Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:11 pm BST

PDB ID	:	5MP3
Title	:	Crystal structure of DC8E8 Fab in the complex with a 30-mer tau peptide at pH 6.5
Authors	:	Skrabana, R.; Novak, M.; Cehlar, O.; Kontsekova, E.
Deposited on	:	2016-12-15
Resolution	:	2.75 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 ①) were used in the production of this report:

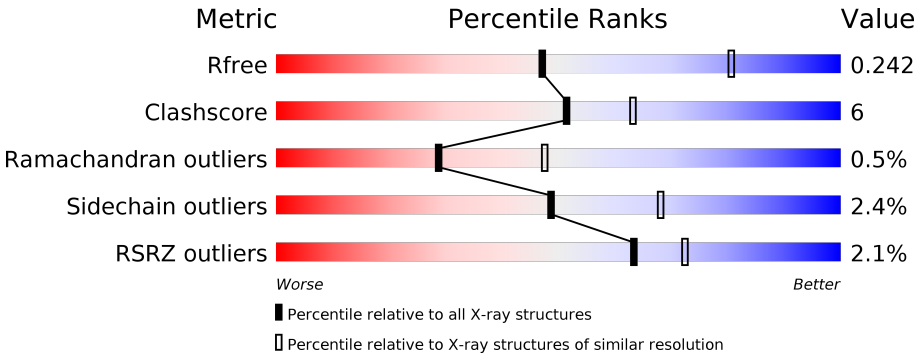
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	220	2% 92% 7%
1	H	220	2% 91% 7%
2	B	218	87% 11%
2	L	218	2% 88% 11%
3	C	30	3% 17% 10% 70%
3	D	30	10% 27% 70%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6842 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 Igh protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	220	Total	C	N	O	S	0	1	0
			1667	1063	267	329	8			
1	A	220	Total	C	N	O	S	0	0	0
			1648	1050	263	327	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	PCA	-	expression tag	UNP Q99LC4
H	9	PRO	ALA	conflict	UNP Q99LC4
H	12	VAL	ALA	conflict	UNP Q99LC4
H	13	LYS	ARG	conflict	UNP Q99LC4
H	16	THR	ALA	conflict	UNP Q99LC4
H	19	LYS	ARG	conflict	UNP Q99LC4
H	20	MET	LEU	conflict	UNP Q99LC4
H	21	PRO	SER	conflict	UNP Q99LC4
H	28	ILE	THR	conflict	UNP Q99LC4
H	31	ASP	GLY	conflict	UNP Q99LC4
H	33	VAL	GLY	conflict	UNP Q99LC4
H	34	ILE	VAL	conflict	UNP Q99LC4
H	48	ILE	VAL	conflict	UNP Q99LC4
H	52	PHE	TYR	conflict	UNP Q99LC4
H	54	ARG	GLY	conflict	UNP Q99LC4
H	57	SER	ASN	conflict	UNP Q99LC4
H	61	ASN	SER	conflict	UNP Q99LC4
H	72	ALA	THR	conflict	UNP Q99LC4
H	77	ASN	SER	conflict	UNP Q99LC4
H	82	GLN	HIS	conflict	UNP Q99LC4
H	86	VAL	LEU	conflict	UNP Q99LC4
H	99	ASP	SER	conflict	UNP Q99LC4
H	100	TYR	SER	conflict	UNP Q99LC4
H	102	GLY	TYR	conflict	UNP Q99LC4
H	103	THR	SER	conflict	UNP Q99LC4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	104	SER	TYR	conflict	UNP Q99LC4
H	105	PHE	ASP	conflict	UNP Q99LC4
H	106	ALA	LEU	conflict	UNP Q99LC4
H	107	MET	PHE	conflict	UNP Q99LC4
H	108	ASP	ALA	conflict	UNP Q99LC4
H	115	SER	LEU	conflict	UNP Q99LC4
H	120	SER	ALA	conflict	UNP Q99LC4
A	1	PCA	-	expression tag	UNP Q99LC4
A	9	PRO	ALA	conflict	UNP Q99LC4
A	12	VAL	ALA	conflict	UNP Q99LC4
A	13	LYS	ARG	conflict	UNP Q99LC4
A	16	THR	ALA	conflict	UNP Q99LC4
A	19	LYS	ARG	conflict	UNP Q99LC4
A	20	MET	LEU	conflict	UNP Q99LC4
A	21	PRO	SER	conflict	UNP Q99LC4
A	28	ILE	THR	conflict	UNP Q99LC4
A	31	ASP	GLY	conflict	UNP Q99LC4
A	33	VAL	GLY	conflict	UNP Q99LC4
A	34	ILE	VAL	conflict	UNP Q99LC4
A	48	ILE	VAL	conflict	UNP Q99LC4
A	52	PHE	TYR	conflict	UNP Q99LC4
A	54	ARG	GLY	conflict	UNP Q99LC4
A	57	SER	ASN	conflict	UNP Q99LC4
A	61	ASN	SER	conflict	UNP Q99LC4
A	72	ALA	THR	conflict	UNP Q99LC4
A	77	ASN	SER	conflict	UNP Q99LC4
A	82	GLN	HIS	conflict	UNP Q99LC4
A	86	VAL	LEU	conflict	UNP Q99LC4
A	99	ASP	SER	conflict	UNP Q99LC4
A	100	TYR	SER	conflict	UNP Q99LC4
A	102	GLY	TYR	conflict	UNP Q99LC4
A	103	THR	SER	conflict	UNP Q99LC4
A	104	SER	TYR	conflict	UNP Q99LC4
A	105	PHE	ASP	conflict	UNP Q99LC4
A	106	ALA	LEU	conflict	UNP Q99LC4
A	107	MET	PHE	conflict	UNP Q99LC4
A	108	ASP	ALA	conflict	UNP Q99LC4
A	115	SER	LEU	conflict	UNP Q99LC4
A	120	SER	ALA	conflict	UNP Q99LC4

