Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:16 pm BST

PDB ID	:	6H0E
Title	:	FAB dmCBTAU-22.1 IN COMPLEX WITH TAU PEPTIDE V1088-23
Authors	:	Juraszek, J.; Steinbacher, S.
Deposited on	:	2018-07-09
Resolution	:	1.95 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 following versions of software and data (see references ⓘ) were used in the production of this report:

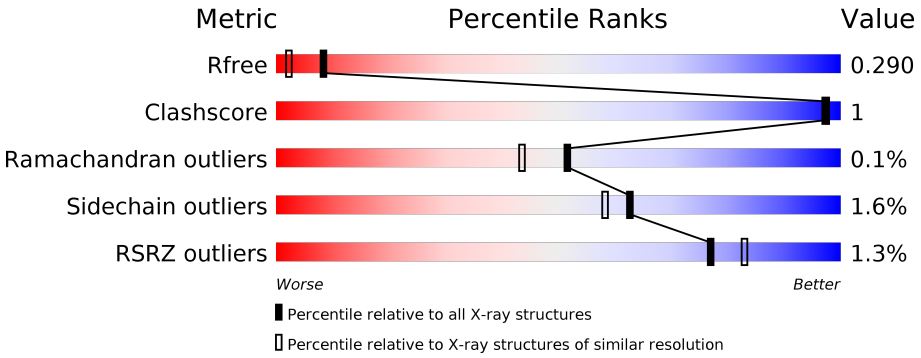
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 on 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	222	93%
1	C	222	95%
1	E	222	94%
1	H	222	95%
2	B	218	97%
2	D	218	4% 94% 6%

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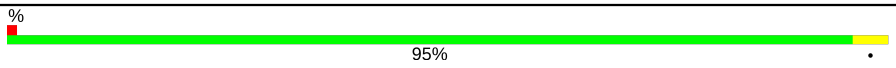
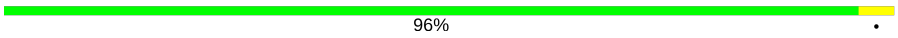
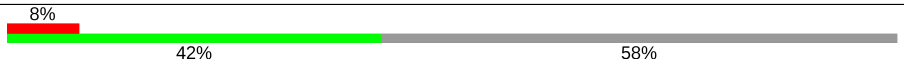
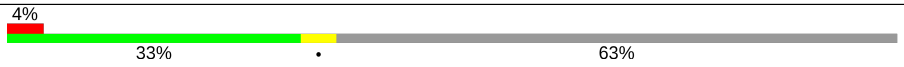
Mol	Chain	Length	Quality of chain
2	F	218	
2	L	218	
3	G	24	
3	I	24	
3	J	24	
3	K	24	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14498 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HUMAN FAB ANTIBODY FRAGMENT OF dmCBTAU-22.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	217	Total	C	N	O	S	0	1	0
			1642	1029	286	317	10			
1	A	216	Total	C	N	O	S	6	0	0
			1630	1023	284	313	10			
1	C	219	Total	C	N	O	S	11	0	0
			1649	1034	288	317	10			
1	E	216	Total	C	N	O	S	7	0	0
			1625	1019	283	313	10			

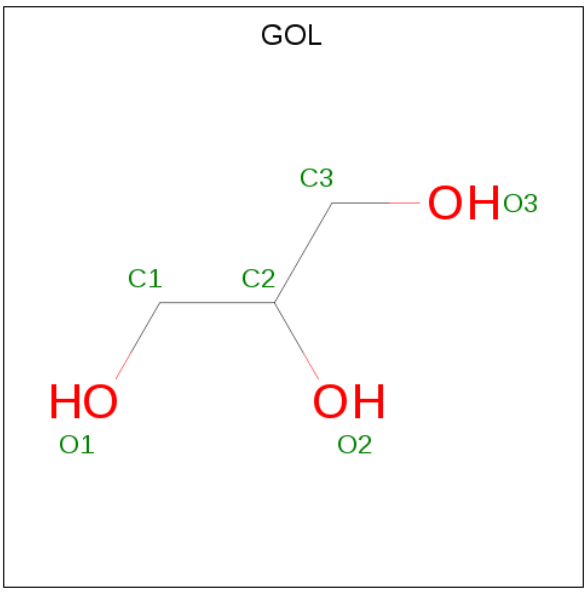
- Molecule 2 is a protein called HUMAN FAB ANTIBODY FRAGMENT OF dmCBTAU-22.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	218	Total	C	N	O	S	0	1	0
			1698	1065	291	336	6			
2	B	218	Total	C	N	O	S	18	2	0
			1702	1068	291	337	6			
2	D	217	Total	C	N	O	S	25	1	0
			1689	1060	290	333	6			
2	F	218	Total	C	N	O	S	22	1	0
			1698	1065	291	336	6			

