



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:07 PM UTC

PDB ID : 4L1U / pdb_0000411u
Title : Crystal Structure of Human Rtf1 Plus3 Domain in Complex with Spt5 CTR Phosphopeptide
Authors : Wier, A.D.; Heroux, A.; VanDemark, A.P.
Deposited on : 2013-06-03
Resolution : 2.42 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

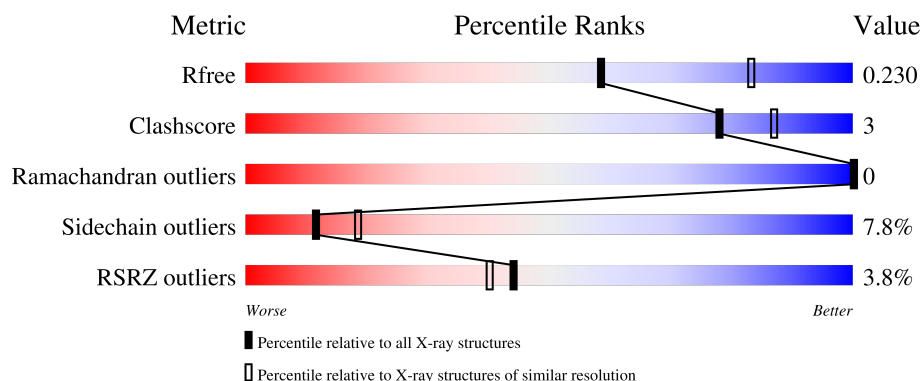
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	138	3% 82% 12% 6%
1	B	138	3% 88% 8% ..
1	C	138	2% 83% 10% 6%
1	D	138	4% 87% 11% ..
1	E	138	4% 83% 12% ..

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Mol	Chain	Length	Quality of chain
1	F	138	3% 84% 12%
2	G	13	8% 46% 15% 38%
2	H	13	23% 69% 15% 15%
2	I	13	23% 15% 62%
2	J	13	8% 31% 8% 62%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13705 atoms, of which 6712 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 RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	130	Total 2123	C 671	H 1067	N 190	O 188	S 7	0	0	0
1	B	134	Total 2183	C 689	H 1095	N 198	O 194	S 7	0	0	0
1	C	130	Total 2125	C 672	H 1069	N 190	O 187	S 7	0	0	0
1	D	136	Total 2182	C 699	H 1078	N 201	O 197	S 7	0	0	0
1	E	134	Total 2190	C 689	H 1102	N 198	O 194	S 7	0	0	0
1	F	134	Total 2178	C 689	H 1090	N 198	O 194	S 7	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	347	GLY	-	expression tag	UNP Q92541
A	348	ASP	-	expression tag	UNP Q92541
A	349	ILE	-	expression tag	UNP Q92541
A	350	THR	-	expression tag	UNP Q92541
A	351	HIS	-	expression tag	UNP Q92541
A	352	MET	-	expression tag	UNP Q92541
B	347	GLY	-	expression tag	UNP Q92541
B	348	ASP	-	expression tag	UNP Q92541
B	349	ILE	-	expression tag	UNP Q92541
B	350	THR	-	expression tag	UNP Q92541
B	351	HIS	-	expression tag	UNP Q92541
B	352	MET	-	expression tag	UNP Q92541
C	347	GLY	-	expression tag	UNP Q92541
C	348	ASP	-	expression tag	UNP Q92541
C	349	ILE	-	expression tag	UNP Q92541
C	350	THR	-	expression tag	UNP Q92541
C	351	HIS	-	expression tag	UNP Q92541

