Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 10:15 PM EDT

PDB ID	:	6F3T
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 (i) 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 (i)) were used in the production of this report:

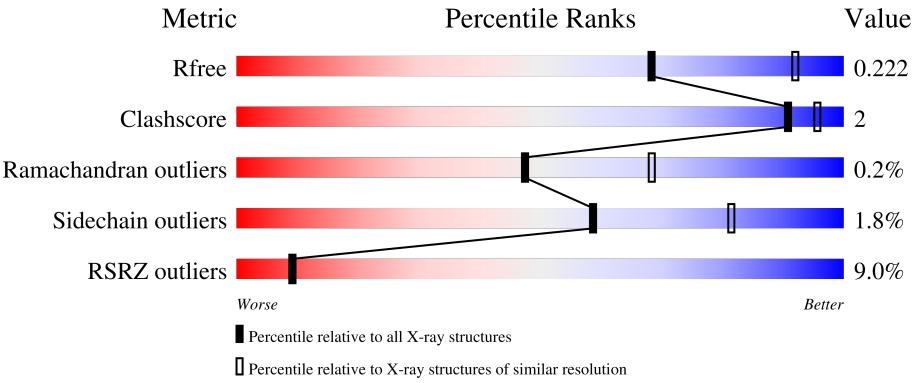
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	7% 86% . 9%
1	B	608	9% 86% . 9%
1	C	608	6% 86% . 9%
1	D	608	12% 84% 6% 10%
2	E	94	4% 95% . .

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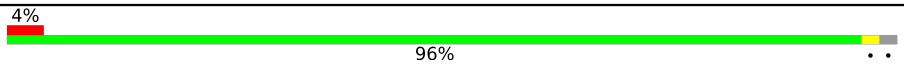
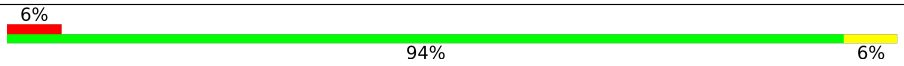
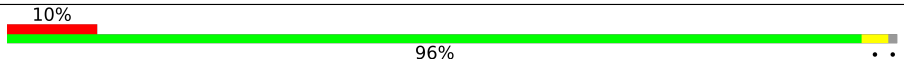
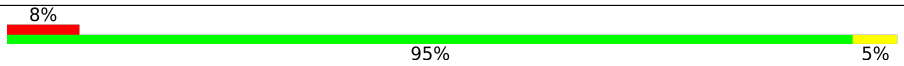
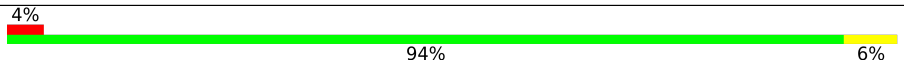
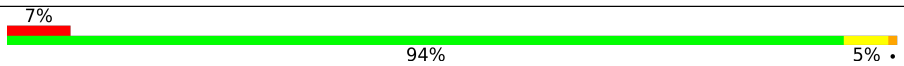
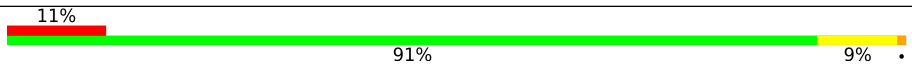
Mol	Chain	Length	Quality of chain
2	G	94	
2	I	94	
2	K	94	
3	F	116	
3	H	116	
3	J	116	
3	L	116	

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 (three-letter code: 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.