- Molecule 3 is a protein called Microtubule-associated protein tau.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	I	9	Total	C	N	O	P	S	6	0	0
			69	40	10	17	1	1			
3	G	10	Total	C	N	O	P	S	0	0	0
			77	44	11	20	1	1			
3	J	8	Total	C	N	O	P	S	0	0	0
			62	36	9	15	1	1			
3	K	8	Total	C	N	O	P	S	0	0	0
			62	36	9	15	1	1			

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	136	Total O 136 136	0	0
5	L	131	Total O 131 131	0	0
5	A	117	Total O 117 117	0	0
5	B	84	Total O 84 84	0	0
5	C	99	Total O 99 99	0	0
5	D	61	Total O 61 61	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	107	Total O 107 107	0	0
5	F	101	Total O 101 101	0	0
5	I	8	Total O 8 8	0	0
5	G	11	Total O 11 11	0	0
5	J	5	Total O 5 5	0	0
5	K	5	Total O 5 5	0	0

3 Residue-property plots (i)

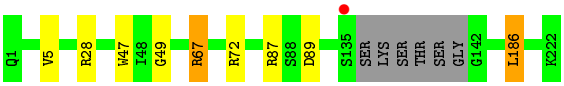
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: HUMAN FAB ANTIBODY FRAGMENT OF dmCBTAU-22.1

Chain H:

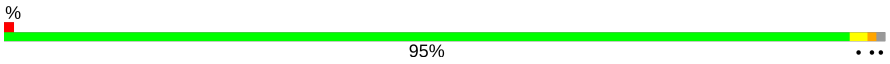
- Molecule 1: HUMAN FAB ANTIBODY FRAGMENT OF dmCBTAU-22.1

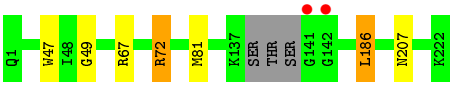
Chain A:



- Molecule 1: HUMAN FAB ANTIBODY FRAGMENT OF dmCBTAU-22.1

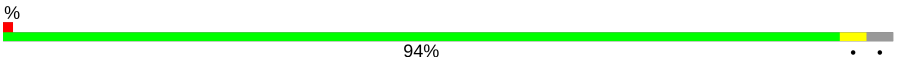
Chain C:

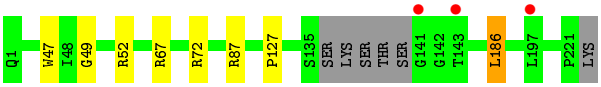




- Molecule 1: HUMAN FAB ANTIBODY FRAGMENT OF dmCBTAU-22.1

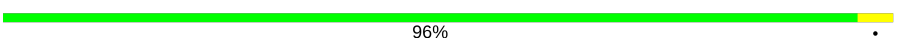
Chain E:

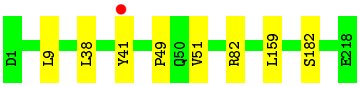




- Molecule 2: HUMAN FAB ANTIBODY FRAGMENT OF dmCBTAU-22.1

Chain L:



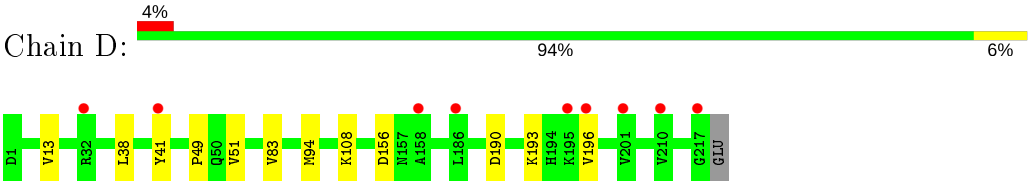


- Molecule 2: HUMAN FAB ANTIBODY FRAGMENT OF dmCBTAU-22.1

Chain B:

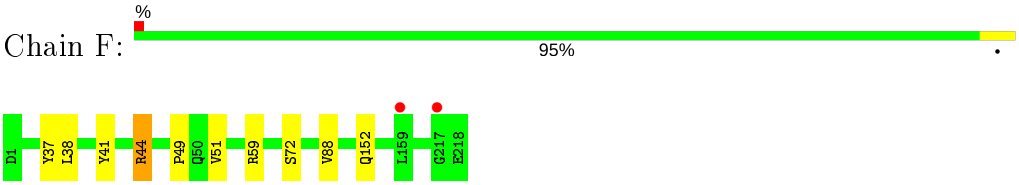
• Molecule 2: HUMAN FAB ANTIBODY FRAGMENT OF dmCBTAU-22.1

Chain D:



• Molecule 2: HUMAN FAB ANTIBODY FRAGMENT OF dmCBTAU-22.1

Chain F:

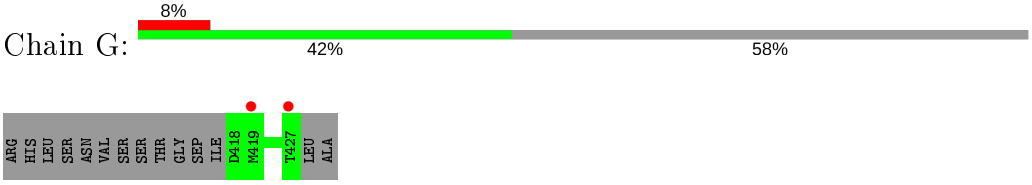


• Molecule 3: Microtubule-associated protein tau

Chain I:

• Molecule 3: Microtubule-associated protein tau

Chain G:

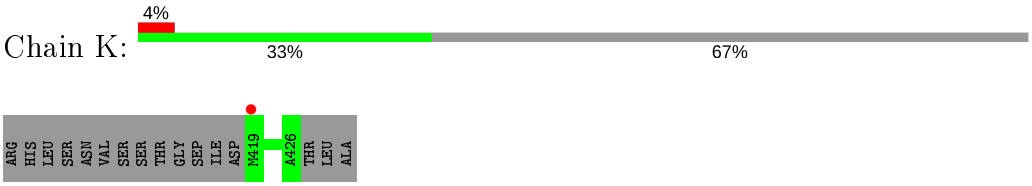


• Molecule 3: Microtubule-associated protein tau

Chain J:

• Molecule 3: Microtubule-associated protein tau

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.55Å 95.50Å 108.32Å 90.00° 112.64° 90.00°	Depositor
Resolution (Å)	99.97 – 1.95 44.29 – 1.95	Depositor EDS
% Data completeness (in resolution range)	93.2 (99.97-1.95) 91.1 (44.29-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.222 , 0.285 0.227 , 0.290	Depositor DCC
R_{free} test set	1866 reflections (1.36%)	wwPDB-VP
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 26.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.169 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14498	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0917e-04.*

[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: GOL, PCA, SEP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.05	0/1663	0.96	7/2264 (0.3%)
1	C	1.01	0/1682	0.92	4/2288 (0.2%)
1	E	1.04	0/1658	0.92	3/2258 (0.1%)
1	H	1.05	0/1675	0.89	3/2280 (0.1%)
2	B	0.97	0/1745	0.85	1/2371 (0.0%)
2	D	0.91	0/1729	0.88	0/2349
2	F	1.04	1/1738 (0.1%)	0.88	2/2361 (0.1%)
2	L	1.02	1/1738 (0.1%)	0.88	1/2361 (0.0%)
3	G	0.85	0/66	0.95	0/87
3	I	1.44	1/58 (1.7%)	1.34	1/76 (1.3%)
3	J	0.69	0/51	0.93	0/66
3	K	0.90	0/51	0.90	0/66
All	All	1.01	3/13854 (0.0%)	0.90	22/18827 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	427	THR	CB-OG1	-7.55	1.28	1.43
2	L	182	SER	CB-OG	5.20	1.49	1.42
2	F	37	TYR	CG-CD1	5.08	1.45	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	186	LEU	CA-CB-CG	8.93	135.83	115.30
1	A	87	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	C	186	LEU	CA-CB-CG	8.20	134.17	115.30
1	C	67	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	C	67	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	E	67	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	28	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	A	186	LEU	CA-CB-CG	6.73	130.78	115.30
1	H	67	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	H	186	LEU	CA-CB-CG	6.53	130.32	115.30
1	H	67	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	C	72	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	F	59	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	B	156	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	67	ARG	NE-CZ-NH2	-5.56	117.52	120.30
3	I	427	THR	CA-CB-CG2	-5.55	104.64	112.40
1	A	67	ARG	NE-CZ-NH1	5.41	123.00	120.30
2	F	44	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	E	87	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	L	82	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	89	ASP	CB-CG-OD1	5.18	122.97	118.30
1	A	87	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	127	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1630	0	1592	2	0
1	C	1649	0	1613	1	0
1	E	1625	0	1582	1	0
1	H	1642	0	1601	1	0
2	B	1702	0	1662	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1689	0	1649	9	0
2	F	1698	0	1655	2	0
2	L	1698	0	1655	3	0
3	G	77	0	67	0	0
3	I	69	0	63	0	0
3	J	62	0	56	0	0
3	K	62	0	56	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	F	6	0	8	0	0
4	H	6	0	8	0	0
5	A	117	0	0	0	0
5	B	84	0	0	0	0
5	C	99	0	0	0	0
5	D	61	0	0	0	0
5	E	107	0	0	0	0
5	F	101	0	0	0	0
5	G	11	0	0	0	0
5	H	136	0	0	0	0
5	I	8	0	0	0	0
5	J	5	0	0	0	0
5	K	5	0	0	0	0
5	L	131	0	0	0	0
All	All	14498	0	13291	21	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 1.

