



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 08:01 AM EDT

PDB ID : 3SZM
Title : STRUCTURE OF HUMAN MICROCEPHALIN (MCPH1) TANDEM BRCT DOMAINS IN COMPLEX WITH A GAMMA-H2AX PHOSPHOPEPTIDE
Authors : Singh, N.; Thompson, J.R.; Mer, G.
Deposited on : 2011-07-19
Resolution : 2.63 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

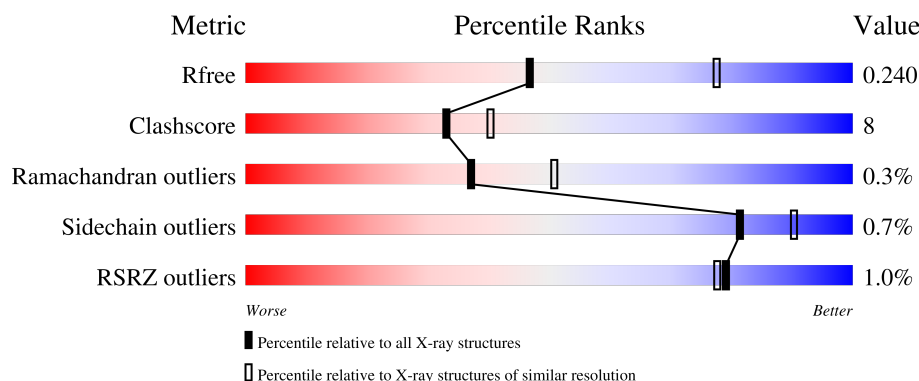
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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}	164625	1851 (2.66-2.62)
Clashscore	180529	1953 (2.66-2.62)
Ramachandran outliers	177936	1929 (2.66-2.62)
Sidechain outliers	177891	1929 (2.66-2.62)
RSRZ outliers	164620	1850 (2.66-2.62)

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	199	
1	B	199	
1	C	199	
1	D	199	
1	E	199	

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Mol	Chain	Length	Quality of chain
1	F	199	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>80%15%5%</div></div></div>
1	G	199	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>80%16%</div></div></div>
1	H	199	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>81%15%5%</div></div></div>
2	I	10	<div><div><div></div><div></div><div></div></div><div>50%10%40%</div></div>
2	J	10	<div><div><div></div><div></div><div></div></div><div>40%10%10%40%</div></div>
2	K	10	<div><div><div></div><div></div><div></div></div><div>40%10%50%</div></div>
2	L	10	<div><div><div></div><div></div><div></div></div><div>40%10%10%40%</div></div>
2	M	10	<div><div><div></div><div></div><div></div></div><div>50%10%40%</div></div>
2	N	10	<div><div><div></div><div></div><div></div></div><div>50%10%40%</div></div>
2	O	10	<div><div><div></div><div></div><div></div></div><div>50%10%40%</div></div>
2	P	10	<div><div><div></div><div></div><div></div></div><div>40%10%50%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24877 atoms, of which 12249 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 Microcephalin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	189	Total	C	H	N	O	S	0	1	0
			2956	946	1488	249	263	10			
1	B	189	Total	C	H	N	O	S	0	1	0
			2958	948	1488	249	262	11			
1	C	191	Total	C	H	N	O	S	0	0	0
			2996	956	1513	253	264	10			
1	D	189	Total	C	H	N	O	S	0	2	0
			2964	952	1488	249	264	11			
1	E	187	Total	C	H	N	O	S	0	3	0
			2937	945	1472	247	262	11			
1	F	189	Total	C	H	N	O	S	0	3	0
			2971	955	1490	251	265	10			
1	G	191	Total	C	H	N	O	S	0	1	0
			3003	960	1514	253	266	10			
1	H	190	Total	C	H	N	O	S	0	2	0
			2982	956	1500	251	264	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	637	GLY	-	expression tag	UNP Q8NEM0
A	638	HIS	-	expression tag	UNP Q8NEM0
A	639	MET	-	expression tag	UNP Q8NEM0
B	637	GLY	-	expression tag	UNP Q8NEM0
B	638	HIS	-	expression tag	UNP Q8NEM0
B	639	MET	-	expression tag	UNP Q8NEM0
C	637	GLY	-	expression tag	UNP Q8NEM0
C	638	HIS	-	expression tag	UNP Q8NEM0
C	639	MET	-	expression tag	UNP Q8NEM0
D	637	GLY	-	expression tag	UNP Q8NEM0
D	638	HIS	-	expression tag	UNP Q8NEM0
D	639	MET	-	expression tag	UNP Q8NEM0
E	637	GLY	-	expression tag	UNP Q8NEM0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	638	HIS	-	expression tag	UNP Q8NEM0
E	639	MET	-	expression tag	UNP Q8NEM0
F	637	GLY	-	expression tag	UNP Q8NEM0
F	638	HIS	-	expression tag	UNP Q8NEM0
F	639	MET	-	expression tag	UNP Q8NEM0
G	637	GLY	-	expression tag	UNP Q8NEM0
G	638	HIS	-	expression tag	UNP Q8NEM0
G	639	MET	-	expression tag	UNP Q8NEM0
H	637	GLY	-	expression tag	UNP Q8NEM0
H	638	HIS	-	expression tag	UNP Q8NEM0
H	639	MET	-	expression tag	UNP Q8NEM0

