Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 07:34 PM EDT

PDB ID	:	4L1U
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:

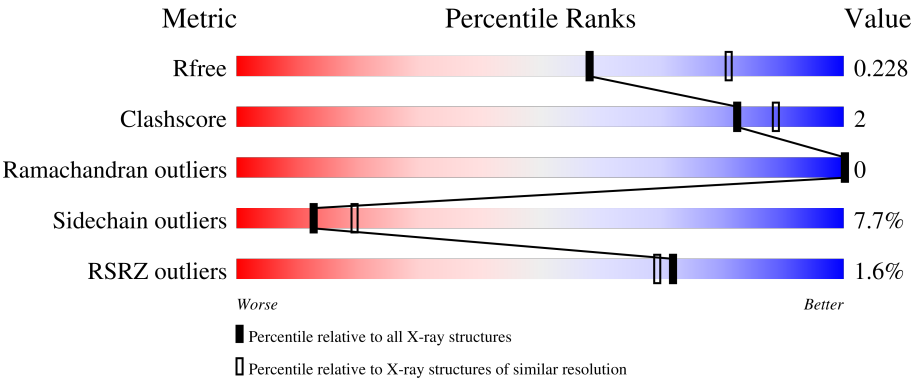
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (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 <=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	82% 12% 6%
1	B	138	% 89% 8% •
1	C	138	% 83% 10% • 6%
1	D	138	2% 86% 12% •
1	E	138	2% 86% 9% • •

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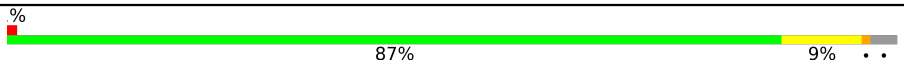
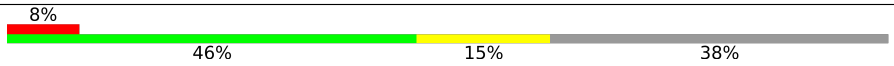
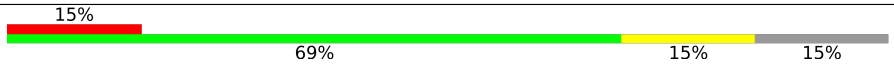
Mol	Chain	Length	Quality of chain
1	F	138	
2	G	13	
2	H	13	
2	I	13	
2	J	13	

2 Entry composition (i)

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

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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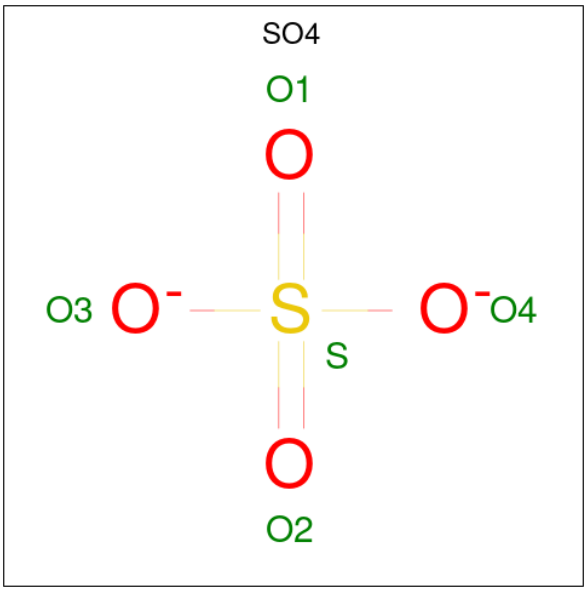
Chain	Residue	Modelled	Actual	Comment	Reference
C	352	MET	-	expression tag	UNP Q92541
D	347	GLY	-	expression tag	UNP Q92541
D	348	ASP	-	expression tag	UNP Q92541
D	349	ILE	-	expression tag	UNP Q92541
D	350	THR	-	expression tag	UNP Q92541
D	351	HIS	-	expression tag	UNP Q92541
D	352	MET	-	expression tag	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 (three-letter code: SO4) (formula: O_4S).