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Chain	Residue	Modelled	Actual	Comment	Reference
C	352	MET	-	expression tag	UNP Q92541
D	347	GLY	-	expression tag	UNP Q92541
D	348	ASP	-	expression tag	UNP Q92541
D	349	ILE	-	expression tag	UNP Q92541
D	350	THR	-	expression tag	UNP Q92541
D	351	HIS	-	expression tag	UNP Q92541
D	352	MET	-	expression tag	UNP Q92541
E	347	GLY	-	expression tag	UNP Q92541
E	348	ASP	-	expression tag	UNP Q92541
E	349	ILE	-	expression tag	UNP Q92541
E	350	THR	-	expression tag	UNP Q92541
E	351	HIS	-	expression tag	UNP Q92541
E	352	MET	-	expression tag	UNP Q92541
F	347	GLY	-	expression tag	UNP Q92541
F	348	ASP	-	expression tag	UNP Q92541
F	349	ILE	-	expression tag	UNP Q92541
F	350	THR	-	expression tag	UNP Q92541
F	351	HIS	-	expression tag	UNP Q92541
F	352	MET	-	expression tag	UNP Q92541

- Molecule 2 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	G	8	Total	C	H	N	O	P	S	0	0	0
			116	36	53	11	14	1	1			
2	H	11	Total	C	H	N	O	P	S	0	0	0
			141	47	57	15	20	1	1			
2	I	5	Total	C	H	N	O	P	S	0	0	0
			80	29	31	8	10	1	1			
2	J	5	Total	C	H	N	O	P	S	0	0	0
			81	23	38	8	10	1	1			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	D	1	Total	C	H	O	0	0
			14	3	8	3		
4	F	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	O	0	0
			13	13		
5	B	25	Total	O	0	0
			25	25		
5	C	15	Total	O	0	0
			15	15		
5	D	18	Total	O	0	0
			18	18		
5	E	13	Total	O	0	0
			13	13		
5	F	16	Total	O	0	0
			16	16		
5	G	3	Total	O	0	0
			3	3		
5	H	1	Total	O	0	0
			1	1		

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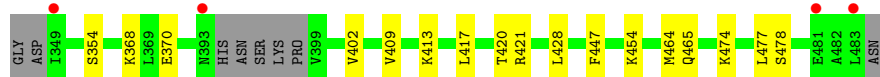
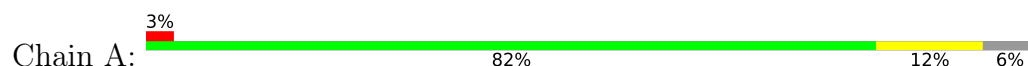
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total	O	0	0
			1	1		

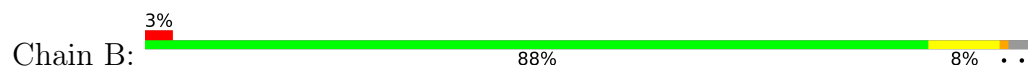
3 Residue-property plots [i](#)

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.

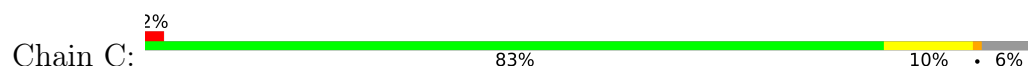
- Molecule 1: RNA polymerase-associated protein RTF1 homolog



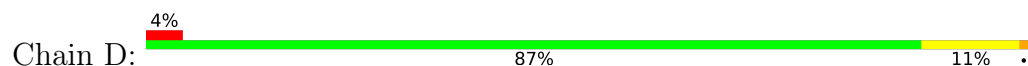
- Molecule 1: RNA polymerase-associated protein RTF1 homolog



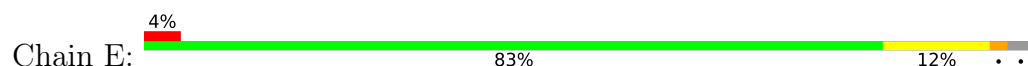
- Molecule 1: RNA polymerase-associated protein RTF1 homolog



