Full wwPDB X-ray Structure Validation Report

Sep 12, 2016 – 05:22 PM EDT

PDB ID	:	5IZQ
Title	:	Crystal structure of human folate receptor alpha in complex with novel antifolate AGF183
Authors	:	Ke, J.; Gu, X.; Brunzelle, J.S.; Xu, H.E.; Melcher, K.
Deposited on	:	2016-03-25
Resolution	:	3.60 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 (i) symbol.

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

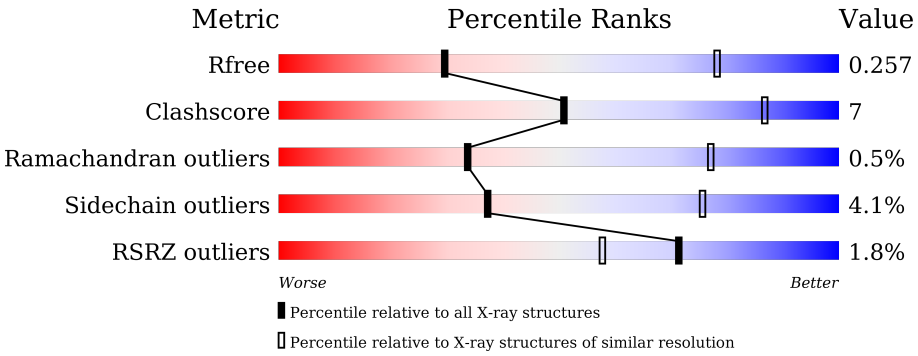
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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 <=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	238	68% 18% 13%
1	B	238	.% 71% 13% • 15%
1	C	238	.% 73% 14% 13%
1	D	238	2% 74% 12% • 12%
1	E	238	2% 65% 20% • 13%
1	F	238	5% 68% 17% • 13%

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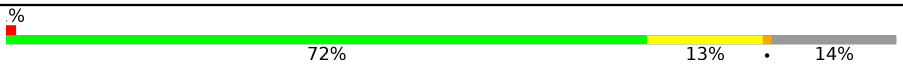
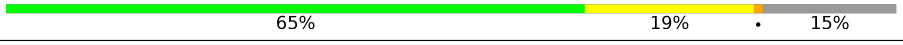
Mol	Chain	Length	Quality of chain
1	G	238	
1	H	238	

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	83A	G	300	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13751 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 Folate receptor alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1697	1064	307	306	20			
1	B	203	Total	C	N	O	S	0	0	0
			1668	1048	300	300	20			
1	C	208	Total	C	N	O	S	0	0	0
			1701	1069	305	307	20			
1	D	209	Total	C	N	O	S	0	0	0
			1710	1075	310	305	20			
1	E	206	Total	C	N	O	S	0	0	0
			1691	1061	306	304	20			
1	F	208	Total	C	N	O	S	0	0	0
			1705	1070	308	307	20			
1	G	205	Total	C	N	O	S	0	0	0
			1686	1058	305	303	20			
1	H	203	Total	C	N	O	S	0	0	0
			1669	1049	300	300	20			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	214	THR	-	expression tag	UNP P15328
A	215	LEU	-	expression tag	UNP P15328
A	216	VAL	-	expression tag	UNP P15328
B	214	THR	-	expression tag	UNP P15328
B	215	LEU	-	expression tag	UNP P15328
B	216	VAL	-	expression tag	UNP P15328
C	214	THR	-	expression tag	UNP P15328
C	215	LEU	-	expression tag	UNP P15328
C	216	VAL	-	expression tag	UNP P15328
D	214	THR	-	expression tag	UNP P15328
D	215	LEU	-	expression tag	UNP P15328
D	216	VAL	-	expression tag	UNP P15328
E	214	THR	-	expression tag	UNP P15328

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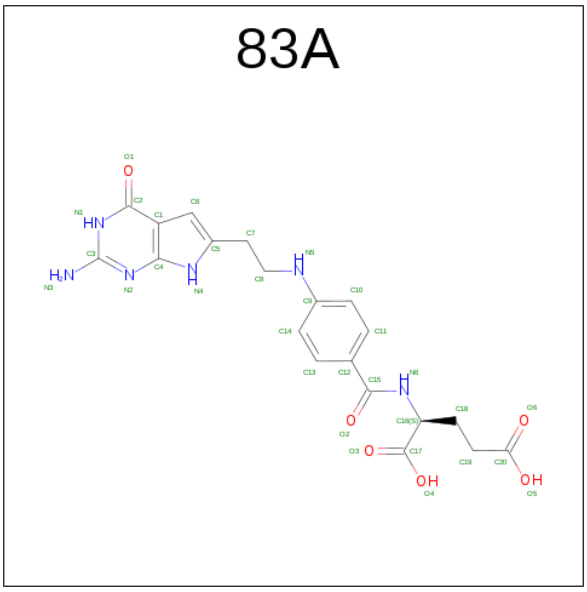
Chain	Residue	Modelled	Actual	Comment	Reference
E	215	LEU	-	expression tag	UNP P15328
E	216	VAL	-	expression tag	UNP P15328
F	214	THR	-	expression tag	UNP P15328
F	215	LEU	-	expression tag	UNP P15328
F	216	VAL	-	expression tag	UNP P15328
G	214	THR	-	expression tag	UNP P15328
G	215	LEU	-	expression tag	UNP P15328
G	216	VAL	-	expression tag	UNP P15328
H	214	THR	-	expression tag	UNP P15328
H	215	LEU	-	expression tag	UNP P15328
H	216	VAL	-	expression tag	UNP P15328

