



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:31 PM UTC

PDB ID : 6F3T / pdb_00006f3t
Title : Crystal structure of the human TAF5-TAF6-TAF9 complex
Authors : Haffke, M.; Berger, I.
Deposited on : 2017-11-28
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

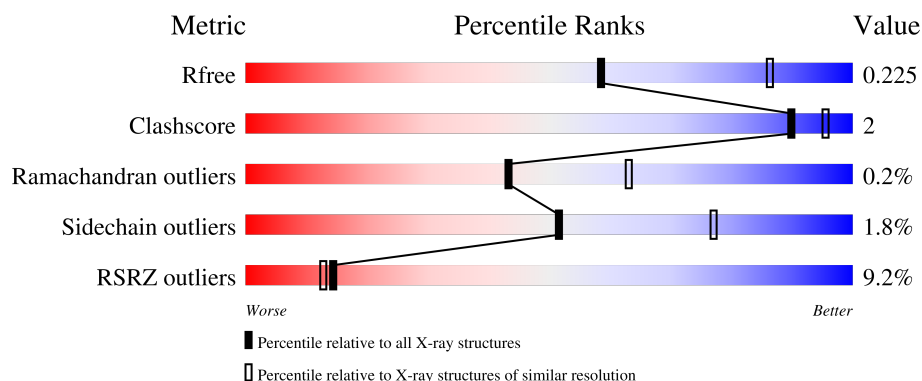
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	608	8% 86% 9%
1	B	608	9% 87% 9%
1	C	608	7% 86% 9%
1	D	608	8% 84% 6% 10%
2	E	94	7% 95% ...

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Mol	Chain	Length	Quality of chain
2	G	94	
2	I	94	
2	K	94	
3	F	116	
3	H	116	
3	J	116	
3	L	116	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 48812 atoms, of which 24044 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 Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	552	Total	C	H	N	O	S	0	0	0
			8717	2799	4299	767	831	21			
1	B	551	Total	C	H	N	O	S	0	0	0
			8698	2794	4289	764	830	21			
1	C	551	Total	C	H	N	O	S	0	0	0
			8698	2794	4289	764	830	21			
1	D	550	Total	C	H	N	O	S	0	0	0
			8689	2792	4283	763	830	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	193	GLY	-	expression tag	UNP Q15542
A	400	SER	PRO	conflict	UNP Q15542
B	193	GLY	-	expression tag	UNP Q15542
B	400	SER	PRO	conflict	UNP Q15542
C	193	GLY	-	expression tag	UNP Q15542
C	400	SER	PRO	conflict	UNP Q15542
D	193	GLY	-	expression tag	UNP Q15542
D	400	SER	PRO	conflict	UNP Q15542

- Molecule 2 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	93	Total	C	H	N	O	S	0	0	0
			1533	475	782	132	139	5			
2	G	92	Total	C	H	N	O	S	0	0	0
			1511	469	769	130	138	5			
2	I	94	Total	C	H	N	O	S	0	0	0
			1555	481	795	134	140	5			
2	K	93	Total	C	H	N	O	S	0	0	0
			1533	475	782	132	139	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	93	ARG	-	expression tag	UNP P49848
E	94	LEU	-	expression tag	UNP P49848
E	95	ARG	-	expression tag	UNP P49848
E	96	ARG	-	expression tag	UNP P49848
E	97	ARG	-	expression tag	UNP P49848
E	98	ALA	-	expression tag	UNP P49848
G	93	ARG	-	expression tag	UNP P49848
G	94	LEU	-	expression tag	UNP P49848
G	95	ARG	-	expression tag	UNP P49848
G	96	ARG	-	expression tag	UNP P49848
G	97	ARG	-	expression tag	UNP P49848
G	98	ALA	-	expression tag	UNP P49848
I	93	ARG	-	expression tag	UNP P49848
I	94	LEU	-	expression tag	UNP P49848
I	95	ARG	-	expression tag	UNP P49848
I	96	ARG	-	expression tag	UNP P49848
I	97	ARG	-	expression tag	UNP P49848
I	98	ALA	-	expression tag	UNP P49848
K	93	ARG	-	expression tag	UNP P49848
K	94	LEU	-	expression tag	UNP P49848
K	95	ARG	-	expression tag	UNP P49848
K	96	ARG	-	expression tag	UNP P49848
K	97	ARG	-	expression tag	UNP P49848
K	98	ALA	-	expression tag	UNP P49848

- Molecule 3 is a protein called Transcription initiation factor TFIID subunit 9.

