Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:22 PM GMT

PDB ID	:	4ELH
Title	:	Structure-activity relationship guides enantiomeric preference among potent inhibitors of B. anthracis dihydrofolate reductase
Authors	:	Bourne, C.R.; Barrow, W.W.
Deposited on	:	2012-04-10
Resolution	:	2.10 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:

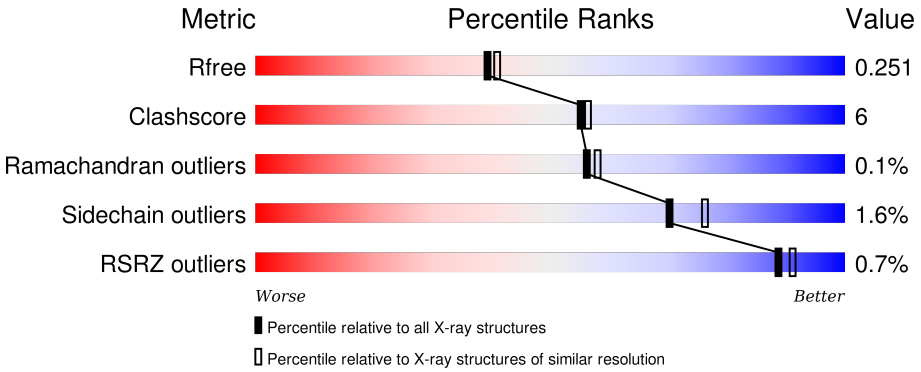
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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.



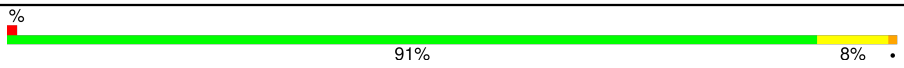
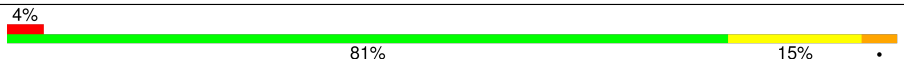
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	166	86% 12%
1	B	166	92% 8%
1	C	166	86% 13%
1	D	166	% 86% 14%
1	E	166	92% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	166	
1	G	166	
1	H	166	

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
3	53I	A	202	-	-	-	X
3	53I	C	202	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12663 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 Dihydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1380	892	228	251	9			
1	H	166	Total	C	N	O	S	0	0	0
			1380	892	228	251	9			
1	C	166	Total	C	N	O	S	0	0	0
			1380	892	228	251	9			
1	B	166	Total	C	N	O	S	0	0	0
			1374	889	225	251	9			
1	G	166	Total	C	N	O	S	0	0	0
			1380	892	228	251	9			
1	F	166	Total	C	N	O	S	0	0	0
			1380	892	228	251	9			
1	D	166	Total	C	N	O	S	0	0	0
			1380	892	228	251	9			
1	E	166	Total	C	N	O	S	0	0	0
			1380	892	228	251	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	163	LEU	-	EXPRESSION TAG	UNP Q81R22
A	164	VAL	-	EXPRESSION TAG	UNP Q81R22
A	165	PRO	-	EXPRESSION TAG	UNP Q81R22
A	166	ARG	-	EXPRESSION TAG	UNP Q81R22
H	163	LEU	-	EXPRESSION TAG	UNP Q81R22
H	164	VAL	-	EXPRESSION TAG	UNP Q81R22
H	165	PRO	-	EXPRESSION TAG	UNP Q81R22
H	166	ARG	-	EXPRESSION TAG	UNP Q81R22
C	163	LEU	-	EXPRESSION TAG	UNP Q81R22
C	164	VAL	-	EXPRESSION TAG	UNP Q81R22
C	165	PRO	-	EXPRESSION TAG	UNP Q81R22
C	166	ARG	-	EXPRESSION TAG	UNP Q81R22
B	163	LEU	-	EXPRESSION TAG	UNP Q81R22

Continued on next page...