- Molecule 2 is a protein called Histone H2A.x.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	I	6	Total	C	H	N	O	P	0	0	0
			94	30	39	8	16	1			
2	J	6	Total	C	H	N	O	P	0	0	0
			94	30	39	8	16	1			
2	K	5	Total	C	H	N	O	P	0	0	0
			77	25	31	6	14	1			
2	L	6	Total	C	H	N	O	P	0	0	0
			94	30	39	8	16	1			
2	M	6	Total	C	H	N	O	P	0	0	0
			94	30	39	8	16	1			
2	N	6	Total	C	H	N	O	P	0	0	0
			94	30	39	8	16	1			
2	O	6	Total	C	H	N	O	P	0	0	0
			94	30	39	8	16	1			
2	P	5	Total	C	H	N	O	P	0	0	0
			77	25	31	6	14	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	56	Total	O	0	0
			56	56		
3	B	27	Total	O	0	0
			27	27		
3	C	48	Total	O	0	0
			48	48		
3	D	38	Total	O	0	0
			38	38		

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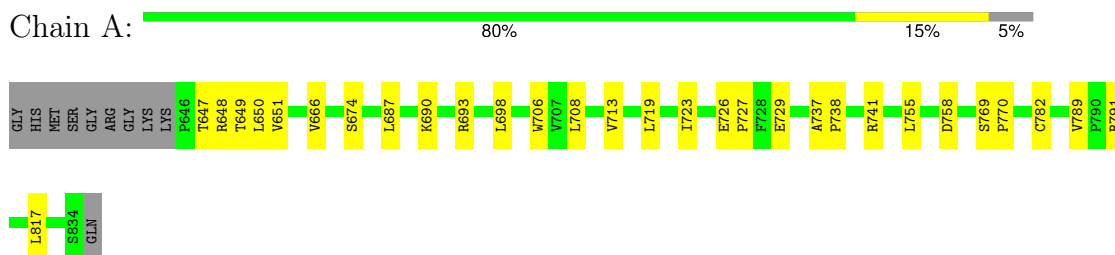
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	37	Total 37	O 37	0	0
3	F	48	Total 48	O 48	0	0
3	G	65	Total 65	O 65	0	0
3	H	38	Total 38	O 38	0	0
3	I	5	Total 5	O 5	0	0
3	J	4	Total 4	O 4	0	0
3	K	2	Total 2	O 2	0	0
3	L	5	Total 5	O 5	0	0
3	M	1	Total 1	O 1	0	0
3	N	6	Total 6	O 6	0	0
3	O	8	Total 8	O 8	0	0
3	P	4	Total 4	O 4	0	0

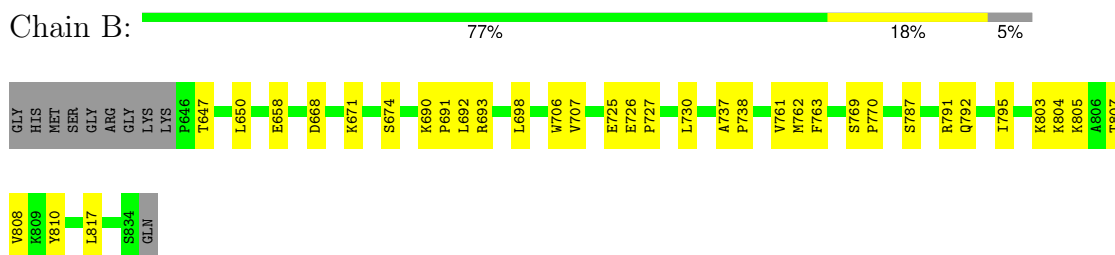
3 Residue-property plots [i](#)

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.

