



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 10:14 AM JST

PDB ID : 7VEC
Title : Crystal structure of GABARAP complexed with the TEX264 LIR phosphorylated at Ser271 and Ser272
Authors : Noda, N.N.
Deposited on : 2021-09-08
Resolution : 3.00 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

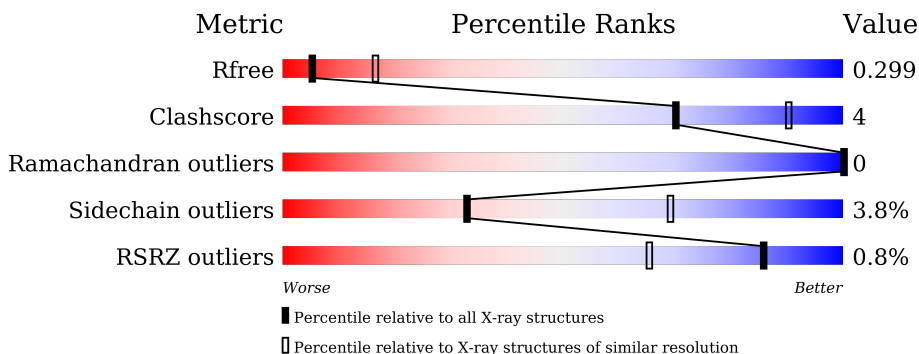
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.






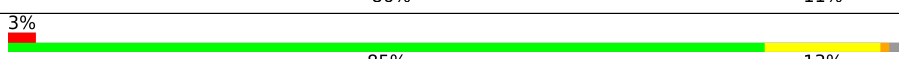
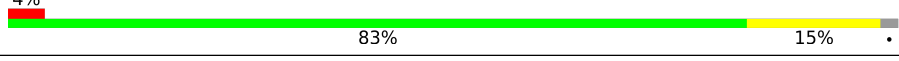



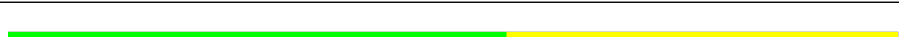



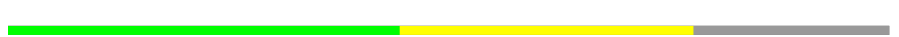
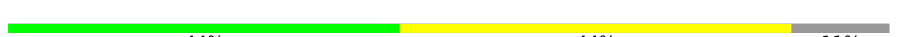


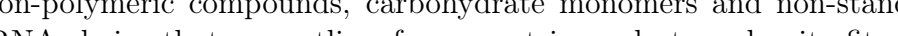
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	118	 84% 14% .
1	B	118	 88% 10% .
1	C	118	 88% 10% .
1	D	118	 81% 16% ..
1	E	118	 86% 12% .
1	F	118	 91% 7% .

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Mol	Chain	Length	Quality of chain
1	G	118	 86% 12%
1	H	118	 83% 14%
1	I	118	 86% 12%
1	J	118	 86% 11%
1	K	118	 85% 13%
1	L	118	 83% 15%
2	M	9	 56% 33% 11%
2	N	9	 67% 22% 11%
2	O	9	 56% 44%
2	P	9	 56% 33% 11%
2	Q	9	 56% 44%
2	R	9	 67% 22% 11%
2	S	9	 56% 33% 11%
2	T	9	 22% 78%
2	U	9	 44% 33% 22%
2	V	9	 44% 44% 11%
2	X	9	 33% 22% 44%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SEP	R	271	-	-	-	X
2	SEP	S	271	-	-	-	X
2	SEP	X	272	-	-	-	X

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 12376 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 Gamma-aminobutyric acid receptor-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	116	962	626	160	174	2	0	0	0
1	B	116	965	629	160	174	2	0	0	0
1	C	116	963	629	158	174	2	0	0	0
1	D	116	957	625	160	170	2	0	0	0
1	E	116	971	632	163	174	2	0	0	0
1	F	115	949	620	160	167	2	0	0	0
1	G	116	975	635	164	174	2	0	0	0
1	H	116	963	627	162	172	2	0	0	0
1	I	116	957	626	161	168	2	0	0	0
1	J	116	975	635	164	174	2	0	0	0
1	K	116	961	626	159	174	2	0	0	0
1	L	116	961	627	160	172	2	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O95166
A	0	PRO	-	expression tag	UNP O95166
B	-1	GLY	-	expression tag	UNP O95166
B	0	PRO	-	expression tag	UNP O95166
C	-1	GLY	-	expression tag	UNP O95166

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	PRO	-	expression tag	UNP O95166
D	-1	GLY	-	expression tag	UNP O95166
D	0	PRO	-	expression tag	UNP O95166
E	-1	GLY	-	expression tag	UNP O95166
E	0	PRO	-	expression tag	UNP O95166
F	-1	GLY	-	expression tag	UNP O95166
F	0	PRO	-	expression tag	UNP O95166
G	-1	GLY	-	expression tag	UNP O95166
G	0	PRO	-	expression tag	UNP O95166
H	-1	GLY	-	expression tag	UNP O95166
H	0	PRO	-	expression tag	UNP O95166
I	-1	GLY	-	expression tag	UNP O95166
I	0	PRO	-	expression tag	UNP O95166
J	-1	GLY	-	expression tag	UNP O95166
J	0	PRO	-	expression tag	UNP O95166
K	-1	GLY	-	expression tag	UNP O95166
K	0	PRO	-	expression tag	UNP O95166
L	-1	GLY	-	expression tag	UNP O95166
L	0	PRO	-	expression tag	UNP O95166