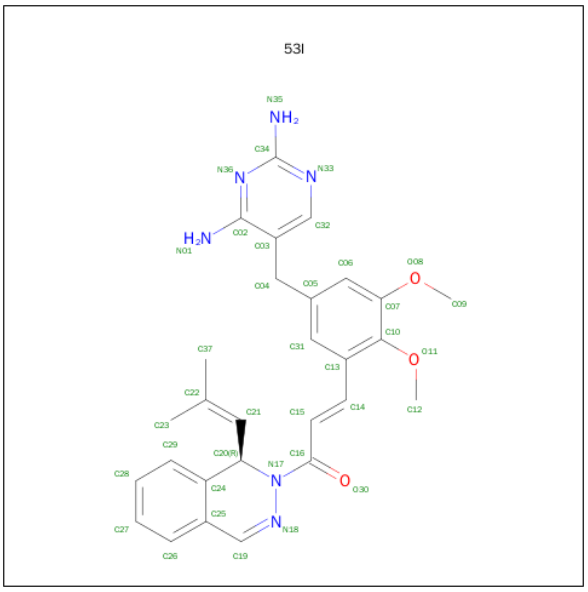
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	164	VAL	-	EXPRESSION TAG	UNP Q81R22
B	165	PRO	-	EXPRESSION TAG	UNP Q81R22
B	166	ARG	-	EXPRESSION TAG	UNP Q81R22
G	163	LEU	-	EXPRESSION TAG	UNP Q81R22
G	164	VAL	-	EXPRESSION TAG	UNP Q81R22
G	165	PRO	-	EXPRESSION TAG	UNP Q81R22
G	166	ARG	-	EXPRESSION TAG	UNP Q81R22
F	163	LEU	-	EXPRESSION TAG	UNP Q81R22
F	164	VAL	-	EXPRESSION TAG	UNP Q81R22
F	165	PRO	-	EXPRESSION TAG	UNP Q81R22
F	166	ARG	-	EXPRESSION TAG	UNP Q81R22
D	163	LEU	-	EXPRESSION TAG	UNP Q81R22
D	164	VAL	-	EXPRESSION TAG	UNP Q81R22
D	165	PRO	-	EXPRESSION TAG	UNP Q81R22
D	166	ARG	-	EXPRESSION TAG	UNP Q81R22
E	163	LEU	-	EXPRESSION TAG	UNP Q81R22
E	164	VAL	-	EXPRESSION TAG	UNP Q81R22
E	165	PRO	-	EXPRESSION TAG	UNP Q81R22
E	166	ARG	-	EXPRESSION TAG	UNP Q81R22

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

- Molecule 3 is (2E)-3-{5-[(2,4-DIAMINOPYRIMIDIN-5-YL)METHYL]-2,3-DIMETHOXYPHENYL}-1-[(1R)-1-(2-METHYLPROP-1-EN-1-YL)PHTHALAZIN-2(1H)-YL]PROP-2-EN-1-ONE (three-letter code: 53I) (formula: $C_{28}H_{30}N_6O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 37 28 6 3	0	0
3	H	1	Total C N O 37 28 6 3	0	0
3	C	1	Total C N O 37 28 6 3	0	0
3	B	1	Total C N O 37 28 6 3	0	0
3	G	1	Total C N O 37 28 6 3	0	0
3	F	1	Total C N O 37 28 6 3	0	0
3	D	1	Total C N O 37 28 6 3	0	1
3	E	1	Total C N O 37 28 6 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

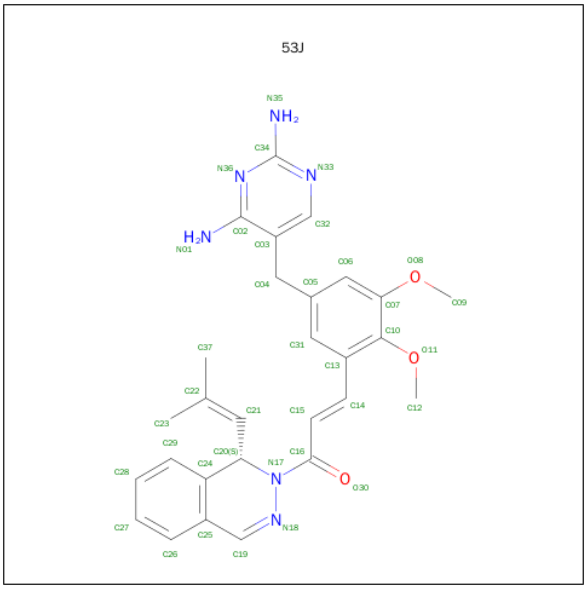
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0

- Molecule 5 is (2E)-3-{5-[(2,4-DIAMINOPYRIMIDIN-5-YL)METHYL]-2,3-DIMETHOXYPHENYL}-1-[(1S)-1-(2-METHYLPROP-1-EN-1-YL)PHTHALAZIN-2(1H)-YL]PROP-2-EN-1-ONE (three-letter code: 53J) (formula: $C_{28}H_{30}N_6O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C N O 37 28 6 3	0	1

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	177	Total O 177 177	0	0
6	H	144	Total O 144 144	0	0
6	C	193	Total O 193 193	0	0

Continued on next page...