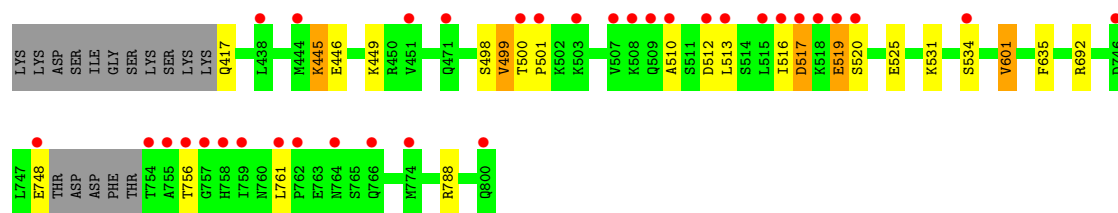
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
3	F	116	Total	C	H	N	O	P	S	0	0	0
			1870	587	939	162	175	1	6			
3	H	116	Total	C	H	N	O	P	S	0	0	0
			1870	587	939	162	175	1	6			
3	J	116	Total	C	H	N	O	P	S	0	0	0
			1870	587	939	162	175	1	6			
3	L	116	Total	C	H	N	O	P	S	0	0	0
			1870	587	939	162	175	1	6			

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

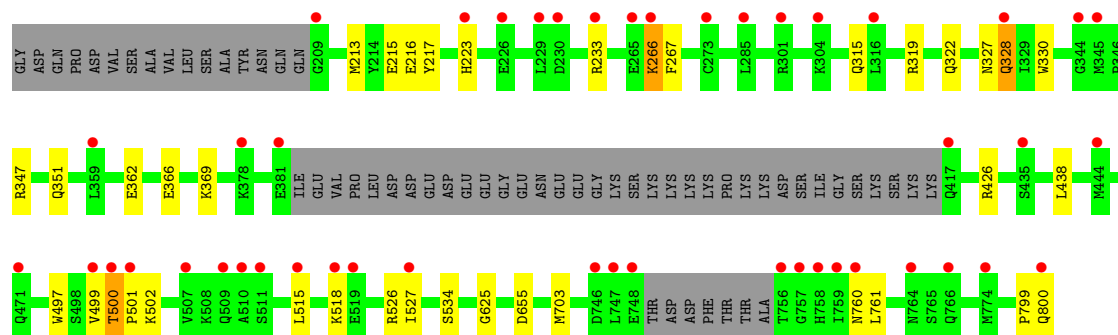
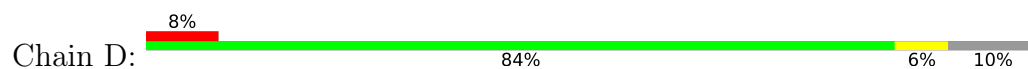
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0
4	B	1	Total Cl 1 1	0	0
4	C	2	Total Cl 2 2	0	0
4	D	2	Total Cl 2 2	0	0

- Molecule 5 is water.

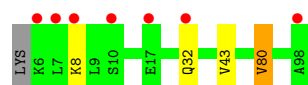
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	65	Total O 65 65	0	0
5	B	52	Total O 52 52	0	0
5	C	108	Total O 108 108	0	0
5	D	74	Total O 74 74	0	0
5	E	11	Total O 11 11	0	0
5	F	12	Total O 12 12	0	0
5	G	10	Total O 10 10	0	0
5	H	6	Total O 6 6	0	0
5	I	14	Total O 14 14	0	0
5	J	23	Total O 23 23	0	0
5	K	6	Total O 6 6	0	0
5	L	10	Total O 10 10	0	0



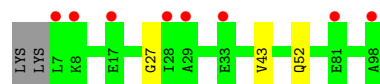
- Molecule 1: Transcription initiation factor TFIID subunit 5



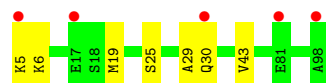
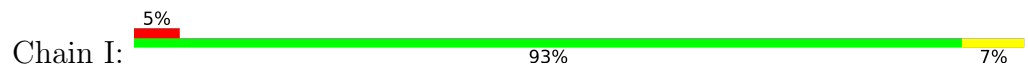
- Molecule 2: Transcription initiation factor TFIID subunit 6



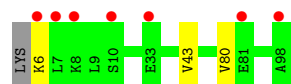
- Molecule 2: Transcription initiation factor TFIID subunit 6



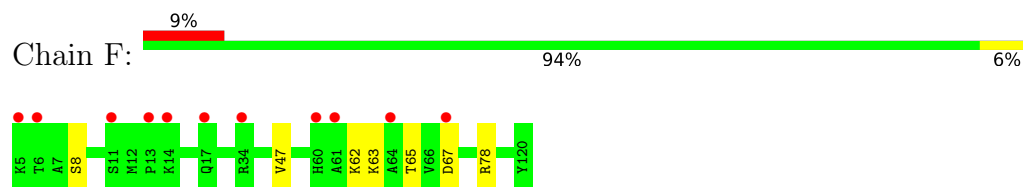
- Molecule 2: Transcription initiation factor TFIID subunit 6