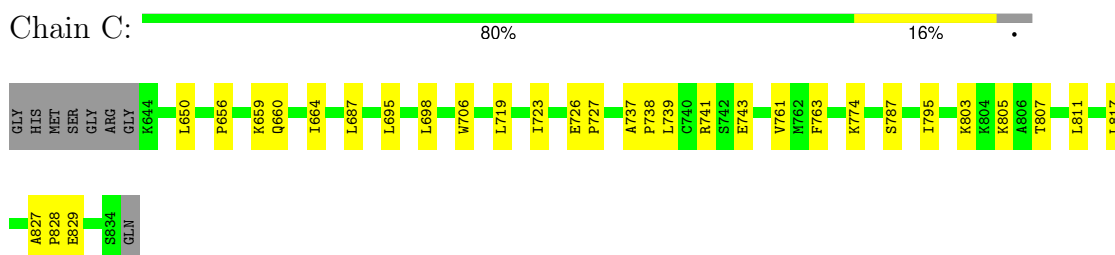
- Molecule 1: Microcephalin



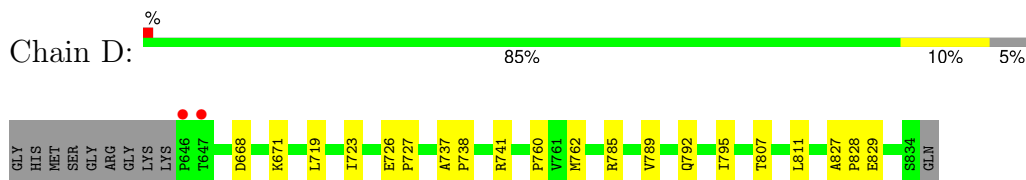
- Molecule 1: Microcephalin



- Molecule 1: Microcephalin

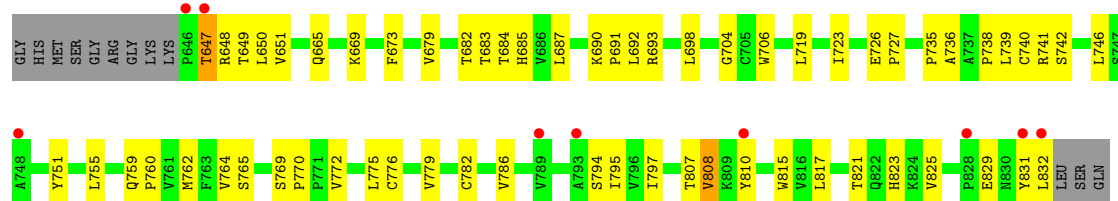


- Molecule 1: Microcephalin




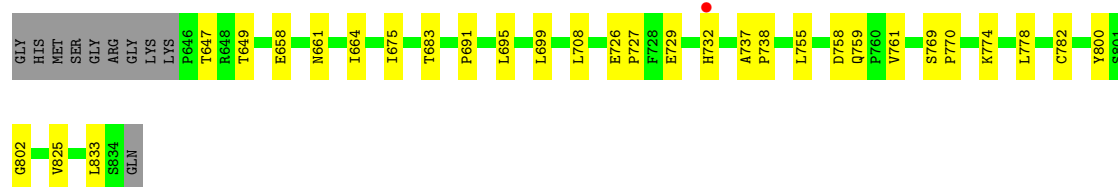
- Molecule 1: Microcephalin

Chain E: 




• Molecule 1: Microcephalin

Chain F: 




• Molecule 1: Microcephalin

Chain G: 



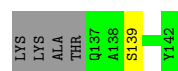
• Molecule 1: Microcephalin

Chain H: 



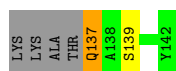
• Molecule 2: Histone H2A.x

Chain I: 



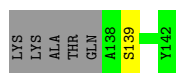
• Molecule 2: Histone H2A.x

Chain J: 



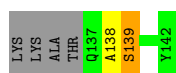
● Molecule 2: Histone H2A.x

Chain K: 



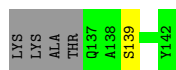
● Molecule 2: Histone H2A.x

Chain L: 



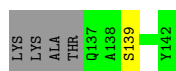
● Molecule 2: Histone H2A.x

Chain M: 



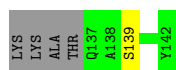
● Molecule 2: Histone H2A.x

Chain N: 



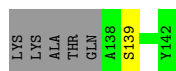
● Molecule 2: Histone H2A.x

Chain O: 



● Molecule 2: Histone H2A.x

Chain P: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.81Å 82.23Å 104.42Å 72.10° 89.87° 80.94°	Depositor
Resolution (Å)	31.37 – 2.63 31.37 – 2.63	Depositor EDS
% Data completeness (in resolution range)	89.7 (31.37-2.63) 89.7 (31.37-2.63)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.1_357)	Depositor
R, R_{free}	0.201 , 0.252 0.199 , 0.240	Depositor DCC
R_{free} test set	572 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 69.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24877	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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

5.1 Standard geometry

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

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	0.44	0/1512	0.54	0/2062
1	B	0.44	0/1514	0.52	0/2064
1	C	0.44	0/1524	0.56	0/2077
1	D	0.46	0/1523	0.58	0/2077
1	E	0.45	0/1515	0.58	0/2066
1	F	0.45	0/1532	0.57	0/2089
1	G	0.55	0/1533	0.59	0/2089
1	H	0.44	0/1529	0.56	0/2084
2	I	0.59	0/44	0.42	0/55
2	J	1.04	0/44	0.64	0/55
2	K	0.35	0/35	0.43	0/43
2	L	0.48	0/44	0.46	0/55
2	M	0.52	0/44	0.56	0/55
2	N	0.99	0/44	0.57	0/55
2	O	0.45	0/44	0.48	0/55
2	P	0.49	0/35	0.41	0/43
All	All	0.47	0/12516	0.56	0/17024

