Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 08:15 am BST

PDB ID	:	6FVN
Title	:	DNA polymerase sliding clamp from Mycobacterium tuberculosis with bound P7 peptide
Authors	:	Martiel, I.; Andre, C.; Olieric, V.; Guichard, G.; Burnouf, D.
Deposited on	:	2018-03-04
Resolution	:	3.14 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

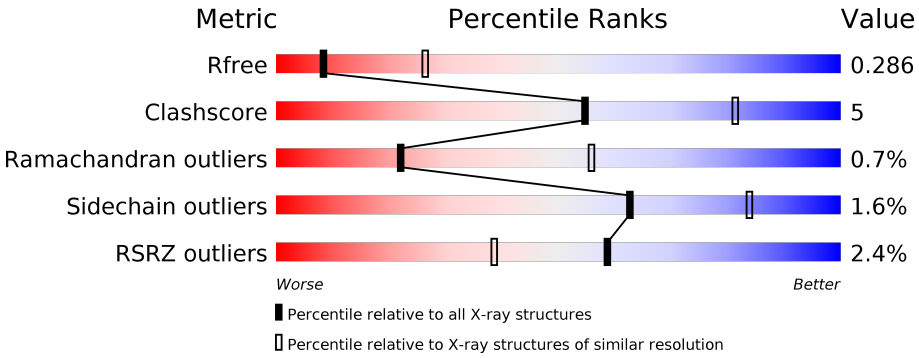
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.14 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	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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	402	85% 8% • 6%
1	B	402	4% 82% 11% 7%
1	C	402	% 83% 9% • 7%
1	D	402	2% 84% 11% 5%
2	H	6	17% 83% 17%
2	I	6	83% 17%

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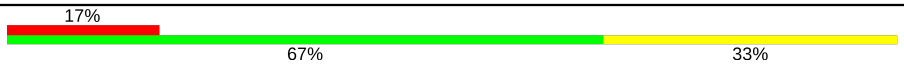
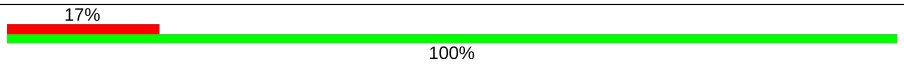
Mol	Chain	Length	Quality of chain
2	J	6	
2	K	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ALC	H	469	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10676 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 Beta sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2659	1691	446	516	6			
1	B	372	Total	C	N	O	S	0	0	0
			2555	1637	430	482	6			
1	C	372	Total	C	N	O	S	0	0	0
			2563	1631	439	487	6			
1	D	380	Total	C	N	O	S	0	0	0
			2636	1679	441	510	6			

- Molecule 2 is a protein called P7 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	6	Total	C	N	O	0	0	0
			51	35	6	10			
2	K	6	Total	C	N	O	0	0	0
			48	32	6	10			
2	H	6	Total	C	N	O	0	0	0
			44	29	6	9			
2	I	6	Total	C	N	O	0	0	0
			51	35	6	10			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	J	2	Total	O	0	0
			2	2		
3	B	10	Total	O	0	0
			10	10		
3	C	9	Total	O	0	0
			9	9		

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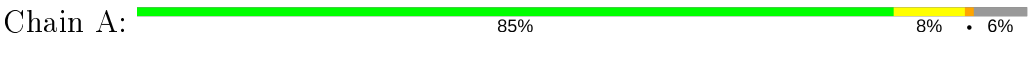
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	22	Total O 22 22	0	0
3	I	1	Total O 1 1	0	0

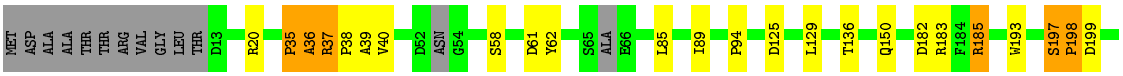
3 Residue-property plots (i)