Continued from previous page...

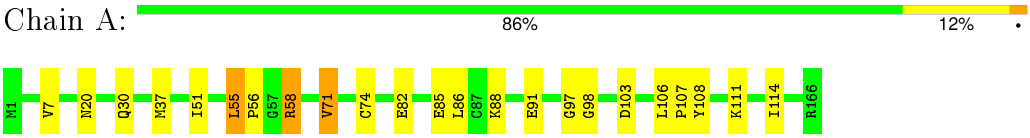
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	183	Total O 183 183	0	0
6	G	167	Total O 167 167	0	0
6	F	163	Total O 163 163	0	0
6	D	131	Total O 131 131	0	0
6	E	122	Total O 122 122	0	0

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.

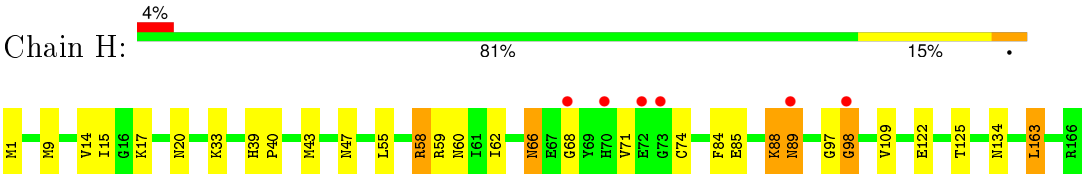
- Molecule 1: Dihydrofolate reductase

Chain A:



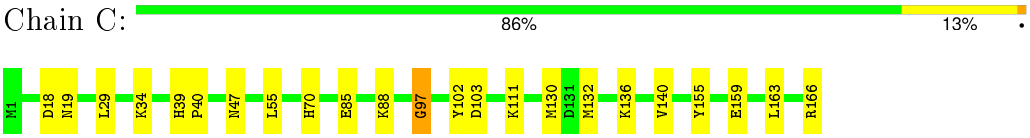
- Molecule 1: Dihydrofolate reductase

Chain H:



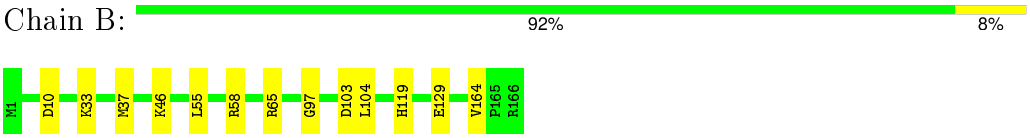
- Molecule 1: Dihydrofolate reductase

Chain C:



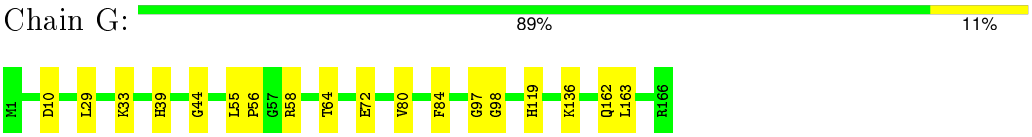
- Molecule 1: Dihydrofolate reductase

Chain B:



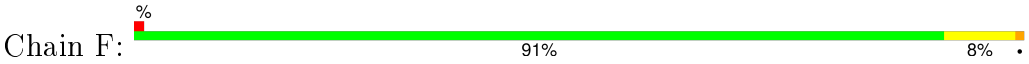
- Molecule 1: Dihydrofolate reductase

Chain G:



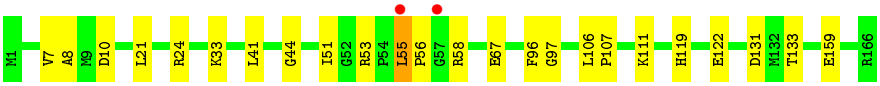
- Molecule 1: Dihydrofolate reductase

Chain F:



• Molecule 1: Dihydrofolate reductase

Chain D:



• Molecule 1: Dihydrofolate reductase

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.35Å 136.03Å 168.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.78 – 2.10 43.78 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.3 (43.78-2.10) 98.3 (43.78-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.25 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.194 , 0.252 0.194 , 0.251	Depositor DCC
R_{free} test set	2000 reflections (2.26%)	DCC
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.634	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	4 of 90499 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12663	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.24 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.9371e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, 53J, 53I, 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	0.40	0/1418	0.54	0/1918
1	B	0.41	0/1412	0.55	0/1911
1	C	0.41	0/1418	0.54	0/1918
1	D	0.38	0/1418	0.52	0/1918
1	E	0.36	0/1418	0.51	1/1918 (0.1%)
1	F	0.37	0/1418	0.54	1/1918 (0.1%)
1	G	0.43	0/1418	0.56	1/1918 (0.1%)
1	H	0.39	0/1418	0.51	1/1918 (0.1%)
All	All	0.39	0/11338	0.53	4/15337 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	8

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	98	GLY	N-CA-C	-5.41	99.59	113.10
1	H	98	GLY	N-CA-C	-5.27	99.93	113.10
1	F	98	GLY	N-CA-C	-5.11	100.34	113.10
1	G	98	GLY	N-CA-C	-5.04	100.49	113.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	97	GLY	Peptide
1	B	97	GLY	Peptide
1	C	97	GLY	Peptide
1	D	97	GLY	Peptide
1	E	97	GLY	Peptide
1	F	97	GLY	Peptide
1	G	97	GLY	Peptide
1	H	97	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1380	0	1346	24	0
1	B	1374	0	1335	11	0
1	C	1380	0	1346	17	0
1	D	1380	0	1346	26	0
1	E	1380	0	1346	10	0
1	F	1380	0	1346	15	0
1	G	1380	0	1346	10	0
1	H	1380	0	1346	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	37	0	30	7	0
3	B	37	0	30	1	0
3	C	37	0	30	4	0
3	D	37	0	30	9	0
3	E	37	0	30	1	0
3	F	37	0	30	4	0
3	G	37	0	30	0	0
3	H	37	0	30	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0
4	E	1	0	0	0	0
4	F	1	0	0	1	0
4	G	1	0	0	1	0
4	H	1	0	0	1	0
5	D	37	0	30	5	0
6	A	177	0	0	4	0
6	B	183	0	0	4	0
6	C	193	0	0	6	0
6	D	131	0	0	1	0
6	E	122	0	0	1	0
6	F	163	0	0	4	0
6	G	167	0	0	2	0
6	H	144	0	0	3	0
All	All	12663	0	11027	142	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 (142) 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:H:60:ASN:ND2	6:H:403:HOH:O	1.94	0.99
1:D:55:LEU:H	1:D:55:LEU:HD12	1.31	0.92
1:D:51:ILE:HG12	5:D:204[B]:53J:H3	1.54	0.89
1:C:130:MET:HB2	1:C:132:MET:CE	2.06	0.86
1:C:70:HIS:HB3	6:C:492:HOH:O	1.82	0.80
1:E:56:PRO:O	1:E:58:ARG:NH1	2.15	0.79
1:H:71:VAL:HG23	1:H:74:CYS:HB2	1.66	0.77
1:B:129:GLU:O	6:B:449:HOH:O	2.02	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LYS:O	1:B:58:ARG:NH2	2.17	0.76
1:D:33:LYS:HB2	3:D:201[A]:53I:H2	1.67	0.75
1:F:13:ARG:NH2	6:F:336:HOH:O	2.20	0.74
1:H:17:LYS:HE2	1:H:122:GLU:HG2	1.69	0.74
1:E:55:LEU:HD12	1:E:56:PRO:HD2	1.69	0.73
3:C:202:53I:N18	3:C:202:53I:H15	2.04	0.73
1:A:20:ASN:ND2	6:A:325:HOH:O	2.14	0.73
1:D:33:LYS:O	1:D:58:ARG:NH2	2.23	0.71
1:A:56:PRO:O	1:A:58:ARG:NH1	2.24	0.70
