



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2016 – 01:33 PM EDT

PDB ID : 5GMZ
Title : Hepatitis B virus core protein Y132A mutant in complex with 4-methyl heteroaryldihydropyrimidine
Authors : Xu, Z.H.; Zhou, Z.
Deposited on : 2016-07-18
Resolution : 1.70 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

<http://wwpdb.org/validation/2016/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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

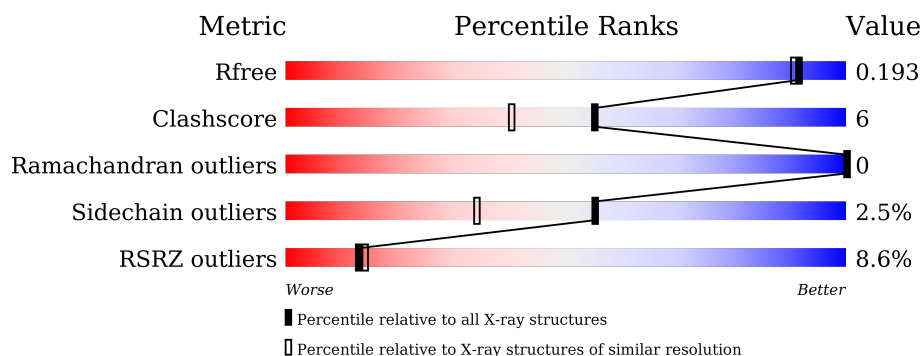
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	155	<div> <div>82%</div> <div>10%</div> <div>8%</div> </div>
1	B	155	<div> <div>3%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
1	C	155	<div> <div>5%</div> <div>78%</div> <div>13%</div> <div>8%</div> </div>
1	D	155	<div> <div>6%</div> <div>88%</div> <div>8%</div> </div>
1	E	155	<div> <div>14%</div> <div>77%</div> <div>14%</div> <div>8%</div> </div>
1	F	155	<div> <div>21%</div> <div>80%</div> <div>13%</div> </div>

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	IPA	A	201	-	-	-	X
2	IPA	A	202	-	-	-	X
2	IPA	A	203	-	-	-	X
2	IPA	A	204	-	-	-	X
2	IPA	C	201	-	-	-	X
2	IPA	D	201	-	-	-	X
2	IPA	E	202	-	-	-	X
2	IPA	E	203	-	-	X	X
2	IPA	E	204	-	-	-	X
3	6XU	A	206	-	-	-	X
4	GOL	B	201	-	-	-	X
4	GOL	F	201	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8136 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 Core protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	2	0
			1147	744	189	209	5			
1	B	148	Total	C	N	O	S	0	3	0
			1204	780	200	219	5			
1	C	143	Total	C	N	O	S	0	4	0
			1161	753	191	212	5			
1	D	150	Total	C	N	O	S	0	4	0
			1227	797	203	222	5			
1	E	143	Total	C	N	O	S	0	2	0
			1147	744	189	209	5			
1	F	150	Total	C	N	O	S	0	2	0
			1211	787	198	221	5			

There are 42 discrepancies between the modelled and reference sequences:

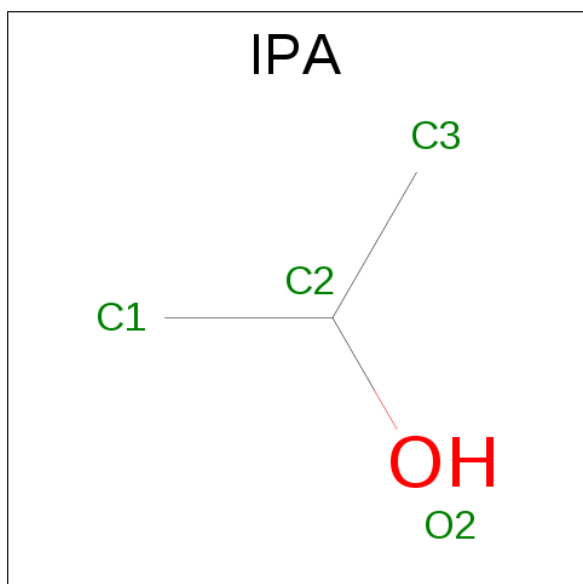
Chain	Residue	Modelled	Actual	Comment	Reference
A	132	ALA	TYR	engineered mutation	UNP L7R9I1
A	150	GLU	-	expression tag	UNP L7R9I1
A	151	ASN	-	expression tag	UNP L7R9I1
A	152	LEU	-	expression tag	UNP L7R9I1
A	153	TYR	-	expression tag	UNP L7R9I1
A	154	PHE	-	expression tag	UNP L7R9I1
A	155	GLN	-	expression tag	UNP L7R9I1
B	132	ALA	TYR	engineered mutation	UNP L7R9I1
B	150	GLU	-	expression tag	UNP L7R9I1
B	151	ASN	-	expression tag	UNP L7R9I1
B	152	LEU	-	expression tag	UNP L7R9I1
B	153	TYR	-	expression tag	UNP L7R9I1
B	154	PHE	-	expression tag	UNP L7R9I1
B	155	GLN	-	expression tag	UNP L7R9I1
C	132	ALA	TYR	engineered mutation	UNP L7R9I1
C	150	GLU	-	expression tag	UNP L7R9I1
C	151	ASN	-	expression tag	UNP L7R9I1