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

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	1468	1488	1493	23	0
1	B	1470	1488	1497	24	0
1	C	1483	1513	1513	23	0
1	D	1476	1488	1503	15	0
1	E	1465	1472	1492	54	0
1	F	1481	1490	1506	18	0
1	G	1489	1514	1519	19	0
1	H	1482	1500	1514	20	0
2	I	55	39	39	0	0
2	J	55	39	39	2	0
2	K	46	31	31	0	0
2	L	55	39	39	1	0
2	M	55	39	39	0	0
2	N	55	39	39	0	0
2	O	55	39	39	0	0
2	P	46	31	30	0	0
3	A	56	0	0	1	0
3	B	27	0	0	0	0
3	C	48	0	0	0	0
3	D	38	0	0	2	0
3	E	37	0	0	5	0
3	F	48	0	0	2	0
3	G	65	0	0	1	0
3	H	38	0	0	0	0
3	I	5	0	0	0	0
3	J	4	0	0	0	0
3	K	2	0	0	0	0
3	L	5	0	0	0	0
3	M	1	0	0	0	0
3	N	6	0	0	0	0
3	O	8	0	0	0	0
3	P	4	0	0	0	0
All	All	12628	12249	12332	189	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 8.

All (189) 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:D:668:ASP:O	1:D:671:LYS:HE2	1.79	0.83
1:C:719:LEU:HD13	1:D:726[B]:GLU:HG2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:726[B]:GLU:HG2	1:H:719:LEU:HD13	1.65	0.79
1:B:792:GLN:HG2	1:D:785:ARG:HB2	1.65	0.76
1:E:693:ARG:HH11	1:E:821:THR:HG21	1.51	0.75
1:B:668:ASP:O	1:B:671:LYS:HE2	1.89	0.71
1:C:803:LYS:HE3	1:C:805:LYS:HE2	1.71	0.71
1:G:660:GLN:O	1:G:664:ILE:HG12	1.90	0.70
1:C:737:ALA:HB3	1:C:738:PRO:HD3	1.74	0.70
2:J:137:GLN:HE21	2:J:137:GLN:N	1.91	0.69
1:E:673:PHE:HZ	1:E:685:HIS:HD1	1.41	0.68
1:H:706:TRP:CH2	1:H:741:ARG:HD2	2.30	0.66
1:C:660:GLN:O	1:C:664:ILE:HG12	1.96	0.66
1:E:776:CYS:SG	1:E:786:VAL:HG11	2.36	0.66
1:D:789:VAL:HB	1:D:792:GLN:HG3	1.78	0.66
1:D:726[A]:GLU:HG2	1:D:727:PRO:HD3	1.78	0.65
1:C:811:LEU:HD21	1:C:828:PRO:HB3	1.78	0.64
1:G:681[B]:GLU:H	1:G:681[B]:GLU:CD	2.00	0.64
1:C:664:ILE:HG13	1:F:664:ILE:HG13	1.79	0.64
1:B:690:LYS:HE3	1:B:692:LEU:HD11	1.81	0.63
1:D:741:ARG:HG2	3:D:59:HOH:O	1.98	0.63
1:C:795:ILE:CG2	1:C:811:LEU:HD12	2.29	0.62
1:B:726:GLU:N	1:B:727:PRO:HD2	2.13	0.62
1:G:658:GLU:O	1:G:661:ASN:HB3	2.02	0.60
1:G:733:HIS:HD2	3:G:137:HOH:O	1.85	0.60
1:E:794:SER:HA	1:E:808:VAL:HG13	1.84	0.60
1:E:690:LYS:HG3	1:E:691:PRO:HD2	1.83	0.59
1:F:664:ILE:HD13	1:F:675:ILE:HD12	1.84	0.58
1:D:807:THR:HB	3:D:339:HOH:O	2.02	0.58
1:D:827:ALA:HB1	1:D:829:GLU:OE1	2.05	0.57
1:E:719:LEU:HD12	1:E:723:ILE:HG21	1.86	0.57
1:G:668:ASP:O	1:G:671:LYS:HE2	2.04	0.57
1:D:719:LEU:HD12	1:D:723:ILE:HG21	1.86	0.56
1:E:673:PHE:HZ	1:E:685:HIS:ND1	2.04	0.56
1:E:736:ALA:CB	1:E:823:HIS:HB2	2.36	0.56
1:G:803:LYS:HD3	1:G:805:LYS:HD3	1.88	0.56
1:E:738:PRO:HA	1:E:741:ARG:HE	1.70	0.55
1:F:758:ASP:HA	1:H:792:GLN:HG2	1.87	0.55
1:A:791:ARG:HD3	1:G:760:PRO:HG3	1.88	0.55
1:B:807:THR:HG21	1:D:792:GLN:HA	1.88	0.55
1:B:690:LYS:HG3	1:B:691:PRO:HD2	1.87	0.55
1:H:737:ALA:HB3	1:H:738:PRO:CD	2.37	0.54