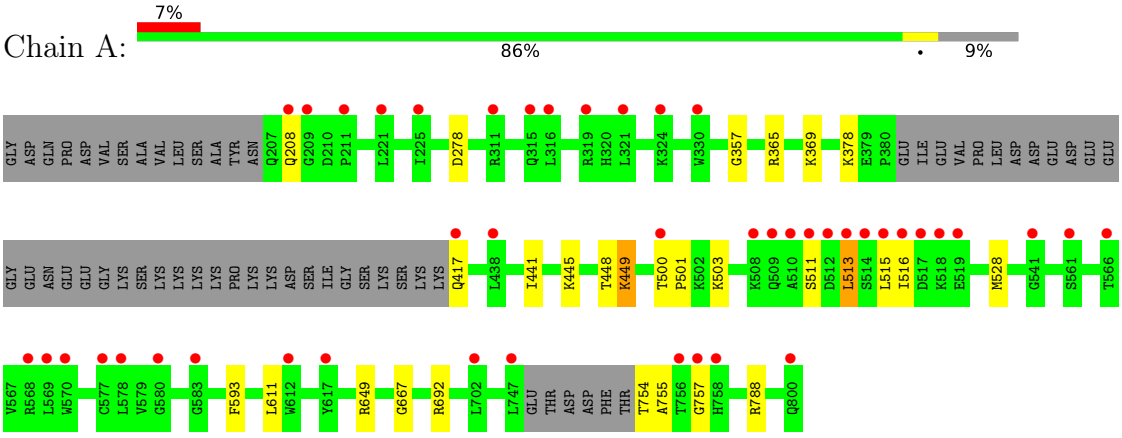
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	65	Total O 65 65	0	0
5	B	52	Total O 52 52	0	0
5	C	108	Total O 108 108	0	0
5	D	74	Total O 74 74	0	0
5	E	11	Total O 11 11	0	0
5	F	12	Total O 12 12	0	0
5	G	10	Total O 10 10	0	0
5	H	6	Total O 6 6	0	0
5	I	14	Total O 14 14	0	0
5	J	23	Total O 23 23	0	0
5	K	6	Total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

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.

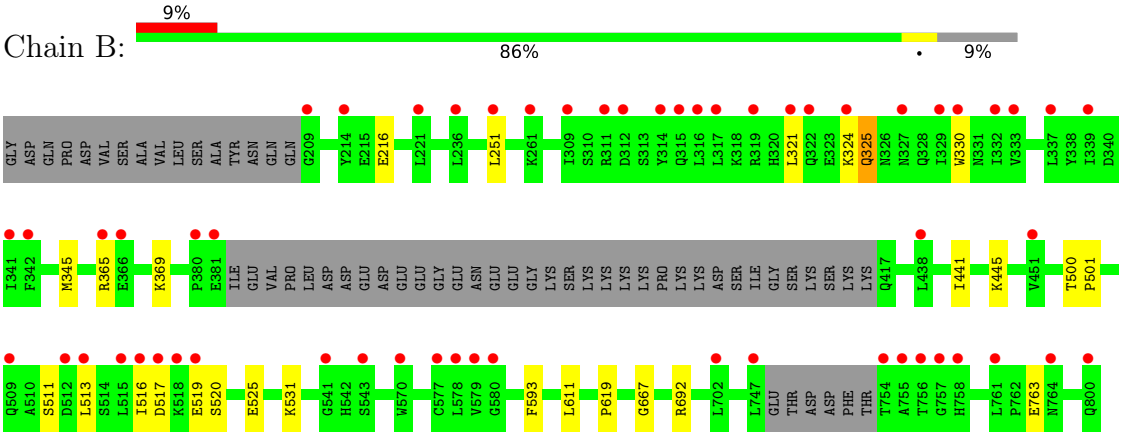
• Molecule 1: Transcription initiation factor TFIID subunit 5

Chain A:



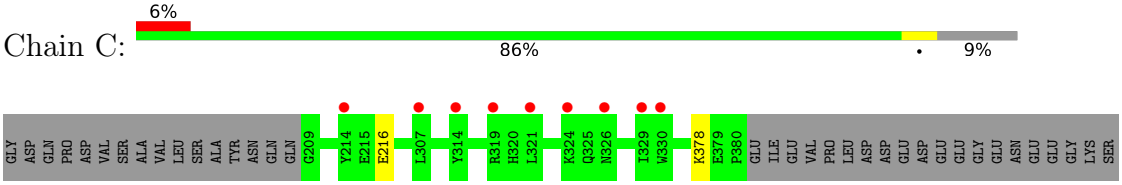
• Molecule 1: Transcription initiation factor TFIID subunit 5