- Molecule 2 is a protein called TEX264 phospho-LIR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	8	Total	C	N	O	P	0	0	0
			73	41	8	22	2			
2	N	8	Total	C	N	O	P	0	0	0
			73	41	8	22	2			
2	O	9	Total	C	N	O	P	0	0	0
			85	50	9	24	2			
2	P	9	Total	C	N	O	P	0	0	0
			85	50	9	24	2			
2	Q	9	Total	C	N	O	P	0	0	0
			85	50	9	24	2			
2	R	8	Total	C	N	O	P	0	0	0
			73	41	8	22	2			
2	S	8	Total	C	N	O	P	0	0	0
			73	41	8	22	2			
2	T	9	Total	C	N	O	P	0	0	0
			85	50	9	24	2			
2	U	7	Total	C	N	O	P	0	0	0
			65	35	7	21	2			
2	V	8	Total	C	N	O	P	0	0	0
			73	41	8	22	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	X	5	47	28	5	13	1	0	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.

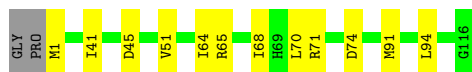
- Molecule 1: Gamma-aminobutyric acid receptor-associated protein

Chain A:  84% 14%




- Molecule 1: Gamma-aminobutyric acid receptor-associated protein

Chain B:  88% 10%




- Molecule 1: Gamma-aminobutyric acid receptor-associated protein

Chain C:  88% 10%




- Molecule 1: Gamma-aminobutyric acid receptor-associated protein

Chain D:  81% 16%




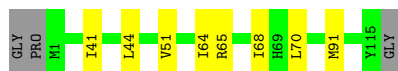
- Molecule 1: Gamma-aminobutyric acid receptor-associated protein

Chain E:  86% 12%

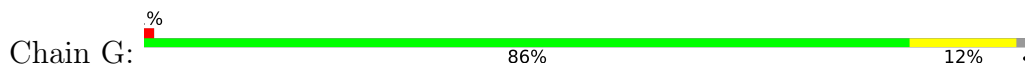


- Molecule 1: Gamma-aminobutyric acid receptor-associated protein

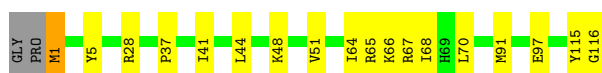
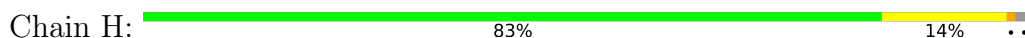
Chain F:  91% 7%



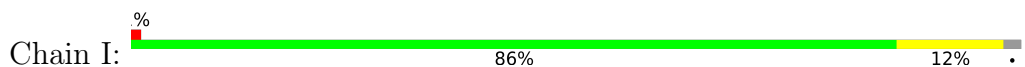
- Molecule 1: Gamma-aminobutyric acid receptor-associated protein



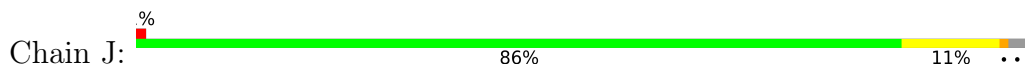
- Molecule 1: Gamma-aminobutyric acid receptor-associated protein



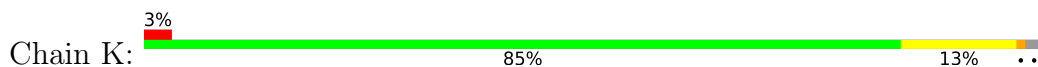
- Molecule 1: Gamma-aminobutyric acid receptor-associated protein



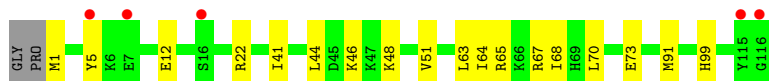
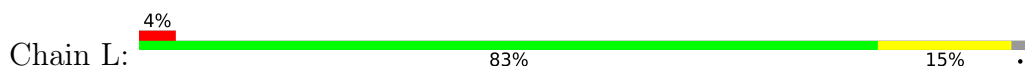
- Molecule 1: Gamma-aminobutyric acid receptor-associated protein