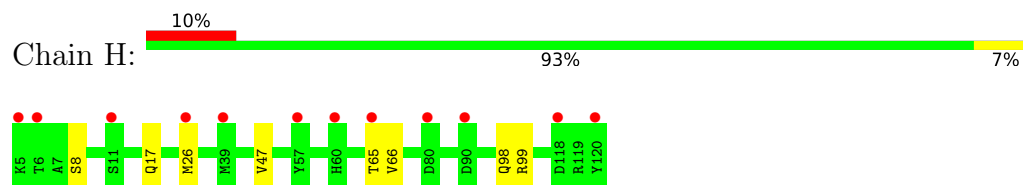
- Molecule 2: Transcription initiation factor TFIID subunit 6



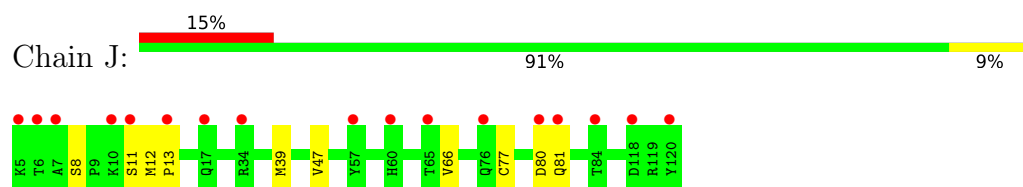
● Molecule 3: Transcription initiation factor TFIID subunit 9



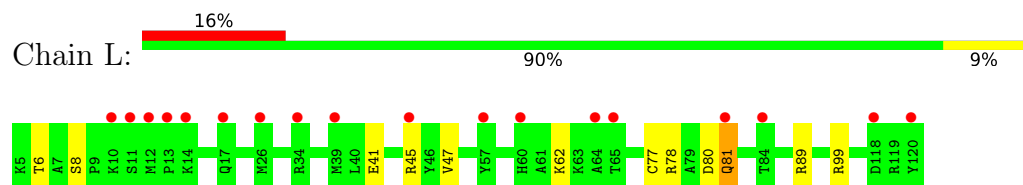
● Molecule 3: Transcription initiation factor TFIID subunit 9



● Molecule 3: Transcription initiation factor TFIID subunit 9



● Molecule 3: Transcription initiation factor TFIID subunit 9



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	339.05Å 339.05Å 339.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.92 – 2.50 79.92 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (79.92-2.50) 99.0 (79.92-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.197 , 0.220 0.203 , 0.225	Depositor DCC
R_{free} test set	10959 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	71.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	48812	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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, 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	0.13	0/4525	0.37	0/6126
1	B	0.15	0/4516	0.36	0/6114
1	C	0.14	0/4516	0.37	0/6114
1	D	0.15	0/4513	0.39	0/6109
2	E	0.13	0/760	0.36	0/1017
2	G	0.13	0/751	0.33	0/1006
2	I	0.17	0/769	0.37	0/1028
2	K	0.14	0/760	0.36	0/1017
3	F	0.17	0/941	0.39	0/1273
3	H	0.17	0/941	0.35	0/1273
3	J	0.23	0/941	0.39	0/1273
3	L	0.15	0/941	0.36	0/1273
All	All	0.15	0/24874	0.37	0/33623

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	4418	4299	4299	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4409	4289	4289	14	0
1	C	4409	4289	4289	17	0
1	D	4406	4283	4283	22	0
2	E	751	782	782	3	0
2	G	742	769	769	4	0
2	I	760	795	795	4	0
2	K	751	782	782	2	0
3	F	931	939	939	3	0
3	H	931	939	939	5	0
3	J	931	939	939	9	0
3	L	931	939	939	6	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	65	0	0	0	0
5	B	52	0	0	0	0
5	C	108	0	0	0	0
5	D	74	0	0	0	0
5	E	11	0	0	0	0
5	F	12	0	0	0	0
5	G	10	0	0	0	0
5	H	6	0	0	0	0
5	I	14	0	0	0	0
5	J	23	0	0	0	0
5	K	6	0	0	0	0
5	L	10	0	0	0	0
All	All	24768	24044	24044	89	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 2.