1:C:103:ASP:OD1	6:C:388:HOH:O	2.07	0.70
1:H:122:GLU:HG3	6:C:481:HOH:O	1.92	0.69
1:A:51:ILE:HG12	3:A:202:53I:H14	1.73	0.68
1:F:82:GLU:OE1	6:F:459:HOH:O	2.11	0.68
1:H:55:LEU:HD22	3:H:201:53I:H1	1.76	0.68
1:A:71:VAL:HG22	1:A:74:CYS:HB2	1.76	0.67
1:D:67:GLU:OE1	6:D:309:HOH:O	2.12	0.67
1:F:55:LEU:HB3	1:F:58:ARG:HH21	1.59	0.67
1:D:51:ILE:HG12	3:D:201[A]:53I:H18	1.77	0.66
1:F:55:LEU:HD21	3:F:201:53I:H1	1.78	0.66
3:C:202:53I:O11	3:C:202:53I:H14	1.96	0.65
1:F:12:ASN:ND2	6:F:386:HOH:O	2.29	0.65
1:A:55:LEU:N	1:A:55:LEU:HD23	2.14	0.63
1:D:55:LEU:H	1:D:55:LEU:CD1	2.06	0.62
1:D:55:LEU:HD23	5:D:204[B]:53J:C26	2.29	0.62
1:A:55:LEU:HD22	3:A:202:53I:C37	2.29	0.62
1:A:103:ASP:OD1	6:A:444:HOH:O	2.16	0.62
1:H:89:ASN:OD1	1:H:89:ASN:N	2.28	0.62
1:A:37:MET:HA	1:A:58:ARG:HE	1.68	0.59
1:D:96:PHE:CZ	5:D:204[B]:53J:H28	2.39	0.58
1:A:51:ILE:HG21	1:A:55:LEU:HD21	1.84	0.57
1:D:55:LEU:N	1:D:55:LEU:HD12	2.11	0.57
1:G:162:GLN:OE1	6:G:311:HOH:O	2.18	0.57
1:G:56:PRO:O	1:G:58:ARG:NH1	2.38	0.56
1:B:46:LYS:NZ	6:B:390:HOH:O	2.36	0.56
1:C:130:MET:HB2	1:C:132:MET:HE3	1.86	0.55
1:H:85:GLU:O	1:H:88:LYS:HE2	2.06	0.55
1:H:62:ILE:HD12	1:H:71:VAL:HG21	1.88	0.54
3:B:202:53I:N18	3:B:202:53I:H15	2.22	0.54
1:A:51:ILE:HG12	3:A:202:53I:C15	2.38	0.54
1:A:7:VAL:CG1	1:A:114:ILE:HG12	2.38	0.54
1:B:33:LYS:NZ	6:B:463:HOH:O	2.35	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:HD22	3:A:202:53I:H11	1.88	0.54
1:F:85:GLU:O	1:F:88:LYS:HG3	2.08	0.54
1:G:33:LYS:O	1:G:58:ARG:NH2	2.36	0.53
1:H:33:LYS:HB2	3:H:201:53I:H2	1.91	0.53
1:G:39:HIS:HD2	6:G:436:HOH:O	1.91	0.53
1:C:111:LYS:HG3	1:C:159:GLU:HG2	1.91	0.53
1:B:164:VAL:O	1:E:65:ARG:HB2	2.10	0.52
3:A:202:53I:H17	3:A:202:53I:O08	2.09	0.52
1:D:33:LYS:HB2	3:D:201[A]:53I:C26	2.38	0.52
1:D:111:LYS:HG3	1:D:159:GLU:HG2	1.91	0.52
1:F:55:LEU:HD21	3:F:201:53I:C19	2.40	0.52
1:H:55:LEU:HD22	3:H:201:53I:C19	2.39	0.51
1:D:131:ASP:OD1	1:D:133:THR:OG1	2.23	0.51
1:H:55:LEU:HD13	3:H:201:53I:H13	1.92	0.51
1:E:33:LYS:HG3	1:E:58:ARG:NH2	2.26	0.51
1:A:111:LYS:NZ	6:A:353:HOH:O	2.41	0.50
1:A:55:LEU:HD22	3:A:202:53I:H12	1.94	0.50
1:A:55:LEU:HD13	3:A:202:53I:H1	1.93	0.50
1:E:147:GLU:CD	1:E:147:GLU:H	2.16	0.49
1:E:85:GLU:OE2	1:E:88:LYS:NZ	2.46	0.49
1:H:40:PRO:HA	1:H:59:ARG:O	2.12	0.49
1:B:65:ARG:HD3	1:F:164:VAL:O	2.14	0.48
1:A:37:MET:HA	1:A:58:ARG:HH21	1.79	0.48
1:H:66:ASN:OD1	1:H:68:GLY:N	2.39	0.47
1:C:29:LEU:O	3:C:202:53I:H2	2.14	0.47
1:H:62:ILE:CD1	1:H:71:VAL:HG21	2.44	0.47
1:H:43:MET:CE	1:H:47:ASN:HD22	2.27	0.47
1:C:29:LEU:HB3	3:C:202:53I:C26	2.44	0.47
1:D:10:ASP:HB2	1:D:119:HIS:O	2.14	0.47
1:F:160:LYS:NZ	6:F:461:HOH:O	2.47	0.47
1:D:122:GLU:HG3	1:D:122:GLU:O	2.15	0.47
1:D:56:PRO:HD2	5:D:204[B]:53J:H26	1.97	0.47
3:D:201[A]:53I:C12	3:D:201[A]:53I:H14	2.44	0.46
1:D:41:LEU:HD22	1:D:55:LEU:HD22	1.97	0.46
1:C:97:GLY:HA3	1:C:102:TYR:CZ	2.50	0.46
1:C:166:ARG:NH2	6:C:446:HOH:O	2.47	0.46
1:B:37:MET:CE	1:B:58:ARG:HH22	2.28	0.46
1:H:43:MET:HE2	1:H:47:ASN:HD22	1.81	0.46
1:D:44:GLY:HA3	4:D:203:CL:CL	2.52	0.46
1:A:98:GLY:HA3	6:A:473:HOH:O	2.14	0.46
1:E:21:LEU:HD23	3:E:201:53I:H20	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:N	1:A:107:PRO:HD2	2.31	0.46
1:G:80:VAL:HG13	1:G:84:PHE:CE2	2.51	0.46