1:B:737:ALA:N	1:B:738:PRO:HD2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:817:LEU:O	1:E:821:THR:HG23	2.07	0.54
1:E:649:THR:N	1:E:682:THR:HG22	2.23	0.54
1:E:755:LEU:HB3	1:E:782:CYS:HB3	1.90	0.54
1:D:811:LEU:HD21	1:D:828:PRO:HB3	1.89	0.53
1:A:758:ASP:HB2	3:A:17:HOH:O	2.08	0.53
1:C:719:LEU:HD12	1:C:723:ILE:HG21	1.90	0.53
1:E:829:GLU:HB2	3:E:335:HOH:O	2.07	0.53
1:A:726:GLU:N	1:A:727:PRO:CD	2.71	0.53
1:B:762[A]:MET:HG2	1:B:795:ILE:HB	1.89	0.53
1:A:719:LEU:HD12	1:A:723:ILE:HG21	1.91	0.53
1:E:649:THR:OG1	1:E:683:THR:CA	2.57	0.53
1:E:649:THR:OG1	1:E:683:THR:N	2.42	0.52
1:B:761:VAL:CG1	1:B:787:SER:HB2	2.39	0.52
1:C:706:TRP:CZ3	1:C:741:ARG:HD2	2.44	0.52
1:E:649:THR:OG1	1:E:683:THR:HA	2.10	0.52
1:C:706:TRP:CH2	1:C:741:ARG:HD2	2.45	0.52
1:B:693:ARG:HD2	1:B:698:LEU:HD21	1.92	0.51
1:H:797:ILE:HD13	1:H:811:LEU:HB2	1.92	0.51
1:E:698:LEU:HD13	1:E:817:LEU:HD22	1.92	0.51
1:E:762[B]:MET:HG2	1:E:795:ILE:HB	1.92	0.50
1:E:739:LEU:HD23	1:E:739:LEU:N	2.26	0.50
1:F:761:VAL:HG21	1:H:807:THR:HG21	1.93	0.50
1:B:804:LYS:HA	1:B:810:TYR:OH	2.12	0.50
1:E:690:LYS:HE3	1:E:692:LEU:HD11	1.93	0.50
1:G:708:LEU:HD21	1:G:725:GLU:HB3	1.94	0.50
1:E:764:VAL:HB	1:E:772:VAL:HG23	1.93	0.49
1:G:800:TYR:CZ	1:G:802:GLY:HA3	2.47	0.49
1:F:800:TYR:CZ	1:F:802:GLY:HA3	2.48	0.49
1:C:650:LEU:HD21	1:C:687:LEU:HD12	1.93	0.49
1:E:738:PRO:O	1:E:741:ARG:HG3	2.13	0.49
1:H:719:LEU:HD12	1:H:723:ILE:HG21	1.94	0.49
1:A:650:LEU:HD11	1:A:687:LEU:HD11	1.94	0.48
1:C:795:ILE:HG23	1:C:811:LEU:HD12	1.93	0.48
1:A:706:TRP:CH2	1:A:741:ARG:HD2	2.48	0.48
1:C:698:LEU:HD13	1:C:817:LEU:HD22	1.95	0.48
1:D:762[A]:MET:HE3	1:D:795:ILE:HG21	1.95	0.48
1:F:737:ALA:HB3	1:F:738:PRO:HD3	1.95	0.48
1:B:726:GLU:N	1:B:727:PRO:CD	2.77	0.48
1:C:650:LEU:HD11	1:C:687:LEU:HD11	1.96	0.48
1:F:649:THR:OG1	1:F:683:THR:HA	2.14	0.48
1:C:706:TRP:CZ3	1:C:741:ARG:CD	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:751:TYR:HA	3:E:334:HOH:O	2.13	0.48
1:F:732[A]:HIS:HB3	3:F:82:HOH:O	2.14	0.47
1:E:665:GLN:O	1:E:669:LYS:HG2	2.14	0.47
1:F:695:LEU:HD21	1:F:774:LYS:HG3	1.96	0.47
1:A:693:ARG:HD2	1:A:698:LEU:HD21	1.97	0.47
2:L:138:ALA:O	2:L:139:SEP:C	2.61	0.47
1:G:698:LEU:HD13	1:G:817:LEU:HD22	1.97	0.47
1:G:664:ILE:HD13	1:G:664:ILE:N	2.30	0.47
1:A:737:ALA:HB3	1:A:738:PRO:HD3	1.95	0.47
1:B:769:SER:HA	1:B:770:PRO:C	2.34	0.47
1:H:706:TRP:CZ3	1:H:741:ARG:CD	2.98	0.46
1:E:815:TRP:HD1	1:E:831:TYR:CD1	2.33	0.46
1:G:719:LEU:HD12	1:G:723:ILE:HG21	1.98	0.46
1:A:649:THR:HA	1:A:674:SER:O	2.16	0.46
1:E:693:ARG:CD	1:E:821:THR:HG21	2.46	0.46
1:A:698:LEU:HD13	1:A:817:LEU:HD22	1.98	0.45
1:E:651:VAL:HG21	1:E:679:VAL:HA	1.98	0.45
1:C:695:LEU:HD21	1:C:774:LYS:HG3	1.97	0.45
1:E:815:TRP:HD1	1:E:831:TYR:HD1	1.63	0.45