- Molecule 1: Gamma-aminobutyric acid receptor-associated protein



- Molecule 1: Gamma-aminobutyric acid receptor-associated protein



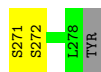
- Molecule 2: TEX264 phospho-LIR

Chain M:  56% 33% 11%



• Molecule 2: TEX264 phospho-LIR

Chain N:  67% 22% 11%



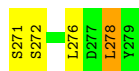
• Molecule 2: TEX264 phospho-LIR

Chain O:  56% 44%



• Molecule 2: TEX264 phospho-LIR

Chain P:  56% 33% 11%



• Molecule 2: TEX264 phospho-LIR

Chain Q:  56% 44%



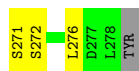
• Molecule 2: TEX264 phospho-LIR

Chain R:  67% 22% 11%

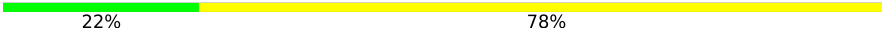


• Molecule 2: TEX264 phospho-LIR

Chain S:  56% 33% 11%



• Molecule 2: TEX264 phospho-LIR

Chain T:  22% 78%

S271
S272
F273
E274
E275
L276
D277
L278
Y279

- Molecule 2: TEX264 phospho-LIR

Chain U:  44% 33% 22%


S271
S272
L276
D277
LEU
TYR

- Molecule 2: TEX264 phospho-LIR

Chain V:  44% 44% 11%

S271
S272
F273
E274
D277
L278
TYR

- Molecule 2: TEX264 phospho-LIR

Chain X:  33% 22% 44%

SEP
S272
L276
ASP
LEU
TYR

4 Data and refinement statistics i

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	200.48Å 201.38Å 211.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.89 – 3.00 30.48 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (28.89-3.00) 98.2 (30.48-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.00Å)	Xtrriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.257 , 0.301 0.257 , 0.299	Depositor DCC
R_{free} test set	2284 reflections (5.34%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtrriage
Anisotropy	0.324	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.023 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	12376	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: 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	0.28	0/989	0.45	0/1335
1	B	0.27	0/992	0.46	0/1337
1	C	0.27	0/990	0.45	0/1334
1	D	0.28	0/984	0.47	0/1327
1	E	0.28	0/998	0.48	0/1344
1	F	0.27	0/975	0.44	0/1315
1	G	0.28	0/1002	0.45	0/1348
1	H	0.27	0/990	0.46	0/1335
1	I	0.27	0/984	0.44	0/1326
1	J	0.28	0/1002	0.48	0/1348
1	K	0.27	0/988	0.46	0/1333
1	L	0.27	0/988	0.44	0/1332
2	M	0.30	0/53	0.45	0/70
2	N	0.28	0/53	0.54	0/70
2	O	0.29	0/66	0.57	0/88
2	P	0.30	0/66	0.62	0/88
2	Q	0.24	0/66	0.37	0/88
2	R	0.28	0/53	0.51	0/70
2	S	0.30	0/53	0.50	0/70
2	T	0.31	0/66	0.55	0/88
2	U	0.33	0/45	0.67	0/59
2	V	0.28	0/53	0.56	0/70
2	X	0.28	0/37	0.36	0/48
All	All	0.27	0/12493	0.46	0/16823

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	962	0	928	8	0
1	B	965	0	944	4	0
1	C	963	0	944	5	0
1	D	957	0	936	10	0
1	E	971	0	955	6	0
1	F	949	0	937	4	0
1	G	975	0	966	7	0
1	H	963	0	940	9	0
1	I	957	0	943	8	0
1	J	975	0	966	10	0
1	K	961	0	933	10	0
1	L	961	0	940	10	0
2	M	73	0	55	1	0
2	N	73	0	55	0	0
2	O	85	0	64	1	0
2	P	85	0	64	1	0
2	Q	85	0	65	1	0
2	R	73	0	55	0	0
2	S	73	0	55	0	0
2	T	85	0	65	3	0
2	U	65	0	45	0	0
2	V	73	0	55	1	0
2	X	47	0	37	1	0
All	All	12376	0	11947	87	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 4.