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

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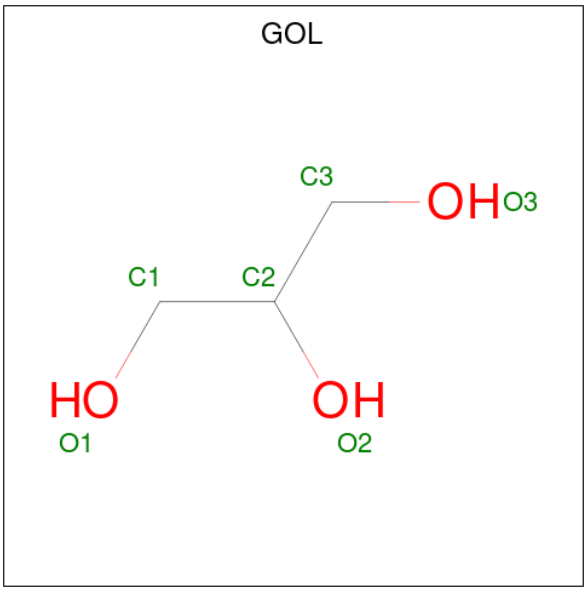
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

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

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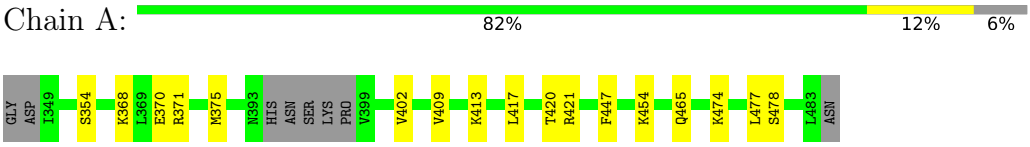
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total O 1 1	0	0

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.

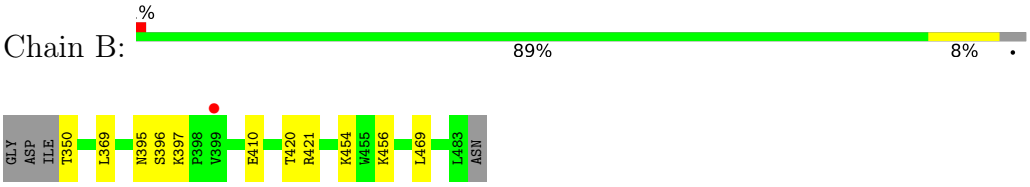
• Molecule 1: RNA polymerase-associated protein RTF1 homolog

Chain A:



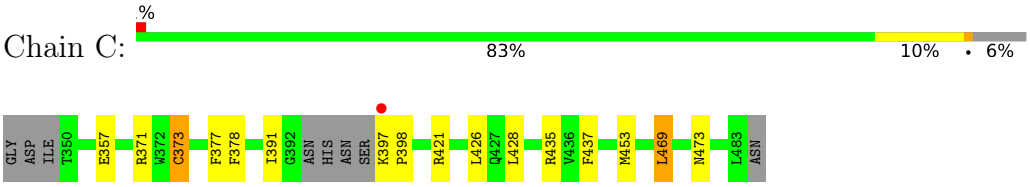
• Molecule 1: RNA polymerase-associated protein RTF1 homolog

Chain B:



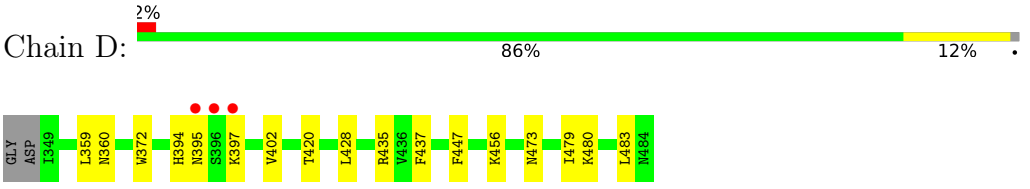
• Molecule 1: RNA polymerase-associated protein RTF1 homolog