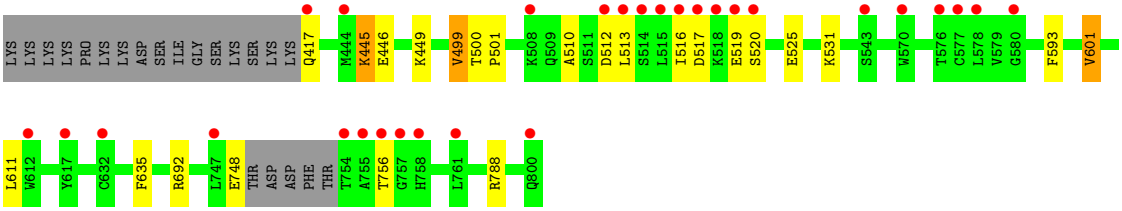
Chain B:



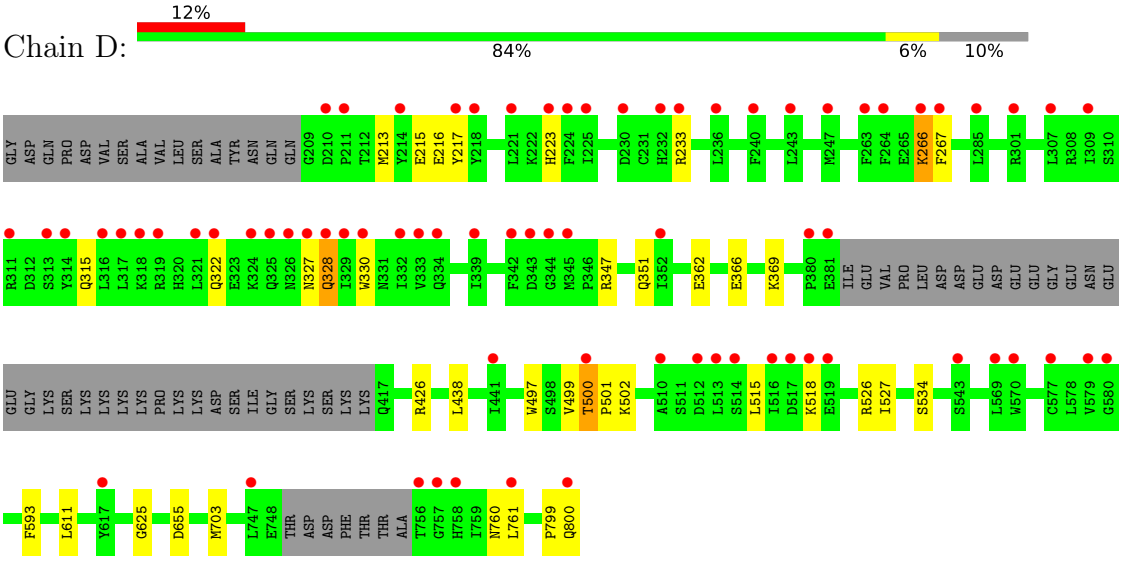
• Molecule 1: Transcription initiation factor TFIID subunit 5

Chain C:

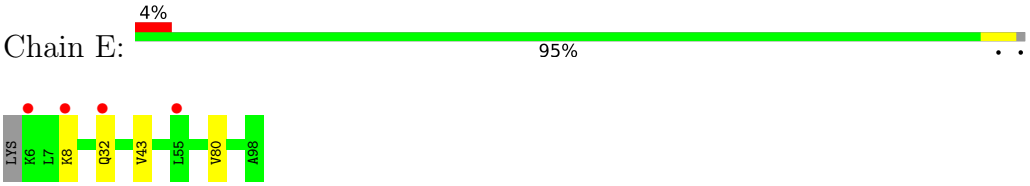




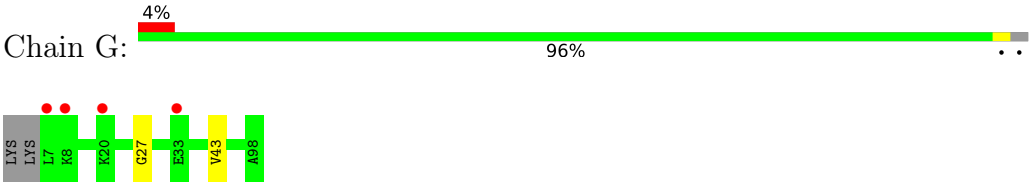
• Molecule 1: Transcription initiation factor TFIID subunit 5