All (89) 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:B:520:SER:OG	1:B:525:GLU:OE2	1.87	0.93
1:D:351:GLN:NE2	1:D:760:ASN:OD1	2.18	0.77
3:J:80:ASP:OD1	3:J:81:GLN:N	2.18	0.77
1:D:499:VAL:O	1:D:501:PRO:HD2	1.84	0.76
1:B:365:ARG:HG3	1:B:369:LYS:HE2	1.70	0.72
3:J:80:ASP:OD1	3:J:81:GLN:HG3	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:LEU:O	1:C:516:ILE:HG22	1.97	0.64
3:J:39:MET:HA	3:J:39:MET:HE2	1.82	0.62
1:B:445:LYS:HG2	1:B:513:LEU:HD11	1.82	0.60
1:D:500:THR:HG23	1:D:501:PRO:HD3	1.84	0.59
1:D:500:THR:HG23	1:D:501:PRO:CD	2.33	0.58
1:C:520:SER:OG	1:C:525:GLU:OE2	2.18	0.58
1:A:448:THR:O	1:A:449:LYS:HB2	2.02	0.57
1:D:216:GLU:N	1:D:216:GLU:OE1	2.36	0.57
1:D:799:PRO:O	1:D:800:GLN:HG3	2.03	0.57
1:C:216:GLU:OE1	1:C:216:GLU:N	2.39	0.56
1:C:499:VAL:HG22	1:C:500:THR:N	2.20	0.56
1:A:357:GLY:O	1:A:649:ARG:NH1	2.39	0.55
2:E:80:VAL:O	3:F:78:ARG:NH1	2.40	0.55
1:A:449:LYS:HD3	1:A:788:ARG:CZ	2.37	0.54
1:A:441:ILE:O	1:A:445:LYS:HD3	2.07	0.54
1:A:667:GLY:O	1:A:692:ARG:NH2	2.41	0.54
1:D:500:THR:H	1:D:526:ARG:HG2	1.74	0.53
3:J:80:ASP:OD1	3:J:80:ASP:C	2.50	0.53
1:D:266:LYS:HE3	1:D:267:PHE:CD2	2.44	0.52
1:A:365:ARG:NE	1:A:369:LYS:HE2	2.23	0.52
1:B:441:ILE:O	1:B:445:LYS:HD3	2.10	0.52
3:L:80:ASP:OD1	3:L:81:GLN:HG3	2.10	0.51
2:G:43:VAL:HG21	3:H:47:VAL:HG22	1.92	0.51
1:A:449:LYS:HD3	1:A:788:ARG:NH1	2.25	0.51
1:B:216:GLU:N	1:B:216:GLU:OE1	2.41	0.51
1:A:500:THR:HB	1:A:501:PRO:HD3	1.91	0.51
1:C:519:GLU:O	1:C:788:ARG:NH1	2.41	0.50
2:K:80:VAL:O	3:L:78:ARG:NH1	2.45	0.49
1:D:215:GLU:HG2	1:D:266:LYS:HZ3	1.78	0.49
1:D:625:GLY:O	3:L:89:ARG:NH1	2.39	0.49
1:A:278:ASP:OD1	1:A:649:ARG:NH2	2.46	0.49
1:B:445:LYS:N	1:B:445:LYS:HD2	2.28	0.48
1:B:500:THR:HB	1:B:501:PRO:HD3	1.94	0.48
1:C:510:ALA:O	1:C:513:LEU:HB3	2.14	0.48
1:A:365:ARG:NE	1:A:757:GLY:HA2	2.28	0.47
1:D:366:GLU:CD	1:D:369:LYS:HD2	2.39	0.47
1:A:501:PRO:C	1:A:503:LYS:H	2.21	0.47
1:D:703:MET:SD	1:D:761:LEU:HD11	2.55	0.47
1:B:531:LYS:HE3	2:I:25:SER:O	2.14	0.47
2:I:43:VAL:HG21	3:J:47:VAL:HG22	1.97	0.47
3:J:77:CYS:O	3:J:80:ASP:OD1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:667:GLY:O	1:B:692:ARG:NH2	2.48	0.46
2:K:43:VAL:HG21	3:L:47:VAL:HG22	1.97	0.46
3:L:77:CYS:O	3:L:80:ASP:OD1	2.34	0.46
1:C:499:VAL:CG2	1:C:500:THR:N	2.79	0.46
2:E:43:VAL:HG21	3:F:47:VAL:HG22	1.98	0.46
1:D:426:ARG:NH2	1:D:655:ASP:OD1	2.50	0.45
1:D:497:TRP:CZ3	1:D:499:VAL:HG22	2.51	0.45
1:B:321:LEU:HB3	1:B:330:TRP:CD1	2.51	0.45
1:C:498:SER:O	1:C:534:SER:OG	2.33	0.45
1:D:347:ARG:NH2	1:D:362:GLU:OE2	2.45	0.45
1:D:217:TYR:CE1	1:D:328:GLN:HG2	2.51	0.45
1:B:445:LYS:HB3	1:B:517:ASP:OD1	2.17	0.44
1:C:449:LYS:HE2	1:C:519:GLU:HG3	1.99	0.44
1:D:215:GLU:CG	1:D:266:LYS:HZ3	2.29	0.44
1:B:619:PRO:O	3:H:99:ARG:HD3	2.17	0.44
1:C:500:THR:CG2	1:C:501:PRO:HD3	2.48	0.43
1:C:531:LYS:HD2	2:G:27:GLY:CA	2.48	0.43
1:D:327:ASN:O	1:D:330:TRP:HB3	2.18	0.43
1:B:324:LYS:O	1:B:325:GLN:HG2	2.18	0.43
1:C:500:THR:HG22	1:C:501:PRO:HD3	2.01	0.43
2:G:52:GLN:HG2	3:H:26:MET:HE3	2.01	0.43
3:J:11:SER:O	3:J:13:PRO:HD3	2.19	0.43
1:C:378:LYS:CE	1:C:417:GLN:N	2.81	0.43
3:H:65:THR:HG22	3:H:66:VAL:N	2.33	0.42
1:C:445:LYS:HD2	1:C:513:LEU:CD1	2.50	0.42
1:D:515:LEU:O	1:D:518:LYS:HG2	2.19	0.42
1:A:378:LYS:HE3	1:A:417:GLN:N	2.34	0.42
1:A:754:THR:O	1:A:755:ALA:HB3	2.19	0.42
1:C:445:LYS:HG2	1:C:516:ILE:HG23	2.01	0.42
1:C:517:ASP:OD1	1:C:517:ASP:C	2.62	0.42
1:A:445:LYS:HB3	1:A:516:ILE:HG21	2.01	0.42
1:B:513:LEU:O	1:B:513:LEU:HD12	2.20	0.41
2:I:43:VAL:HG21	3:J:47:VAL:CG2	2.50	0.41
1:A:513:LEU:HD22	1:A:513:LEU:O	2.20	0.41
1:C:601:VAL:HG22	1:C:635:PHE:CE2	2.55	0.41
1:D:213:MET:HE3	1:D:216:GLU:HB2	2.03	0.41
2:G:43:VAL:HG21	3:H:47:VAL:CG2	2.51	0.40
2:E:43:VAL:HG21	3:F:47:VAL:CG2	2.51	0.40
1:D:266:LYS:HE2	1:D:266:LYS:HB3	1.86	0.40
2:I:19:MET:HE1	3:J:12:MET:HE1	2.03	0.40
1:D:502:LYS:CG	1:D:534:SER:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:41:GLU:HB3	3:L:45:ARG:NH1	2.36	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	546/608 (90%)	522 (96%)	23 (4%)	1 (0%)	43	63
1	B	545/608 (90%)	525 (96%)	19 (4%)	1 (0%)	43	63
1	C	545/608 (90%)	528 (97%)	17 (3%)	0	100	100
1	D	544/608 (90%)	529 (97%)	14 (3%)	1 (0%)	43	63
2	E	91/94 (97%)	90 (99%)	1 (1%)	0	100	100
2	G	90/94 (96%)	89 (99%)	1 (1%)	0	100	100
2	I	92/94 (98%)	88 (96%)	2 (2%)	2 (2%)	5	9
2	K	91/94 (97%)	89 (98%)	2 (2%)	0	100	100
3	F	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
3	H	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
3	J	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
3	L	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
All	All	2996/3272 (92%)	2900 (97%)	91 (3%)	5 (0%)	43	63