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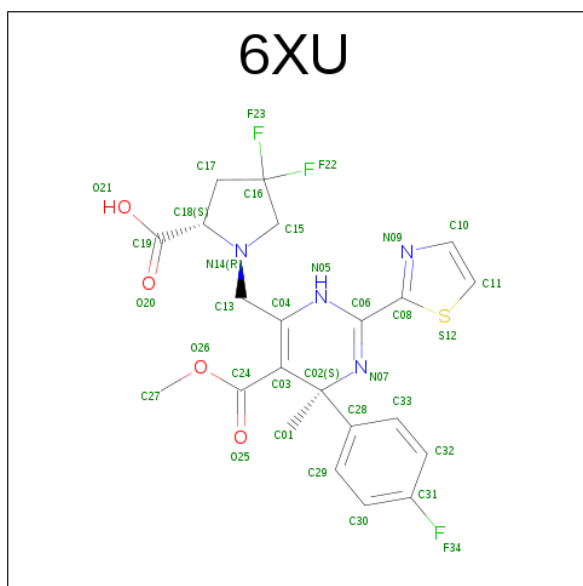
Chain	Residue	Modelled	Actual	Comment	Reference
C	152	LEU	-	expression tag	UNP L7R9I1
C	153	TYR	-	expression tag	UNP L7R9I1
C	154	PHE	-	expression tag	UNP L7R9I1
C	155	GLN	-	expression tag	UNP L7R9I1
D	132	ALA	TYR	engineered mutation	UNP L7R9I1
D	150	GLU	-	expression tag	UNP L7R9I1
D	151	ASN	-	expression tag	UNP L7R9I1
D	152	LEU	-	expression tag	UNP L7R9I1
D	153	TYR	-	expression tag	UNP L7R9I1
D	154	PHE	-	expression tag	UNP L7R9I1
D	155	GLN	-	expression tag	UNP L7R9I1
E	132	ALA	TYR	engineered mutation	UNP L7R9I1
E	150	GLU	-	expression tag	UNP L7R9I1
E	151	ASN	-	expression tag	UNP L7R9I1
E	152	LEU	-	expression tag	UNP L7R9I1
E	153	TYR	-	expression tag	UNP L7R9I1
E	154	PHE	-	expression tag	UNP L7R9I1
E	155	GLN	-	expression tag	UNP L7R9I1
F	132	ALA	TYR	engineered mutation	UNP L7R9I1
F	150	GLU	-	expression tag	UNP L7R9I1
F	151	ASN	-	expression tag	UNP L7R9I1
F	152	LEU	-	expression tag	UNP L7R9I1
F	153	TYR	-	expression tag	UNP L7R9I1
F	154	PHE	-	expression tag	UNP L7R9I1
F	155	GLN	-	expression tag	UNP L7R9I1

- Molecule 2 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



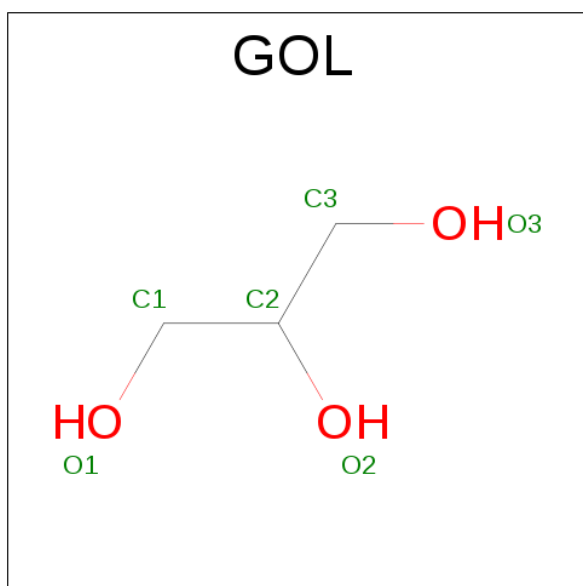
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 3 1	0	0
2	A	1	Total C O 4 3 1	0	0
2	A	1	Total C O 4 3 1	0	0
2	A	1	Total C O 4 3 1	0	0
2	C	1	Total C O 4 3 1	0	0
2	D	1	Total C O 4 3 1	0	0
2	D	1	Total C O 4 3 1	0	0
2	E	1	Total C O 4 3 1	0	0
2	E	1	Total C O 4 3 1	0	0
2	E	1	Total C O 4 3 1	0	0
2	E	1	Total C O 4 3 1	0	0

- Molecule 3 is (2S)-4,4-difluoro-1-[[[(4S)-4-(4-fluorophenyl)-5-methoxycarbonyl-4-methyl-2-(1,3-thiazol-2-yl)-1H-pyrimidin-6-yl]methyl]pyrrolidine-2-carboxylic acid (three-letter code: 6XU) (formula: C₂₂H₂₁F₃N₄O₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			34	22	3	4	4	1		
3	A	1	Total	C	F	N	O	S	0	0
			34	22	3	4	4	1		
3	B	1	Total	C	F	N	O	S	0	0
			34	22	3	4	4	1		
3	C	1	Total	C	F	N	O	S	0	0
			34	22	3	4	4	1		
3	D	1	Total	C	F	N	O	S	0	0
			34	22	3	4	4	1		
3	E	1	Total	C	F	N	O	S	0	0
			34	22	3	4	4	1		
3	F	1	Total	C	F	N	O	S	0	0
			34	22	3	4	4	1		