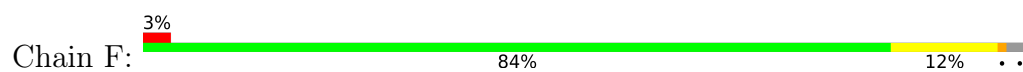
- Molecule 1: RNA polymerase-associated protein RTF1 homolog



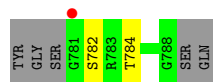
- Molecule 1: RNA polymerase-associated protein RTF1 homolog



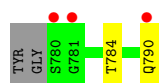
- Molecule 1: RNA polymerase-associated protein RTF1 homolog



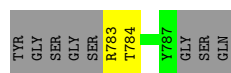
- Molecule 2: Transcription elongation factor SPT5



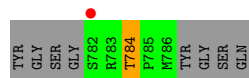
- Molecule 2: Transcription elongation factor SPT5



- Molecule 2: Transcription elongation factor SPT5



- Molecule 2: Transcription elongation factor SPT5



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.93Å 172.51Å 58.48Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	46.92 – 2.42 46.92 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.92-2.42) 95.8 (46.92-2.42)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.178 , 0.226 0.183 , 0.230	Depositor DCC
R_{free} test set	1990 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13705	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, TPO, SO4

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	0.65	0/1075	0.80	0/1442
1	B	0.67	0/1110	0.75	0/1491
1	C	0.68	0/1076	0.76	0/1443
1	D	0.57	0/1126	0.76	0/1513
1	E	0.61	0/1110	0.78	0/1491
1	F	0.58	0/1110	0.74	0/1491
2	G	0.40	0/52	0.56	0/65
2	H	0.38	0/73	0.64	0/93
2	I	0.25	0/38	0.42	0/47
2	J	0.29	0/31	0.60	0/37
All	All	0.62	0/6801	0.76	0/9113

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1056	1067	1068	3	0
1	B	1088	1095	1096	2	0
1	C	1056	1069	1071	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1104	1078	1113	9	0
1	E	1088	1102	1096	8	0
1	F	1088	1090	1096	6	0
2	G	63	53	54	0	0
2	H	84	57	72	0	0
2	I	49	31	43	2	0
2	J	43	38	39	1	0
3	A	15	0	0	0	0
3	B	35	0	0	0	0
3	C	20	0	0	0	0
3	D	35	0	0	1	0
3	E	25	0	0	0	0
3	F	15	0	0	0	0
4	A	6	8	8	1	0
4	C	6	8	8	1	0
4	D	6	8	8	0	0
4	F	6	8	8	0	0
5	A	13	0	0	0	0
5	B	25	0	0	0	0
5	C	15	0	0	1	0
5	D	18	0	0	0	0
5	E	13	0	0	2	0
5	F	16	0	0	0	0
5	G	3	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	1	0
All	All	6993	6712	6780	38	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 3.