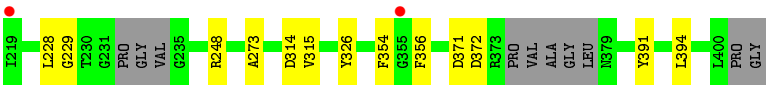
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Beta sliding clamp

Chain A:

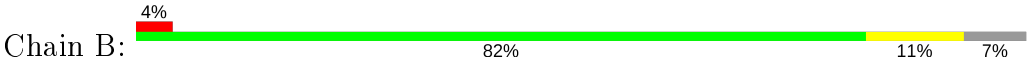


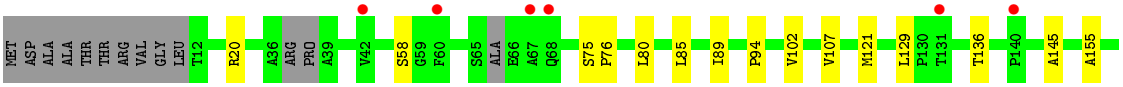


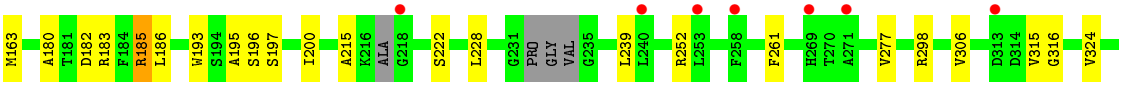


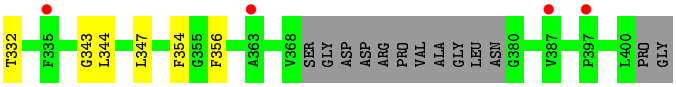
- Molecule 1: Beta sliding clamp

Chain B:



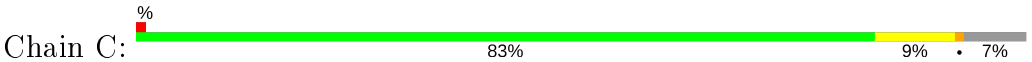


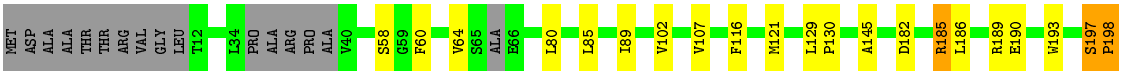


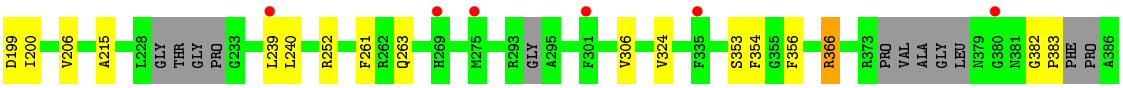


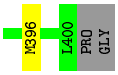
- Molecule 1: Beta sliding clamp

Chain C:



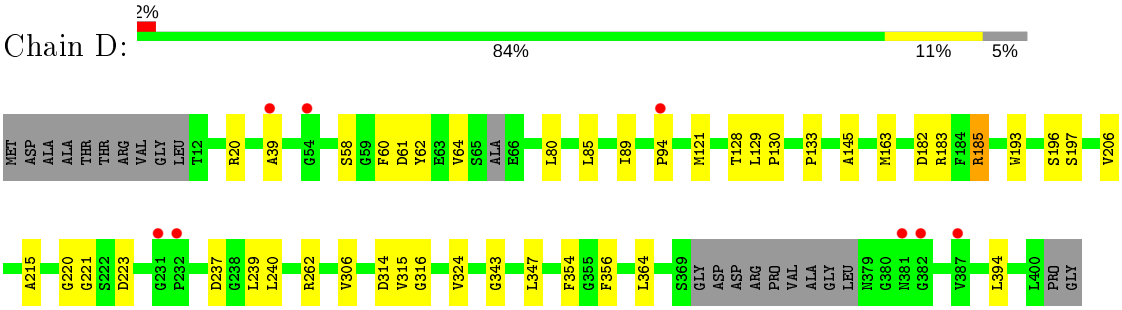






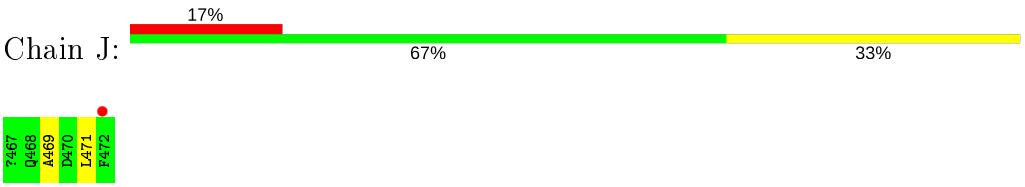
• Molecule 1: Beta sliding clamp

Chain D:



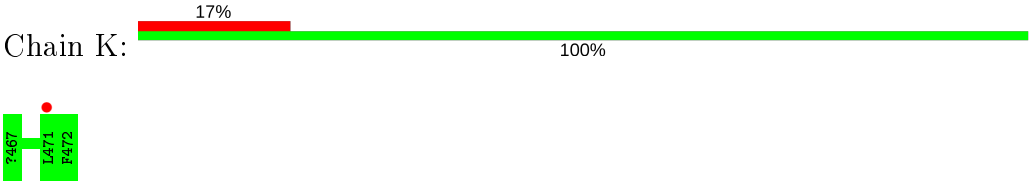
• Molecule 2: P7 peptide

Chain J:



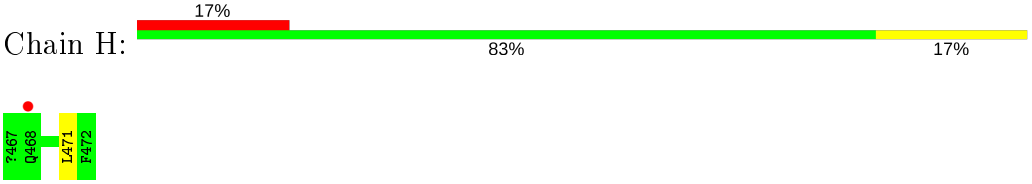
• Molecule 2: P7 peptide

Chain K:



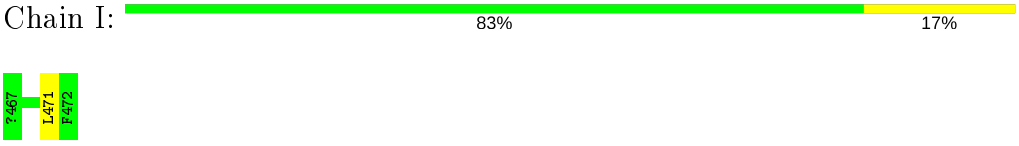
• Molecule 2: P7 peptide

Chain H:



• Molecule 2: P7 peptide

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.45Å 126.76Å 171.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.84 – 3.14 101.84 – 3.14	Depositor EDS
% Data completeness (in resolution range)	88.0 (101.84-3.14) 88.0 (101.84-3.14)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 3.13Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.256 , 0.291 0.259 , 0.286	Depositor DCC
R_{free} test set	1351 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	80.3	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 57.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	10676	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: ALC, ACE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/2703	0.50	0/3705
1	B	0.25	0/2595	0.47	0/3558
1	C	0.29	0/2599	0.49	0/3555
1	D	0.27	0/2680	0.50	0/3680
2	H	0.18	0/29	0.37	0/37
2	I	0.23	0/37	0.33	0/46
2	J	0.23	0/37	0.32	0/46
2	K	0.25	0/34	0.26	0/42
All	All	0.27	0/10714	0.49	0/14669