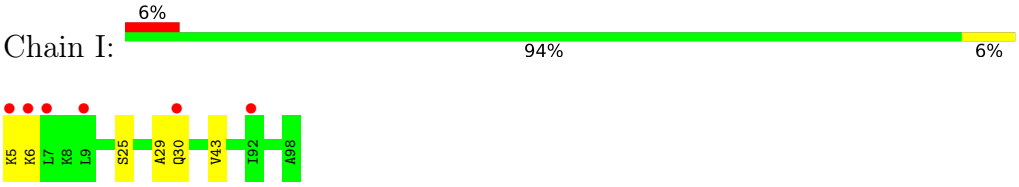
• Molecule 2: Transcription initiation factor TFIID subunit 6



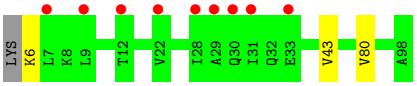
• Molecule 2: Transcription initiation factor TFIID subunit 6



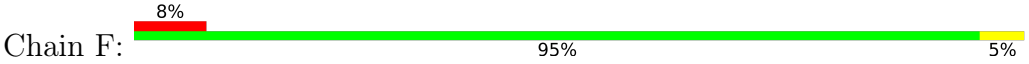
• Molecule 2: Transcription initiation factor TFIID subunit 6

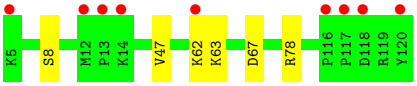


• Molecule 2: Transcription initiation factor TFIID subunit 6

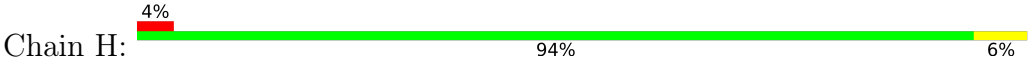


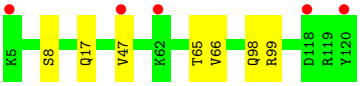
• Molecule 3: Transcription initiation factor TFIID subunit 9



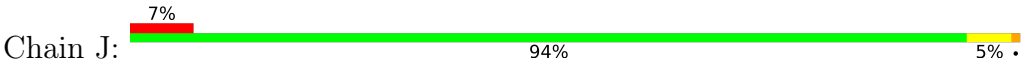


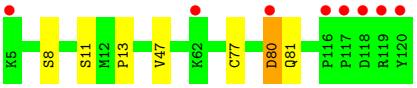
• Molecule 3: Transcription initiation factor TFIID subunit 9



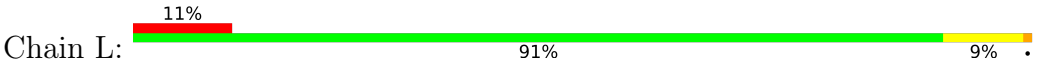


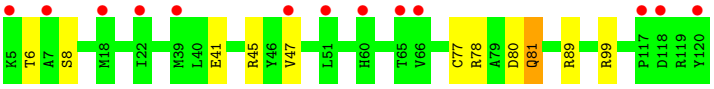
• Molecule 3: Transcription initiation factor TFIID subunit 9





• Molecule 3: Transcription initiation factor TFIID subunit 9





4 Data and refinement statistics (i)

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 90.61 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (79.92-2.50) 99.0 (90.61-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.197 , 0.220 0.198 , 0.222	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)	0.37 , 58.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.26	0/4525	0.48	0/6126
1	B	0.26	0/4516	0.48	0/6114
1	C	0.26	0/4516	0.48	0/6114
1	D	0.26	0/4513	0.49	0/6109
2	E	0.25	0/760	0.45	0/1017
2	G	0.25	0/751	0.44	0/1006
2	I	0.27	0/769	0.45	0/1028
2	K	0.26	0/760	0.45	0/1017
3	F	0.27	0/941	0.47	0/1273
3	H	0.27	0/941	0.44	0/1273
3	J	0.29	0/941	0.49	1/1273 (0.1%)
3	L	0.26	0/941	0.44	0/1273
All	All	0.26	0/24874	0.47	1/33623 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	80	ASP	CB-CG-OD1	-5.33	113.50	118.30