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	449	LYS
1	D	500	THR
1	B	325	GLN

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Mol	Chain	Res	Type
2	I	29	ALA
2	I	30	GLN

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	485/535 (91%)	478 (99%)	7 (1%)	59	81
1	B	484/535 (90%)	479 (99%)	5 (1%)	68	86
1	C	484/535 (90%)	473 (98%)	11 (2%)	44	72
1	D	484/535 (90%)	475 (98%)	9 (2%)	50	76
2	E	83/84 (99%)	80 (96%)	3 (4%)	31	58
2	G	82/84 (98%)	82 (100%)	0	100	100
2	I	84/84 (100%)	82 (98%)	2 (2%)	43	70
2	K	83/84 (99%)	82 (99%)	1 (1%)	63	83
3	F	102/102 (100%)	98 (96%)	4 (4%)	28	55
3	H	102/102 (100%)	100 (98%)	2 (2%)	48	75
3	J	102/102 (100%)	101 (99%)	1 (1%)	68	86
3	L	102/102 (100%)	98 (96%)	4 (4%)	28	55
All	All	2677/2884 (93%)	2628 (98%)	49 (2%)	51	77

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

Mol	Chain	Res	Type
1	A	208	GLN
1	A	216	GLU
1	A	511	SER
1	A	513	LEU
1	A	515	LEU
1	A	528	MET
1	A	761	LEU
1	B	251	LEU