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	2659	0	2558	30	0
1	B	2555	0	2454	21	0
1	C	2563	0	2436	30	0
1	D	2636	0	2511	27	0
2	H	44	0	42	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	51	0	49	1	0
2	J	51	0	49	2	0
2	K	48	0	40	0	0
3	A	25	0	0	0	0
3	B	10	0	0	0	0
3	C	9	0	0	0	0
3	D	22	0	0	0	0
3	I	1	0	0	0	0
3	J	2	0	0	0	0
All	All	10676	0	10139	107	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 5.

All (107) 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:C:198:PRO:HA	1:C:199:ASP:HB3	1.24	1.18
1:C:197:SER:CB	1:C:198:PRO:CB	2.22	1.17
1:C:60:PHE:CD2	1:C:64:VAL:HG12	1.83	1.14
1:C:197:SER:CB	1:C:198:PRO:CA	2.26	1.12
1:D:61:ASP:OD1	1:D:62:TYR:N	1.89	1.05
1:C:197:SER:CB	1:C:198:PRO:HA	1.94	0.96
1:C:60:PHE:CG	1:C:64:VAL:HG12	2.05	0.91
1:A:197:SER:CB	1:A:198:PRO:CD	2.49	0.90
1:A:198:PRO:HB2	1:A:199:ASP:CB	2.02	0.89
1:A:198:PRO:HB2	1:A:199:ASP:CA	2.03	0.88
1:C:60:PHE:CD2	1:C:64:VAL:CG1	2.56	0.87
1:D:61:ASP:CG	1:D:62:TYR:H	1.82	0.83
1:C:198:PRO:CA	1:C:199:ASP:HB3	2.08	0.80
1:A:198:PRO:HB2	1:A:199:ASP:C	2.03	0.79
1:A:197:SER:CB	1:A:198:PRO:HD3	2.13	0.79
1:D:60:PHE:CD1	1:D:61:ASP:N	2.53	0.76
1:C:58:SER:HB3	1:C:129:LEU:HD11	1.68	0.75
1:A:35:PRO:O	1:A:36:ALA:HB2	1.86	0.74
1:B:58:SER:HB3	1:B:129:LEU:HD11	1.67	0.74
1:A:62:TYR:HA	1:D:39:ALA:HB2	1.71	0.72
1:D:64:VAL:HG11	1:D:130:PRO:HD2	1.72	0.70
1:D:60:PHE:HD1	1:D:61:ASP:H	1.41	0.67
1:A:228:LEU:H	1:A:229:GLY:HA2	1.59	0.67
1:C:198:PRO:HA	1:C:199:ASP:CB	2.05	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:PRO:HB2	1:A:199:ASP:O	1.96	0.63
1:B:145:ALA:HA	1:B:215:ALA:HB1	1.82	0.61
1:B:195:ALA:HB1	1:B:200:ILE:HD11	1.82	0.61
1:A:58:SER:HB3	1:A:129:LEU:HD11	1.86	0.57
1:A:35:PRO:O	1:A:36:ALA:CB	2.53	0.57
1:C:64:VAL:HG11	1:C:130:PRO:HD2	1.87	0.57
1:D:182:ASP:O	1:D:183:ARG:HB2	2.06	0.55
1:A:39:ALA:HA	1:A:40:VAL:C	2.27	0.54
