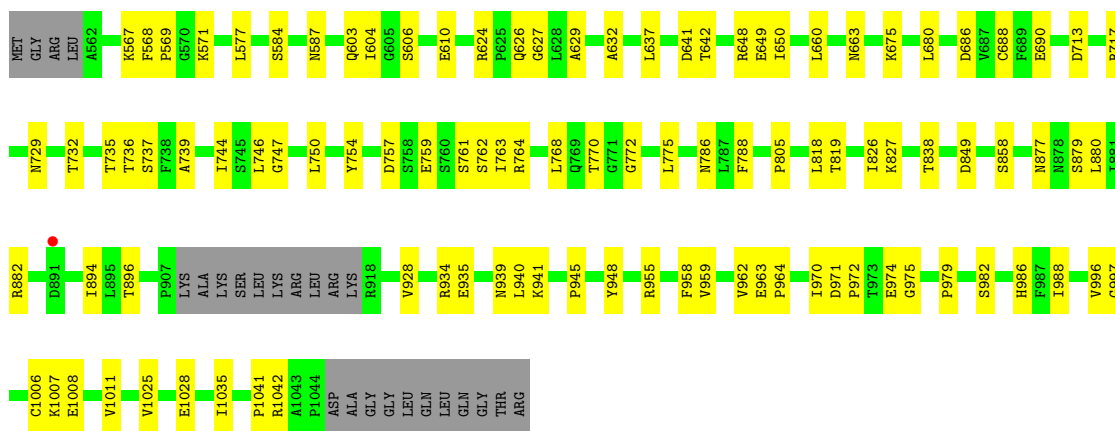
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	26	Total 26	O 26	0	0
4	A	12	Total 12	O 12	0	0
4	B	15	Total 15	O 15	0	0

3 Residue-property plots [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.

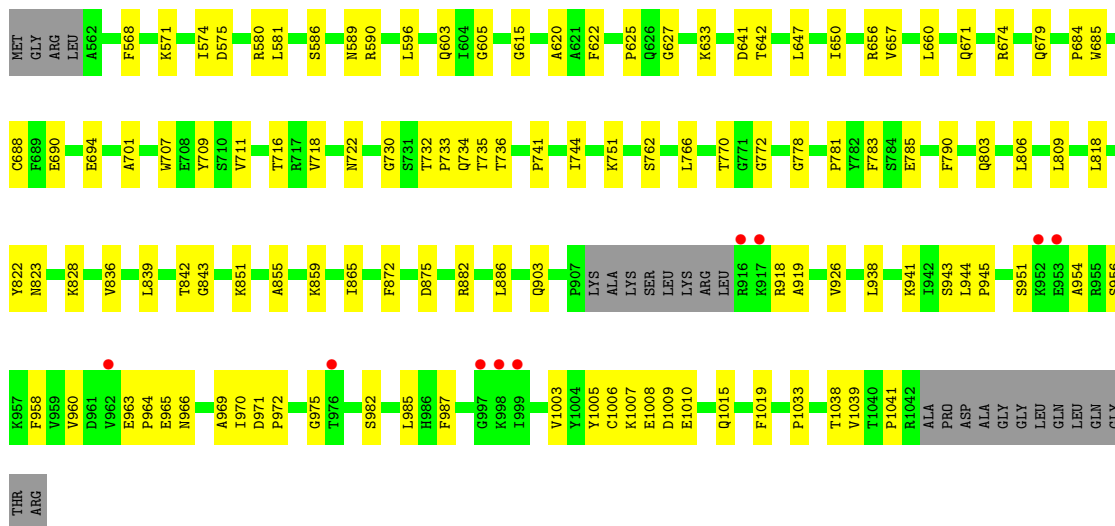
- Molecule 1: Protein SUPPRESSOR OF QUENCHING 1, chloroplastic

Chain C: 