All (87) 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:41:ILE:HD11	1:D:70:LEU:HD11	1.63	0.81
1:L:41:ILE:HD11	1:L:70:LEU:HD11	1.72	0.71
1:K:41:ILE:HG13	1:K:70:LEU:HD21	1.76	0.68
1:K:65:ARG:NH2	1:K:74:ASP:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:ARG:NH2	2:T:274:GLU:OE2	2.32	0.63
1:E:41:ILE:HD11	1:E:70:LEU:HD11	1.82	0.61
1:H:41:ILE:HD11	1:H:70:LEU:HD11	1.83	0.61
1:L:44:LEU:HD11	1:L:67:ARG:HB3	1.83	0.60
1:J:112:GLU:OE2	1:L:99:HIS:NE2	2.35	0.59
1:I:41:ILE:HD11	1:I:70:LEU:HD11	1.85	0.59
1:J:44:LEU:HD11	1:J:67:ARG:HB3	1.86	0.57
1:L:64:ILE:O	1:L:68:ILE:HG12	2.05	0.57
1:K:64:ILE:O	1:K:68:ILE:HG12	2.05	0.56
1:H:28:ARG:HH22	2:T:275:GLU:HB3	1.71	0.56
1:G:41:ILE:HD11	1:G:70:LEU:HD11	1.86	0.55
1:I:64:ILE:O	1:I:68:ILE:HG12	2.06	0.55
1:J:64:ILE:O	1:J:68:ILE:HG13	2.06	0.54
1:K:51:VAL:HG11	1:K:91:MET:HG3	1.88	0.54
1:E:64:ILE:O	1:E:68:ILE:HG12	2.07	0.54
1:C:41:ILE:HD11	1:C:70:LEU:HD11	1.89	0.54
1:B:41:ILE:HD11	1:B:70:LEU:HD11	1.90	0.53
1:H:64:ILE:O	1:H:68:ILE:HG12	2.08	0.53
1:K:41:ILE:CG1	1:K:70:LEU:HD21	2.38	0.53
1:L:63:LEU:HD13	2:X:276:LEU:HD13	1.89	0.53
1:G:64:ILE:O	1:G:68:ILE:HG12	2.07	0.53
1:B:51:VAL:HG11	1:B:91:MET:HG3	1.91	0.53
1:F:44:LEU:HD13	1:F:68:ILE:HG23	1.90	0.53
1:D:5:TYR:OH	1:D:48:LYS:HD3	2.09	0.52
1:F:64:ILE:O	1:F:68:ILE:HG12	2.10	0.52
1:D:64:ILE:O	1:D:68:ILE:HG12	2.10	0.52
1:I:44:LEU:HD13	1:I:68:ILE:HG23	1.91	0.52
1:B:64:ILE:O	1:B:68:ILE:HG12	2.09	0.52
1:E:51:VAL:HG11	1:E:91:MET:HG3	1.92	0.52
1:F:41:ILE:HD11	1:F:70:LEU:HD11	1.93	0.51
1:L:51:VAL:HG11	1:L:91:MET:HG3	1.92	0.51
1:A:48:LYS:HB3	2:M:273:PHE:CD1	2.46	0.51
1:I:51:VAL:HG11	1:I:91:MET:HG3	1.91	0.51
1:A:64:ILE:O	1:A:68:ILE:HG12	2.11	0.50
1:G:37:PRO:HG2	1:G:116:GLY:OXT	2.12	0.50
1:J:51:VAL:HG11	1:J:91:MET:HG3	1.92	0.50
1:A:51:VAL:HG11	1:A:91:MET:HG3	1.94	0.49
1:F:51:VAL:HG11	1:F:91:MET:HG3	1.95	0.49
1:C:64:ILE:O	1:C:68:ILE:HG13	2.13	0.48
1:K:44:LEU:HD13	1:K:68:ILE:HG23	1.95	0.48
1:J:112:GLU:CD	1:L:99:HIS:HE2	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:5:TYR:OH	1:J:48:LYS:HD3	2.14	0.47
1:C:28:ARG:NH1	2:O:277:ASP:OD1	2.48	0.46
1:C:44:LEU:HD11	1:C:67:ARG:HB3	1.97	0.46
1:C:51:VAL:HG11	1:C:91:MET:HG3	1.96	0.46
1:E:67:ARG:NH2	2:Q:274:GLU:OE2	2.50	0.45
1:J:67:ARG:NH2	2:V:274:GLU:OE2	2.25	0.45
1:H:44:LEU:HD13	1:H:68:ILE:HG23	1.98	0.45
1:A:41:ILE:HD11	1:A:70:LEU:HD11	1.99	0.44
1:B:71:ARG:HG3	1:B:74:ASP:OD2	2.17	0.44
1:J:66:LYS:HD2	1:J:66:LYS:HA	1.74	0.44
1:I:44:LEU:HD12	1:I:44:LEU:HA	1.83	0.44
1:G:70:LEU:HD23	1:G:70:LEU:HA	1.86	0.43
1:D:59:GLN:HG2	2:P:278:LEU:HD11	2.00	0.43
1:D:35:LYS:HG2	1:D:36:ALA:O	2.19	0.43
1:K:37:PRO:HG2	1:K:116:GLY:OXT	2.19	0.43
1:J:44:LEU:HD12	1:J:44:LEU:HA	1.71	0.42
1:K:44:LEU:HD11	1:K:67:ARG:HB3	2.01	0.42
1:D:51:VAL:HG11	1:D:91:MET:HG3	2.01	0.42
1:D:1:MET:HB3	1:D:115:TYR:CE2	2.55	0.42
1:D:37:PRO:HG2	1:D:116:GLY:OXT	2.19	0.42
1:H:5:TYR:OH	1:H:48:LYS:HD3	2.19	0.42
1:I:66:LYS:HD3	1:I:66:LYS:HA	1.74	0.42
2:T:278:LEU:HD23	2:T:278:LEU:HA	1.78	0.42
1:A:72:ALA:HB2	1:L:73:GLU:HG2	2.02	0.41