1:B:182:ASP:O	1:B:183:ARG:HB2	2.07	0.54
1:D:133:PRO:HD3	1:D:239:LEU:HD11	1.88	0.54
1:C:102:VAL:HG22	1:C:107:VAL:HG22	1.88	0.54
1:A:182:ASP:O	1:A:183:ARG:HB2	2.08	0.54
1:C:353:SER:HB3	1:C:366:ARG:HG3	1.90	0.53
1:D:145:ALA:HA	1:D:215:ALA:HB1	1.91	0.53
1:A:36:ALA:O	1:A:37:ARG:CB	2.57	0.53
1:D:58:SER:HB3	1:D:129:LEU:HD11	1.89	0.53
1:B:136:THR:OG1	1:B:228:LEU:HB2	2.09	0.52
1:D:306:VAL:HB	1:D:324:VAL:HG21	1.90	0.52
1:A:394:LEU:HD21	2:J:471:LEU:HD21	1.91	0.52
1:D:220:GLY:HA3	1:D:221:GLY:O	2.08	0.52
1:B:80:LEU:HD23	1:B:121:MET:HB2	1.91	0.52
1:B:354:PHE:HB3	1:B:356:PHE:CE2	2.44	0.52
1:D:394:LEU:HD21	2:I:471:LEU:HD21	1.91	0.52
1:A:198:PRO:CB	1:A:199:ASP:CB	2.83	0.52
1:C:85:LEU:O	1:C:89:ILE:HG12	2.10	0.52
1:A:85:LEU:O	1:A:89:ILE:HG12	2.10	0.51
1:C:80:LEU:HD23	1:C:121:MET:HB2	1.93	0.51
1:B:306:VAL:HB	1:B:324:VAL:HG21	1.93	0.51
1:B:239:LEU:HD23	1:B:252:ARG:HA	1.92	0.51
1:B:85:LEU:O	1:B:89:ILE:HG12	2.11	0.50
1:D:85:LEU:O	1:D:89:ILE:HG12	2.11	0.49
1:D:354:PHE:HB3	1:D:356:PHE:CE2	2.47	0.49
1:B:315:VAL:HG13	1:B:316:GLY:H	1.78	0.49
1:D:315:VAL:HG13	1:D:316:GLY:H	1.77	0.48
1:C:189:ARG:NH1	1:C:190:GLU:O	2.44	0.48
1:C:60:PHE:CB	1:C:64:VAL:HG12	2.44	0.48
1:D:80:LEU:HD23	1:D:121:MET:HB2	1.96	0.48
1:A:228:LEU:N	1:A:229:GLY:HA2	2.23	0.47
1:B:277:VAL:HG13	1:B:344:LEU:HB3	1.95	0.47
1:A:125:ASP:OD1	1:D:128:THR:HG22	2.14	0.47
1:B:196:SER:HA	1:B:197:SER:HA	1.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:GLN:N	1:C:263:GLN:OE1	2.42	0.47
1:A:354:PHE:HB3	1:A:356:PHE:CE2	2.50	0.46
1:B:182:ASP:OD1	1:B:185:ARG:HG2	2.16	0.46
1:A:197:SER:CB	1:A:198:PRO:HD2	2.40	0.46
1:C:182:ASP:OD1	1:C:185:ARG:HG2	2.16	0.46
1:C:197:SER:CA	1:C:198:PRO:CB	2.89	0.46
1:D:61:ASP:CG	1:D:62:TYR:N	2.49	0.46
1:C:198:PRO:CB	1:C:200:ILE:H	2.29	0.45
1:C:396:MET:HG2	2:H:471:LEU:HG	1.99	0.45
1:D:343:GLY:O	1:D:347:LEU:HG	2.17	0.45