- Molecule 2 is N-(4-{[2-(2-amino-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidin-6-yl)ethyl]amino}benzene-1-carbonyl)-L-glutamic acid (three-letter code: 83A) (formula: $C_{20}H_{22}N_6O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	20	6	6		
2	B	1	Total	C	N	O	0	0
			32	20	6	6		
2	C	1	Total	C	N	O	0	0
			32	20	6	6		
2	E	1	Total	C	N	O	0	0
			32	20	6	6		
2	F	1	Total	C	N	O	0	0
			32	20	6	6		

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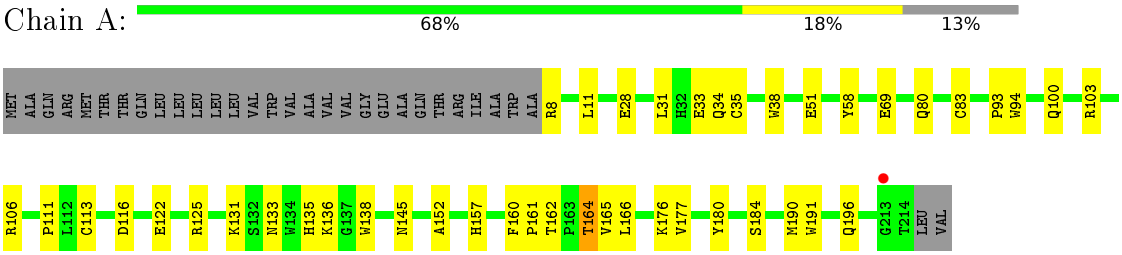
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	N	O	0	0
			32	20	6	6		
2	H	1	Total	C	N	O	0	0
			32	20	6	6		

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.

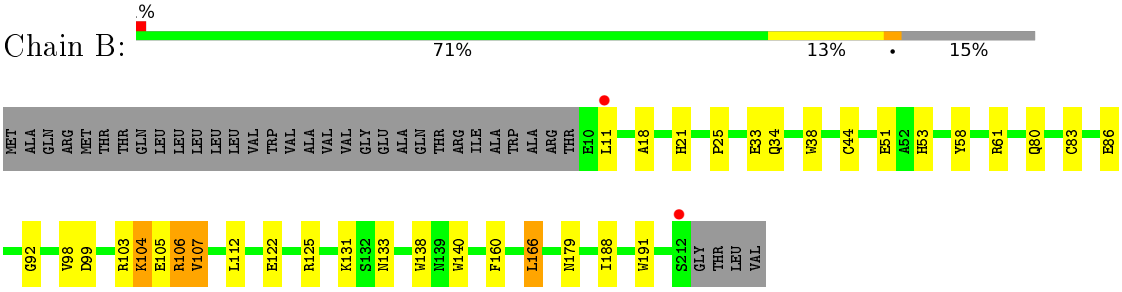
- Molecule 1: Folate receptor alpha

Chain A:



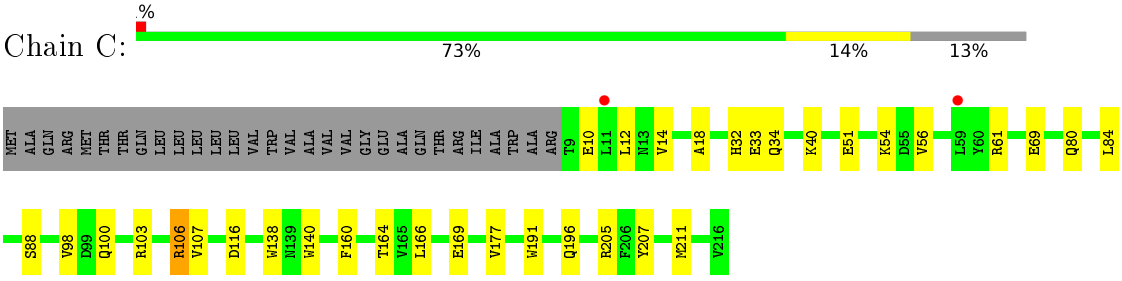
- Molecule 1: Folate receptor alpha

Chain B:



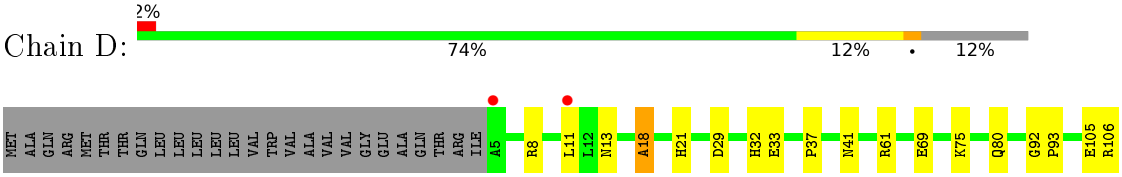
- Molecule 1: Folate receptor alpha

Chain C:



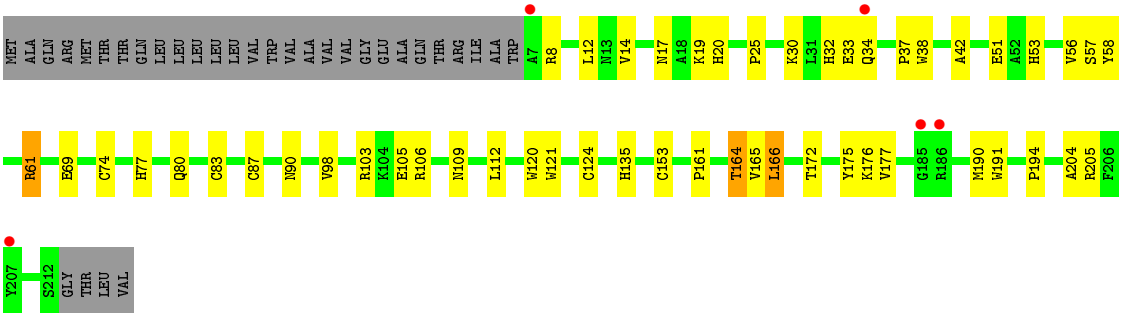
- Molecule 1: Folate receptor alpha

Chain D:



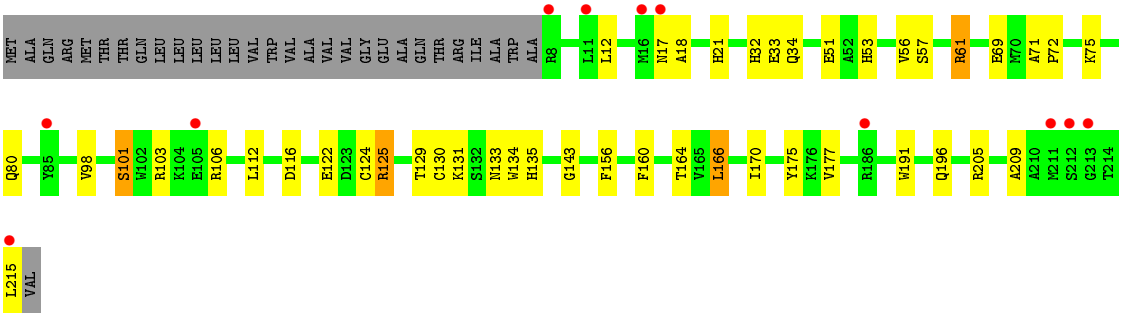
• Molecule 1: Folate receptor alpha

Chain E:



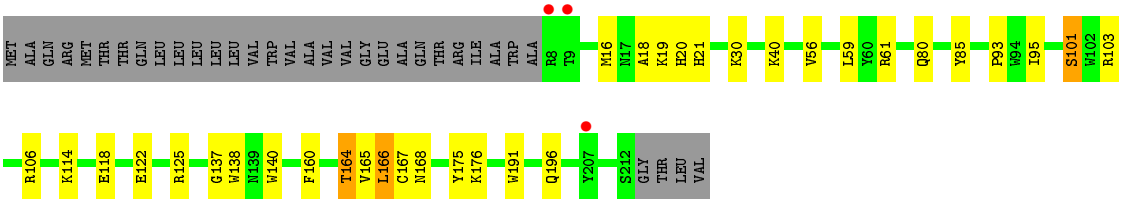
• Molecule 1: Folate receptor alpha

Chain F:



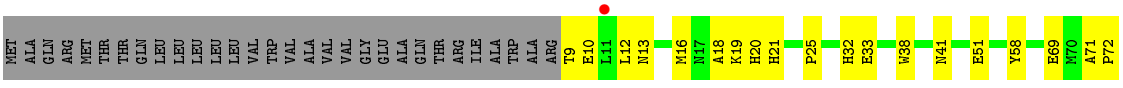
• Molecule 1: Folate receptor alpha

Chain G:



• Molecule 1: Folate receptor alpha

Chain H:




Q80
C83
L84
S88
I95
V98
D99
Q100
R106
L112
E122
R125
W140
F144
N145
K146
F156
F160
P161
T162
P163
T164
V165
L166
I170
W171
S174
Y175
G183
Q189
M190
W191
M211
SER
GLY
THR
LEU
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.79Å 144.98Å 211.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.11 – 3.60 47.11 – 3.56	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.11-3.60) 99.3 (47.11-3.56)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.216 , 0.257 0.212 , 0.257	Depositor DCC
R_{free} test set	1601 reflections (4.88%)	DCC
Wilson B-factor (Å^2)	71.1	Xtriage
Anisotropy	0.888	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 35.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	13751	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: 83A

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	0.33	0/1755	0.53	2/2384 (0.1%)
1	B	0.29	0/1726	0.61	5/2345 (0.2%)
1	C	0.28	0/1759	0.46	1/2391 (0.0%)
1	D	0.27	0/1770	0.46	1/2406 (0.0%)
1	E	0.30	0/1749	0.46	0/2376
1	F	0.28	0/1763	0.45	0/2395
1	G	0.28	0/1744	0.44	0/2369
1	H	0.35	0/1727	0.48	0/2347
All	All	0.30	0/13993	0.49	9/19013 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	98	VAL	N-CA-C	-14.37	72.20	111.00
1	B	104	LYS	CB-CA-C	-8.46	93.47	110.40
1	A	33	GLU	CB-CA-C	-6.95	96.51	110.40
1	B	105	GLU	N-CA-CB	6.87	122.96	110.60
1	B	99	ASP	N-CA-CB	-6.71	98.52	110.60
1	A	33	GLU	N-CA-C	6.66	128.97	111.00
1	B	99	ASP	N-CA-C	-5.98	94.85	111.00
1	D	18	ALA	CB-CA-C	-5.21	102.28	110.10
1	C	33	GLU	N-CA-C	5.17	124.96	111.00

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	1697	0	1555	28	0
1	B	1668	0	1525	20	0
1	C	1701	0	1562	19	0
1	D	1710	0	1564	20	0
1	E	1691	0	1550	27	0
1	F	1705	0	1566	25	0
1	G	1686	0	1545	19	0
1	H	1669	0	1527	24	0
2	A	32	0	0	1	0
2	B	32	0	0	0	0
2	C	32	0	0	0	0
2	E	32	0	0	0	0
2	F	32	0	0	0	0
2	G	32	0	0	1	0
2	H	32	0	0	0	0
All	All	13751	0	12394	179	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 7.