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	4418	4299	4299	15	0
1	B	4409	4289	4289	14	0
1	C	4409	4289	4289	16	0
1	D	4406	4283	4283	21	0
2	E	751	782	782	3	0
2	G	742	769	769	3	0
2	I	760	795	795	3	0
2	K	751	782	782	2	0
3	F	931	939	939	3	0
3	H	931	939	939	4	0
3	J	931	939	939	7	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	84	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 (84) 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
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
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: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
3:J:80:ASP:OD1	3:J:80:ASP:C	2.50	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:215:GLU:CG	1:D:266:LYS:HZ3	2.29	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:B:619:PRO:O	3:H:99:ARG:HD3	2.17	0.44
1:A:501:PRO:C	1:A:503:LYS:H	2.21	0.44
1:D:213:MET:HE3	1:D:216:GLU:HB2	2.01	0.43
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
1:D:366:GLU:CD	1:D:369:LYS:HD2	2.39	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:378:LYS:HZ1	1:C:417:GLN:N	2.18	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
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
1:D:502:LYS:CG	1:D:534:SER:HB3	2.51	0.40
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%)	47 68
1	B	545/608 (90%)	525 (96%)	19 (4%)	1 (0%)	47 68
1	C	545/608 (90%)	528 (97%)	17 (3%)	0	100 100
1	D	544/608 (90%)	529 (97%)	14 (3%)	1 (0%)	47 68
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%)	6 10
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%)	47 68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	449	LYS
1	D	500	THR
1	B	325	GLN
2	I	29	ALA
2	I	30	GLN

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	485/535 (91%)	478 (99%)	7 (1%)	67	86
1	B	484/535 (90%)	476 (98%)	8 (2%)	60	82
1	C	484/535 (90%)	473 (98%)	11 (2%)	50	76
1	D	484/535 (90%)	474 (98%)	10 (2%)	53	78
2	E	83/84 (99%)	81 (98%)	2 (2%)	49	74
2	G	82/84 (98%)	82 (100%)	0	100	100
2	I	84/84 (100%)	82 (98%)	2 (2%)	49	74
2	K	83/84 (99%)	82 (99%)	1 (1%)	71	88
3	F	102/102 (100%)	99 (97%)	3 (3%)	42	69
3	H	102/102 (100%)	100 (98%)	2 (2%)	55	79
3	J	102/102 (100%)	102 (100%)	0	100	100
3	L	102/102 (100%)	99 (97%)	3 (3%)	42	69
All	All	2677/2884 (93%)	2628 (98%)	49 (2%)	59	81

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

Mol	Chain	Res	Type
1	A	208	GLN
1	A	511	SER
1	A	513	LEU
1	A	515	LEU
1	A	528	MET
1	A	593	PHE
1	A	611	LEU
1	B	251	LEU
1	B	345	MET
1	B	511	SER
1	B	516	ILE
1	B	519	GLU
1	B	593	PHE
1	B	611	LEU
1	B	763	GLU
1	C	445	LYS
1	C	446	GLU
1	C	499	VAL
1	C	512	ASP

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Mol	Chain	Res	Type
1	C	517	ASP
1	C	593	PHE
1	C	601	VAL
1	C	611	LEU
1	C	692	ARG
1	C	748	GLU
1	C	756	THR
1	D	223	HIS
1	D	233	ARG
1	D	266	LYS
1	D	315	GLN
1	D	322	GLN
1	D	328	GLN
1	D	438	LEU
1	D	527	ILE
1	D	593	PHE
1	D	611	LEU
2	E	8	LYS
2	E	32	GLN
3	F	62	LYS
3	F	63	LYS
3	F	67	ASP
3	H	17	GLN
3	H	98	GLN
2	I	5	LYS
2	I	6	LYS
2	K	6	LYS
3	L	6	THR
3	L	81	GLN
3	L	99	ARG