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



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Cl	0	0
			1	1		

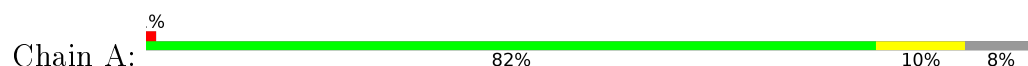
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	129	Total 129	O 129	0	0
6	B	153	Total 153	O 153	0	0
6	C	125	Total 125	O 125	0	0
6	D	139	Total 139	O 139	0	0
6	E	96	Total 96	O 96	0	0
6	F	102	Total 102	O 102	0	0

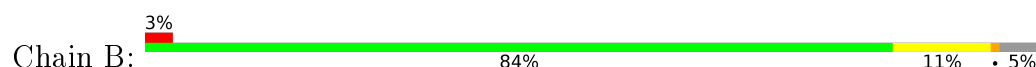
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

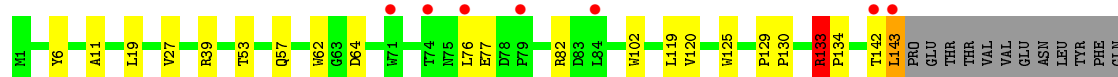
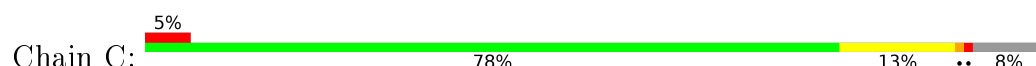
• Molecule 1: Core protein



• Molecule 1: Core protein



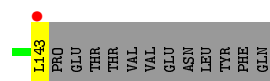
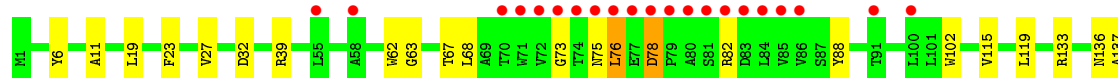
• Molecule 1: Core protein



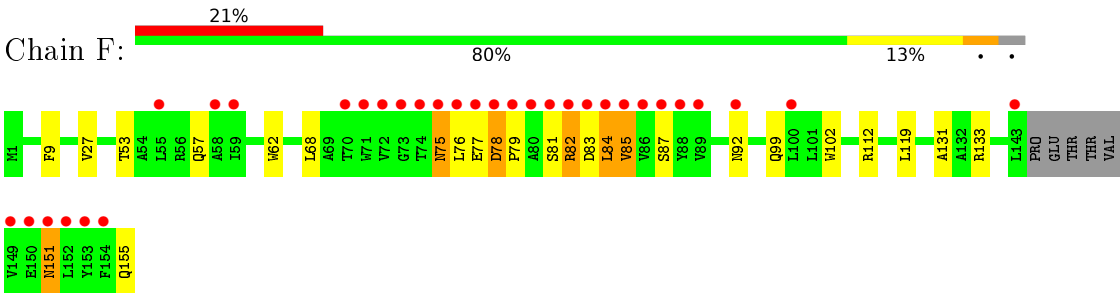
• Molecule 1: Core protein



• Molecule 1: Core protein



● Molecule 1: Core protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.02Å 67.22Å 87.67Å 68.10° 68.43° 83.07°	Depositor
Resolution (Å)	33.31 – 1.70 33.31 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.3 (33.31-1.70) 79.1 (33.31-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 1.70Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.174 , 0.196 0.169 , 0.193	Depositor DCC
R_{free} test set	3034 reflections (2.43%)	DCC
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8136	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6XU, GOL, IPA, CL