1:G:51:VAL:HG11	1:G:91:MET:HG3	2.02	0.41
1:A:44:LEU:HD13	1:A:68:ILE:HG23	2.01	0.41
1:D:77:PHE:O	1:D:109:TYR:HA	2.21	0.41
1:E:37:PRO:HG2	1:E:116:GLY:OXT	2.20	0.41
1:H:51:VAL:HG11	1:H:91:MET:HG3	2.01	0.41
1:H:37:PRO:HG2	1:H:116:GLY:OXT	2.21	0.41
1:I:37:PRO:HG2	1:I:116:GLY:OXT	2.20	0.41
1:I:46:LYS:HE3	1:I:46:LYS:HB3	1.93	0.41
1:D:44:LEU:HD11	1:D:67:ARG:HB3	2.02	0.41
1:E:5:TYR:OH	1:E:48:LYS:HD3	2.20	0.41
1:L:5:TYR:OH	1:L:48:LYS:HD3	2.21	0.41
1:G:5:TYR:OH	1:G:48:LYS:HD3	2.21	0.41
1:A:50:LEU:HD23	1:A:50:LEU:HA	1.99	0.40
1:J:114:VAL:HG22	1:L:22:ARG:HH21	1.86	0.40
1:K:70:LEU:HA	1:K:70:LEU:HD23	1.70	0.40
1:A:84:ILE:HB	1:G:26:PRO:HB3	2.04	0.40
1:K:25:TYR:HB3	1:K:28:ARG:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1:MET:HB3	1:H:115:TYR:CE2	2.56	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	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
1	B	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
1	C	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
1	D	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
1	E	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
1	F	113/118 (96%)	112 (99%)	1 (1%)	0	100	100
1	G	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
1	H	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
1	I	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
1	J	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
1	K	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
1	L	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
2	M	5/9 (56%)	5 (100%)	0	0	100	100
2	N	5/9 (56%)	5 (100%)	0	0	100	100
2	O	6/9 (67%)	6 (100%)	0	0	100	100
2	P	6/9 (67%)	6 (100%)	0	0	100	100
2	Q	6/9 (67%)	6 (100%)	0	0	100	100
2	R	5/9 (56%)	5 (100%)	0	0	100	100
2	S	5/9 (56%)	5 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	6/9 (67%)	6 (100%)	0	0	100	100
2	U	4/9 (44%)	4 (100%)	0	0	100	100
2	V	5/9 (56%)	5 (100%)	0	0	100	100
2	X	3/9 (33%)	3 (100%)	0	0	100	100
All	All	1423/1515 (94%)	1411 (99%)	12 (1%)	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	100/106 (94%)	94 (94%)	6 (6%)	19	53
1	B	102/106 (96%)	98 (96%)	4 (4%)	32	69
1	C	102/106 (96%)	99 (97%)	3 (3%)	42	76
1	D	100/106 (94%)	98 (98%)	2 (2%)	55	83
1	E	103/106 (97%)	100 (97%)	3 (3%)	42	76
1	F	100/106 (94%)	99 (99%)	1 (1%)	76	91
1	G	104/106 (98%)	101 (97%)	3 (3%)	42	76
1	H	101/106 (95%)	97 (96%)	4 (4%)	31	68
1	I	100/106 (94%)	97 (97%)	3 (3%)	41	75
1	J	104/106 (98%)	100 (96%)	4 (4%)	33	69
1	K	101/106 (95%)	98 (97%)	3 (3%)	41	75
1	L	101/106 (95%)	97 (96%)	4 (4%)	31	68
2	M	6/7 (86%)	6 (100%)	0	100	100
2	N	6/7 (86%)	6 (100%)	0	100	100
2	O	7/7 (100%)	6 (86%)	1 (14%)	3	15
2	P	7/7 (100%)	5 (71%)	2 (29%)	0	2
2	Q	7/7 (100%)	6 (86%)	1 (14%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	6/7 (86%)	6 (100%)	0	100	100
2	S	6/7 (86%)	5 (83%)	1 (17%)	2	11
2	T	7/7 (100%)	5 (71%)	2 (29%)	0	2
2	U	5/7 (71%)	4 (80%)	1 (20%)	1	7
2	V	6/7 (86%)	5 (83%)	1 (17%)	2	11
2	X	4/7 (57%)	4 (100%)	0	100	100
All	All	1285/1349 (95%)	1236 (96%)	49 (4%)	33	69