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Mol	Chain	Res	Type
1	B	511	SER
1	B	516	ILE
1	B	519	GLU
1	B	763	GLU
1	C	445	LYS
1	C	446	GLU
1	C	499	VAL
1	C	512	ASP
1	C	517	ASP
1	C	519	GLU
1	C	601	VAL
1	C	692	ARG
1	C	748	GLU
1	C	756	THR
1	C	761	LEU
1	D	223	HIS
1	D	233	ARG
1	D	266	LYS
1	D	315	GLN
1	D	319	ARG
1	D	322	GLN
1	D	328	GLN
1	D	438	LEU
1	D	527	ILE
2	E	8	LYS
2	E	32	GLN
2	E	80	VAL
3	F	62	LYS
3	F	63	LYS
3	F	65	THR
3	F	67	ASP
3	H	17	GLN
3	H	98	GLN
2	I	5	LYS
2	I	6	LYS
3	J	66	VAL
2	K	6	LYS
3	L	6	THR
3	L	62	LYS
3	L	81	GLN
3	L	99	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	782	HIS
1	B	232	HIS
1	B	673	HIS
1	B	782	HIS
1	C	320	HIS
1	C	351	GLN
1	C	585	ASN
1	C	673	HIS
1	C	758	HIS
1	C	782	HIS
1	D	232	HIS
1	D	351	GLN
1	D	471	GLN
1	D	782	HIS
3	F	81	GLN
3	H	37	ASN
2	I	32	GLN
3	J	37	ASN
3	J	81	GLN
3	L	37	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
3	SEP	H	8	3	8,9,10	1.61	1 (12%)	7,12,14	1.40	1 (14%)
3	SEP	L	8	3	8,9,10	1.61	1 (12%)	7,12,14	1.29	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SEP	J	8	3	8,9,10	1.61	1 (12%)	7,12,14	1.33	1 (14%)
3	SEP	F	8	3	8,9,10	1.61	1 (12%)	7,12,14	1.58	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
3	SEP	H	8	3	-	0/6/8/10	-
3	SEP	L	8	3	-	0/6/8/10	-
3	SEP	J	8	3	-	0/6/8/10	-
3	SEP	F	8	3	-	0/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	8	SEP	P-O1P	3.54	1.61	1.50
3	L	8	SEP	P-O1P	3.52	1.61	1.50
3	J	8	SEP	P-O1P	3.52	1.61	1.50
3	F	8	SEP	P-O1P	3.50	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	8	SEP	OG-CB-CA	3.61	111.66	108.14
3	H	8	SEP	OG-CB-CA	3.08	111.14	108.14
3	J	8	SEP	OG-CB-CA	2.79	110.86	108.14
3	L	8	SEP	OG-CB-CA	2.71	110.78	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	552/608 (90%)	0.43	48 (8%) 16 14	63, 88, 151, 230	0
1	B	551/608 (90%)	0.54	56 (10%) 12 10	62, 91, 163, 228	0
1	C	551/608 (90%)	0.24	43 (7%) 19 17	54, 76, 144, 224	0
1	D	550/608 (90%)	0.44	46 (8%) 17 15	58, 88, 161, 196	0
2	E	93/94 (98%)	0.43	7 (7%) 20 18	67, 87, 131, 154	0
2	G	92/94 (97%)	0.47	8 (8%) 16 14	68, 90, 128, 163	0
2	I	94/94 (100%)	0.49	5 (5%) 32 28	64, 88, 133, 184	0
2	K	93/94 (98%)	0.68	7 (7%) 20 18	75, 106, 147, 174	0
3	F	115/116 (99%)	0.68	11 (9%) 13 11	67, 95, 148, 172	0
3	H	115/116 (99%)	0.69	12 (10%) 11 10	72, 95, 142, 168	0
3	J	115/116 (99%)	0.82	17 (14%) 5 4	63, 94, 144, 178	0
3	L	115/116 (99%)	0.85	18 (15%) 5 4	68, 113, 149, 171	0
All	All	3036/3272 (92%)	0.48	278 (9%) 14 13	54, 89, 154, 230	0