Chain C:



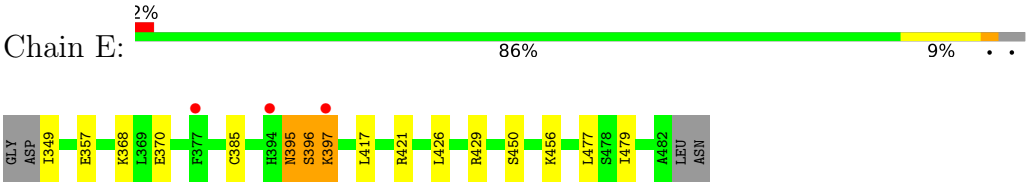
• Molecule 1: RNA polymerase-associated protein RTF1 homolog

Chain D:



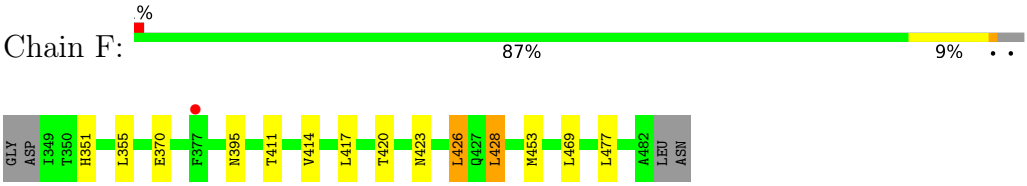
• Molecule 1: RNA polymerase-associated protein RTF1 homolog

Chain E:



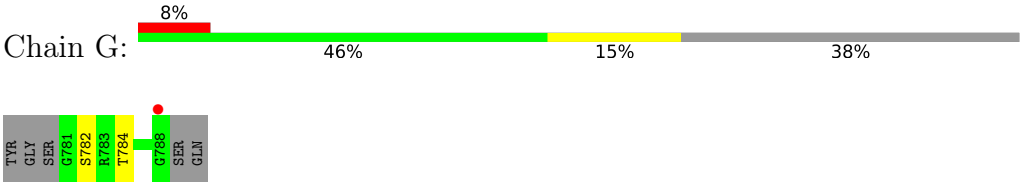
• Molecule 1: RNA polymerase-associated protein RTF1 homolog

Chain F:



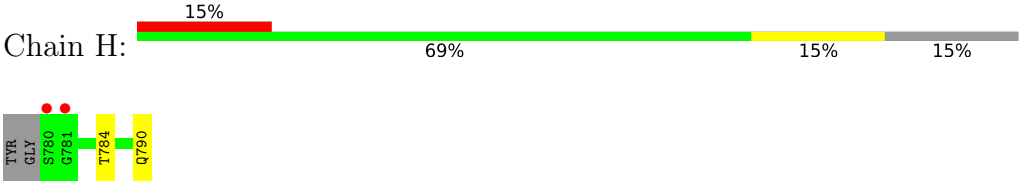
• Molecule 2: Transcription elongation factor SPT5

Chain G:



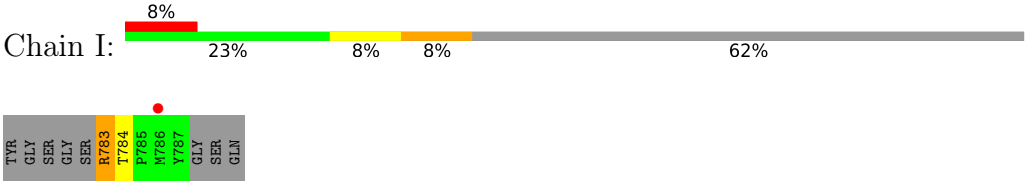
• Molecule 2: Transcription elongation factor SPT5

Chain H:



• Molecule 2: Transcription elongation factor SPT5

Chain I:



• Molecule 2: Transcription elongation factor SPT5

Chain J:

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.10 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.178 , 0.226 0.180 , 0.228	Depositor DCC
R_{free} test set	1990 reflections (4.94%)	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)	0.40 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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: TPO, SO4, GOL

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	0.52	0/1075	0.61	0/1442
1	B	0.54	0/1110	0.61	0/1491
1	C	0.59	1/1076 (0.1%)	0.59	0/1443
1	D	0.47	0/1126	0.60	0/1513
1	E	0.51	0/1110	0.59	0/1491
1	F	0.46	0/1110	0.60	0/1491
2	G	0.37	0/52	0.40	0/65
2	H	0.37	0/73	0.50	0/93
2	I	0.30	0/38	0.43	0/47
2	J	0.31	0/31	0.58	0/37
All	All	0.51	1/6801 (0.0%)	0.60	0/9113

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	373	CYS	CB-SG	-6.05	1.72	1.82

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
1	D	1104	1078	1113	9	0
1	E	1088	1102	1096	7	0
1	F	1088	1090	1096	4	0
2	G	63	53	54	0	0
2	H	84	57	72	0	0
2	I	49	31	43	1	0
2	J	43	38	39	0	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	34	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 (34) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
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 (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	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 (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	115/122 (94%)	104 (90%)	11 (10%)	8	11
1	B	119/122 (98%)	112 (94%)	7 (6%)	19	30
1	C	115/122 (94%)	108 (94%)	7 (6%)	18	29
1	D	121/122 (99%)	113 (93%)	8 (7%)	16	25
1	E	119/122 (98%)	109 (92%)	10 (8%)	11	16
1	F	119/122 (98%)	110 (92%)	9 (8%)	13	20
2	G	5/9 (56%)	4 (80%)	1 (20%)	1	1
2	H	8/9 (89%)	7 (88%)	1 (12%)	4	5
2	I	4/9 (44%)	3 (75%)	1 (25%)	0	0
2	J	4/9 (44%)	3 (75%)	1 (25%)	0	0
All	All	729/768 (95%)	673 (92%)	56 (8%)	13	19

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	354	SER
1	A	368	LYS
1	A	371	ARG
1	A	375	MET
1	A	409	VAL
1	A	413	LYS
1	A	454	LYS
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	454	LYS
1	B	456	LYS
1	B	469	LEU
1	C	357	GLU
1	C	391	ILE
1	C	421	ARG
1	C	426	LEU
1	C	435	ARG
1	C	453	MET
1	C	469	LEU
1	D	359	LEU
1	D	360	ASN
1	D	394	HIS
1	D	420	THR
1	D	435	ARG
1	D	456	LYS
1	D	479	ILE
1	D	480	LYS
1	E	349	ILE
1	E	357	GLU
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

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Mol	Chain	Res	Type
1	E	477	LEU
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
2	G	782	SER
2	H	790	GLN
2	I	783	ARG
2	J	783	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	465	GLN
1	F	374	HIS
1	F	394	HIS

5.3.3 RNA (i)

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	$\#\|Z\| > 2$
2	TPO	I	784	2	8,10,11	1.33	1 (12%)	10,14,16	1.43	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	TPO	H	784	2	8,10,11	1.19	0	10,14,16	1.63	1 (10%)
2	TPO	G	784	2	8,10,11	1.28	0	10,14,16	1.57	1 (10%)
2	TPO	J	784	2	8,10,11	1.19	1 (12%)	10,14,16	1.84	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	I	784	2	-	0/9/11/13	-
2	TPO	H	784	2	-	0/9/11/13	-
2	TPO	G	784	2	-	0/9/11/13	-
2	TPO	J	784	2	-	0/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	784	TPO	P-O2P	2.12	1.63	1.54
2	J	784	TPO	P-O2P	2.01	1.62	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	784	TPO	P-OG1-CB	-4.68	109.07	123.21
2	G	784	TPO	P-OG1-CB	-4.06	110.94	123.21
2	H	784	TPO	P-OG1-CB	-4.03	111.04	123.21
2	I	784	TPO	P-OG1-CB	-3.34	113.12	123.21
2	J	784	TPO	O-C-CA	-2.27	118.84	124.78
2	J	784	TPO	CG2-CB-CA	-2.04	109.14	113.16