1:D:364:LEU:HD11	1:D:394:LEU:HD12	1.99	0.44
1:C:206:VAL:HG21	1:C:240:LEU:HD22	1.99	0.44
1:A:150:GLN:HB3	1:A:391:TYR:CE1	2.52	0.44
1:C:145:ALA:HA	1:C:215:ALA:HB1	1.99	0.44
1:A:314:ASP:OD2	1:A:315:VAL:N	2.50	0.44
1:A:61:ASP:OD1	1:A:62:TYR:N	2.48	0.44
1:C:186:LEU:HD21	1:C:261:PHE:HB2	1.98	0.44
1:B:102:VAL:HG22	1:B:107:VAL:HG22	2.00	0.44
1:D:20:ARG:HD3	1:D:94:PRO:O	2.18	0.44
1:A:182:ASP:OD1	1:A:185:ARG:HG2	2.18	0.43
1:C:239:LEU:HD23	1:C:252:ARG:HA	1.99	0.43
1:D:182:ASP:OD1	1:D:185:ARG:HG2	2.18	0.43
2:J:469:ALC:HD23	2:J:469:ALC:HA	1.88	0.43
1:A:136:THR:OG1	1:A:228:LEU:HB2	2.19	0.43
1:B:186:LEU:HD21	1:B:261:PHE:HB2	2.01	0.43
1:B:343:GLY:O	1:B:347:LEU:HG	2.19	0.43
1:D:314:ASP:OD2	1:D:315:VAL:N	2.52	0.43
1:D:196:SER:HA	1:D:197:SER:HA	1.70	0.42
1:C:354:PHE:HB3	1:C:356:PHE:CE2	2.55	0.42
1:D:60:PHE:CD1	1:D:64:VAL:HG12	2.54	0.42
1:B:155:ALA:HB2	1:B:180:ALA:HB1	2.03	0.41
1:A:197:SER:O	1:A:198:PRO:O	2.37	0.41
1:C:89:ILE:HD12	1:C:116:PHE:CE2	2.56	0.41
1:A:198:PRO:CB	1:A:199:ASP:C	2.84	0.41
1:C:306:VAL:HB	1:C:324:VAL:HG21	2.03	0.41
1:B:298:ARG:HE	1:B:332:THR:HG21	1.85	0.41
1:A:20:ARG:HD3	1:A:94:PRO:O	2.20	0.40
1:D:206:VAL:HG21	1:D:240:LEU:HD22	2.03	0.40
1:C:382:GLY:HA2	1:C:383:PRO:HD3	1.91	0.40
1:B:20:ARG:HD3	1:B:94:PRO:O	2.21	0.40
1:A:273:ALA:HB2	1:A:326:TYR:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:SER:HA	1:B:76:PRO:HD3	1.96	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	371/402 (92%)	354 (95%)	11 (3%)	6 (2%)	9 35
1	B	364/402 (90%)	353 (97%)	10 (3%)	1 (0%)	41 72
1	C	360/402 (90%)	344 (96%)	14 (4%)	2 (1%)	25 59
1	D	376/402 (94%)	361 (96%)	14 (4%)	1 (0%)	41 72
2	H	3/6 (50%)	3 (100%)	0	0	100 100
2	I	3/6 (50%)	3 (100%)	0	0	100 100
2	J	3/6 (50%)	3 (100%)	0	0	100 100
2	K	3/6 (50%)	3 (100%)	0	0	100 100
All	All	1483/1632 (91%)	1424 (96%)	49 (3%)	10 (1%)	22 56