1:H:39:HIS:O	1:H:58:ARG:HB2	2.16	0.46
1:F:33:LYS:HG3	1:F:58:ARG:HH12	1.81	0.45
1:A:107:PRO:HG2	1:A:108:TYR:CE2	2.51	0.45
1:B:55:LEU:HD12	1:B:55:LEU:N	2.31	0.45
1:F:55:LEU:HB3	1:F:58:ARG:NH2	2.28	0.45
1:B:10:ASP:HB2	1:B:119:HIS:O	2.17	0.45
1:E:85:GLU:O	1:E:88:LYS:HB2	2.17	0.45
1:H:66:ASN:C	1:H:66:ASN:OD1	2.54	0.45
1:G:10:ASP:HB2	1:G:119:HIS:O	2.18	0.44
1:D:53:ARG:NH2	3:D:201[A]:53I:H13	2.33	0.44
1:H:98:GLY:HA3	4:H:203:CL:CL	2.55	0.44
1:D:24:ARG:NH2	1:E:88:LYS:HG2	2.33	0.44
1:B:103:ASP:OD1	6:B:453:HOH:O	2.21	0.44
1:B:104:LEU:HD23	1:F:162:GLN:HG2	1.99	0.44
1:D:56:PRO:O	1:D:58:ARG:NH1	2.51	0.43
1:D:21:LEU:HG	5:D:204[B]:53J:O08	2.19	0.43
1:G:44:GLY:HA3	4:G:203:CL:CL	2.55	0.43
1:C:34:LYS:HE2	6:C:357:HOH:O	2.19	0.43
1:H:33:LYS:HD2	3:H:201:53I:H3	1.99	0.43
1:A:106:LEU:N	1:A:107:PRO:CD	2.82	0.43
1:H:109:VAL:O	6:H:417:HOH:O	2.21	0.43
1:C:136:LYS:NZ	6:C:450:HOH:O	2.38	0.43
1:A:82:GLU:O	1:A:86:LEU:HD13	2.18	0.42
1:F:44:GLY:HA3	4:F:203:CL:CL	2.56	0.42
1:D:51:ILE:HG12	3:D:201[A]:53I:H14	2.01	0.42
1:A:7:VAL:HG13	1:A:114:ILE:HA	2.01	0.42
1:D:7:VAL:HG22	1:D:8:ALA:N	2.35	0.42
1:D:106:LEU:N	1:D:107:PRO:CD	2.82	0.42
1:H:15:ILE:HG13	1:H:125:THR:HG23	2.01	0.42
1:G:163:LEU:HA	1:G:163:LEU:HD23	1.78	0.42
1:E:46:LYS:HE3	6:E:418:HOH:O	2.19	0.41
1:C:18:ASP:O	1:C:19:ASN:HB2	2.19	0.41
1:H:163:LEU:H	1:H:163:LEU:HG	1.71	0.41
3:D:201[A]:53I:O11	3:D:201[A]:53I:C15	2.68	0.41
1:C:39:HIS:HA	1:C:40:PRO:HD3	1.89	0.41
1:C:130:MET:HB2	1:C:132:MET:HE2	1.94	0.41
1:C:163:LEU:HA	1:C:163:LEU:HD23	1.86	0.41
1:F:53:ARG:CZ	3:F:201:53I:H11	2.51	0.41
1:A:85:GLU:OE2	1:A:88:LYS:NZ	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:GLU:OE2	1:C:88:LYS:NZ	2.42	0.41
1:C:140:VAL:HA	1:C:155:TYR:O	2.21	0.41
1:H:1:MET:HE3	1:H:84:PHE:CE1	2.56	0.41
1:G:55:LEU:HD12	1:G:56:PRO:CD	2.51	0.40
1:F:33:LYS:HB2	3:F:201:53I:H2	2.03	0.40
1:H:9:MET:HA	1:H:14:VAL:O	2.21	0.40
1:G:29:LEU:HD23	1:G:29:LEU:HA	1.85	0.40
3:D:201[A]:53I:H14	3:D:201[A]:53I:H18	2.04	0.40
1:H:1:MET:O	6:H:398:HOH:O	2.21	0.40
1:D:96:PHE:CZ	3:D:201[A]:53I:H30	2.55	0.40
1:A:7:VAL:HG11	1:A:114:ILE:HG12	2.04	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	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	B	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	C	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
1	D	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
1	E	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	F	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
1	G	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	H	164/166 (99%)	157 (96%)	6 (4%)	1 (1%)	30	24
All	All	1312/1328 (99%)	1287 (98%)	24 (2%)	1 (0%)	56	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	66	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	150/150 (100%)	145 (97%)	5 (3%)	45 47
1	B	149/150 (99%)	149 (100%)	0	100 100
1	C	150/150 (100%)	148 (99%)	2 (1%)	76 82
1	D	150/150 (100%)	149 (99%)	1 (1%)	88 92
1	E	150/150 (100%)	149 (99%)	1 (1%)	88 92
1	F	150/150 (100%)	149 (99%)	1 (1%)	88 92
1	G	150/150 (100%)	147 (98%)	3 (2%)	63 68
1	H	150/150 (100%)	144 (96%)	6 (4%)	38 38
All	All	1199/1200 (100%)	1180 (98%)	19 (2%)	70 76