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	0.35	0/1181	0.50	0/1620
1	B	0.36	0/1239	0.51	0/1694
1	C	0.37	0/1195	0.56	1/1639 (0.1%)
1	D	0.36	0/1263	0.52	0/1729
1	E	0.34	0/1181	0.50	0/1619
1	F	0.34	0/1246	0.51	0/1706
All	All	0.35	0/7305	0.52	1/10007 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	ARG	NE-CZ-NH2	5.74	123.17	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1147	0	1131	12	0
1	B	1204	0	1175	13	0
1	C	1161	0	1145	20	0
1	D	1227	0	1204	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1147	0	1130	21	0
1	F	1211	0	1185	22	0
2	A	16	0	32	0	0
2	C	4	0	8	0	0
2	D	8	0	16	0	0
2	E	16	0	32	7	0
3	A	68	0	0	0	0
3	B	34	0	0	0	0
3	C	34	0	0	0	0
3	D	34	0	0	0	0
3	E	34	0	0	0	0
3	F	34	0	0	0	0
4	B	6	0	8	0	0
4	F	6	0	8	2	0
5	D	1	0	0	0	0
6	A	129	0	0	1	0
6	B	153	0	0	1	0
6	C	125	0	0	3	0
6	D	139	0	0	2	0
6	E	96	0	0	2	0
6	F	102	0	0	2	0
All	All	8136	0	7074	91	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 (91) 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:A:19[B]:LEU:HD11	1:A:119:LEU:HD22	1.53	0.90
1:C:19[A]:LEU:HD11	1:C:119[A]:LEU:HD22	1.62	0.79
1:E:136:ASN:HA	2:E:204:IPA:H2	1.69	0.74
1:E:32:ASP:OD2	6:E:301:HOH:O	2.07	0.72
1:E:137:ALA:H	2:E:204:IPA:H33	1.57	0.69
1:A:19[B]:LEU:HD11	1:A:119:LEU:CD2	2.25	0.67
1:E:19:LEU:HD11	1:E:119[A]:LEU:HD22	1.78	0.66
1:D:150:GLU:N	6:D:303:HOH:O	2.28	0.65
1:F:151:ASN:N	1:F:151:ASN:OD1	2.31	0.64
1:D:28:ARG:NH1	6:D:302:HOH:O	2.30	0.64
1:B:112[B]:ARG:NH1	6:B:301:HOH:O	2.31	0.63
1:D:137:ALA:H	2:E:203:IPA:H32	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:PRO:HA	1:F:82:ARG:HG3	1.81	0.61
1:C:64:ASP:OD1	6:C:301:HOH:O	2.16	0.61
1:E:102:TRP:CZ3	1:E:119[A]:LEU:HD21	2.36	0.60
1:C:142:THR:O	1:C:143:LEU:HB2	2.02	0.59
1:F:77:GLU:HG3	1:F:78:ASP:H	1.67	0.59
1:C:19[B]:LEU:HD21	1:C:119[B]:LEU:HG	1.85	0.59
1:A:36:ALA:O	6:A:301:HOH:O	2.17	0.57
1:C:19[B]:LEU:CD2	1:C:119[B]:LEU:HG	2.35	0.57
1:B:37:LEU:HD21	1:C:120:VAL:HG11	1.87	0.56
1:A:102:TRP:CZ3	1:A:119:LEU:HD21	2.41	0.56
1:B:19:LEU:HD21	1:B:119[B]:LEU:HG	1.88	0.56
1:B:70:THR:O	1:B:74:THR:HG23	2.06	0.56
1:E:115:VAL:O	1:E:119[A]:LEU:HG	2.06	0.55
1:E:73:GLY:O	1:E:82:ARG:NE	2.26	0.55
1:F:77:GLU:HG3	1:F:78:ASP:N	2.22	0.55
1:F:131:ALA:O	4:F:201:GOL:H32	2.07	0.54
1:A:70:THR:O	1:A:74:THR:HG23	2.07	0.54
1:F:102:TRP:CZ3	1:F:119[A]:LEU:HD21	2.43	0.53
1:A:39:ARG:HG3	1:B:1:MET:HG2	1.90	0.53
1:E:143:LEU:O	6:E:302:HOH:O	2.19	0.53
1:D:19:LEU:CD2	1:D:119[A]:LEU:HG	2.39	0.53
1:F:155:GLN:HG3	6:F:329:HOH:O	2.08	0.52
1:D:19:LEU:HD21	1:D:119[A]:LEU:HG	1.91	0.52
1:F:79:PRO:HA	1:F:82:ARG:CG	2.40	0.52
1:E:19:LEU:HD11	1:E:119[A]:LEU:CD2	2.40	0.52
1:A:45:PRO:HG3	1:B:7:LYS:HE2	1.92	0.52
1:E:102:TRP:HZ3	1:E:119[A]:LEU:HD21	1.76	0.51
1:B:19:LEU:CD2	1:B:119[B]:LEU:HG	2.40	0.50
1:D:139:ILE:O	1:D:142:THR:HG22	2.10	0.50
1:E:75:ASN:OD1	1:E:76:LEU:N	2.45	0.50
1:E:133:ARG:O	2:E:203:IPA:H33	2.11	0.50
1:C:102:TRP:CZ3	1:C:119[A]:LEU:HD21	2.47	0.50
1:F:82:ARG:HE	1:F:83:ASP:HB2	1.77	0.49
1:D:136:ASN:HA	2:E:203:IPA:H32	1.94	0.49
1:F:75:ASN:N	1:F:75:ASN:OD1	2.46	0.49
1:E:78:ASP:OD1	1:E:78:ASP:N	2.46	0.48
1:C:39:ARG:NH2	6:C:307:HOH:O	2.46	0.48
1:D:10:GLY:HA3	1:D:112:ARG:HE	1.79	0.48
1:B:102:TRP:CZ3	1:B:119[A]:LEU:HD21	2.49	0.48
1:F:112:ARG:HH21	1:F:112:ARG:HB3	1.79	0.48
1:A:46:GLU:HB3	1:B:155:GLN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:TRP:CD1	1:C:133:ARG:HG3	2.49	0.47
1:E:27:VAL:HG11	1:E:62:TRP:CE2	2.48	0.47
1:F:81:SER:O	1:F:85:VAL:HG12	2.14	0.47
1:C:76:LEU:O	1:C:82:ARG:NH1	2.48	0.47
1:C:133:ARG:HD3	6:C:372:HOH:O	2.15	0.46
1:C:102:TRP:HZ3	1:C:119[A]:LEU:HD21	1.79	0.46
1:C:53:THR:O	1:C:57:GLN:HG2	2.15	0.46
1:B:53:THR:O	1:B:57:GLN:HG2	2.16	0.45
1:F:84:LEU:O	1:F:87:SER:OG	2.34	0.45
1:D:102:TRP:CZ3	1:D:119[B]:LEU:HD21	2.52	0.45
1:C:19[A]:LEU:HD11	1:C:119[A]:LEU:CD2	2.41	0.45
1:B:87:SER:O	1:B:91:THR:HG23	2.17	0.45
1:D:137:ALA:H	2:E:203:IPA:C3	2.30	0.44
1:C:133:ARG:HG2	1:C:134:PRO:O	2.18	0.43
1:A:102:TRP:HZ3	1:A:119:LEU:HD21	1.83	0.43
1:E:19:LEU:HD13	1:E:23:PHE:CE1	2.53	0.43
1:B:27:VAL:HG11	1:B:62:TRP:CE2	2.55	0.42
1:C:125:TRP:NE1	1:C:133:ARG:HG3	2.33	0.42
1:E:63:GLY:O	1:E:67:THR:HG23	2.19	0.42
1:F:53:THR:O	1:F:57:GLN:HG2	2.20	0.42
1:E:68:LEU:CD2	1:F:68:LEU:HD12	2.49	0.42
1:E:88:TYR:HE2	1:F:68:LEU:HD23	1.84	0.42
1:F:99:GLN:NE2	6:F:301:HOH:O	2.28	0.42
1:C:133:ARG:HG2	1:C:134:PRO:N	2.31	0.42
1:C:27:VAL:HG11	1:C:62:TRP:CE2	2.55	0.42
1:F:133:ARG:O	4:F:201:GOL:H31	2.20	0.42
1:C:129:PRO:HA	1:C:130:PRO:HD3	1.96	0.42
1:E:39:ARG:HB3	2:E:201:IPA:H11	2.01	0.42
1:E:88:TYR:CE2	1:F:68:LEU:HD23	2.55	0.41
1:F:112:ARG:HB3	1:F:112:ARG:NH2	2.35	0.41
1:A:115:VAL:O	1:A:119:LEU:HG	2.19	0.41
1:B:129:PRO:HA	1:B:130:PRO:HD3	1.99	0.41
1:E:6:TYR:HB3	1:E:11:ALA:HB3	2.02	0.41
1:A:27:VAL:HG11	1:A:62:TRP:CE2	2.56	0.41
1:F:9:PHE:O	1:F:112:ARG:HD2	2.21	0.41
1:C:6:TYR:HB3	1:C:11:ALA:HB3	2.04	0.40
1:A:53:THR:O	1:A:57:GLN:HG2	2.22	0.40
1:F:27:VAL:HG11	1:F:62:TRP:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	143/155 (92%)	141 (99%)	2 (1%)	0	100	100
1	B	147/155 (95%)	144 (98%)	3 (2%)	0	100	100
1	C	145/155 (94%)	143 (99%)	2 (1%)	0	100	100
1	D	150/155 (97%)	148 (99%)	2 (1%)	0	100	100
1	E	143/155 (92%)	141 (99%)	2 (1%)	0	100	100
1	F	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
All	All	876/930 (94%)	860 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/137 (93%)	125 (98%)	2 (2%)	70	54
1	B	132/137 (96%)	130 (98%)	2 (2%)	72	56
1	C	129/137 (94%)	126 (98%)	3 (2%)	58	37
1	D	135/137 (98%)	132 (98%)	3 (2%)	60	39
1	E	127/137 (93%)	125 (98%)	2 (2%)	70	54
1	F	133/137 (97%)	125 (94%)	8 (6%)	24	7
All	All	783/822 (95%)	763 (97%)	20 (3%)	55	32