1:B:698:LEU:HD13	1:B:817:LEU:HD22	1.98	0.45
1:H:726:GLU:N	1:H:727:PRO:CD	2.79	0.45
1:A:737:ALA:N	1:A:738:PRO:HD2	2.31	0.45
1:E:759:GLN:HG2	3:E:350:HOH:O	2.16	0.45
1:B:761:VAL:HG11	1:B:787:SER:HB2	1.97	0.45
1:E:650:LEU:HD21	1:E:687:LEU:HD12	1.99	0.44
1:B:706:TRP:CE2	1:B:725:GLU:HG3	2.52	0.44
1:H:698:LEU:HD13	1:H:817:LEU:HD22	1.99	0.44
1:H:737:ALA:N	1:H:738:PRO:HD2	2.32	0.44
1:D:762[B]:MET:HG2	1:D:795:ILE:HB	2.00	0.44
1:E:741:ARG:HD2	1:E:742:SER:N	2.33	0.44
1:E:815:TRP:HA	1:E:831:TYR:CE1	2.52	0.44
1:F:833:LEU:HD12	3:F:284:HOH:O	2.18	0.44
1:E:769:SER:HA	1:E:770:PRO:C	2.37	0.44
1:A:666:VAL:HG21	1:A:713:VAL:HG13	2.00	0.44
1:A:713:VAL:O	1:A:713:VAL:CG1	2.66	0.44
1:B:650:LEU:C	1:B:650:LEU:HD23	2.37	0.44
1:D:737:ALA:N	1:D:738:PRO:HD2	2.33	0.44
1:E:719:LEU:HD12	1:E:723:ILE:CG2	2.48	0.44
1:G:803:LYS:CD	1:G:805:LYS:HD3	2.48	0.44
2:J:137:GLN:N	2:J:137:GLN:NE2	2.63	0.44
1:A:650:LEU:HD23	1:A:650:LEU:C	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:VAL:HG12	1:A:791:ARG:H	1.83	0.44
1:H:769:SER:HA	1:H:770:PRO:C	2.37	0.44
1:H:827:ALA:HB1	1:H:829:GLU:OE2	2.18	0.43
1:C:763:PHE:HD1	1:C:787:SER:O	2.01	0.43
1:E:765:SER:HB2	1:E:797:ILE:O	2.18	0.43
1:E:648:ARG:HA	1:E:682:THR:HG22	1.99	0.43
1:E:704:GLY:HA2	1:E:740:CYS:HB3	1.99	0.43
1:E:738:PRO:HA	1:E:741:ARG:CG	2.49	0.43
1:E:742:SER:O	1:E:746:LEU:HG	2.18	0.43
1:E:794:SER:C	1:E:808:VAL:CG1	2.86	0.43
1:E:832:LEU:HD11	3:E:192:HOH:O	2.17	0.43
1:B:763:PHE:HD1	1:B:787:SER:O	2.01	0.43
1:C:739:LEU:O	1:C:743:GLU:HG3	2.18	0.43
1:E:685:HIS:CD2	1:E:706:TRP:HB2	2.53	0.43
1:A:647:THR:HG22	1:A:648:ARG:N	2.34	0.43
1:A:737:ALA:HB3	1:A:738:PRO:CD	2.49	0.43
1:B:707:VAL:HG12	1:B:730:LEU:HD12	2.01	0.43
1:C:827:ALA:HB1	1:C:829:GLU:OE2	2.19	0.43
1:F:699:LEU:HD23	1:F:778:LEU:CD2	2.49	0.43
1:F:708:LEU:HD23	1:F:729:GLU:HA	1.99	0.42
1:C:656:PRO:HD2	1:C:659:LYS:HD2	2.01	0.42
1:H:711:ASP:HB2	1:H:728:PHE:CD2	2.55	0.42
1:E:825:VAL:HG21	3:E:350:HOH:O	2.19	0.42
1:F:759:GLN:NE2	1:F:825:VAL:HG11	2.35	0.42
1:B:791:ARG:HG2	1:D:760:PRO:HA	2.01	0.42
1:B:725:GLU:C	1:B:727:PRO:HD2	2.40	0.42
1:A:706:TRP:CE3	1:A:741:ARG:HD3	2.55	0.42
1:A:706:TRP:CZ3	1:A:741:ARG:CD	3.03	0.42
1:E:726[B]:GLU:OE2	1:H:721:HIS:NE2	2.50	0.42
1:E:810:TYR:O	1:E:832:LEU:HD23	2.19	0.42
1:F:755:LEU:HB3	1:F:782:CYS:HB3	2.02	0.41
1:G:647:THR:O	1:G:648:ARG:C	2.59	0.41
1:E:650:LEU:C	1:E:650:LEU:HD23	2.40	0.41
1:H:737:ALA:HB3	1:H:738:PRO:HD3	2.03	0.41
1:A:708:LEU:HD23	1:A:729:GLU:HA	2.02	0.41
1:C:761:VAL:HG11	1:C:787:SER:HB2	2.01	0.41
1:A:755:LEU:HB3	1:A:782:CYS:HB3	2.02	0.41
1:E:760:PRO:HB2	1:E:794:SER:HB3	2.03	0.41
1:F:737:ALA:HB3	1:F:738:PRO:CD	2.50	0.41
1:F:769:SER:HA	1:F:770:PRO:C	2.40	0.41