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	55	LEU
1	A	58	ARG
1	A	71	VAL
1	A	91	GLU
1	H	20	ASN
1	H	58	ARG
1	H	88	LYS
1	H	89	ASN
1	H	134	ASN
1	H	163	LEU
1	C	47	ASN
1	C	55	LEU
1	G	64	THR
1	G	72	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	136	LYS
1	F	162	GLN
1	D	55	LEU
1	E	166	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	47	ASN
1	E	66	ASN

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 25 ligands modelled in this entry, 16 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
3	53I	A	202	-	39,40,40	3.03	12 (30%)	47,56,56	2.37	15 (31%)
3	53I	B	202	-	39,40,40	3.18	13 (33%)	47,56,56	2.35	15 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	53I	C	202	-	39,40,40	3.17	14 (35%)	47,56,56	2.20	15 (31%)
3	53I	D	201[A]	-	39,40,40	3.04	13 (33%)	47,56,56	2.05	14 (29%)
5	53J	D	204[B]	-	39,40,40	2.72	11 (28%)	47,56,56	1.97	14 (29%)
3	53I	E	201	-	39,40,40	2.96	13 (33%)	47,56,56	2.26	16 (34%)
3	53I	F	201	-	39,40,40	3.02	12 (30%)	47,56,56	2.32	16 (34%)
3	53I	G	201	-	39,40,40	3.00	13 (33%)	47,56,56	2.32	16 (34%)
3	53I	H	201	-	39,40,40	2.95	12 (30%)	47,56,56	2.44	15 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	53I	A	202	-	-	1/19/34/34	0/3/4/4
3	53I	B	202	-	-	0/19/34/34	0/3/4/4
3	53I	C	202	-	-	0/19/34/34	0/3/4/4
3	53I	D	201[A]	-	-	1/19/34/34	0/3/4/4
5	53J	D	204[B]	-	-	2/19/34/34	0/3/4/4
3	53I	E	201	-	-	0/19/34/34	0/3/4/4
3	53I	F	201	-	-	0/19/34/34	0/3/4/4
3	53I	G	201	-	-	0/19/34/34	0/3/4/4
3	53I	H	201	-	-	0/19/34/34	0/3/4/4