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	112	ARG
1	B	112[A]	ARG
1	B	112[B]	ARG
1	C	77	GLU
1	C	133	ARG
1	C	143	LEU
1	D	74	THR
1	D	142	THR
1	D	155	GLN
1	E	76	LEU
1	E	78	ASP
1	F	75	ASN
1	F	76	LEU
1	F	78	ASP
1	F	82	ARG
1	F	84	LEU
1	F	85	VAL
1	F	92	ASN
1	F	151	ASN

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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

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	IPA	A	201	-	3,3,3	0.59	0	3,3,3	0.18	0
2	IPA	A	202	-	3,3,3	0.59	0	3,3,3	0.17	0
2	IPA	A	203	-	3,3,3	0.60	0	3,3,3	0.40	0
2	IPA	A	204	-	3,3,3	0.56	0	3,3,3	0.28	0
3	6XU	A	205	-	24,37,37	2.08	8 (33%)	28,56,56	1.96	7 (25%)
3	6XU	A	206	-	24,37,37	3.54	9 (37%)	28,56,56	2.46	11 (39%)
4	GOL	B	201	-	5,5,5	0.35	0	5,5,5	0.45	0
3	6XU	B	202	-	24,37,37	2.05	6 (25%)	28,56,56	1.92	8 (28%)
2	IPA	C	201	-	3,3,3	0.53	0	3,3,3	0.25	0
3	6XU	C	202	-	24,37,37	1.72	4 (16%)	28,56,56	2.01	10 (35%)
2	IPA	D	201	-	3,3,3	0.53	0	3,3,3	0.31	0
2	IPA	D	202	-	3,3,3	0.56	0	3,3,3	0.26	0
3	6XU	D	204	-	24,37,37	1.88	7 (29%)	28,56,56	1.98	9 (32%)
2	IPA	E	201	-	3,3,3	0.51	0	3,3,3	0.29	0
2	IPA	E	202	-	3,3,3	0.53	0	3,3,3	0.31	0
2	IPA	E	203	-	3,3,3	0.55	0	3,3,3	0.36	0
2	IPA	E	204	-	3,3,3	0.61	0	3,3,3	0.11	0
3	6XU	E	205	-	24,37,37	1.82	5 (20%)	28,56,56	2.08	8 (28%)
4	GOL	F	201	-	5,5,5	0.29	0	5,5,5	0.60	0
3	6XU	F	202	-	24,37,37	1.84	7 (29%)	28,56,56	2.15	11 (39%)