All (179) 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:B:104:LYS:HG2	1:B:104:LYS:O	1.64	0.92
1:C:10:GLU:HG3	1:C:12:LEU:H	1.49	0.77
1:H:13:ASN:OD1	1:H:41:ASN:ND2	2.17	0.77
1:A:122:GLU:OE2	1:A:125:ARG:NH1	2.21	0.74
1:G:122:GLU:OE2	1:G:125:ARG:NH1	2.21	0.74
1:D:80:GLN:NE2	1:D:190:MET:O	2.21	0.72
1:C:12:LEU:HD21	1:C:205:ARG:HG2	1.76	0.67
1:F:12:LEU:HD21	1:F:205:ARG:HG3	1.78	0.65
1:A:80:GLN:HG3	1:A:191:TRP:CZ2	2.33	0.63
1:G:85:TYR:OH	1:G:103:ARG:NH1	2.30	0.63
1:A:51:GLU:HG3	1:A:58:TYR:HB3	1.83	0.61
1:A:161:PRO:HD2	1:A:165:VAL:HG11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:PHE:CD1	1:D:166:LEU:HA	2.37	0.60
1:C:56:VAL:HG12	1:C:61:ARG:HG3	1.84	0.60
1:B:104:LYS:CG	1:B:104:LYS:O	2.36	0.60
1:B:103:ARG:CZ	1:B:106:ARG:HG3	2.32	0.59
1:C:80:GLN:HG3	1:C:191:TRP:CZ2	2.39	0.58
1:E:135:HIS:ND1	1:E:172:THR:OG1	2.34	0.57
1:C:160:PHE:CD1	1:C:166:LEU:HA	2.39	0.57
1:H:51:GLU:HG3	1:H:58:TYR:HB3	1.86	0.57
1:G:160:PHE:HD1	1:G:165:VAL:HG12	1.68	0.57
1:E:51:GLU:OE1	1:E:58:TYR:N	2.33	0.56
1:H:80:GLN:HG3	1:H:191:TRP:CZ2	2.40	0.56
1:B:80:GLN:HG3	1:B:191:TRP:CZ2	2.40	0.56
1:F:164:THR:HA	1:F:177:VAL:HG21	1.86	0.56
1:C:138:TRP:HB2	1:C:140:TRP:HE1	1.71	0.55
1:H:144:PHE:CE1	1:H:146:LYS:HE3	2.41	0.55
1:E:161:PRO:HD2	1:E:165:VAL:HG11	1.89	0.55
1:G:80:GLN:HG3	1:G:191:TRP:CZ2	2.42	0.55
1:C:138:TRP:HB2	1:C:140:TRP:NE1	2.21	0.55
1:F:80:GLN:HG3	1:F:191:TRP:CH2	2.42	0.55
1:H:122:GLU:OE2	1:H:125:ARG:NH1	2.39	0.55
1:F:122:GLU:OE2	1:F:125:ARG:NH1	2.39	0.54
1:A:38:TRP:CZ3	1:A:83:CYS:HB3	2.42	0.54
1:B:33:GLU:HG3	1:B:53:HIS:CD2	2.42	0.54
1:G:20:HIS:NE2	1:G:59:LEU:O	2.38	0.54
1:E:103:ARG:CZ	1:E:106:ARG:HD2	2.37	0.54
1:D:160:PHE:CG	1:D:166:LEU:HD23	2.43	0.54
1:C:12:LEU:HD11	1:C:205:ARG:HA	1.90	0.54
1:D:80:GLN:HG3	1:D:191:TRP:CZ2	2.42	0.54
1:E:80:GLN:HG3	1:E:191:TRP:CZ2	2.43	0.53
1:F:160:PHE:CD1	1:F:166:LEU:HA	2.44	0.53
1:F:80:GLN:HG3	1:F:191:TRP:CZ2	2.44	0.53
1:F:18:ALA:HB3	1:F:21:HIS:ND1	2.24	0.52
1:D:32:HIS:CG	1:D:33:GLU:H	2.27	0.52
1:D:11:LEU:O	1:D:92:GLY:HA3	2.08	0.52
1:A:80:GLN:NE2	1:A:190:MET:O	2.42	0.52
1:A:152:ALA:HA	1:B:191:TRP:CZ3	2.45	0.52
1:D:80:GLN:HG3	1:D:191:TRP:CH2	2.45	0.52
1:B:38:TRP:CZ3	1:B:83:CYS:HB3	2.44	0.52
1:E:112:LEU:HB2	1:E:175:TYR:HD2	1.73	0.52
1:E:164:THR:HA	1:E:177:VAL:HG21	1.91	0.52
1:E:98:VAL:HG11	1:E:106:ARG:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:GLN:HB2	1:F:53:HIS:NE2	2.25	0.51
1:H:140:TRP:CZ2	1:H:145:ASN:HB3	2.45	0.51
1:H:84:LEU:HD12	1:H:88:SER:HB2	1.92	0.51
1:D:11:LEU:HD22	1:D:93:PRO:HA	1.92	0.51
1:E:38:TRP:O	1:E:42:ALA:HB2	2.10	0.51
1:F:98:VAL:HG11	1:F:106:ARG:HD3	1.93	0.51
1:G:164:THR:O	1:G:168:ASN:ND2	2.42	0.51
1:H:98:VAL:HG21	1:H:106:ARG:HD3	1.93	0.51
1:A:80:GLN:HG3	1:A:191:TRP:CE2	2.46	0.50