All (21) 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)
2:D:13:VAL:HB	2:D:83:VAL:HG11	1.73	0.71
2:D:83:VAL:HG13	2:D:83:VAL:O	2.03	0.58
2:D:156:ASP:HA	2:D:196:VAL:HG12	1.85	0.58
2:F:41[B]:TYR:CE2	2:F:51:VAL:HG22	2.40	0.57
2:D:13:VAL:CG1	2:D:83:VAL:HG11	2.35	0.56
2:L:41[A]:TYR:CD1	2:L:49:PRO:HB3	2.42	0.54
2:D:13:VAL:CB	2:D:83:VAL:HG11	2.38	0.53
2:B:41[B]:TYR:CE2	2:B:51:VAL:HG22	2.44	0.53
2:D:41[A]:TYR:CD1	2:D:49:PRO:HB3	2.46	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41[A]:TYR:CD1	2:B:49:PRO:HB3	2.48	0.49
1:C:47:TRP:CH2	1:C:49:GLY:HA2	2.48	0.48
1:A:47:TRP:CH2	1:A:49:GLY:HA2	2.49	0.47
2:F:44:ARG:NH1	2:F:88:VAL:O	2.48	0.47
2:D:190:ASP:HA	2:D:193:LYS:HG2	1.97	0.46
2:L:9:LEU:HD21	1:A:5:VAL:HG21	1.98	0.44
1:E:47:TRP:CH2	1:E:49:GLY:HA2	2.53	0.44
2:D:41[B]:TYR:CE1	2:D:94:MET:SD	3.11	0.43
2:B:41[B]:TYR:CE1	2:B:94:MET:SD	3.12	0.43
1:H:47:TRP:CH2	1:H:49:GLY:HA2	2.55	0.42
2:L:41[B]:TYR:CE2	2:L:51:VAL:HG22	2.54	0.41
2:D:41[B]:TYR:CE2	2:D:51:VAL:HG22	2.56	0.41

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	212/222 (96%)	210 (99%)	2 (1%)	0	100	100
1	C	215/222 (97%)	212 (99%)	3 (1%)	0	100	100
1	E	212/222 (96%)	210 (99%)	2 (1%)	0	100	100
1	H	214/222 (96%)	209 (98%)	5 (2%)	0	100	100
2	B	218/218 (100%)	215 (99%)	3 (1%)	0	100	100
2	D	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
2	F	217/218 (100%)	213 (98%)	3 (1%)	1 (0%)	29	17
2	L	217/218 (100%)	214 (99%)	3 (1%)	0	100	100
3	G	7/24 (29%)	6 (86%)	1 (14%)	0	100	100
3	I	6/24 (25%)	6 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	J	5/24 (21%)	5 (100%)	0	0	100 100
3	K	5/24 (21%)	5 (100%)	0	0	100 100
All	All	1744/1856 (94%)	1714 (98%)	29 (2%)	1 (0%)	51 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	72	SER