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	IPA	A	201	-	-	0/0/0/0	0/0/0/0
2	IPA	A	202	-	-	0/0/0/0	0/0/0/0
2	IPA	A	203	-	-	0/0/0/0	0/0/0/0
2	IPA	A	204	-	-	0/0/0/0	0/0/0/0
3	6XU	A	205	-	-	0/14/57/57	0/4/4/4
3	6XU	A	206	-	-	0/14/57/57	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	201	-	-	0/4/4/4	0/0/0/0
3	6XU	B	202	-	-	0/14/57/57	0/4/4/4
2	IPA	C	201	-	-	0/0/0/0	0/0/0/0
3	6XU	C	202	-	-	0/14/57/57	0/4/4/4
2	IPA	D	201	-	-	0/0/0/0	0/0/0/0
2	IPA	D	202	-	-	0/0/0/0	0/0/0/0
3	6XU	D	204	-	-	0/14/57/57	0/4/4/4
2	IPA	E	201	-	-	0/0/0/0	0/0/0/0
2	IPA	E	202	-	-	0/0/0/0	0/0/0/0
2	IPA	E	203	-	-	0/0/0/0	0/0/0/0
2	IPA	E	204	-	-	0/0/0/0	0/0/0/0
3	6XU	E	205	-	-	0/14/57/57	0/4/4/4
4	GOL	F	201	-	-	0/4/4/4	0/0/0/0
3	6XU	F	202	-	-	0/14/57/57	0/4/4/4

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	205	6XU	F23-C16	-5.20	1.31	1.38
3	A	206	6XU	F23-C16	-4.47	1.32	1.38
3	E	205	6XU	F23-C16	-4.42	1.32	1.38
3	C	202	6XU	F23-C16	-4.29	1.32	1.38
3	B	202	6XU	F22-C16	-4.01	1.33	1.38
3	A	205	6XU	C08-C06	-3.86	1.43	1.48
3	F	202	6XU	F23-C16	-3.82	1.33	1.38
3	D	204	6XU	F23-C16	-3.53	1.33	1.38
3	D	204	6XU	F22-C16	-3.49	1.33	1.38
3	B	202	6XU	F23-C16	-3.40	1.33	1.38
3	B	202	6XU	C08-C06	-2.76	1.44	1.48
3	A	205	6XU	F22-C16	-2.76	1.34	1.38
3	B	202	6XU	C13-N14	-2.67	1.40	1.48
3	C	202	6XU	C08-C06	-2.57	1.44	1.48
3	A	205	6XU	F34-C31	-2.45	1.30	1.36
3	A	206	6XU	F22-C16	-2.34	1.35	1.38
3	E	205	6XU	C17-C18	-2.34	1.51	1.54
3	E	205	6XU	C08-C06	-2.18	1.45	1.48
3	F	202	6XU	F22-C16	-2.18	1.35	1.38
3	D	204	6XU	C08-C06	-2.17	1.45	1.48
3	A	205	6XU	C17-C18	-2.04	1.51	1.54
3	B	202	6XU	C17-C18	-2.03	1.51	1.54
3	A	205	6XU	C30-C31	2.01	1.41	1.37
3	A	205	6XU	C32-C31	2.04	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	204	6XU	C33-C28	2.08	1.42	1.39
3	F	202	6XU	C29-C28	2.10	1.42	1.39
3	C	202	6XU	C32-C31	2.12	1.41	1.37
3	E	205	6XU	C02-C28	2.15	1.56	1.52
3	A	206	6XU	C30-C31	2.17	1.41	1.37
3	F	202	6XU	C32-C31	2.22	1.41	1.37
3	F	202	6XU	C30-C31	2.29	1.41	1.37
3	F	202	6XU	C02-C28	2.56	1.57	1.52
3	D	204	6XU	C02-C28	2.68	1.57	1.52
3	D	204	6XU	C32-C31	2.76	1.42	1.37
3	A	206	6XU	C04-N05	3.06	1.42	1.37
3	A	206	6XU	O26-C24	3.11	1.41	1.33
3	C	202	6XU	C08-S12	3.65	1.78	1.73
3	D	204	6XU	C08-S12	3.80	1.78	1.73
3	E	205	6XU	C08-S12	4.02	1.79	1.73
3	A	206	6XU	C02-C28	4.31	1.60	1.52
3	A	206	6XU	C24-C03	4.40	1.57	1.48
3	A	205	6XU	C08-S12	4.41	1.79	1.73
3	F	202	6XU	C08-S12	4.42	1.79	1.73
3	B	202	6XU	C08-S12	4.77	1.80	1.73
3	A	206	6XU	C08-S12	8.28	1.85	1.73
3	A	206	6XU	C08-C06	11.04	1.62	1.48