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	40	ARG
1	A	65	ARG
1	A	71	ARG
1	A	73	GLU
1	A	97	GLU
1	B	1	MET
1	B	45	ASP
1	B	65	ARG
1	B	94	LEU
1	C	1	MET
1	C	2	LYS
1	C	65	ARG
1	D	1	MET
1	D	65	ARG
1	E	1	MET
1	E	12	GLU
1	E	65	ARG
1	F	65	ARG
1	G	1	MET
1	G	40	ARG
1	G	65	ARG
1	H	1	MET
1	H	65	ARG
1	H	66	LYS
1	H	97	GLU
1	I	1	MET
1	I	27	ASP
1	I	65	ARG

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Mol	Chain	Res	Type
1	J	1	MET
1	J	40	ARG
1	J	65	ARG
1	J	66	LYS
1	K	1	MET
1	K	65	ARG
1	K	73	GLU
1	L	1	MET
1	L	12	GLU
1	L	46	LYS
1	L	65	ARG
2	O	278	LEU
2	P	276	LEU
2	P	278	LEU
2	Q	277	ASP
2	S	276	LEU
2	T	276	LEU
2	T	279	TYR
2	U	276	LEU
2	V	277	ASP

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](#)

21 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	V	272	2	8,9,10	1.56	1 (12%)	8,12,14	1.57	1 (12%)
2	SEP	O	271	2	8,9,10	1.56	1 (12%)	8,12,14	1.79	2 (25%)
2	SEP	P	271	2	8,9,10	1.57	1 (12%)	8,12,14	1.65	2 (25%)
2	SEP	V	271	2	8,9,10	1.57	1 (12%)	8,12,14	1.37	2 (25%)
2	SEP	R	272	2	8,9,10	1.56	1 (12%)	8,12,14	1.38	2 (25%)
2	SEP	T	271	2	8,9,10	1.56	1 (12%)	8,12,14	2.12	2 (25%)
2	SEP	N	271	2	8,9,10	1.60	1 (12%)	8,12,14	1.82	2 (25%)
2	SEP	M	272	2	8,9,10	1.54	1 (12%)	8,12,14	1.00	1 (12%)
2	SEP	R	271	2	8,9,10	1.57	1 (12%)	8,12,14	1.62	2 (25%)
2	SEP	Q	271	2	8,9,10	1.57	1 (12%)	8,12,14	1.66	2 (25%)
2	SEP	S	272	2	8,9,10	1.59	1 (12%)	8,12,14	1.14	1 (12%)
2	SEP	U	272	2	8,9,10	1.58	1 (12%)	8,12,14	1.48	1 (12%)
2	SEP	T	272	2	8,9,10	1.57	1 (12%)	8,12,14	1.12	1 (12%)
2	SEP	O	272	2	8,9,10	1.56	1 (12%)	8,12,14	1.31	1 (12%)
2	SEP	X	272	2	8,9,10	1.69	1 (12%)	8,12,14	1.60	2 (25%)
2	SEP	P	272	2	8,9,10	1.58	1 (12%)	8,12,14	0.82	0
2	SEP	N	272	2	8,9,10	1.58	1 (12%)	8,12,14	0.92	1 (12%)
2	SEP	Q	272	2	8,9,10	1.56	1 (12%)	8,12,14	1.19	1 (12%)
2	SEP	M	271	2	8,9,10	1.59	1 (12%)	8,12,14	1.83	2 (25%)
2	SEP	U	271	2	8,9,10	1.56	1 (12%)	8,12,14	2.21	2 (25%)
2	SEP	S	271	2	8,9,10	1.58	1 (12%)	8,12,14	1.56	2 (25%)

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	V	272	2	-	3/5/8/10	-
2	SEP	O	271	2	-	4/5/8/10	-
2	SEP	P	271	2	-	3/5/8/10	-
2	SEP	V	271	2	-	3/5/8/10	-
2	SEP	R	272	2	-	2/5/8/10	-
2	SEP	T	271	2	-	3/5/8/10	-
2	SEP	N	271	2	-	4/5/8/10	-
2	SEP	M	272	2	-	3/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	R	271	2	-	3/5/8/10	-
2	SEP	Q	271	2	-	4/5/8/10	-
2	SEP	S	272	2	-	3/5/8/10	-
2	SEP	U	272	2	-	3/5/8/10	-
2	SEP	T	272	2	-	3/5/8/10	-
2	SEP	O	272	2	-	3/5/8/10	-
2	SEP	X	272	2	-	0/5/8/10	-
2	SEP	P	272	2	-	1/5/8/10	-
2	SEP	N	272	2	-	3/5/8/10	-
2	SEP	Q	272	2	-	3/5/8/10	-
2	SEP	M	271	2	-	2/5/8/10	-
2	SEP	U	271	2	-	4/5/8/10	-
2	SEP	S	271	2	-	4/5/8/10	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	272	SEP	P-O1P	3.59	1.62	1.50
2	N	271	SEP	P-O1P	3.52	1.61	1.50
2	S	272	SEP	P-O1P	3.50	1.61	1.50
2	M	271	SEP	P-O1P	3.50	1.61	1.50
2	V	271	SEP	P-O1P	3.47	1.61	1.50
2	U	272	SEP	P-O1P	3.47	1.61	1.50
2	Q	271	SEP	P-O1P	3.45	1.61	1.50
2	P	272	SEP	P-O1P	3.44	1.61	1.50
2	S	271	SEP	P-O1P	3.44	1.61	1.50
2	O	271	SEP	P-O1P	3.43	1.61	1.50
2	N	272	SEP	P-O1P	3.43	1.61	1.50
2	R	271	SEP	P-O1P	3.42	1.61	1.50
2	P	271	SEP	P-O1P	3.41	1.61	1.50
2	R	272	SEP	P-O1P	3.41	1.61	1.50
2	T	272	SEP	P-O1P	3.41	1.61	1.50
2	O	272	SEP	P-O1P	3.39	1.61	1.50
2	M	272	SEP	P-O1P	3.36	1.61	1.50
2	T	271	SEP	P-O1P	3.35	1.61	1.50
2	U	271	SEP	P-O1P	3.35	1.61	1.50
2	V	272	SEP	P-O1P	3.34	1.61	1.50
2	Q	272	SEP	P-O1P	3.34	1.61	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	271	SEP	OG-CB-CA	4.65	112.67	108.14
2	T	271	SEP	OG-CB-CA	4.51	112.54	108.14
2	O	271	SEP	P-OG-CB	-3.94	107.44	118.30
2	V	272	SEP	P-OG-CB	-3.79	107.86	118.30
2	N	271	SEP	OG-CB-CA	3.66	111.71	108.14
2	U	271	SEP	P-OG-CB	-3.61	108.34	118.30
2	M	271	SEP	OG-CB-CA	3.40	111.46	108.14
2	T	271	SEP	P-OG-CB	-3.38	109.00	118.30
2	Q	271	SEP	OG-CB-CA	3.35	111.41	108.14
2	R	271	SEP	OG-CB-CA	3.18	111.24	108.14
2	X	272	SEP	OG-CB-CA	3.10	111.16	108.14
2	S	271	SEP	OG-CB-CA	3.09	111.15	108.14
2	P	271	SEP	OG-CB-CA	3.07	111.14	108.14
2	M	271	SEP	P-OG-CB	-3.05	109.88	118.30
2	N	271	SEP	P-OG-CB	-3.05	109.89	118.30
2	P	271	SEP	P-OG-CB	-2.99	110.06	118.30
2	X	272	SEP	P-OG-CB	-2.78	110.63	118.30
2	R	271	SEP	P-OG-CB	-2.77	110.68	118.30
2	V	271	SEP	P-OG-CB	-2.69	110.88	118.30
2	Q	271	SEP	P-OG-CB	-2.68	110.91	118.30
2	Q	272	SEP	P-OG-CB	-2.65	110.99	118.30
2	S	271	SEP	P-OG-CB	-2.65	111.01	118.30
2	U	272	SEP	OG-CB-CA	2.54	110.62	108.14
2	O	271	SEP	OG-CB-CA	2.51	110.59	108.14
2	R	272	SEP	P-OG-CB	-2.45	111.53	118.30
2	R	272	SEP	OG-CB-CA	2.35	110.43	108.14
2	S	272	SEP	P-OG-CB	-2.31	111.94	118.30
2	V	271	SEP	OG-CB-CA	2.20	110.28	108.14
2	M	272	SEP	P-OG-CB	-2.18	112.29	118.30
2	T	272	SEP	P-OG-CB	-2.11	112.48	118.30
2	N	272	SEP	P-OG-CB	-2.06	112.61	118.30
2	O	272	SEP	OG-CB-CA	2.00	110.09	108.14