- Molecule 2 is a protein called ENSMUSG00000076577 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	218	Total	C	N	O	S	0	0	0
			1682	1050	284	341	7			
2	B	218	Total	C	N	O	S	0	0	0
			1683	1051	284	341	7			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	15	ALA	VAL	conflict	UNP Q52L64
L	31	ASN	TYR	conflict	UNP Q52L64
L	33	ARG	TYR	conflict	UNP Q52L64
L	34	THR	ASN	conflict	UNP Q52L64
L	35	ARG	GLN	conflict	UNP Q52L64
L	67	ARG	HIS	conflict	UNP Q52L64
L	69	THR	SER	conflict	UNP Q52L64
L	85	GLN	LYS	conflict	UNP Q52L64
L	91	VAL	LEU	conflict	UNP Q52L64
L	95	LYS	GLN	conflict	UNP Q52L64
L	?	-	TYR	deletion	UNP Q52L64
L	97	SER	TYR	conflict	UNP Q52L64
L	98	PHE	ASN	conflict	UNP Q52L64
L	100	LEU	PRO	conflict	UNP Q52L64
L	101	ARG	LEU	conflict	UNP Q52L64
L	105	GLY	ALA	conflict	UNP Q52L64
L	111	ILE	LEU	conflict	UNP Q52L64
L	112	LYS	ARG	conflict	UNP Q52L64
L	152	ARG	LYS	conflict	UNP Q52L64
B	15	ALA	VAL	conflict	UNP Q52L64
B	31	ASN	TYR	conflict	UNP Q52L64
B	33	ARG	TYR	conflict	UNP Q52L64
B	34	THR	ASN	conflict	UNP Q52L64
B	35	ARG	GLN	conflict	UNP Q52L64
B	67	ARG	HIS	conflict	UNP Q52L64
B	69	THR	SER	conflict	UNP Q52L64
B	85	GLN	LYS	conflict	UNP Q52L64
B	91	VAL	LEU	conflict	UNP Q52L64
B	95	LYS	GLN	conflict	UNP Q52L64
B	?	-	TYR	deletion	UNP Q52L64
B	97	SER	TYR	conflict	UNP Q52L64
B	98	PHE	ASN	conflict	UNP Q52L64
B	100	LEU	PRO	conflict	UNP Q52L64
B	101	ARG	LEU	conflict	UNP Q52L64
B	105	GLY	ALA	conflict	UNP Q52L64