1:H:160:PHE:CD1	1:H:166:LEU:HA	2.46	0.50
1:E:19:LYS:HE2	1:E:20:HIS:NE2	2.27	0.50
1:B:51:GLU:HG3	1:B:58:TYR:HB3	1.93	0.49
1:E:8:ARG:HH21	1:E:14:VAL:HG21	1.78	0.49
1:A:160:PHE:CD1	1:A:166:LEU:HA	2.47	0.49
1:A:131:LYS:NZ	1:A:133:ASN:O	2.45	0.49
1:B:112:LEU:HD12	1:B:188:ILE:O	2.12	0.49
1:H:32:HIS:CG	1:H:33:GLU:H	2.30	0.49
1:H:80:GLN:NE2	1:H:190:MET:O	2.46	0.49
1:A:28:GLU:O	1:A:31:LEU:HG	2.13	0.48
1:E:34:GLN:O	1:E:80:GLN:NE2	2.46	0.48
1:D:18:ALA:HB3	1:D:21:HIS:ND1	2.28	0.48
1:A:152:ALA:HA	1:B:191:TRP:HZ3	1.78	0.48
1:D:113:CYS:HB2	1:D:116:ASP:OD1	2.14	0.48
1:G:160:PHE:CD1	1:G:166:LEU:HA	2.49	0.48
1:C:84:LEU:HD12	1:C:88:SER:HB2	1.96	0.48
1:B:138:TRP:HB2	1:B:140:TRP:NE1	2.29	0.48
1:E:33:GLU:HG3	1:E:53:HIS:CD2	2.49	0.47
1:C:164:THR:HA	1:C:177:VAL:HG21	1.95	0.47
1:E:80:GLN:HG3	1:E:191:TRP:CH2	2.49	0.47
1:F:51:GLU:HB3	1:F:57:SER:HB2	1.96	0.47
1:H:162:THR:OG1	1:H:165:VAL:HG23	2.13	0.47
1:H:80:GLN:HG3	1:H:191:TRP:CH2	2.50	0.47
1:B:160:PHE:CD1	1:B:166:LEU:HA	2.49	0.47
1:A:103:ARG:CZ	1:A:106:ARG:HD2	2.45	0.47
1:D:186:ARG:HB3	1:D:186:ARG:HH11	1.79	0.47
1:B:122:GLU:OE2	1:B:125:ARG:NH1	2.48	0.46
1:C:160:PHE:CG	1:C:166:LEU:HD23	2.50	0.46
1:A:35:CYS:O	1:A:38:TRP:HE3	1.99	0.46
1:C:207:TYR:O	1:C:211:MET:HG2	2.15	0.46
1:E:56:VAL:HG12	1:E:61:ARG:HG3	1.97	0.46
1:A:136:LYS:HE2	2:A:300:83A:O5	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:PRO:HA	1:D:194:PRO:HB3	1.97	0.46
1:E:12:LEU:HD21	1:E:205:ARG:HA	1.96	0.46
1:A:80:GLN:HG3	1:A:191:TRP:CH2	2.51	0.46
1:F:209:ALA:HB1	1:F:215:LEU:HA	1.97	0.46
1:C:34:GLN:OE1	1:C:80:GLN:HG2	2.16	0.45
1:F:32:HIS:CG	1:F:33:GLU:H	2.33	0.45
1:A:164:THR:HA	1:A:177:VAL:HG21	1.98	0.45
1:A:180:TYR:HB3	1:A:184:SER:OG	2.16	0.45
1:F:56:VAL:HG12	1:F:61:ARG:HG3	1.99	0.45
1:B:106:ARG:HD3	1:B:107:VAL:O	2.17	0.45
1:E:109:ASN:HA	1:E:176:LYS:HB2	1.98	0.45
1:G:164:THR:HG22	1:G:168:ASN:ND2	2.32	0.45
1:A:34:GLN:OE1	1:A:80:GLN:HG2	2.17	0.45
1:C:169:GLU:HB3	1:F:196:GLN:OE1	2.16	0.45
1:H:12:LEU:HD12	1:H:12:LEU:H	1.82	0.45
1:G:18:ALA:HB3	1:G:21:HIS:ND1	2.32	0.45
1:C:40:LYS:HE2	1:C:40:LYS:HB3	1.73	0.44
1:F:112:LEU:HB2	1:F:175:TYR:CD1	2.51	0.44
1:F:129:THR:OG1	1:F:130:CYS:N	2.50	0.44
1:C:18:ALA:HA	1:C:103:ARG:HB2	2.00	0.44
1:C:98:VAL:HG11	1:C:106:ARG:HD3	1.99	0.44
1:G:56:VAL:HG12	1:G:61:ARG:HG3	1.99	0.44
1:E:77:HIS:HB3	1:E:120:TRP:CD1	2.53	0.44
1:F:131:LYS:HE3	1:F:133:ASN:O	2.18	0.44
1:G:114:LYS:O	1:G:118:GLU:HG3	2.18	0.43
1:F:34:GLN:OE1	1:F:80:GLN:HG2	2.19	0.43
1:D:171:TRP:HB2	1:D:174:SER:HB2	2.00	0.43
1:G:80:GLN:HG3	1:G:191:TRP:CH2	2.54	0.43
1:C:12:LEU:O	1:C:14:VAL:HG13	2.19	0.43
1:F:103:ARG:CZ	1:F:106:ARG:HD2	2.48	0.43
1:C:51:GLU:OE2	1:C:54:LYS:HD3	2.19	0.43
1:H:144:PHE:HE1	1:H:146:LYS:HE3	1.81	0.43
1:G:168:ASN:OD1	1:G:176:LYS:HA	2.19	0.42