All (278) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	754	THR	7.1
1	B	516	ILE	6.7
1	C	515	LEU	6.3
3	J	5	LYS	6.2
1	A	500	THR	6.2
2	I	98	ALA	6.1
1	C	507	VAL	6.1
2	K	98	ALA	6.0
1	B	510	ALA	5.8
1	B	756	THR	5.8
1	A	513	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	756	THR	5.6
1	C	510	ALA	5.3
2	E	98	ALA	5.3
3	J	81	GLN	5.2
1	B	513	LEU	5.1
1	A	515	LEU	5.1
3	J	80	ASP	5.0
1	B	755	ALA	5.0
1	D	500	THR	5.0
1	C	500	THR	4.9
1	C	380	PRO	4.9
1	C	501	PRO	4.9
1	D	758	HIS	4.9
1	A	755	ALA	4.8
1	C	755	ALA	4.8
1	B	754	THR	4.8
1	A	516	ILE	4.8
1	C	209	GLY	4.7
1	B	500	THR	4.7
2	G	98	ALA	4.7
2	E	7	LEU	4.6
3	J	65	THR	4.6
1	B	758	HIS	4.6
1	B	451	VAL	4.6
1	A	762	PRO	4.5
1	A	209	GLY	4.4
1	D	800	GLN	4.4
1	B	316	LEU	4.4
1	D	759	ILE	4.4
1	B	209	GLY	4.3
1	C	513	LEU	4.3
1	B	501	PRO	4.3
1	A	508	LYS	4.3
1	A	754	THR	4.2
3	J	6	THR	4.2
1	A	510	ALA	4.2
3	J	60	HIS	4.2
1	C	508	LYS	4.1
3	H	5	LYS	4.1
1	A	380	PRO	4.0
1	C	512	ASP	4.0
1	B	330	TRP	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	519	GLU	3.9
2	E	32	GLN	3.9
2	G	7	LEU	3.8
2	G	29	ALA	3.8
1	A	519	GLU	3.8
3	J	57	TYR	3.7
1	D	444	MET	3.7
1	A	758	HIS	3.7
1	D	316	LEU	3.7
3	L	13	PRO	3.7
3	H	6	THR	3.7
2	I	81	GLU	3.7
1	D	515	LEU	3.7
3	H	120	TYR	3.7
1	C	758	HIS	3.6
1	D	209	GLY	3.6
1	B	507	VAL	3.6
1	D	509	GLN	3.6
1	B	762	PRO	3.6
1	C	516	ILE	3.5
1	A	448	THR	3.5
1	D	328	GLN	3.5
1	A	507	VAL	3.4
1	D	748	GLU	3.4
3	L	14	LYS	3.4
1	B	380	PRO	3.4
3	F	13	PRO	3.4
1	A	517	ASP	3.4
1	A	501	PRO	3.3
1	D	285	LEU	3.3
1	B	759	ILE	3.3
1	D	510	ALA	3.3
1	C	319	ARG	3.3
3	F	64	ALA	3.3
1	D	757	GLY	3.3
3	F	6	THR	3.3
1	A	449	LYS	3.3
3	J	118	ASP	3.2
2	K	7	LEU	3.2
1	A	756	THR	3.2
1	B	515	LEU	3.2
1	D	507	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	517	ASP	3.2
1	B	321	LEU	3.2
1	A	528	MET	3.2
3	F	11	SER	3.2
1	C	762	PRO	3.2
1	D	266	LYS	3.2
1	B	440	LYS	3.1
1	B	746	ASP	3.1
3	L	120	TYR	3.1
1	B	509	GLN	3.1
1	C	748	GLU	3.0
1	C	518	LYS	3.0
2	G	8	LYS	3.0
1	A	330	TRP	3.0
1	C	756	THR	3.0
3	H	65	THR	3.0
2	G	33	GLU	3.0
1	D	223	HIS	3.0
1	D	265	GLU	3.0
3	H	57	TYR	3.0
2	E	10	SER	3.0
1	A	471	GLN	3.0
1	C	800	GLN	3.0
2	I	17	GLU	2.9
1	A	514	SER	2.9
1	A	207	GLN	2.9
3	H	60	HIS	2.9
3	L	11	SER	2.9
1	B	319	ARG	2.9
1	B	518	LYS	2.9
1	B	519	GLU	2.9
1	C	759	ILE	2.9
1	A	512	ASP	2.9
1	A	208	GLN	2.9
3	L	17	GLN	2.9
1	B	366	GLU	2.9
1	B	520	SER	2.8
2	K	6	LYS	2.8
3	F	60	HIS	2.8
1	A	747	LEU	2.8
1	A	509	GLN	2.8
1	B	308	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	8	LYS	2.8
1	A	301	ARG	2.8
1	B	324	LYS	2.8
1	C	324	LYS	2.8
3	L	118	ASP	2.8
1	A	760	ASN	2.8
1	C	520	SER	2.8
1	C	451	VAL	2.8
1	A	273	CYS	2.8
1	D	417	GLN	2.8
1	B	512	ASP	2.8
1	D	435	SER	2.7
1	B	223	HIS	2.7
1	D	233	ARG	2.7
1	C	517	ASP	2.7
1	D	344	GLY	2.7
1	D	760	ASN	2.7
1	B	444	MET	2.7
1	C	444	MET	2.7
1	D	229	LEU	2.7
1	D	359	LEU	2.7
1	D	774	MET	2.7
1	D	381	GLU	2.7
1	A	746	ASP	2.7
2	I	5	LYS	2.7
1	B	289	GLU	2.7
1	C	746	ASP	2.6
2	K	8	LYS	2.6
1	B	800	GLN	2.6
1	C	360	ALA	2.6
1	C	471	GLN	2.6
3	J	76	GLN	2.6
3	F	67	ASP	2.6
1	C	764	ASN	2.6
2	I	30	GLN	2.6
1	A	503	LYS	2.6
1	C	378	LYS	2.6
3	F	5	LYS	2.6
1	B	528	MET	2.6
1	A	761	LEU	2.6
2	K	10	SER	2.6
3	L	84	THR	2.6