1:G:695:LEU:HD21	1:G:774:LYS:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:SER:HA	1:A:770:PRO:C	2.41	0.41
1:E:775:LEU:O	1:E:779:VAL:HG23	2.20	0.41
1:C:726:GLU:N	1:C:727:PRO:CD	2.84	0.41
1:F:658:GLU:O	1:F:661:ASN:HB3	2.21	0.41
1:G:645:LYS:HA	1:G:646:PRO:HD3	1.85	0.41
1:H:659:LYS:HG2	1:H:710:TYR:CZ	2.56	0.41
1:H:660:GLN:O	1:H:661:ASN:C	2.59	0.41
1:G:827:ALA:HA	1:G:828:PRO:HD3	1.91	0.41
1:E:648:ARG:HA	1:E:682:THR:CG2	2.51	0.40
1:F:726:GLU:N	1:F:727:PRO:CD	2.84	0.40
1:G:726:GLU:N	1:G:727:PRO:CD	2.84	0.40
1:B:737:ALA:HB3	1:B:738:PRO:HD3	2.03	0.40
1:B:805:LYS:HB2	1:B:808:VAL:HG23	2.02	0.40
1:C:795:ILE:HG21	1:C:811:LEU:HD12	2.04	0.40
1:B:658:GLU:H	1:B:658:GLU:CD	2.25	0.40
1:G:694:THR:OG1	1:G:697:VAL:HG23	2.21	0.40
1:H:772:VAL:HG13	1:H:773:ALA:N	2.36	0.40
1:E:735:PRO:O	1:E:738:PRO:HD2	2.21	0.40
1:H:811:LEU:HA	1:H:831:TYR:O	2.21	0.40
1:A:650:LEU:HD23	1:A:651:VAL:N	2.37	0.40
1:E:647:THR:O	1:E:682:THR:HG23	2.22	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	188/199 (94%)	176 (94%)	12 (6%)	0	100	100
1	B	188/199 (94%)	179 (95%)	8 (4%)	1 (0%)	25	37
1	C	189/199 (95%)	186 (98%)	3 (2%)	0	100	100
1	D	189/199 (95%)	184 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	188/199 (94%)	180 (96%)	8 (4%)	0	100	100
1	F	190/199 (96%)	184 (97%)	4 (2%)	2 (1%)	12	17
1	G	190/199 (96%)	186 (98%)	4 (2%)	0	100	100
1	H	190/199 (96%)	184 (97%)	5 (3%)	1 (0%)	25	37
2	I	3/10 (30%)	3 (100%)	0	0	100	100
2	J	3/10 (30%)	3 (100%)	0	0	100	100
2	K	2/10 (20%)	2 (100%)	0	0	100	100
2	L	3/10 (30%)	3 (100%)	0	0	100	100
2	M	3/10 (30%)	3 (100%)	0	0	100	100
2	N	3/10 (30%)	3 (100%)	0	0	100	100
2	O	3/10 (30%)	3 (100%)	0	0	100	100
2	P	2/10 (20%)	2 (100%)	0	0	100	100
All	All	1534/1672 (92%)	1481 (96%)	49 (3%)	4 (0%)	37	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	647	THR
1	F	647	THR
1	F	691	PRO
1	H	691	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	168/174 (97%)	167 (99%)	1 (1%)	84	92
1	B	168/174 (97%)	166 (99%)	2 (1%)	67	82
1	C	169/174 (97%)	168 (99%)	1 (1%)	84	92
1	D	169/174 (97%)	169 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	168/174 (97%)	164 (98%)	4 (2%)	44	64
1	F	170/174 (98%)	170 (100%)	0	100	100
1	G	170/174 (98%)	170 (100%)	0	100	100
1	H	170/174 (98%)	170 (100%)	0	100	100
2	I	4/7 (57%)	4 (100%)	0	100	100
2	J	4/7 (57%)	3 (75%)	1 (25%)	0	0
2	K	3/7 (43%)	3 (100%)	0	100	100
2	L	4/7 (57%)	4 (100%)	0	100	100
2	M	4/7 (57%)	4 (100%)	0	100	100
2	N	4/7 (57%)	4 (100%)	0	100	100
2	O	4/7 (57%)	4 (100%)	0	100	100
2	P	3/7 (43%)	3 (100%)	0	100	100
All	All	1382/1448 (95%)	1373 (99%)	9 (1%)	81	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	690	LYS
1	B	674	SER
1	B	803	LYS
1	C	807	THR
1	E	647	THR
1	E	684	THR
1	E	807	THR
1	E	808	VAL
2	J	137	GLN