1:G:16:MET:HB3	1:G:95:ILE:HD13	2.00	0.42
1:A:135:HIS:HB3	1:A:136:LYS:HE3	2.01	0.42
1:E:121:TRP:HA	1:E:166:LEU:HD12	2.00	0.42
1:G:103:ARG:NH2	1:G:106:ARG:HD2	2.34	0.42
1:H:38:TRP:CZ3	1:H:83:CYS:HB3	2.54	0.42
1:H:71:ALA:HA	1:H:72:PRO:HD3	1.91	0.42
1:G:138:TRP:HB2	1:G:140:TRP:HE1	1.84	0.42
1:A:138:TRP:HB3	1:A:145:ASN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:PRO:HG3	1:E:194:PRO:HD3	2.00	0.42
1:B:103:ARG:NH2	1:B:106:ARG:HG3	2.33	0.42
1:E:74:CYS:HB2	1:E:124:CYS:HA	2.02	0.42
1:E:8:ARG:NH1	1:E:105:GLU:OE2	2.53	0.42
1:F:124:CYS:HB3	1:F:156:PHE:CD2	2.54	0.42
1:H:19:LYS:HG2	1:H:20:HIS:CE1	2.55	0.42
1:A:94:TRP:NE1	1:A:111:PRO:HD3	2.35	0.42
1:F:103:ARG:NH2	1:F:106:ARG:HD2	2.34	0.42
1:G:160:PHE:CD2	1:G:166:LEU:HD23	2.55	0.42
1:H:183:GLY:H	1:H:189:GLN:HE21	1.67	0.42
1:G:137:GLY:H	2:G:300:83A:C17	2.33	0.42
1:H:80:GLN:HG3	1:H:191:TRP:CE2	2.55	0.42
1:E:112:LEU:HB2	1:E:175:TYR:CD2	2.54	0.42
1:E:90:ASN:HB3	1:E:204:ALA:HB2	2.02	0.42
1:A:111:PRO:HA	1:A:176:LYS:O	2.19	0.41
1:B:18:ALA:HB3	1:B:21:HIS:ND1	2.35	0.41
1:B:34:GLN:HB2	1:B:53:HIS:NE2	2.35	0.41
1:F:61:ARG:HG2	1:F:143:GLY:O	2.21	0.41
1:H:170:ILE:HG23	1:H:171:TRP:CD1	2.55	0.41
1:A:113:CYS:HB2	1:A:116:ASP:OD1	2.20	0.41
1:F:71:ALA:HA	1:F:72:PRO:HD3	1.92	0.41
1:E:51:GLU:HB3	1:E:57:SER:HB2	2.03	0.41
1:H:18:ALA:HB3	1:H:21:HIS:ND1	2.35	0.41
1:D:80:GLN:HE21	1:D:80:GLN:HB3	1.71	0.41
1:D:160:PHE:CD2	1:D:166:LEU:HD23	2.56	0.41
1:D:75:LYS:HE3	1:D:75:LYS:HB2	1.88	0.41
1:F:75:LYS:HE3	1:F:75:LYS:HB2	1.84	0.41
1:B:131:LYS:HE3	1:B:133:ASN:O	2.21	0.41
1:B:44:CYS:HB3	1:B:86:GLU:O	2.20	0.40
1:D:8:ARG:NH1	1:D:105:GLU:OE2	2.54	0.40
1:A:138:TRP:CG	1:A:145:ASN:HB2	2.56	0.40
1:D:13:ASN:OD1	1:D:41:ASN:ND2	2.53	0.40
1:E:83:CYS:O	1:E:87:CYS:HB2	2.22	0.40
1:A:125:ARG:HB2	1:A:157:HIS:CE1	2.56	0.40
1:A:162:THR:OG1	1:A:164:THR:HG23	2.20	0.40
1:D:29:ASP:OD1	1:D:29:ASP:N	2.53	0.40
1:E:30:LYS:HA	1:E:30:LYS:HD3	1.84	0.40
1:H:112:LEU:HB2	1:H:175:TYR:CD1	2.56	0.40
1:A:160:PHE:CG	1:A:166:LEU:HD23	2.57	0.40
1:D:129:THR:HG23	1:D:159:TYR:HD2	1.86	0.40
1:F:134:TRP:CE3	1:F:170:ILE:HD11	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:CYS:O	1:G:175:TYR:HB2	2.21	0.40
1:H:16:MET:HB3	1:H:95:ILE:HD13	2.02	0.40
1:B:11:LEU:O	1:B:92:GLY:HA3	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	205/238 (86%)	184 (90%)	20 (10%)	1 (0%)	34 77
1	B	201/238 (84%)	181 (90%)	19 (10%)	1 (0%)	34 77
1	C	206/238 (87%)	191 (93%)	15 (7%)	0	100 100
1	D	207/238 (87%)	193 (93%)	14 (7%)	0	100 100
1	E	204/238 (86%)	184 (90%)	19 (9%)	1 (0%)	34 77
1	F	206/238 (87%)	185 (90%)	20 (10%)	1 (0%)	34 77
1	G	203/238 (85%)	184 (91%)	16 (8%)	3 (2%)	13 57
1	H	201/238 (84%)	187 (93%)	13 (6%)	1 (0%)	34 77
All	All	1633/1904 (86%)	1489 (91%)	136 (8%)	8 (0%)	34 77