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	181/186 (97%)	178 (98%)	3 (2%)	60 55
1	C	183/186 (98%)	179 (98%)	4 (2%)	52 44
1	E	180/186 (97%)	177 (98%)	3 (2%)	60 55
1	H	183/186 (98%)	179 (98%)	4 (2%)	52 44
2	B	195/193 (101%)	192 (98%)	3 (2%)	65 60
2	D	193/193 (100%)	191 (99%)	2 (1%)	76 74
2	F	194/193 (100%)	191 (98%)	3 (2%)	65 60
2	L	194/193 (100%)	192 (99%)	2 (1%)	76 74
3	G	8/19 (42%)	8 (100%)	0	100 100
3	I	7/19 (37%)	7 (100%)	0	100 100
3	J	6/19 (32%)	5 (83%)	1 (17%)	2 0
3	K	6/19 (32%)	6 (100%)	0	100 100
All	All	1530/1592 (96%)	1505 (98%)	25 (2%)	62 58

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	67	ARG

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Mol	Chain	Res	Type
1	H	72	ARG
1	H	186	LEU
1	H	217	LYS
2	L	38	LEU
2	L	159	LEU
1	A	67	ARG
1	A	72	ARG
1	A	186	LEU
2	B	38	LEU
2	B	49	PRO
2	B	132	SER
1	C	72	ARG
1	C	81	MET
1	C	186	LEU
1	C	207	ASN
2	D	38	LEU
2	D	108	LYS
1	E	52	ARG
1	E	72	ARG
1	E	186	LEU
2	F	38	LEU
2	F	49	PRO
2	F	152	GLN
3	J	420	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 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	K	422	3	8,9,10	1.17	0	8,12,14	2.13	2 (25%)
1	PCA	E	1	1	7,8,9	0.89	0	9,10,12	1.92	3 (33%)
1	PCA	A	1	1	7,8,9	0.58	0	9,10,12	2.03	2 (22%)
1	PCA	C	1	1	7,8,9	0.97	0	9,10,12	1.45	2 (22%)
3	SEP	G	422	3	8,9,10	0.83	0	8,12,14	2.18	3 (37%)
3	SEP	J	422	3	8,9,10	0.88	0	8,12,14	1.63	2 (25%)
3	SEP	I	422	3	8,9,10	1.05	0	8,12,14	2.39	3 (37%)
1	PCA	H	1	1	7,8,9	1.21	1 (14%)	9,10,12	2.33	2 (22%)

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	K	422	3	-	0/5/8/10	-
1	PCA	E	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
3	SEP	G	422	3	-	0/5/8/10	-
3	SEP	J	422	3	-	0/5/8/10	-
3	SEP	I	422	3	-	0/5/8/10	-
1	PCA	H	1	1	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	1	PCA	OE-CD	-2.59	1.18	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	1	PCA	CB-CA-C	-5.75	104.79	112.70
3	K	422	SEP	OG-CB-CA	4.68	112.70	108.14
3	G	422	SEP	OG-CB-CA	4.58	112.60	108.14
3	I	422	SEP	OG-CB-CA	4.35	112.38	108.14
1	A	1	PCA	OE-CD-CG	-4.06	119.68	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1	PCA	CB-CA-C	-3.81	107.46	112.70
3	I	422	SEP	O3P-P-O2P	3.75	121.97	107.64
1	A	1	PCA	CB-CA-C	-3.55	107.81	112.70
3	I	422	SEP	OG-P-O1P	-3.02	98.01	106.47
1	E	1	PCA	OE-CD-CG	-2.89	121.72	126.76
3	J	422	SEP	O3P-P-O2P	2.75	118.15	107.64
3	K	422	SEP	O3P-P-O2P	2.53	117.29	107.64
1	C	1	PCA	OE-CD-CG	-2.41	122.56	126.76
3	G	422	SEP	O3P-P-O2P	2.38	116.75	107.64
1	E	1	PCA	CB-CG-CD	-2.33	100.66	104.40
1	H	1	PCA	O-C-CA	-2.25	118.88	124.78
3	J	422	SEP	OG-CB-CA	2.25	110.33	108.14
3	G	422	SEP	OG-P-O1P	-2.23	100.20	106.47
1	C	1	PCA	O-C-CA	-2.14	119.18	124.78