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)

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	A	503	-	4,4,4	0.15	0	6,6,6	0.16	0
3	SO4	C	504	-	4,4,4	0.25	0	6,6,6	0.55	0
3	SO4	A	502	-	4,4,4	0.13	0	6,6,6	0.19	0
3	SO4	B	505	-	4,4,4	0.17	0	6,6,6	0.34	0
4	GOL	D	508	-	5,5,5	0.31	0	5,5,5	0.24	0
3	SO4	D	502	-	4,4,4	0.18	0	6,6,6	0.38	0
3	SO4	F	503	-	4,4,4	0.15	0	6,6,6	0.13	0
3	SO4	F	501	-	4,4,4	0.11	0	6,6,6	0.19	0
3	SO4	A	501	-	4,4,4	0.12	0	6,6,6	0.18	0
3	SO4	E	504	-	4,4,4	0.19	0	6,6,6	0.33	0
3	SO4	B	506	-	4,4,4	0.13	0	6,6,6	0.14	0
3	SO4	E	501	-	4,4,4	0.17	0	6,6,6	0.23	0
3	SO4	D	505	-	4,4,4	0.13	0	6,6,6	0.23	0
3	SO4	C	501	-	4,4,4	0.15	0	6,6,6	0.28	0
3	SO4	E	502	-	4,4,4	0.16	0	6,6,6	0.16	0
3	SO4	D	504	-	4,4,4	0.12	0	6,6,6	0.16	0
3	SO4	D	506	-	4,4,4	0.16	0	6,6,6	0.10	0
3	SO4	B	503	-	4,4,4	0.13	0	6,6,6	0.11	0
3	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.13	0
3	SO4	B	504	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SO4	E	505	-	4,4,4	0.15	0	6,6,6	0.16	0
3	SO4	B	501	-	4,4,4	0.23	0	6,6,6	0.26	0
3	SO4	F	502	-	4,4,4	0.15	0	6,6,6	0.07	0
3	SO4	B	502	-	4,4,4	0.14	0	6,6,6	0.23	0
3	SO4	D	503	-	4,4,4	0.13	0	6,6,6	0.10	0
3	SO4	E	503	-	4,4,4	0.14	0	6,6,6	0.15	0
3	SO4	D	501	-	4,4,4	0.17	0	6,6,6	0.25	0
4	GOL	C	505	-	5,5,5	0.42	0	5,5,5	0.82	0
4	GOL	F	504	-	5,5,5	0.35	0	5,5,5	0.21	0
4	GOL	A	504	-	5,5,5	0.35	0	5,5,5	0.41	0
3	SO4	D	507	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	C	503	-	4,4,4	0.15	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	B	507	-	4,4,4	0.13	0	6,6,6	0.07	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	A	504	-	-	2/4/4/4	-
4	GOL	C	505	-	-	4/4/4/4	-
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
3	D	504	SO4	1	0
4	C	505	GOL	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, 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	130/138 (94%)	0.18	0 100 100	26, 47, 78, 96	0
1	B	134/138 (97%)	0.21	1 (0%) 87 86	25, 43, 72, 97	0
1	C	130/138 (94%)	0.22	1 (0%) 86 84	27, 43, 67, 87	0
1	D	136/138 (98%)	0.27	3 (2%) 62 59	26, 45, 81, 117	0
1	E	134/138 (97%)	0.25	3 (2%) 62 59	30, 47, 81, 95	0
1	F	134/138 (97%)	0.26	1 (0%) 87 86	33, 52, 84, 109	0
2	G	7/13 (53%)	0.93	1 (14%) 2 2	42, 55, 76, 79	0
2	H	10/13 (76%)	1.24	2 (20%) 1 0	46, 64, 94, 98	0
2	I	4/13 (30%)	1.20	1 (25%) 0 0	68, 73, 79, 95	0
2	J	4/13 (30%)	1.19	0 100 100	71, 74, 104, 105	0
All	All	823/880 (93%)	0.26	13 (1%) 72 69	25, 47, 79, 117	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	397	LYS	2.8
1	F	377	PHE	2.7
2	H	780	SER	2.6
1	E	377	PHE	2.6
1	D	396	SER	2.6
2	H	781	GLY	2.6
1	B	399	VAL	2.5
1	D	397	LYS	2.5
2	G	788	GLY	2.5
1	E	394	HIS	2.4
1	E	397	LYS	2.4
2	I	786	MET	2.3
1	D	395	ASN	2.1