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

Mol	Chain	Res	Type
1	C	665	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SEP	P	139	2	8,9,10	1.46	1 (12%)	7,12,14	1.40	2 (28%)
2	SEP	I	139	2	8,9,10	1.62	1 (12%)	7,12,14	1.04	0
2	SEP	K	139	2	8,9,10	1.79	2 (25%)	7,12,14	1.22	1 (14%)
2	SEP	O	139	2	8,9,10	1.52	2 (25%)	7,12,14	0.72	0
2	SEP	J	139	2	8,9,10	1.64	1 (12%)	7,12,14	0.63	0
2	SEP	N	139	2	8,9,10	1.62	1 (12%)	7,12,14	1.11	1 (14%)
2	SEP	M	139	2	8,9,10	1.61	1 (12%)	7,12,14	2.18	2 (28%)
2	SEP	L	139	2	8,9,10	1.40	1 (12%)	7,12,14	1.18	1 (14%)

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	SEP	P	139	2	-	0/6/8/10	-
2	SEP	I	139	2	-	0/6/8/10	-
2	SEP	K	139	2	-	0/6/8/10	-
2	SEP	O	139	2	-	0/6/8/10	-
2	SEP	J	139	2	-	0/6/8/10	-
2	SEP	N	139	2	-	0/6/8/10	-
2	SEP	M	139	2	-	2/6/8/10	-
2	SEP	L	139	2	-	4/6/8/10	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	139	SEP	P-O1P	3.84	1.62	1.50
2	J	139	SEP	P-O1P	3.76	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	139	SEP	P-O1P	3.70	1.62	1.50
2	M	139	SEP	P-O1P	3.64	1.61	1.50
2	N	139	SEP	P-O1P	3.54	1.61	1.50
2	O	139	SEP	P-O1P	3.21	1.60	1.50
2	L	139	SEP	P-O1P	3.15	1.60	1.50
2	P	139	SEP	P-O1P	2.95	1.59	1.50
2	O	139	SEP	P-O2P	2.14	1.62	1.54
2	K	139	SEP	P-O3P	2.13	1.62	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	139	SEP	OG-CB-CA	5.01	113.02	108.14
2	P	139	SEP	OG-CB-CA	2.53	110.61	108.14
2	L	139	SEP	OG-CB-CA	2.45	110.53	108.14
2	M	139	SEP	O2P-P-OG	2.43	113.00	106.67
2	K	139	SEP	OG-CB-CA	2.32	110.40	108.14
2	P	139	SEP	OG-P-O1P	2.11	112.15	106.44
2	N	139	SEP	OG-CB-CA	2.07	110.16	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	139	SEP	C-CA-CB-OG
2	L	139	SEP	CB-OG-P-O1P
2	M	139	SEP	N-CA-CB-OG
2	M	139	SEP	C-CA-CB-OG
2	L	139	SEP	N-CA-CB-OG
2	L	139	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	139	SEP	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	189/199 (94%)	-0.32	0 100 100	39, 65, 104, 128	1 (0%)
1	B	189/199 (94%)	-0.09	0 100 100	41, 74, 123, 138	1 (0%)
1	C	191/199 (95%)	-0.20	0 100 100	40, 63, 108, 124	0
1	D	189/199 (94%)	-0.13	2 (1%) 77 76	32, 63, 125, 141	2 (1%)
1	E	187/199 (93%)	0.37	9 (4%) 36 35	35, 94, 151, 185	3 (1%)
1	F	189/199 (94%)	-0.38	1 (0%) 87 86	32, 55, 93, 124	3 (1%)
1	G	191/199 (95%)	-0.38	2 (1%) 79 78	29, 54, 102, 138	1 (0%)
1	H	190/199 (95%)	-0.13	2 (1%) 77 76	41, 66, 108, 125	2 (1%)
2	I	5/10 (50%)	-0.26	0 100 100	41, 54, 72, 112	0
2	J	5/10 (50%)	-0.29	0 100 100	41, 51, 82, 106	0
2	K	4/10 (40%)	0.13	0 100 100	41, 58, 64, 79	0
2	L	5/10 (50%)	-0.36	0 100 100	36, 43, 67, 115	0
2	M	5/10 (50%)	-0.35	0 100 100	37, 50, 84, 116	0
2	N	5/10 (50%)	-0.34	0 100 100	40, 48, 70, 116	0
2	O	5/10 (50%)	-0.10	0 100 100	36, 43, 87, 115	0
2	P	4/10 (40%)	-0.17	0 100 100	48, 59, 76, 89	0
All	All	1553/1672 (92%)	-0.16	16 (1%) 79 78	29, 65, 121, 185	13 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	732[A]	HIS	4.8
1	G	833	LEU	3.2
1	E	646	PRO	3.0
1	G	830	ASN	3.0
1	E	789	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	793	ALA	2.5
1	D	646	PRO	2.4
1	H	807	THR	2.4
1	E	810	TYR	2.4
1	E	832	LEU	2.3
1	E	828	PRO	2.2
1	E	831	TYR	2.2
1	D	647	THR	2.1
1	H	761	VAL	2.1
1	E	748	ALA	2.1
1	E	647	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SEP	I	139	10/11	0.96	0.07	26,41,55,55	0
2	SEP	M	139	10/11	0.96	0.08	42,61,75,102	0
2	SEP	N	139	10/11	0.97	0.06	26,42,52,53	0
2	SEP	L	139	10/11	0.98	0.05	26,34,40,45	0
2	SEP	J	139	10/11	0.98	0.06	28,45,66,66	0
2	SEP	K	139	10/11	0.98	0.06	20,49,68,68	0
2	SEP	O	139	10/11	0.98	0.05	22,33,53,53	0
2	SEP	P	139	10/11	0.98	0.06	31,61,74,74	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.