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
4	GOL	B	301	-	5,5,5	0.61	0	5,5,5	0.56	0
4	GOL	H	301	-	5,5,5	0.59	0	5,5,5	0.65	0
4	GOL	C	301	-	5,5,5	0.61	0	5,5,5	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	F	301	-	5,5,5	1.09	0	5,5,5	0.65	0
4	GOL	A	301	-	5,5,5	0.66	0	5,5,5	1.06	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	B	301	-	-	2/4/4/4	-
4	GOL	H	301	-	-	4/4/4/4	-
4	GOL	C	301	-	-	2/4/4/4	-
4	GOL	F	301	-	-	0/4/4/4	-
4	GOL	A	301	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	GOL	O1-C1-C2-C3
4	H	301	GOL	O1-C1-C2-C3
4	C	301	GOL	C1-C2-C3-O3
4	A	301	GOL	O1-C1-C2-C3
4	H	301	GOL	O1-C1-C2-O2
4	H	301	GOL	C1-C2-C3-O3
4	C	301	GOL	O2-C2-C3-O3
4	A	301	GOL	O1-C1-C2-O2
4	H	301	GOL	O2-C2-C3-O3
4	B	301	GOL	O1-C1-C2-O2
4	A	301	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	215/222 (96%)	-0.18	1 (0%) 91 94	20, 31, 61, 84	2 (0%)
1	C	218/222 (98%)	-0.13	2 (0%) 84 89	23, 36, 57, 76	4 (1%)
1	E	215/222 (96%)	-0.18	3 (1%) 75 82	21, 31, 59, 85	2 (0%)
1	H	216/222 (97%)	-0.27	0 100 100	21, 30, 47, 65	0
2	B	218/218 (100%)	-0.09	1 (0%) 91 94	25, 38, 59, 79	7 (3%)
2	D	217/218 (99%)	0.16	9 (4%) 37 46	24, 45, 76, 87	8 (3%)
2	F	218/218 (100%)	-0.12	2 (0%) 84 89	21, 35, 63, 96	6 (2%)
2	L	218/218 (100%)	-0.23	1 (0%) 91 94	21, 31, 55, 77	0
3	G	9/24 (37%)	1.23	2 (22%) 0 0	34, 49, 97, 99	0
3	I	8/24 (33%)	0.66	1 (12%) 3 6	30, 41, 68, 84	3 (37%)
3	J	7/24 (29%)	0.68	0 100 100	32, 50, 71, 73	0
3	K	7/24 (29%)	0.85	1 (14%) 2 4	46, 51, 64, 87	0
All	All	1766/1856 (95%)	-0.11	23 (1%) 77 83	20, 34, 64, 99	32 (1%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	419	MET	5.6
3	I	427	THR	5.5
3	K	419	MET	4.3
1	E	197	LEU	4.2
1	C	141	GLY	3.8
3	G	427	THR	3.3
1	A	135	SER	2.8
2	D	196	VAL	2.5
2	D	32	ARG	2.2
2	F	159	LEU	2.2
1	E	141	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	195	LYS	2.2
2	D	217	GLY	2.1
2	L	41[A]	TYR	2.1
2	D	41[A]	TYR	2.1
1	C	142	GLY	2.1
2	F	217	GLY	2.1
2	D	186	LEU	2.1
2	B	32	ARG	2.0
2	D	201	VAL	2.0
2	D	158	ALA	2.0
1	E	143	THR	2.0
2	D	210	VAL	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
1	PCA	E	1	8/9	0.93	0.10	26,29,37,50	0
1	PCA	H	1	8/9	0.94	0.08	26,36,44,66	0
1	PCA	C	1	8/9	0.95	0.10	22,32,39,53	0
1	PCA	A	1	8/9	0.95	0.11	29,35,47,58	0
3	SEP	G	422	10/11	0.96	0.09	26,29,35,35	0
3	SEP	I	422	10/11	0.98	0.07	25,26,30,30	0
3	SEP	J	422	10/11	0.98	0.09	25,28,32,37	0
3	SEP	K	422	10/11	0.99	0.09	27,31,40,41	0

6.3 Carbohydrates (i)

There are no carbohydrates 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	B	301	6/6	0.83	0.18	51,58,61,76	0
4	GOL	F	301	6/6	0.87	0.13	25,39,46,49	0
4	GOL	H	301	6/6	0.89	0.14	26,42,51,55	0
4	GOL	C	301	6/6	0.91	0.18	51,57,75,80	0
4	GOL	A	301	6/6	0.95	0.09	29,33,35,40	0

6.5 Other polymers (i)

There are no such residues in this entry.