All (38) 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:395:ASN:HB2	1:D:397:LYS:HE3	1.54	0.89
1:C:397:LYS:N	1:C:398:PRO:CD	2.45	0.79
1:C:397:LYS:N	1:C:398:PRO:HD3	1.98	0.79
1:D:395:ASN:CB	1:D:397:LYS:HE3	2.14	0.78
1:D:428:LEU:HD12	1:D:437:PHE:CD2	2.25	0.71
1:E:421:ARG:NH2	5:E:613:HOH:O	2.30	0.62
1:C:371:ARG:NH1	5:C:610:HOH:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:ARG:NE	5:E:608:HOH:O	2.42	0.52
2:I:783:ARG:HD2	5:I:801:HOH:O	2.10	0.50
1:E:395:ASN:O	1:E:396:SER:HB2	2.11	0.50
1:B:395:ASN:O	1:B:396:SER:OG	2.26	0.48
1:A:420:THR:OG1	1:A:421:ARG:N	2.47	0.47
4:A:504:GOL:O1	4:A:504:GOL:O3	2.18	0.47
1:E:385:CYS:SG	1:E:479:ILE:HD11	2.54	0.47
1:A:370:GLU:HG2	1:A:417:LEU:HG	1.95	0.47
1:E:459:MET:SD	1:E:464:MET:HE2	2.56	0.46
1:B:420:THR:OG1	1:B:421:ARG:N	2.48	0.45
1:D:473:ASN:ND2	3:D:504:SO4:O1	2.44	0.45
1:F:426:LEU:HB3	1:F:428:LEU:HD13	1.98	0.45
1:C:469:LEU:HD13	1:C:473:ASN:ND2	2.32	0.45
1:A:402:VAL:HG22	1:A:447:PHE:CD1	2.52	0.44
1:D:428:LEU:HD12	1:D:437:PHE:HD2	1.81	0.44
1:E:370:GLU:HG2	1:E:417:LEU:HG	1.99	0.44
1:F:370:GLU:HG2	1:F:417:LEU:HG	2.01	0.43
1:C:373:CYS:HA	1:C:378:PHE:CD1	2.54	0.43
1:E:397:LYS:HB2	1:E:397:LYS:HE3	1.79	0.43
1:E:395:ASN:HB3	1:E:397:LYS:HD3	2.00	0.42
1:F:372:TRP:CZ2	1:F:482:ALA:C	2.97	0.42
1:D:395:ASN:HB3	1:D:397:LYS:HE3	1.99	0.42
1:D:372:TRP:CZ2	1:D:483:LEU:HD21	2.56	0.41
1:C:428:LEU:HD12	1:C:437:PHE:CD1	2.55	0.41
1:D:395:ASN:HB2	1:D:397:LYS:CE	2.39	0.41
1:F:414:VAL:HG22	1:F:423:ASN:ND2	2.36	0.41
2:I:783:ARG:HD3	2:I:783:ARG:C	2.46	0.41
1:F:443:SER:OG	2:J:784:TPO:O3P	2.35	0.41
1:F:411:THR:HG22	1:F:423:ASN:HA	2.02	0.40
1:D:402:VAL:HG22	1:D:447:PHE:CD1	2.56	0.40
1:C:377:PHE:HA	4:C:505:GOL:O2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	126/138 (91%)	124 (98%)	2 (2%)	0	100	100
1	B	132/138 (96%)	129 (98%)	3 (2%)	0	100	100
1	C	126/138 (91%)	124 (98%)	2 (2%)	0	100	100
1	D	134/138 (97%)	132 (98%)	2 (2%)	0	100	100
1	E	132/138 (96%)	131 (99%)	1 (1%)	0	100	100
1	F	132/138 (96%)	129 (98%)	3 (2%)	0	100	100
2	G	5/13 (38%)	5 (100%)	0	0	100	100
2	H	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	I	2/13 (15%)	2 (100%)	0	0	100	100
2	J	2/13 (15%)	2 (100%)	0	0	100	100
All	All	799/880 (91%)	785 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	115/122 (94%)	104 (90%)	11 (10%)	8	12
1	B	119/122 (98%)	110 (92%)	9 (8%)	12	19
1	C	115/122 (94%)	109 (95%)	6 (5%)	21	34
1	D	121/122 (99%)	113 (93%)	8 (7%)	15	25
1	E	119/122 (98%)	108 (91%)	11 (9%)	8	13
1	F	119/122 (98%)	109 (92%)	10 (8%)	10	16
2	G	5/9 (56%)	4 (80%)	1 (20%)	1	1
2	H	8/9 (89%)	7 (88%)	1 (12%)	4	6
2	I	4/9 (44%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	4/9 (44%)	4 (100%)	0	100	100
All	All	729/768 (95%)	672 (92%)	57 (8%)	11	18