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	271	SEP	N-CA-CB-OG
2	M	271	SEP	CB-OG-P-O2P
2	N	271	SEP	N-CA-CB-OG
2	N	271	SEP	CB-OG-P-O2P
2	O	271	SEP	N-CA-CB-OG
2	O	271	SEP	CB-OG-P-O1P

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Mol	Chain	Res	Type	Atoms
2	O	271	SEP	CB-OG-P-O2P
2	O	271	SEP	CB-OG-P-O3P
2	P	271	SEP	N-CA-CB-OG
2	P	271	SEP	CB-OG-P-O2P
2	Q	271	SEP	N-CA-CB-OG
2	Q	271	SEP	CB-OG-P-O2P
2	Q	271	SEP	CB-OG-P-O3P
2	R	271	SEP	N-CA-CB-OG
2	R	271	SEP	CB-OG-P-O2P
2	R	271	SEP	CB-OG-P-O3P
2	S	271	SEP	N-CA-CB-OG
2	S	271	SEP	CB-OG-P-O1P
2	S	271	SEP	CB-OG-P-O2P
2	S	271	SEP	CB-OG-P-O3P
2	T	271	SEP	N-CA-CB-OG
2	T	271	SEP	CB-OG-P-O2P
2	T	271	SEP	CB-OG-P-O3P
2	U	271	SEP	CB-OG-P-O1P
2	U	271	SEP	CB-OG-P-O2P
2	V	271	SEP	N-CA-CB-OG
2	V	271	SEP	CB-OG-P-O1P
2	V	271	SEP	CB-OG-P-O2P
2	M	272	SEP	CB-OG-P-O1P
2	M	272	SEP	CB-OG-P-O2P
2	M	272	SEP	CB-OG-P-O3P
2	N	272	SEP	CB-OG-P-O1P
2	N	272	SEP	CB-OG-P-O2P
2	N	272	SEP	CB-OG-P-O3P
2	O	272	SEP	CB-OG-P-O1P
2	O	272	SEP	CB-OG-P-O2P
2	O	272	SEP	CB-OG-P-O3P
2	Q	272	SEP	CB-OG-P-O1P
2	Q	272	SEP	CB-OG-P-O2P
2	Q	272	SEP	CB-OG-P-O3P
2	R	272	SEP	CB-OG-P-O1P
2	S	272	SEP	CB-OG-P-O1P
2	S	272	SEP	CB-OG-P-O2P
2	S	272	SEP	CB-OG-P-O3P
2	T	272	SEP	CB-OG-P-O1P
2	T	272	SEP	CB-OG-P-O2P
2	T	272	SEP	CB-OG-P-O3P
2	U	272	SEP	CB-OG-P-O1P