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Chain	Residue	Modelled	Actual	Comment	Reference
B	111	ILE	LEU	conflict	UNP Q52L64
B	112	LYS	ARG	conflict	UNP Q52L64
B	152	ARG	LYS	conflict	UNP Q52L64

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			52	31	11	10			
3	D	9	Total	C	N	O	0	0	0
			52	31	11	10			

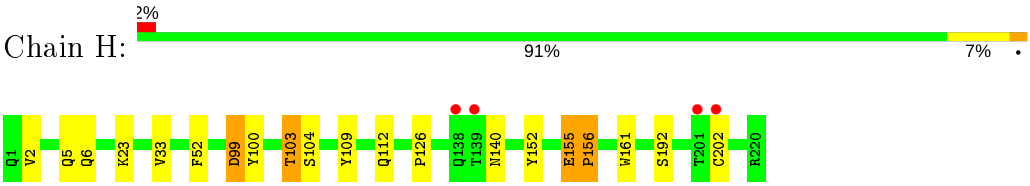
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	9	Total	O	0	0
			9	9		
4	L	12	Total	O	0	0
			12	12		
4	A	17	Total	O	0	0
			17	17		
4	B	19	Total	O	0	0
			19	19		
4	D	1	Total	O	0	0
			1	1		

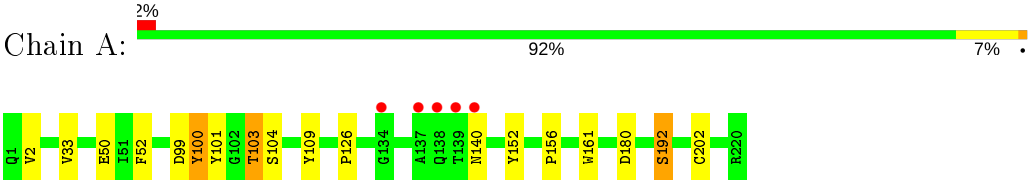
3 Residue-property plots (i)

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.

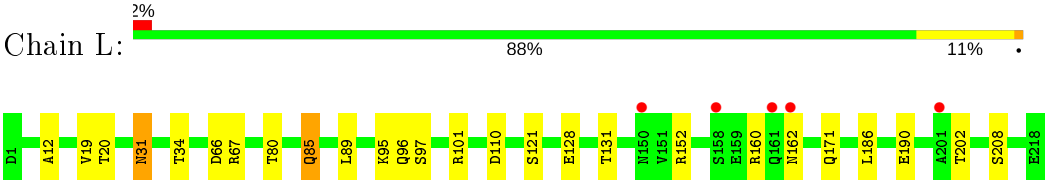
- Molecule 1: Igh protein



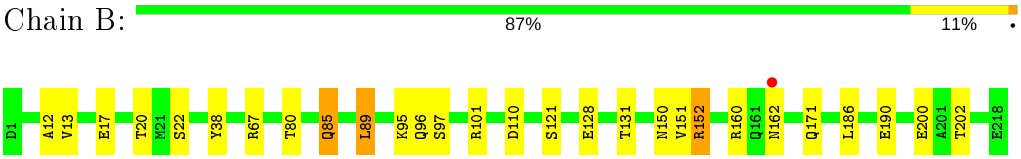
- Molecule 1: Igh protein



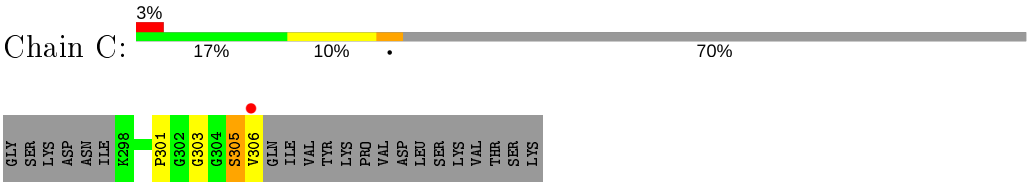
- Molecule 2: ENSMUSG00000076577 protein