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
2	TPO	I	784	11/12	0.94	0.26	60,75,83,98	0
2	TPO	J	784	11/12	0.94	0.17	66,82,90,99	0
2	TPO	H	784	11/12	0.98	0.15	30,47,56,61	0
2	TPO	G	784	11/12	0.99	0.14	37,43,52,52	0

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	GOL	C	505	6/6	0.81	0.27	66,79,89,93	0
3	SO4	D	507	5/5	0.85	0.17	111,111,112,114	0
3	SO4	F	503	5/5	0.87	0.17	111,113,115,116	0
3	SO4	D	503	5/5	0.87	0.13	92,94,94,95	0
3	SO4	D	506	5/5	0.88	0.20	99,100,100,102	0
3	SO4	F	501	5/5	0.88	0.18	68,76,81,82	0
3	SO4	B	507	5/5	0.89	0.17	98,100,100,101	0
3	SO4	C	501	5/5	0.89	0.18	89,90,91,93	0
3	SO4	E	505	5/5	0.90	0.17	97,98,98,99	0
3	SO4	C	502	5/5	0.90	0.27	94,97,98,98	0
3	SO4	A	503	5/5	0.90	0.14	95,98,99,99	0
4	GOL	A	504	6/6	0.90	0.26	64,77,87,88	0
3	SO4	E	502	5/5	0.90	0.16	87,89,91,93	0
3	SO4	E	501	5/5	0.91	0.18	83,86,87,89	0
4	GOL	F	504	6/6	0.91	0.08	59,72,85,86	0
3	SO4	E	503	5/5	0.92	0.13	92,94,95,96	0
3	SO4	A	501	5/5	0.92	0.27	92,95,96,97	0
3	SO4	D	505	5/5	0.92	0.34	90,94,95,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	F	502	5/5	0.92	0.12	99,99,100,102	0
3	SO4	E	504	5/5	0.93	0.23	87,91,92,92	0
3	SO4	B	505	5/5	0.93	0.31	95,98,99,100	0
3	SO4	C	503	5/5	0.93	0.21	84,85,86,90	0
3	SO4	B	506	5/5	0.93	0.16	102,104,104,106	0
3	SO4	D	501	5/5	0.94	0.14	73,76,78,78	0
4	GOL	D	508	6/6	0.94	0.23	56,68,79,81	0
3	SO4	B	503	5/5	0.94	0.26	82,85,90,90	0
3	SO4	C	504	5/5	0.95	0.26	50,51,54,59	0
3	SO4	B	502	5/5	0.97	0.17	65,67,68,70	0
3	SO4	A	502	5/5	0.97	0.19	39,45,47,48	0
3	SO4	D	502	5/5	0.97	0.16	41,44,49,52	0
3	SO4	B	504	5/5	0.97	0.15	93,94,95,96	0
3	SO4	D	504	5/5	0.97	0.14	63,65,68,72	0
3	SO4	B	501	5/5	0.98	0.25	47,51,52,55	0

6.5 Other polymers (i)

There are no such residues in this entry.