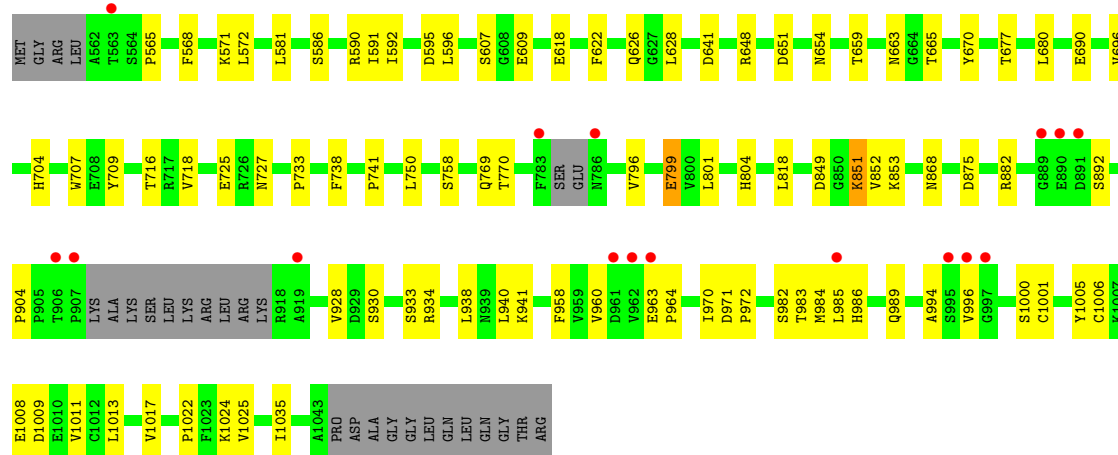
- Molecule 1: Protein SUPPRESSOR OF QUENCHING 1, chloroplastic

Chain A: 



- Molecule 1: Protein SUPPRESSOR OF QUENCHING 1, chloroplastic

Chain B:  3% 76% 18% 6%



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)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.168 , 0.226 0.168 , 0.226	Depositor DCC
R_{free} test set	2131 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	65.3	Xtrriage
Anisotropy	0.597	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: CL, NA

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	0.53	0/3711	0.74	0/5025
1	B	0.54	0/3680	0.73	0/4984
1	C	0.53	0/3718	0.74	0/5036
All	All	0.53	0/11109	0.74	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	85	0
1	B	3614	0	3553	61	0
1	C	3644	0	3595	70	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	213	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 (213) 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: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
1:A:842:THR:HG23	1:A:855:ALA:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:618:GLU:H	1:B:618:GLU:CD	2.16	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:783:PHE:C	1:A:785:GLU:H	2.21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:790:PHE:CD1	1:A:790:PHE:C	2.94	0.41
1:A:965:GLU:OE2	1:A:966:ASN:N	2.48	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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%)	400 (100%)	2 (0%)	88	95
1	B	398/417 (95%)	394 (99%)	4 (1%)	76	90
1	C	402/417 (96%)	398 (99%)	4 (1%)	76	90
All	All	1202/1251 (96%)	1192 (99%)	10 (1%)	81	92

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	584	SER
1	C	675	LYS
1	C	690	GLU
1	C	717	ARG
1	A	690	GLU
1	A	818	LEU
1	B	727	ASN
1	B	799	GLU
1	B	818	LEU
1	B	851	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	473/498 (94%)	0.13	9 (1%) 66 49	50, 71, 98, 119	0
1	B	470/498 (94%)	0.02	16 (3%) 45 29	47, 65, 94, 116	0
1	C	473/498 (94%)	-0.07	1 (0%) 95 90	47, 63, 91, 109	0
All	All	1416/1494 (94%)	0.03	26 (1%) 68 51	47, 66, 95, 119	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	906	THR	4.0
1	B	786	ASN	3.5
1	B	907	PRO	3.4
1	B	919	ALA	3.3
1	B	996	VAL	2.9
1	B	962	VAL	2.6
1	A	962	VAL	2.5
1	A	997	GLY	2.5
1	C	891	ASP	2.5
1	A	976	THR	2.5
1	B	891	ASP	2.4
1	B	995	SER	2.4
1	B	985	LEU	2.4
1	A	998	LYS	2.4
1	A	916	ARG	2.3
1	B	997	GLY	2.3
1	B	890	GLU	2.3
1	A	953	GLU	2.2
1	A	952	LYS	2.2
1	B	889	GLY	2.2
1	B	961	ASP	2.2
1	B	963	GLU	2.2
1	B	563	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	999	ILE	2.1
1	A	917	LYS	2.1
1	B	783	PHE	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 monosaccharides 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
2	CL	A	1102	1/1	0.77	0.26	83,83,83,83	0
2	CL	A	1101	1/1	0.88	0.15	100,100,100,100	0
3	NA	B	1101	1/1	0.95	0.56	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.