- Molecule 2: ENSMUSG00000076577 protein

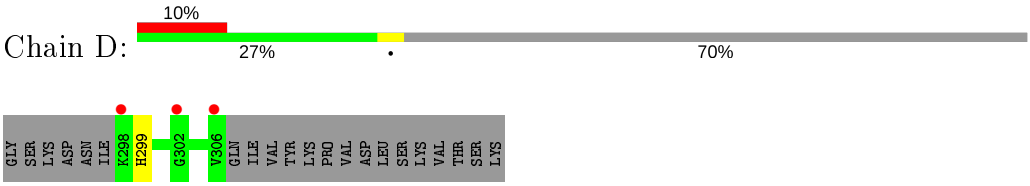


- Molecule 3: Microtubule-associated protein



- Molecule 3: Microtubule-associated protein

Chain D:


10%
27%
70%
GLY
SER
LYS
ASP
ASN
ILE
K298
H299
G302
V306
GLN
ILE
VAL
TYR
LYS
PRO
VAL
ASP
LEU
SER
LYS
VAL
THR
SER
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.85Å 89.89Å 83.60Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	44.94 – 2.75 44.95 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.94-2.75) 99.4 (44.95-2.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.199 , 0.249 0.200 , 0.242	Depositor DCC
R_{free} test set	1142 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
Reported twinning fraction	0.912 for H, K, L 0.088 for -h,-k,l	Depositor
Outliers	0 of 23944 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6842	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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: PCA

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	0.72	0/1686	0.81	2/2307 (0.1%)
1	H	0.71	0/1706	0.89	2/2334 (0.1%)
2	B	0.71	0/1719	0.82	0/2331
2	L	0.67	0/1718	0.82	2/2330 (0.1%)
3	C	0.73	0/53	0.93	0/71
3	D	0.69	0/53	0.93	0/71
All	All	0.70	0/6935	0.84	6/9444 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	155	GLU	C-N-CD	-16.86	83.51	120.60
1	A	50	GLU	OE1-CD-OE2	-6.08	116.01	123.30
1	H	99	ASP	CB-CG-OD2	-5.67	113.20	118.30
2	L	66	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	180	ASP	CB-CG-OD1	5.43	123.19	118.30
2	L	152	ARG	NE-CZ-NH1	5.12	122.86	120.30

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	1648	0	1592	10	0
1	H	1667	0	1616	16	0
2	B	1683	0	1620	27	0
2	L	1682	0	1618	19	0
3	C	52	0	40	4	0
3	D	52	0	40	1	0
4	A	17	0	0	1	0
4	B	19	0	0	2	0
4	D	1	0	0	0	0
4	H	9	0	0	1	0
4	L	12	0	0	2	0
All	All	6842	0	6526	75	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 6.