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	101	SER
1	E	25	PRO
1	F	101	SER
1	G	19	LYS
1	G	93	PRO
1	A	93	PRO
1	B	25	PRO

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Mol	Chain	Res	Type
1	H	25	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	184/209 (88%)	178 (97%)	6 (3%)	45 80
1	B	181/209 (87%)	176 (97%)	5 (3%)	51 82
1	C	185/209 (88%)	178 (96%)	7 (4%)	40 77
1	D	183/209 (88%)	174 (95%)	9 (5%)	31 71
1	E	183/209 (88%)	175 (96%)	8 (4%)	35 74
1	F	185/209 (88%)	177 (96%)	8 (4%)	35 75
1	G	183/209 (88%)	177 (97%)	6 (3%)	45 80
1	H	181/209 (87%)	170 (94%)	11 (6%)	23 65
All	All	1465/1672 (88%)	1405 (96%)	60 (4%)	37 75

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	11	LEU
1	A	69	GLU
1	A	100	GLN
1	A	164	THR
1	A	196	GLN
1	B	61	ARG
1	B	106	ARG
1	B	107	VAL
1	B	166	LEU
1	B	179	ASN
1	C	32	HIS
1	C	69	GLU
1	C	100	GLN

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Mol	Chain	Res	Type
1	C	106	ARG
1	C	107	VAL
1	C	116	ASP
1	C	196	GLN
1	D	61	ARG
1	D	69	GLU
1	D	106	ARG
1	D	107	VAL
1	D	164	THR
1	D	166	LEU
1	D	174	SER
1	D	179	ASN
1	D	186	ARG
1	E	17	ASN
1	E	32	HIS
1	E	61	ARG
1	E	69	GLU
1	E	153	CYS
1	E	164	THR
1	E	166	LEU
1	E	190	MET
1	F	17	ASN
1	F	61	ARG
1	F	69	GLU
1	F	101	SER
1	F	116	ASP
1	F	125	ARG
1	F	135	HIS
1	F	166	LEU
1	G	30	LYS
1	G	40	LYS
1	G	101	SER
1	G	164	THR
1	G	166	LEU
1	G	196	GLN
1	H	9	THR
1	H	10	GLU
1	H	69	GLU
1	H	88	SER
1	H	99	ASP
1	H	100	GLN
1	H	106	ARG

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Mol	Chain	Res	Type
1	H	156	PHE
1	H	164	THR
1	H	166	LEU
1	H	174	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	80	GLN
1	D	119	GLN
1	E	17	ASN
1	E	90	ASN
1	F	17	ASN
1	F	32	HIS
1	H	100	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

7 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	$\#\|Z\|>2$
2	83A	A	300	-	26,34,34	1.45	3 (11%)	25,47,47	2.24	5 (20%)
2	83A	B	300	-	26,34,34	1.47	3 (11%)	25,47,47	2.23	7 (28%)
2	83A	C	300	-	26,34,34	1.49	4 (15%)	25,47,47	2.20	7 (28%)
2	83A	E	300	-	26,34,34	1.47	5 (19%)	25,47,47	2.24	5 (20%)
2	83A	F	300	-	26,34,34	1.41	4 (15%)	25,47,47	2.01	5 (20%)
2	83A	G	300	-	26,34,34	1.44	4 (15%)	25,47,47	2.12	6 (24%)
2	83A	H	300	-	26,34,34	1.43	4 (15%)	25,47,47	2.22	6 (24%)

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	83A	A	300	-	-	0/16/23/23	0/3/3/3
2	83A	B	300	-	-	0/16/23/23	0/3/3/3
2	83A	C	300	-	-	0/16/23/23	0/3/3/3
2	83A	E	300	-	-	0/16/23/23	0/3/3/3
2	83A	F	300	-	-	0/16/23/23	0/3/3/3
2	83A	G	300	-	-	0/16/23/23	0/3/3/3
2	83A	H	300	-	-	0/16/23/23	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	300	83A	C16-N6	-3.53	1.41	1.46
2	A	300	83A	C16-N6	-3.41	1.41	1.46
2	F	300	83A	C16-N6	-2.68	1.42	1.46
2	G	300	83A	C16-N6	-2.55	1.43	1.46
2	E	300	83A	C16-N6	-2.38	1.43	1.46
2	H	300	83A	C12-C15	2.06	1.54	1.50
2	C	300	83A	C9-N5	2.11	1.45	1.38
2	G	300	83A	C12-C15	2.14	1.54	1.50
2	F	300	83A	C12-C15	2.28	1.54	1.50
2	B	300	83A	C12-C15	2.35	1.54	1.50
2	E	300	83A	C9-N5	2.41	1.45	1.38
2	C	300	83A	C12-C15	2.44	1.55	1.50
2	E	300	83A	C12-C15	2.51	1.55	1.50
2	H	300	83A	C15-N6	2.84	1.40	1.34
2	G	300	83A	C15-N6	3.28	1.41	1.34
2	A	300	83A	C15-N6	3.34	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	300	83A	C3-N3	3.54	1.41	1.34
2	A	300	83A	C3-N3	3.55	1.41	1.34
2	F	300	83A	C15-N6	3.57	1.42	1.34
2	B	300	83A	C3-N3	3.63	1.41	1.34
2	E	300	83A	C15-N6	3.64	1.42	1.34
2	H	300	83A	C3-N3	3.65	1.41	1.34
2	F	300	83A	C3-N3	3.74	1.42	1.34
2	C	300	83A	C3-N3	3.78	1.42	1.34
2	G	300	83A	C3-N3	3.93	1.42	1.34
2	B	300	83A	C15-N6	4.03	1.43	1.34
2	C	300	83A	C15-N6	4.18	1.43	1.34