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	354	SER
1	A	368	LYS
1	A	409	VAL
1	A	413	LYS
1	A	428	LEU
1	A	454	LYS
1	A	464	MET
1	A	465	GLN
1	A	474	LYS
1	A	477	LEU
1	A	478	SER
1	B	350	THR
1	B	369	LEU
1	B	397	LYS
1	B	410	GLU
1	B	421	ARG
1	B	454	LYS
1	B	456	LYS
1	B	469	LEU
1	B	483	LEU
1	C	357	GLU
1	C	391	ILE
1	C	421	ARG
1	C	426	LEU
1	C	453	MET
1	C	469	LEU
1	D	359	LEU
1	D	360	ASN
1	D	394	HIS
1	D	397	LYS
1	D	420	THR
1	D	435	ARG
1	D	479	ILE
1	D	480	LYS
1	E	349	ILE
1	E	357	GLU

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Mol	Chain	Res	Type
1	E	368	LYS
1	E	395	ASN
1	E	396	SER
1	E	397	LYS
1	E	426	LEU
1	E	450	SER
1	E	456	LYS
1	E	477	LEU
1	E	480	LYS
1	F	351	HIS
1	F	355	LEU
1	F	395	ASN
1	F	420	THR
1	F	426	LEU
1	F	428	LEU
1	F	453	MET
1	F	469	LEU
1	F	477	LEU
1	F	479	ILE
2	G	782	SER
2	H	790	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	GLN
1	C	445	GLN
1	D	445	GLN
1	E	367	HIS
1	E	393	ASN
1	E	423	ASN
1	E	465	GLN
1	F	374	HIS
1	F	393	ASN
1	F	394	HIS

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
2	TPO	G	784	2	8,10,11	1.32	2 (25%)	10,14,16	1.73	1 (10%)
2	TPO	I	784	2	8,10,11	1.37	1 (12%)	10,14,16	1.57	1 (10%)
2	TPO	H	784	2	8,10,11	1.24	1 (12%)	10,14,16	1.78	1 (10%)
2	TPO	J	784	2	8,10,11	1.22	1 (12%)	10,14,16	2.01	3 (30%)

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	TPO	G	784	2	-	0/9/11/13	-
2	TPO	I	784	2	-	0/9/11/13	-
2	TPO	H	784	2	-	0/9/11/13	-
2	TPO	J	784	2	-	0/9/11/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	784	TPO	P-O2P	2.21	1.63	1.54
2	J	784	TPO	P-O2P	2.10	1.62	1.54
2	G	784	TPO	P-O3P	2.07	1.62	1.54
2	G	784	TPO	P-O2P	2.07	1.62	1.54
2	H	784	TPO	P-O2P	2.02	1.62	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	784	TPO	P-OG1-CB	-5.25	109.07	123.33
2	G	784	TPO	P-OG1-CB	-4.56	110.94	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	784	TPO	P-OG1-CB	-4.52	111.04	123.33
2	I	784	TPO	P-OG1-CB	-3.76	113.12	123.33
2	J	784	TPO	O-C-CA	-2.31	118.84	124.77
2	J	784	TPO	CG2-CB-CA	-2.11	109.14	113.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	784	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