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

Mol	Chain	Res	Type
3	J	81	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	L	8	3	8,9,10	1.55	1 (12%)	8,12,14	1.51	2 (25%)
3	SEP	J	8	3	8,9,10	1.55	1 (12%)	8,12,14	1.53	2 (25%)
3	SEP	H	8	3	8,9,10	1.55	1 (12%)	8,12,14	1.63	2 (25%)
3	SEP	F	8	3	8,9,10	1.55	1 (12%)	8,12,14	1.78	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
3	SEP	L	8	3	-	0/5/8/10	-
3	SEP	J	8	3	-	0/5/8/10	-
3	SEP	H	8	3	-	0/5/8/10	-
3	SEP	F	8	3	-	0/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	8	SEP	P-O1P	3.40	1.61	1.50
3	L	8	SEP	P-O1P	3.38	1.61	1.50
3	J	8	SEP	P-O1P	3.37	1.61	1.50
3	F	8	SEP	P-O1P	3.36	1.61	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	F	8	SEP	P-OG-CB	-2.88	110.37	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	8	SEP	P-OG-CB	-2.83	110.50	118.30
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
3	L	8	SEP	P-OG-CB	-2.67	110.94	118.30
3	J	8	SEP	P-OG-CB	-2.59	111.15	118.30

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.66	45 (8%) 11 11	58, 80, 136, 217	0
1	B	551/608 (90%)	0.80	57 (10%) 6 6	57, 83, 148, 207	0
1	C	551/608 (90%)	0.67	38 (6%) 16 17	50, 70, 131, 206	0
1	D	550/608 (90%)	0.93	74 (13%) 3 2	53, 81, 149, 177	0
2	E	93/94 (98%)	0.55	4 (4%) 35 38	62, 78, 121, 136	0
2	G	92/94 (97%)	0.60	4 (4%) 35 38	62, 82, 117, 145	0
2	I	94/94 (100%)	0.65	6 (6%) 19 20	59, 80, 125, 165	0
2	K	93/94 (98%)	0.84	9 (9%) 7 7	69, 94, 135, 158	0
3	F	115/116 (99%)	0.69	9 (7%) 13 13	61, 85, 135, 158	0
3	H	115/116 (99%)	0.60	5 (4%) 35 38	66, 86, 128, 147	0
3	J	115/116 (99%)	0.74	8 (6%) 16 16	57, 83, 134, 160	0
3	L	115/116 (99%)	0.75	13 (11%) 5 4	62, 103, 136, 154	0
All	All	3036/3272 (92%)	0.74	272 (8%) 9 9	50, 81, 140, 217	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	516	ILE	8.3
1	D	321	LEU	7.8
1	B	517	ASP	7.4
1	B	516	ILE	7.2
1	B	321	LEU	7.2
1	D	344	GLY	6.8
3	J	5	LYS	6.4
1	D	329	ILE	6.4
1	D	326	ASN	6.4
1	C	513	LEU	6.3
1	B	754	THR	6.3