All (75) 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:B:150:ASN:ND2	2:B:152:ARG:HD2	1.49	1.25
2:B:152:ARG:NH2	2:B:200:GLU:O	1.69	1.23
2:B:150:ASN:ND2	2:B:152:ARG:CD	2.14	1.10
2:B:150:ASN:HD21	2:B:152:ARG:HD2	0.97	1.03
2:L:31:ASN:ND2	2:L:34:THR:OG1	1.95	0.97
2:B:152:ARG:NH1	2:B:202:THR:OG1	2.02	0.93
1:H:140:ASN:O	1:H:192:SER:HB2	1.77	0.85
2:B:150:ASN:HD21	2:B:152:ARG:CD	1.81	0.82
1:H:52[A]:PHE:HB2	3:D:299:HIS:CD2	2.18	0.79
2:B:150:ASN:ND2	2:B:152:ARG:NE	2.30	0.79
2:B:151:VAL:C	2:B:152:ARG:HD3	2.06	0.75
3:C:301:PRO:CD	3:C:306:VAL:HA	2.16	0.75
2:B:150:ASN:HD22	2:B:152:ARG:NE	1.84	0.74
3:C:301:PRO:HD2	3:C:305:SER:O	1.89	0.73
1:H:140:ASN:O	1:H:192:SER:CB	2.37	0.72
2:L:89:LEU:HD11	2:L:171:GLN:HE21	1.56	0.70
2:B:152:ARG:HH22	2:B:200:GLU:C	1.94	0.69
2:L:31:ASN:HD21	2:L:34:THR:H	1.40	0.68
3:C:301:PRO:HD2	3:C:306:VAL:HA	1.75	0.68
2:L:31:ASN:ND2	2:L:34:THR:H	1.92	0.67
2:B:152:ARG:HH21	2:B:152:ARG:N	1.95	0.65
1:A:33:VAL:HG22	1:A:99:ASP:HB3	1.82	0.62
2:B:95:LYS:NZ	4:B:301:HOH:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:VAL:HG22	1:H:99:ASP:HB3	1.83	0.61
1:A:103:THR:OG1	1:A:104:SER:N	2.35	0.59
1:H:103:THR:OG1	1:H:104:SER:N	2.35	0.58
2:B:38:TYR:CD2	3:C:303:GLY:HA3	2.40	0.57
2:L:128:GLU:O	2:L:131:THR:HB	2.07	0.55
1:A:33:VAL:CG2	1:A:99:ASP:HB3	2.37	0.55
2:B:152:ARG:N	2:B:152:ARG:HD3	2.23	0.54
1:H:52[B]:PHE:N	1:H:52[B]:PHE:CD1	2.76	0.53
1:A:101:TYR:HB3	4:A:303:HOH:O	2.10	0.52
2:B:89:LEU:HD11	2:B:171:GLN:HB3	1.92	0.52
1:H:33:VAL:CG2	1:H:99:ASP:HB3	2.39	0.52
2:L:89:LEU:HD11	2:L:171:GLN:HB3	1.92	0.51
2:L:186:LEU:HD23	2:L:190:GLU:HG3	1.93	0.50
4:H:301:HOH:O	2:L:95:LYS:NZ	2.44	0.50
1:H:2:VAL:HG11	1:H:109:TYR:CE1	2.46	0.50
2:L:160:ARG:NH1	2:L:162:ASN:O	2.45	0.49
1:A:161:TRP:CZ3	1:A:202:CYS:HB3	2.48	0.49
1:H:2:VAL:HG13	1:H:109:TYR:CE2	2.48	0.49
2:L:12:ALA:HA	2:L:110:ASP:O	2.13	0.49
1:A:2:VAL:HG13	1:A:109:TYR:CE2	2.49	0.48
1:A:2:VAL:HG11	1:A:109:TYR:CE1	2.48	0.48
2:B:151:VAL:CA	2:B:152:ARG:HH21	2.27	0.48
2:B:160:ARG:NH1	2:B:162:ASN:O	2.47	0.48
1:H:161:TRP:CZ3	1:H:202:CYS:HB3	2.48	0.48
2:L:89:LEU:CD1	2:L:171:GLN:NE2	2.77	0.47
2:B:20:THR:HG22	2:B:80:THR:HG23	1.97	0.47
1:A:140:ASN:O	1:A:192:SER:HB2	2.14	0.47
2:B:13:VAL:HB	2:B:17:GLU:OE1	2.16	0.46
2:L:89:LEU:HD11	2:L:171:GLN:NE2	2.27	0.46
2:B:186:LEU:HD23	2:B:190:GLU:HG3	1.97	0.46
2:L:202:THR:N	4:L:301:HOH:O	2.48	0.46
2:L:67:ARG:CZ	2:L:85:GLN:HG3	2.45	0.46
2:L:20:THR:HG22	2:L:80:THR:HG23	1.99	0.45
1:H:2:VAL:HG12	4:B:317:HOH:O	2.17	0.45
2:B:151:VAL:HA	2:B:152:ARG:NH2	2.32	0.44
1:H:126:PRO:HB3	1:H:152:TYR:HB3	1.99	0.44
2:B:151:VAL:HA	2:B:152:ARG:HH21	1.83	0.44
2:L:96:GLN:O	2:L:101:ARG:HA	2.17	0.44
1:H:2:VAL:HG13	1:H:109:TYR:CD2	2.53	0.43
1:A:126:PRO:HB3	1:A:152:TYR:HB3	2.01	0.43
2:B:67:ARG:CZ	2:B:85:GLN:HG3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:67:ARG:HA	4:L:307:HOH:O	2.18	0.43
1:H:6:GLN:O	1:H:112:GLN:NE2	2.51	0.43
2:B:96:GLN:O	2:B:101:ARG:HA	2.19	0.42
1:H:5:GLN:HB3	1:H:23:LYS:HB3	2.01	0.42
2:B:151:VAL:C	2:B:152:ARG:HH21	2.23	0.42
2:B:128:GLU:O	2:B:131:THR:HB	2.20	0.41
2:L:89:LEU:CD1	2:L:171:GLN:HE21	2.26	0.41
1:H:155:GLU:HA	1:H:156:PRO:HA	1.82	0.41
1:A:2:VAL:HG13	1:A:109:TYR:CD2	2.56	0.41
2:L:67:ARG:NH2	2:L:85:GLN:HG3	2.36	0.41
2:B:12:ALA:HA	2:B:110:ASP:O	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	218/220 (99%)	209 (96%)	7 (3%)	2 (1%)	17 31
1	H	219/220 (100%)	210 (96%)	8 (4%)	1 (0%)	29 47
2	B	216/218 (99%)	207 (96%)	9 (4%)	0	100 100
2	L	216/218 (99%)	206 (95%)	10 (5%)	0	100 100
3	C	7/30 (23%)	5 (71%)	1 (14%)	1 (14%)	0 0
3	D	7/30 (23%)	5 (71%)	2 (29%)	0	100 100
All	All	883/936 (94%)	842 (95%)	37 (4%)	4 (0%)	29 47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	156	PRO