33 ligands 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	SO4	B	506	-	4,4,4	0.23	0	6,6,6	0.15	0
3	SO4	D	506	-	4,4,4	0.26	0	6,6,6	0.13	0
3	SO4	D	505	-	4,4,4	0.22	0	6,6,6	0.24	0
3	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	B	507	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	F	502	-	4,4,4	0.26	0	6,6,6	0.06	0
3	SO4	E	505	-	4,4,4	0.25	0	6,6,6	0.19	0
3	SO4	A	503	-	4,4,4	0.25	0	6,6,6	0.18	0
3	SO4	F	501	-	4,4,4	0.23	0	6,6,6	0.18	0
4	GOL	C	505	-	5,5,5	0.43	0	5,5,5	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	F	503	-	4,4,4	0.25	0	6,6,6	0.09	0
4	GOL	D	508	-	5,5,5	0.31	0	5,5,5	0.27	0
3	SO4	C	501	-	4,4,4	0.25	0	6,6,6	0.30	0
3	SO4	E	503	-	4,4,4	0.23	0	6,6,6	0.17	0
3	SO4	D	504	-	4,4,4	0.21	0	6,6,6	0.17	0
3	SO4	A	502	-	4,4,4	0.22	0	6,6,6	0.17	0
3	SO4	C	503	-	4,4,4	0.24	0	6,6,6	0.18	0
3	SO4	D	507	-	4,4,4	0.25	0	6,6,6	0.11	0
3	SO4	E	501	-	4,4,4	0.27	0	6,6,6	0.26	0
4	GOL	A	504	-	5,5,5	0.36	0	5,5,5	0.45	0
4	GOL	F	504	-	5,5,5	0.36	0	5,5,5	0.23	0
3	SO4	A	501	-	4,4,4	0.19	0	6,6,6	0.15	0
3	SO4	B	502	-	4,4,4	0.22	0	6,6,6	0.19	0
3	SO4	B	504	-	4,4,4	0.24	0	6,6,6	0.05	0
3	SO4	B	505	-	4,4,4	0.25	0	6,6,6	0.36	0
3	SO4	D	502	-	4,4,4	0.28	0	6,6,6	0.34	0
3	SO4	B	503	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	B	501	-	4,4,4	0.22	0	6,6,6	0.27	0
3	SO4	E	502	-	4,4,4	0.26	0	6,6,6	0.17	0
3	SO4	D	501	-	4,4,4	0.28	0	6,6,6	0.28	0
3	SO4	C	504	-	4,4,4	0.23	0	6,6,6	0.47	0
3	SO4	E	504	-	4,4,4	0.28	0	6,6,6	0.29	0
3	SO4	D	503	-	4,4,4	0.23	0	6,6,6	0.11	0

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
4	GOL	D	508	-	-	2/4/4/4	-
4	GOL	C	505	-	-	4/4/4/4	-
4	GOL	A	504	-	-	2/4/4/4	-
4	GOL	F	504	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	GOL	O1-C1-C2-O2
4	A	504	GOL	O1-C1-C2-C3
4	C	505	GOL	O1-C1-C2-C3
4	C	505	GOL	C1-C2-C3-O3
4	F	504	GOL	O1-C1-C2-C3
4	D	508	GOL	O1-C1-C2-C3
4	C	505	GOL	O2-C2-C3-O3
4	D	508	GOL	O1-C1-C2-O2
4	F	504	GOL	O1-C1-C2-O2
4	C	505	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	505	GOL	1	0
3	D	504	SO4	1	0
4	A	504	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	130/138 (94%)	-0.04	4 (3%) 51 48	29, 51, 83, 104	0
1	B	134/138 (97%)	-0.14	4 (2%) 52 49	27, 47, 78, 106	0
1	C	130/138 (94%)	-0.21	3 (2%) 61 57	29, 47, 73, 95	0
1	D	136/138 (98%)	-0.02	5 (3%) 45 41	29, 49, 91, 117	0
1	E	134/138 (97%)	0.04	6 (4%) 38 34	33, 52, 91, 104	0
1	F	134/138 (97%)	0.12	4 (2%) 52 49	36, 57, 88, 122	0
2	G	7/13 (53%)	0.96	1 (14%) 6 4	45, 62, 81, 84	0
2	H	10/13 (76%)	1.15	3 (30%) 1 1	50, 67, 96, 106	0
2	I	4/13 (30%)	1.28	0 100 100	74, 82, 88, 95	0
2	J	4/13 (30%)	1.41	1 (25%) 2 1	78, 80, 112, 116	0
All	All	823/880 (93%)	-0.00	31 (3%) 44 40	27, 51, 88, 122	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	349	ILE	4.4
1	E	377	PHE	3.8
1	B	483	LEU	3.7
1	A	349	ILE	3.4
2	G	781	GLY	3.3
1	A	483	LEU	3.3
1	D	394	HIS	2.9
1	C	392	GLY	2.9
1	E	482	ALA	2.9
1	F	482	ALA	2.8
1	C	350	THR	2.7
2	H	781	GLY	2.7
1	D	395	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	396	SER	2.6
1	D	484	ASN	2.5
1	B	377	PHE	2.5
1	E	351	HIS	2.5
2	H	790	GLN	2.4
1	F	349	ILE	2.3
1	A	481	GLU	2.3
2	H	780	SER	2.3
1	F	469	LEU	2.3
1	B	432	ASN	2.3
1	F	372	TRP	2.3
1	E	470	ASP	2.2
1	C	483	LEU	2.2
2	J	782	SER	2.1
1	A	393	ASN	2.1
1	E	397	LYS	2.1
1	D	397	LYS	2.0
1	B	350	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TPO	I	784	11/12	0.95	0.12	60,75,83,98	0
2	TPO	J	784	11/12	0.95	0.10	66,82,90,99	0
2	TPO	H	784	11/12	0.98	0.08	30,47,56,61	0
2	TPO	G	784	11/12	0.99	0.06	37,43,52,52	0