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	206	6XU	O26-C24-O25	-5.45	112.61	123.57
3	E	205	6XU	O26-C24-O25	-4.41	114.70	123.57
3	F	202	6XU	O26-C24-O25	-4.07	115.38	123.57
3	A	205	6XU	O26-C24-O25	-3.90	115.73	123.57
3	B	202	6XU	O26-C24-O25	-3.69	116.15	123.57
3	D	204	6XU	O26-C24-O25	-3.58	116.37	123.57
3	C	202	6XU	O26-C24-O25	-3.57	116.38	123.57
3	A	206	6XU	N05-C06-N07	-2.93	119.72	123.03
3	C	202	6XU	C30-C31-C32	-2.71	118.91	122.87
3	F	202	6XU	C30-C31-C32	-2.65	119.00	122.87
3	E	205	6XU	C30-C31-C32	-2.60	119.08	122.87
3	B	202	6XU	C30-C31-C32	-2.49	119.23	122.87
3	D	204	6XU	C30-C31-C32	-2.40	119.37	122.87
3	A	206	6XU	C30-C31-C32	-2.35	119.45	122.87
3	A	206	6XU	C29-C28-C33	-2.14	114.78	117.95
3	F	202	6XU	C29-C28-C33	-2.01	114.98	117.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	205	6XU	C11-C10-N09	2.02	115.62	109.52
3	D	204	6XU	C11-C10-N09	2.04	115.69	109.52
3	A	206	6XU	C01-C02-N07	2.06	110.41	107.67
3	B	202	6XU	C11-C10-N09	2.10	115.87	109.52
3	C	202	6XU	C32-C33-C28	2.11	124.02	121.26
3	A	205	6XU	C11-C10-N09	2.11	115.89	109.52
3	C	202	6XU	C11-C10-N09	2.11	115.89	109.52
3	A	206	6XU	C11-C10-N09	2.12	115.91	109.52
3	D	204	6XU	C27-O26-C24	2.12	120.02	115.89
3	D	204	6XU	C29-C30-C31	2.17	120.65	118.34
3	F	202	6XU	C11-C10-N09	2.19	116.12	109.52
3	A	205	6XU	C32-C33-C28	2.25	124.21	121.26
3	B	202	6XU	C32-C33-C28	2.38	124.38	121.26
3	F	202	6XU	C29-C28-C02	2.39	124.79	120.62
3	A	206	6XU	C32-C33-C28	2.39	124.39	121.26
3	E	205	6XU	C32-C33-C28	2.45	124.47	121.26
3	A	206	6XU	C27-O26-C24	2.46	120.69	115.89
3	B	202	6XU	C29-C30-C31	2.48	120.98	118.34
3	F	202	6XU	C01-C02-N07	2.52	111.03	107.67
3	F	202	6XU	C29-C30-C31	2.54	121.05	118.34
3	D	204	6XU	C01-C02-N07	2.55	111.07	107.67
3	C	202	6XU	C27-O26-C24	2.63	121.02	115.89
3	C	202	6XU	C01-C02-N07	2.69	111.26	107.67
3	E	205	6XU	C29-C30-C31	2.71	121.23	118.34
3	E	205	6XU	C02-N07-C06	2.72	123.46	115.01
3	A	205	6XU	C27-O26-C24	2.80	121.34	115.89
3	F	202	6XU	C32-C33-C28	2.87	125.01	121.26
3	D	204	6XU	C02-N07-C06	2.90	124.03	115.01
3	B	202	6XU	C02-N07-C06	2.91	124.06	115.01
3	A	205	6XU	C02-N07-C06	2.91	124.06	115.01
3	C	202	6XU	C02-N07-C06	2.92	124.09	115.01
3	C	202	6XU	C29-C30-C31	2.93	121.47	118.34
3	F	202	6XU	C02-N07-C06	2.98	124.27	115.01
3	A	206	6XU	C02-N07-C06	3.43	125.68	115.01
3	B	202	6XU	C10-N09-C08	3.75	113.17	103.97
3	C	202	6XU	C10-N09-C08	3.93	113.61	103.97
3	F	202	6XU	C10-N09-C08	3.98	113.74	103.97
3	A	205	6XU	C10-N09-C08	4.03	113.85	103.97
3	E	205	6XU	C10-N09-C08	4.08	113.97	103.97
3	D	204	6XU	C10-N09-C08	4.20	114.28	103.97
3	C	202	6XU	O26-C24-C03	4.87	119.15	111.91
3	A	206	6XU	C10-N09-C08	4.93	116.06	103.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	205	6XU	O26-C24-C03	5.08	119.47	111.91
3	B	202	6XU	O26-C24-C03	5.08	119.47	111.91
3	D	204	6XU	O26-C24-C03	5.14	119.56	111.91
3	F	202	6XU	O26-C24-C03	5.88	120.65	111.91
3	E	205	6XU	O26-C24-C03	5.90	120.69	111.91
3	A	206	6XU	O26-C24-C03	6.86	122.11	111.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	201	IPA	1	0
2	E	203	IPA	4	0
2	E	204	IPA	2	0
4	F	201	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	143/155 (92%)	-0.23	1 (0%) 89 91	21, 33, 51, 87	0
1	B	148/155 (95%)	-0.15	4 (2%) 58 62	22, 31, 52, 110	0
1	C	143/155 (92%)	0.12	7 (4%) 33 36	22, 30, 78, 101	0
1	D	150/155 (96%)	-0.04	9 (6%) 25 27	22, 31, 66, 87	0
1	E	143/155 (92%)	0.74	22 (15%) 3 3	27, 37, 114, 141	0
1	F	150/155 (96%)	1.08	32 (21%) 1 1	26, 39, 137, 163	0
All	All	877/930 (94%)	0.26	75 (8%) 13 14	21, 33, 87, 163	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	84	LEU	14.7
1	E	76	LEU	12.7
1	F	79	PRO	11.7
1	F	80	ALA	11.1
1	F	85	VAL	10.9
1	F	77	GLU	9.2
1	F	76	LEU	8.8
1	C	143	LEU	8.4
1	F	81	SER	8.2
1	F	82	ARG	7.8
1	F	86	VAL	7.5
1	E	77	GLU	7.3
1	E	79	PRO	7.0
1	E	71	TRP	6.5
1	E	143	LEU	6.5
1	E	74	THR	6.4
1	E	84	LEU	6.2
1	F	143	LEU	6.2
1	E	80	ALA	6.1