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Mol	Chain	Res	Type	RSRZ
1	B	317	LEU	6.3
1	C	515	LEU	6.3
1	B	755	ALA	6.1
1	A	515	LEU	6.1
1	B	756	THR	6.1
1	D	758	HIS	6.0
1	D	225	ILE	5.9
1	A	512	ASP	5.9
3	L	118	ASP	5.7
1	D	756	THR	5.7
1	B	513	LEU	5.7
1	D	757	GLY	5.6
1	D	221	LEU	5.3
3	J	118	ASP	5.3
3	H	120	TYR	5.2
1	A	516	ILE	5.0
1	D	324	LYS	4.9
3	H	118	ASP	4.9
1	B	515	LEU	4.8
1	C	517	ASP	4.8
2	K	30	GLN	4.8
1	A	519	GLU	4.7
1	C	519	GLU	4.6
1	D	345	MET	4.6
1	A	517	ASP	4.5
1	D	218	TYR	4.5
3	H	5	LYS	4.4
1	B	319	ARG	4.4
1	A	500	THR	4.4
1	D	330	TRP	4.4
1	D	314	TYR	4.4
3	F	118	ASP	4.2
2	E	6	LYS	4.2
1	A	513	LEU	4.2
1	B	314	TYR	4.2
1	B	757	GLY	4.2
1	C	512	ASP	4.2
1	D	513	LEU	4.2
2	K	7	LEU	4.1
1	B	758	HIS	4.0
1	D	328	GLN	4.0
1	D	211	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	381	GLU	3.9
1	D	236	LEU	3.9
1	D	322	GLN	3.9
1	D	325	GLN	3.9
1	C	800	GLN	3.8
1	A	756	THR	3.7
1	C	508	LYS	3.7
1	A	509	GLN	3.6
1	D	266	LYS	3.6
1	D	342	PHE	3.6
1	D	214	TYR	3.6
1	D	343	ASP	3.6
1	C	319	ARG	3.5
2	K	31	ILE	3.5
1	A	514	SER	3.5
3	L	120	TYR	3.5
1	D	267	PHE	3.4
1	A	508	LYS	3.4
1	B	800	GLN	3.4
1	D	517	ASP	3.4
3	L	65	THR	3.4
2	K	9	LEU	3.3
1	C	755	ALA	3.3
3	J	120	TYR	3.3
1	A	758	HIS	3.3
1	D	516	ILE	3.3
1	D	327	ASN	3.3
2	K	29	ALA	3.3
2	G	8	LYS	3.3
1	B	512	ASP	3.3
1	C	321	LEU	3.3
2	K	28	ILE	3.3
1	D	318	LYS	3.2
2	I	5	LYS	3.2
1	B	381	GLU	3.2
1	B	380	PRO	3.1
1	D	232	HIS	3.1
1	A	577	CYS	3.1
1	B	509	GLN	3.1
1	C	754	THR	3.1
1	A	319	ARG	3.1
1	C	577	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	800	GLN	3.1
1	A	757	GLY	3.1
1	D	747	LEU	3.1
1	A	209	GLY	3.0
1	B	261	LYS	3.0
1	B	330	TRP	3.0
3	F	120	TYR	3.0
1	D	333	VAL	3.0
1	C	756	THR	3.0
1	C	514	SER	2.9
1	B	577	CYS	2.9
1	D	224	PHE	2.9
3	L	7	ALA	2.9
1	A	511	SER	2.9
1	D	317	LEU	2.9
1	D	339	ILE	2.9
1	A	747	LEU	2.9
1	D	223	HIS	2.9
1	A	518	LYS	2.8
1	C	758	HIS	2.8
1	B	341	ILE	2.8
1	C	330	TRP	2.8
1	D	580	GLY	2.8
1	B	339	ILE	2.8
3	H	47	VAL	2.8
1	D	309	ILE	2.8
1	B	519	GLU	2.8
1	D	579	VAL	2.8
3	J	80	ASP	2.8
1	C	307	LEU	2.8
1	B	309	ILE	2.7
1	D	240	PHE	2.7
1	B	579	VAL	2.7
3	L	66	VAL	2.7
1	C	324	LYS	2.7
1	B	541	GLY	2.7
1	B	702	LEU	2.7
1	B	311	ARG	2.7
1	C	326	ASN	2.7
1	C	761	LEU	2.7
1	A	417	GLN	2.7
1	D	577	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	800	GLN	2.7
1	D	332	ILE	2.7
3	F	62	LYS	2.7
3	F	13	PRO	2.7
1	B	337	LEU	2.6
1	D	316	LEU	2.6
3	L	47	VAL	2.6
1	C	444	MET	2.6
2	I	6	LYS	2.6
1	B	451	VAL	2.6
1	C	580	GLY	2.6
1	D	243	LEU	2.6
1	A	583	GLY	2.6
1	D	380	PRO	2.6
1	C	329	ILE	2.6
1	B	764	ASN	2.6
1	B	580	GLY	2.6
1	D	500	THR	2.5
1	C	417	GLN	2.5
1	A	330	TRP	2.5
2	I	30	GLN	2.5
1	B	366	GLU	2.5
1	A	324	LYS	2.5
1	D	313	SER	2.5