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(Å ²)	Q<0.9
3	SO4	D	507	5/5	0.71	0.10	111,111,112,114	0
3	SO4	F	503	5/5	0.73	0.13	111,113,115,116	0
4	GOL	F	504	6/6	0.76	0.15	59,72,85,86	0
3	SO4	E	502	5/5	0.77	0.12	87,89,91,93	0
3	SO4	B	506	5/5	0.79	0.11	102,104,104,106	0
3	SO4	F	501	5/5	0.80	0.14	68,76,81,82	0
3	SO4	F	502	5/5	0.80	0.09	99,99,100,102	0
3	SO4	B	503	5/5	0.81	0.12	82,85,90,90	0
3	SO4	D	503	5/5	0.81	0.12	92,94,94,95	0
3	SO4	E	503	5/5	0.82	0.11	92,94,95,96	0
3	SO4	D	506	5/5	0.83	0.09	99,100,100,102	0
4	GOL	A	504	6/6	0.83	0.15	64,77,87,88	0
3	SO4	B	504	5/5	0.83	0.11	93,94,95,96	0
3	SO4	E	501	5/5	0.84	0.13	83,86,87,89	0
4	GOL	C	505	6/6	0.84	0.17	66,79,89,93	0
3	SO4	C	501	5/5	0.84	0.11	89,90,91,93	0
3	SO4	E	505	5/5	0.85	0.09	97,98,98,99	0
3	SO4	A	503	5/5	0.86	0.08	95,98,99,99	0
4	GOL	D	508	6/6	0.86	0.21	56,68,79,81	0
3	SO4	B	507	5/5	0.86	0.09	98,100,100,101	0
3	SO4	C	502	5/5	0.89	0.11	94,97,98,98	0
3	SO4	D	501	5/5	0.89	0.11	73,76,78,78	0
3	SO4	C	503	5/5	0.90	0.08	84,85,86,90	0
3	SO4	B	505	5/5	0.90	0.18	95,98,99,100	0
3	SO4	D	505	5/5	0.91	0.17	90,94,95,98	0
3	SO4	B	502	5/5	0.93	0.08	65,67,68,70	0
3	SO4	A	501	5/5	0.94	0.15	92,95,96,97	0
3	SO4	C	504	5/5	0.94	0.13	50,51,54,59	0
3	SO4	D	504	5/5	0.95	0.07	63,65,68,72	0
3	SO4	E	504	5/5	0.95	0.14	87,91,92,92	0
3	SO4	D	502	5/5	0.96	0.07	41,44,49,52	0
3	SO4	A	502	5/5	0.96	0.07	39,45,47,48	0
3	SO4	B	501	5/5	0.97	0.11	47,51,52,55	0

6.5 Other polymers ⓘ

There are no such residues in this entry.