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Mol	Chain	Res	Type
3	C	305	SER
1	A	100	TYR
1	A	156	PRO

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	184/189 (97%)	180 (98%)	4 (2%)	52	70
1	H	187/189 (99%)	185 (99%)	2 (1%)	73	84
2	B	190/194 (98%)	184 (97%)	6 (3%)	39	59
2	L	190/194 (98%)	184 (97%)	6 (3%)	39	59
3	C	4/26 (15%)	4 (100%)	0	100	100
3	D	4/26 (15%)	4 (100%)	0	100	100
All	All	759/818 (93%)	741 (98%)	18 (2%)	49	68

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	100	TYR
1	H	103	THR
2	L	19	VAL
2	L	31	ASN
2	L	85	GLN
2	L	97	SER
2	L	121	SER
2	L	208	SER
1	A	52	PHE
1	A	100	TYR
1	A	103	THR
1	A	192	SER
2	B	22	SER
2	B	85	GLN
2	B	89	LEU

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Mol	Chain	Res	Type
2	B	97	SER
2	B	121	SER
2	B	152	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	31	ASN
2	L	171	GLN
1	A	43	GLN
2	B	143	ASN
2	B	150	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 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	$\#\|Z\| > 2$
1	PCA	A	1	1	7,8,9	0.62	0	9,10,12	1.06	1 (11%)
1	PCA	H	1	1	7,8,9	0.49	0	9,10,12	1.04	1 (11%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	H	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	1	PCA	CB-CA-C	2.84	116.61	112.70
1	A	1	PCA	CB-CA-C	2.17	115.69	112.70

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)

There are no ligands in this entry.

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	219/220 (99%)	-0.13	5 (2%)	60	69	25, 41, 71, 154	0
1	H	219/220 (99%)	-0.06	4 (1%)	68	76	28, 48, 85, 142	0
2	B	218/218 (100%)	-0.16	1 (0%)	91	94	29, 41, 65, 94	0
2	L	218/218 (100%)	0.01	5 (2%)	60	69	31, 48, 80, 116	0
3	C	9/30 (30%)	1.13	1 (11%)	5	6	63, 71, 81, 81	0
3	D	9/30 (30%)	1.48	3 (33%)	0	0	55, 65, 80, 85	9 (100%)
All	All	892/936 (95%)	-0.06	19 (2%)	63	72	25, 44, 77, 154	9 (1%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	306	VAL	5.5
1	H	139	THR	4.2
1	A	138	GLN	4.0
1	H	138	GLN	3.8
3	D	302	GLY	3.5
1	A	139	THR	3.5
1	A	137	ALA	3.2
1	A	134	GLY	2.7
2	L	162	ASN	2.4
3	D	306	VAL	2.4
2	L	158	SER	2.3
1	H	201	THR	2.2
2	B	162	ASN	2.2
1	A	140	ASN	2.1
1	H	202	CYS	2.1
2	L	150	ASN	2.1
2	L	161	GLN	2.0
2	L	201	ALA	2.0
3	D	298	LYS	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	H	1	8/9	0.92	0.19	49,56,59,66	0
1	PCA	A	1	8/9	0.94	0.26	47,53,57,62	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.