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Mol	Chain	Res	Type	RSRZ
3	H	80	ASP	2.6
1	B	747	LEU	2.6
1	C	766	GLN	2.5
1	A	757	GLY	2.5
1	D	230	ASP	2.5
1	A	345	MET	2.5
3	L	81	GLN	2.5
1	A	511	SER	2.5
1	A	444	MET	2.5
3	L	57	TYR	2.5
1	A	451	VAL	2.5
1	D	301	ARG	2.5
3	J	11	SER	2.5
1	D	226	GLU	2.4
3	L	34	ARG	2.4
3	L	64	ALA	2.4
1	B	532	THR	2.4
3	F	34	ARG	2.4
1	A	774	MET	2.4
3	J	13	PRO	2.4
1	B	508	LYS	2.4
1	A	452	ARG	2.4
1	B	343	ASP	2.4
1	D	766	GLN	2.3
1	D	345	MET	2.3
1	C	301	ARG	2.3
3	F	17	GLN	2.3
3	F	14	LYS	2.3
2	E	17	GLU	2.3
1	B	365	ARG	2.3
1	B	700	HIS	2.3
1	C	345	MET	2.3
1	D	499	VAL	2.3
2	K	33	GLU	2.3
2	K	81	GLU	2.3
1	B	760	ASN	2.3
1	C	509	GLN	2.3
1	D	511	SER	2.3
1	B	774	MET	2.3
2	E	6	LYS	2.3
3	L	10	LYS	2.3
1	D	471	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	355	MET	2.2
1	C	761	LEU	2.2
1	A	439	ASP	2.2
1	D	746	ASP	2.2
2	G	17	GLU	2.2
3	F	61	ALA	2.2
1	D	273	CYS	2.2
1	A	344	GLY	2.2
3	H	26	MET	2.2
3	L	26	MET	2.2
3	H	90	ASP	2.2
3	J	120	TYR	2.2
1	B	355	MET	2.2
1	B	307	LEU	2.2
3	H	11	SER	2.2
2	G	81	GLU	2.2
1	D	501	PRO	2.2
1	D	378	LYS	2.2
3	J	10	LYS	2.2
1	B	351	GLN	2.2
3	L	12	MET	2.2
1	D	527	ILE	2.2
1	C	503	LYS	2.2
1	D	304	LYS	2.2
1	B	764	ASN	2.1
1	D	764	ASN	2.1
3	H	39	MET	2.1
3	J	7	ALA	2.1
3	J	17	GLN	2.1
1	C	438	LEU	2.1
1	B	449	LYS	2.1
1	D	518	LYS	2.1
1	B	328	GLN	2.1
1	C	328	GLN	2.1
1	C	774	MET	2.1
3	L	60	HIS	2.1
1	D	747	LEU	2.1
3	J	84	THR	2.1
1	B	284	SER	2.1
1	B	503	LYS	2.1
1	C	757	GLY	2.1
1	B	514	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	H	118	ASP	2.1
1	A	763	GLU	2.1
1	D	519	GLU	2.1
3	L	65	THR	2.1
1	B	309	ILE	2.1
1	A	460	SER	2.1
3	L	39	MET	2.1
1	B	315	GLN	2.0
1	A	319	ARG	2.0
3	L	45	ARG	2.0
1	A	211	PRO	2.0
1	B	765	SER	2.0
3	J	34	ARG	2.0
2	G	28	ILE	2.0
1	C	534	SER	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
3	SEP	H	8	10/11	0.81	0.13	84,93,111,116	4
3	SEP	L	8	10/11	0.83	0.13	102,105,125,127	4
3	SEP	J	8	10/11	0.87	0.11	96,101,116,122	4
3	SEP	F	8	10/11	0.87	0.12	92,98,117,117	4

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	A	902	1/1	0.82	0.27	107,107,107,107	0
4	CL	A	901	1/1	0.96	0.14	73,73,73,73	0
4	CL	C	902	1/1	0.97	0.07	76,76,76,76	0
4	CL	C	901	1/1	0.98	0.08	71,71,71,71	0
4	CL	B	901	1/1	0.98	0.11	73,73,73,73	0
4	CL	D	901	1/1	0.98	0.06	70,70,70,70	0
4	CL	D	902	1/1	0.98	0.09	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.