1	D	319	ARG	2.5
2	G	33	GLU	2.5
1	D	617	TYR	2.5
1	B	761	LEU	2.5
1	C	520	SER	2.5
3	F	14	LYS	2.5
3	F	117	PRO	2.5
1	B	322	GLN	2.5
1	D	247	MET	2.5
2	E	8	LYS	2.5
1	B	747	LEU	2.5
1	D	311	ARG	2.5
3	H	62	LYS	2.5
1	D	230	ASP	2.5
1	C	518	LYS	2.4
1	A	221	LEU	2.4
1	D	264	PHE	2.4
1	D	519	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	G	7	LEU	2.4
2	G	20	LYS	2.4
1	B	221	LEU	2.4
1	D	285	LEU	2.4
1	D	514	SER	2.4
3	J	62	LYS	2.4
1	A	580	GLY	2.4
1	B	327	ASN	2.4
1	A	211	PRO	2.4
2	K	33	GLU	2.4
1	D	512	ASP	2.4
1	B	365	ARG	2.4
1	B	315	GLN	2.4
1	C	570	TRP	2.4
1	B	543	SER	2.4
1	C	757	GLY	2.4
1	D	543	SER	2.4
2	K	22	VAL	2.3
1	C	617	TYR	2.3
1	B	578	LEU	2.3
1	A	617	TYR	2.3
1	C	214	TYR	2.3
1	D	510	ALA	2.3
1	B	236	LEU	2.3
1	D	441	ILE	2.3
1	B	438	LEU	2.3
1	B	324	LYS	2.3
1	B	333	VAL	2.3
3	F	116	PRO	2.3
1	B	570	TRP	2.3
1	D	307	LEU	2.3
1	D	352	ILE	2.2
1	A	702	LEU	2.2
1	D	233	ARG	2.2
2	E	32	GLN	2.2
3	F	12	MET	2.2
1	B	332	ILE	2.2
1	A	321	LEU	2.2
1	C	578	LEU	2.2
1	A	208	GLN	2.2
3	L	39	MET	2.2
1	D	334	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
3	J	117	PRO	2.2
1	C	543	SER	2.2
3	J	119	ARG	2.2
3	L	60	HIS	2.2
1	A	578	LEU	2.2
1	D	210	ASP	2.2
2	I	9	LEU	2.2
1	A	510	ALA	2.2
1	A	541	GLY	2.2
3	L	117	PRO	2.2
1	D	301	ARG	2.2
1	A	316	LEU	2.2
1	C	747	LEU	2.2
3	L	51	LEU	2.2
1	D	217	TYR	2.1
3	L	18	MET	2.1
2	I	92	ILE	2.1
1	B	251	LEU	2.1
1	A	315	GLN	2.1
1	A	570	TRP	2.1
1	B	329	ILE	2.1
3	F	5	LYS	2.1
1	A	566	THR	2.1
1	A	438	LEU	2.1
1	A	568	ARG	2.1
1	B	214	TYR	2.1
3	J	116	PRO	2.1
1	D	570	TRP	2.1
1	D	761	LEU	2.1
1	A	561	SER	2.1
1	D	518	LYS	2.1
1	A	311	ARG	2.1
1	A	225	ILE	2.1
1	C	632	CYS	2.1
2	E	55	LEU	2.1
1	D	263	PHE	2.1
1	D	569	LEU	2.1
1	A	612	TRP	2.1
1	C	576	THR	2.0
2	K	12	THR	2.0
1	B	342	PHE	2.0
3	L	5	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	612	TRP	2.0
1	B	312	ASP	2.0
1	B	209	GLY	2.0
1	C	314	TYR	2.0
2	I	7	LEU	2.0
3	L	22	ILE	2.0
1	B	518	LYS	2.0
1	A	569	LEU	2.0
1	B	316	LEU	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, 95^{th} 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	0.87	0.15	84,93,111,116	4
3	SEP	L	8	10/11	0.89	0.16	102,105,125,127	4
3	SEP	F	8	10/11	0.92	0.13	92,98,117,117	4
3	SEP	J	8	10/11	0.94	0.11	96,101,116,122	4

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
4	CL	A	902	1/1	0.82	0.19	107,107,107,107	0
4	CL	D	902	1/1	0.92	0.12	83,83,83,83	0
4	CL	A	901	1/1	0.95	0.14	73,73,73,73	0
4	CL	B	901	1/1	0.96	0.22	73,73,73,73	0
4	CL	D	901	1/1	0.97	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	C	901	1/1	0.97	0.23	71,71,71,71	0
4	CL	C	902	1/1	0.98	0.12	76,76,76,76	0

6.5 Other polymers (i)

There are no such residues in this entry.