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	300	83A	C6-C5-N4	-6.43	100.68	111.48
2	C	300	83A	C6-C5-N4	-6.14	101.16	111.48
2	A	300	83A	C6-C5-N4	-5.67	101.96	111.48
2	G	300	83A	C6-C5-N4	-5.58	102.10	111.48
2	H	300	83A	N2-C3-N1	-5.50	120.08	127.56
2	F	300	83A	C6-C5-N4	-5.43	102.36	111.48
2	B	300	83A	N2-C3-N1	-5.34	120.29	127.56
2	C	300	83A	N2-C3-N1	-5.17	120.52	127.56
2	A	300	83A	N2-C3-N1	-5.13	120.57	127.56
2	H	300	83A	C6-C5-N4	-5.09	102.92	111.48
2	E	300	83A	N2-C3-N1	-5.08	120.65	127.56
2	G	300	83A	N2-C3-N1	-5.03	120.71	127.56
2	F	300	83A	N2-C3-N1	-4.94	120.84	127.56
2	B	300	83A	C6-C5-N4	-4.63	103.71	111.48
2	A	300	83A	C18-C16-N6	-2.82	105.52	109.92
2	B	300	83A	C8-C7-C5	-2.63	101.18	112.69
2	G	300	83A	C10-C9-N5	-2.44	116.18	121.04
2	G	300	83A	C11-C12-C15	-2.38	113.04	120.62
2	F	300	83A	C17-C16-N6	-2.23	108.49	112.93
2	A	300	83A	C14-C13-C12	-2.14	118.24	120.76
2	C	300	83A	O2-C15-C12	-2.09	117.37	120.95
2	H	300	83A	C8-C7-C5	-2.04	103.75	112.69
2	H	300	83A	C10-C9-N5	-2.04	116.99	121.04
2	B	300	83A	C7-C8-N5	-2.02	108.24	111.25
2	E	300	83A	N3-C3-N1	2.23	120.88	117.20
2	C	300	83A	C18-C19-C20	2.24	122.19	113.05
2	C	300	83A	C7-C8-N5	2.37	114.78	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	300	83A	N3-C3-N1	2.48	121.28	117.20
2	H	300	83A	N3-C3-N1	2.71	121.67	117.20
2	G	300	83A	N3-C3-N1	2.82	121.84	117.20
2	F	300	83A	N3-C3-N1	3.12	122.35	117.20
2	B	300	83A	N3-C3-N1	3.18	122.44	117.20
2	B	300	83A	C8-N5-C9	3.18	129.41	123.07
2	G	300	83A	C2-N1-C3	3.75	120.27	115.88
2	E	300	83A	C7-C8-N5	4.06	117.30	111.25
2	F	300	83A	C2-N1-C3	4.13	120.72	115.88
2	C	300	83A	C2-N1-C3	4.31	120.93	115.88
2	B	300	83A	C2-N1-C3	4.85	121.56	115.88
2	E	300	83A	C2-N1-C3	5.02	121.77	115.88
2	A	300	83A	C2-N1-C3	5.02	121.77	115.88
2	H	300	83A	C2-N1-C3	5.08	121.83	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	83A	1	0
2	G	300	83A	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	207/238 (86%)	-0.11	1 (0%)	91	86	40, 65, 107, 173	0
1	B	203/238 (85%)	-0.09	2 (0%)	84	73	58, 88, 121, 144	0
1	C	208/238 (87%)	0.04	2 (0%)	84	73	74, 98, 121, 139	0
1	D	209/238 (87%)	0.04	5 (2%)	62	47	66, 98, 127, 166	0
1	E	206/238 (86%)	0.09	5 (2%)	62	47	54, 90, 125, 161	0
1	F	208/238 (87%)	0.16	11 (5%)	30	21	68, 106, 136, 151	0
1	G	205/238 (86%)	0.01	3 (1%)	76	64	67, 97, 129, 167	0
1	H	203/238 (85%)	-0.19	1 (0%)	91	86	45, 64, 99, 134	0
All	All	1649/1904 (86%)	-0.00	30 (1%)	71	58	40, 90, 128, 173	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	213	GLY	4.3
1	F	211	MET	3.8
1	E	186	ARG	3.4
1	A	213	GLY	3.4
1	F	105	GLU	3.2
1	F	186	ARG	3.2
1	F	11	LEU	3.1
1	F	85	TYR	2.8
1	D	210	ALA	2.7
1	D	186	ARG	2.7
1	G	8	ARG	2.7
1	C	11	LEU	2.7
1	D	213	GLY	2.7
1	E	185	GLY	2.6
1	H	11	LEU	2.6
1	G	9	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	215	LEU	2.4
1	E	34	GLN	2.4
1	E	207	TYR	2.3
1	G	207	TYR	2.3
1	B	11	LEU	2.3
1	F	16	MET	2.2
1	C	59	LEU	2.2
1	B	212	SER	2.2
1	F	8	ARG	2.2
1	D	5	ALA	2.2
1	E	7	ALA	2.1
1	D	11	LEU	2.1
1	F	212	SER	2.1
1	F	17	ASN	2.0

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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	83A	G	300	32/32	0.83	0.41	1.29	86,94,109,113	0
2	83A	B	300	32/32	0.89	0.30	1.13	64,85,109,112	0
2	83A	C	300	32/32	0.87	0.37	0.69	93,102,111,119	0
2	83A	E	300	32/32	0.91	0.32	0.57	61,76,99,107	0
2	83A	A	300	32/32	0.91	0.24	0.13	51,63,96,107	0
2	83A	F	300	32/32	0.84	0.30	-0.19	88,96,115,117	0
2	83A	H	300	32/32	0.94	0.22	-0.31	48,62,96,107	0

6.5 Other polymers (i)

There are no such residues in this entry.