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Mol	Chain	Res	Type	RSRZ
1	E	81	SER	5.9
1	F	154	PHE	5.9
1	F	78	ASP	5.6
1	E	72	VAL	5.3
1	F	74	THR	5.1
1	F	83	ASP	5.1
1	F	149	VAL	4.7
1	E	73	GLY	4.7
1	F	71	TRP	4.6
1	F	153	TYR	4.4
1	F	73	GLY	4.3
1	E	82	ARG	4.3
1	E	75	ASN	4.2
1	E	78	ASP	4.2
1	F	152	LEU	4.1
1	D	143	LEU	4.1
1	F	88	TYR	4.0
1	F	151	ASN	3.9
1	F	72	VAL	3.9
1	E	85	VAL	3.9
1	C	79	PRO	3.8
1	D	84	LEU	3.7
1	A	143	LEU	3.6
1	B	150	GLU	3.5
1	E	83	ASP	3.4
1	F	150	GLU	3.2
1	C	71	TRP	3.2
1	E	70	THR	3.1
1	D	87	SER	3.1
1	F	58	ALA	3.0
1	F	87	SER	3.0
1	E	86	VAL	3.0
1	D	79	PRO	2.9
1	B	152	LEU	2.8
1	F	92	ASN	2.8
1	C	84	LEU	2.8
1	B	151	ASN	2.7
1	D	80	ALA	2.7
1	F	75	ASN	2.7
1	D	91	THR	2.7
1	E	58	ALA	2.6
1	D	83	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	144	PRO	2.6
1	F	55	LEU	2.6
1	B	154	PHE	2.6
1	C	76	LEU	2.6
1	E	55	LEU	2.5
1	F	89	VAL	2.5
1	E	91	THR	2.5
1	F	70	THR	2.4
1	C	142	THR	2.4
1	E	100	LEU	2.4
1	D	28	ARG	2.4
1	C	74	THR	2.4
1	F	100	LEU	2.1
1	F	59	ILE	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	IPA	A	203	4/4	0.65	0.27	17.58	41,42,43,53	0
2	IPA	E	203	4/4	0.76	0.24	16.83	28,45,46,48	0
4	GOL	F	201	6/6	0.93	0.24	15.49	38,49,51,55	0
2	IPA	E	204	4/4	0.75	0.17	9.12	26,35,52,53	0
4	GOL	B	201	6/6	0.93	0.14	3.81	36,43,54,60	0
3	6XU	A	206	34/34	0.81	0.21	3.74	60,69,88,93	0
2	IPA	A	201	4/4	0.75	0.23	3.65	34,34,45,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	IPA	E	202	4/4	0.92	0.29	3.30	36,41,41,47	0
2	IPA	C	201	4/4	0.87	0.21	2.99	32,34,44,46	0
2	IPA	A	204	4/4	0.88	0.14	2.75	52,62,64,65	0
2	IPA	A	202	4/4	0.94	0.18	2.44	31,32,35,41	0
2	IPA	D	201	4/4	0.95	0.18	2.15	32,32,34,36	0
2	IPA	E	201	4/4	0.69	0.17	1.68	55,58,58,71	0
2	IPA	D	202	4/4	0.82	0.14	0.70	44,50,54,60	0
3	6XU	F	202	34/34	0.96	0.07	0.02	22,28,33,33	0
3	6XU	A	205	34/34	0.97	0.06	-0.18	22,26,31,32	0
3	6XU	D	204	34/34	0.97	0.06	-0.42	21,25,30,33	0
3	6XU	C	202	34/34	0.98	0.06	-0.49	21,25,29,33	0
3	6XU	B	202	34/34	0.98	0.06	-0.84	19,25,32,33	0
3	6XU	E	205	34/34	0.98	0.05	-0.88	20,27,32,38	0
5	CL	D	203	1/1	0.87	0.28	-	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.