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Mol	Chain	Res	Type	Atoms
2	U	272	SEP	CB-OG-P-O2P
2	U	272	SEP	CB-OG-P-O3P
2	V	272	SEP	CB-OG-P-O1P
2	V	272	SEP	CB-OG-P-O2P
2	V	272	SEP	CB-OG-P-O3P
2	N	271	SEP	CB-OG-P-O1P
2	Q	271	SEP	CB-OG-P-O1P
2	N	271	SEP	CB-OG-P-O3P
2	P	271	SEP	CB-OG-P-O3P
2	U	271	SEP	N-CA-CB-OG
2	P	272	SEP	CB-OG-P-O1P
2	U	271	SEP	CB-OG-P-O3P
2	R	272	SEP	CB-OG-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 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	116/118 (98%)	-0.54	0 100 100	8, 26, 54, 75	0
1	B	116/118 (98%)	-0.55	0 100 100	9, 30, 60, 75	0
1	C	116/118 (98%)	-0.60	0 100 100	6, 18, 50, 65	0
1	D	116/118 (98%)	-0.54	0 100 100	5, 25, 63, 80	0
1	E	116/118 (98%)	-0.47	0 100 100	10, 30, 64, 88	0
1	F	115/118 (97%)	-0.45	0 100 100	9, 30, 57, 67	0
1	G	116/118 (98%)	-0.49	1 (0%) 84 63	7, 26, 64, 72	0
1	H	116/118 (98%)	-0.45	0 100 100	7, 26, 63, 80	0
1	I	116/118 (98%)	-0.29	1 (0%) 84 63	11, 37, 67, 87	0
1	J	116/118 (98%)	-0.42	1 (0%) 84 63	8, 29, 65, 86	0
1	K	116/118 (98%)	0.25	4 (3%) 45 19	16, 56, 88, 100	0
1	L	116/118 (98%)	0.43	5 (4%) 35 13	34, 69, 98, 112	0
2	M	6/9 (66%)	-0.17	0 100 100	27, 30, 39, 52	0
2	N	6/9 (66%)	-0.11	0 100 100	27, 36, 39, 46	0
2	O	7/9 (77%)	-0.11	0 100 100	27, 31, 41, 54	0
2	P	7/9 (77%)	-0.16	0 100 100	27, 28, 47, 58	0
2	Q	7/9 (77%)	-0.38	0 100 100	32, 36, 39, 49	0
2	R	6/9 (66%)	-0.18	0 100 100	36, 39, 43, 49	0
2	S	6/9 (66%)	-0.10	0 100 100	30, 39, 49, 55	0
2	T	7/9 (77%)	-0.17	0 100 100	26, 32, 51, 58	0
2	U	5/9 (55%)	0.26	0 100 100	56, 60, 65, 85	0
2	V	6/9 (66%)	0.19	0 100 100	22, 32, 34, 48	0
2	X	4/9 (44%)	1.10	0 100 100	73, 77, 78, 89	0
All	All	1458/1515 (96%)	-0.33	12 (0%) 86 65	5, 33, 78, 112	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	116	GLY	4.1
1	J	45	ASP	2.8
1	L	7	GLU	2.8
1	I	116	GLY	2.7
1	K	69	HIS	2.4
1	L	115	TYR	2.4
1	G	45	ASP	2.3
1	K	53	SER	2.2
1	K	27	ASP	2.1
1	L	5	TYR	2.1
1	L	16	SER	2.1
1	K	54	ASP	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	R	272	10/11	0.67	0.34	55,89,130,133	0
2	SEP	R	271	10/11	0.69	0.49	69,82,109,113	0
2	SEP	M	271	10/11	0.72	0.28	69,88,123,129	0
2	SEP	N	271	10/11	0.72	0.32	51,73,101,105	0
2	SEP	X	272	10/11	0.72	0.44	43,73,113,119	0
2	SEP	S	271	10/11	0.75	0.48	62,79,92,93	0
2	SEP	S	272	10/11	0.77	0.32	47,73,100,100	0
2	SEP	Q	271	10/11	0.77	0.32	57,68,87,101	0
2	SEP	U	272	10/11	0.78	0.22	56,84,117,118	0
2	SEP	P	271	10/11	0.79	0.32	38,71,89,89	0
2	SEP	Q	272	10/11	0.81	0.31	49,67,89,90	0
2	SEP	T	272	10/11	0.83	0.21	30,56,91,91	0
2	SEP	O	271	10/11	0.86	0.24	39,51,67,72	0
2	SEP	M	272	10/11	0.86	0.20	38,56,69,70	0
2	SEP	T	271	10/11	0.87	0.27	42,52,67,71	0
2	SEP	V	271	10/11	0.88	0.35	48,70,93,95	0
2	SEP	U	271	10/11	0.89	0.20	58,67,74,82	0
2	SEP	O	272	10/11	0.90	0.21	35,48,65,66	0
2	SEP	V	272	10/11	0.92	0.24	30,63,85,87	0
2	SEP	N	272	10/11	0.92	0.21	26,46,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SEP	P	272	10/11	0.93	0.21	28,34,51,53	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.