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	SER
1	A	198	PRO
1	C	197	SER
1	C	198	PRO
1	A	36	ALA
1	A	38	PRO
1	B	222	SER
1	D	223	ASP
1	A	37	ARG

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Mol	Chain	Res	Type
1	A	35	PRO

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	258/316 (82%)	253 (98%)	5 (2%)	57 80
1	B	236/316 (75%)	233 (99%)	3 (1%)	69 86
1	C	236/316 (75%)	233 (99%)	3 (1%)	69 86
1	D	249/316 (79%)	244 (98%)	5 (2%)	55 79
2	H	3/4 (75%)	3 (100%)	0	100 100
2	I	4/4 (100%)	4 (100%)	0	100 100
2	J	4/4 (100%)	4 (100%)	0	100 100
2	K	3/4 (75%)	3 (100%)	0	100 100
All	All	993/1280 (78%)	977 (98%)	16 (2%)	62 84

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	ARG
1	A	193	TRP
1	A	248	ARG
1	A	371	ASP
1	A	372	ASP
1	B	163	MET
1	B	185	ARG
1	B	193	TRP
1	C	185	ARG
1	C	193	TRP
1	C	366	ARG
1	D	163	MET
1	D	185	ARG
1	D	193	TRP

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Mol	Chain	Res	Type
1	D	237	ASP
1	D	262	ARG

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

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	ALC	H	469	2	9,11,12	0.20	0	10,13,15	0.97	1 (10%)
2	ALC	J	469	2	9,11,12	0.19	0	10,13,15	0.85	1 (10%)
2	ALC	I	469	2	9,11,12	0.20	0	10,13,15	0.97	1 (10%)
2	ALC	K	469	2	9,11,12	0.19	0	10,13,15	0.99	1 (10%)

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	ALC	H	469	2	-	0/5/14/16	0/1/1/1
2	ALC	J	469	2	-	0/5/14/16	0/1/1/1
2	ALC	I	469	2	-	0/5/14/16	0/1/1/1
2	ALC	K	469	2	-	0/5/14/16	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	469	ALC	CB-CA-N	3.08	117.19	110.32
2	I	469	ALC	CB-CA-N	3.03	117.06	110.32
2	H	469	ALC	CB-CA-N	3.02	117.05	110.32
2	J	469	ALC	CB-CA-N	2.64	116.21	110.32

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	469	ALC	1	0

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	379/402 (94%)	0.22	2 (0%) 91 83	37, 56, 86, 103	0
1	B	372/402 (92%)	0.38	17 (4%) 32 15	52, 76, 99, 114	0
1	C	372/402 (92%)	0.25	6 (1%) 72 53	47, 65, 96, 119	0
1	D	380/402 (94%)	0.26	8 (2%) 63 44	37, 61, 93, 117	0
2	H	4/6 (66%)	1.34	1 (25%) 0 0	79, 83, 87, 88	3 (75%)
2	I	4/6 (66%)	0.98	0 100 100	71, 72, 80, 81	0
2	J	4/6 (66%)	0.74	1 (25%) 0 0	62, 65, 65, 73	0
2	K	4/6 (66%)	1.97	1 (25%) 0 0	80, 86, 88, 102	2 (50%)
All	All	1519/1632 (93%)	0.29	36 (2%) 59 38	37, 65, 95, 119	5 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	382	GLY	5.3
1	D	232	PRO	5.1
2	K	471	LEU	3.6
1	A	219	ILE	3.2
1	B	313	ASP	3.0
1	C	269	HIS	3.0
1	B	240	LEU	2.9
1	C	275	MET	2.8
1	B	42	VAL	2.8
1	A	355	GLY	2.6
1	D	94	PRO	2.6
1	C	301	PHE	2.6
1	B	363	ALA	2.5
1	B	253	LEU	2.5
1	B	68	GLN	2.5
1	D	387	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	335	PHE	2.4
1	B	258	PHE	2.4
1	B	269	HIS	2.3
1	B	131	THR	2.3
1	D	231	GLY	2.3
1	D	54	GLY	2.3
1	C	335	PHE	2.2
2	H	468	GLN	2.2
1	B	140	PRO	2.1
1	B	387	VAL	2.1
1	B	60	PHE	2.1
1	D	39	ALA	2.1
1	C	380	GLY	2.1
1	B	271	ALA	2.1
1	B	397	PRO	2.1
1	D	381	ASN	2.1
1	C	239	LEU	2.1
1	B	67	ALA	2.1
2	J	472	PHE	2.0
1	B	218	GLY	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
2	ALC	K	469	11/12	0.70	0.39	79,89,94,98	0
2	ALC	H	469	11/12	0.75	0.74	86,89,93,99	11
2	ALC	I	469	11/12	0.91	0.32	68,71,76,83	0
2	ALC	J	469	11/12	0.92	0.30	56,62,70,75	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.