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	53I	C25-C24	-6.56	1.32	1.40
3	G	201	53I	C25-C24	-6.03	1.33	1.40
5	D	204[B]	53J	C25-C24	-6.02	1.33	1.40
3	C	202	53I	C25-C24	-6.01	1.33	1.40
3	D	201[A]	53I	C25-C24	-6.01	1.33	1.40
3	H	201	53I	C25-C24	-5.90	1.33	1.40
3	F	201	53I	C25-C24	-5.75	1.33	1.40
3	E	201	53I	C25-C24	-5.69	1.33	1.40
3	A	202	53I	C25-C24	-5.55	1.33	1.40
3	C	202	53I	O11-C10	2.00	1.42	1.38
3	E	201	53I	C32-C03	2.00	1.42	1.37
3	D	201[A]	53I	C15-C14	2.01	1.38	1.32
3	G	201	53I	C25-C19	2.01	1.47	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	201[A]	53I	C32-C03	2.02	1.42	1.37
3	H	201	53I	C25-C19	2.04	1.47	1.44
5	D	204[B]	53J	C25-C19	2.04	1.47	1.44
3	E	201	53I	C25-C19	2.07	1.47	1.44
3	B	202	53I	O08-C07	2.11	1.40	1.37
3	F	201	53I	C25-C19	2.14	1.47	1.44
3	A	202	53I	C32-C03	2.14	1.42	1.37
3	C	202	53I	C25-C19	2.21	1.47	1.44
3	B	202	53I	C25-C19	2.25	1.48	1.44
3	G	201	53I	O11-C10	2.29	1.42	1.38
3	C	202	53I	C32-C03	2.31	1.42	1.37
3	B	202	53I	C21-C22	2.31	1.36	1.33
3	C	202	53I	C21-C22	2.33	1.36	1.33
3	C	202	53I	O08-C07	2.33	1.40	1.37
3	B	202	53I	C32-C03	2.35	1.42	1.37
3	D	201[A]	53I	C32-N33	2.36	1.39	1.34
3	E	201	53I	O08-C07	2.38	1.41	1.37
3	D	201[A]	53I	O08-C07	2.42	1.41	1.37
3	H	201	53I	C21-C22	2.43	1.36	1.33
3	A	202	53I	C06-C07	2.43	1.43	1.38
3	D	201[A]	53I	C06-C07	2.44	1.43	1.38
3	F	201	53I	C32-N33	2.47	1.39	1.34
3	A	202	53I	C32-N33	2.47	1.39	1.34
3	E	201	53I	C32-N33	2.49	1.39	1.34
3	D	201[A]	53I	C21-C22	2.49	1.36	1.33
3	G	201	53I	C32-N33	2.50	1.39	1.34
3	A	202	53I	O08-C07	2.55	1.41	1.37
3	G	201	53I	C21-C22	2.59	1.37	1.33
3	E	201	53I	C21-C22	2.62	1.37	1.33
3	E	201	53I	C06-C07	2.64	1.43	1.38
5	D	204[B]	53J	O08-C07	2.65	1.41	1.37
3	A	202	53I	C21-C22	2.67	1.37	1.33
3	F	201	53I	C21-C22	2.67	1.37	1.33
3	C	202	53I	C32-N33	2.68	1.40	1.34
3	B	202	53I	C06-C07	2.70	1.43	1.38
3	G	201	53I	O08-C07	2.71	1.41	1.37
5	D	204[B]	53J	C15-C16	2.73	1.52	1.48
3	C	202	53I	C06-C07	2.84	1.44	1.38
3	H	201	53I	C32-N33	2.84	1.40	1.34
3	H	201	53I	C06-C07	2.89	1.44	1.38
3	B	202	53I	C32-N33	2.89	1.40	1.34
3	F	201	53I	O08-C07	2.89	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	201	53I	O08-C07	2.93	1.41	1.37
3	G	201	53I	C06-C07	2.97	1.44	1.38
3	F	201	53I	C06-C07	3.08	1.44	1.38
5	D	204[B]	53J	C29-C24	3.16	1.44	1.39
5	D	204[B]	53J	C02-N01	3.38	1.42	1.34
3	A	202	53I	C02-N01	3.74	1.43	1.34
3	H	201	53I	C02-N01	3.83	1.43	1.34
5	D	204[B]	53J	C21-C22	3.99	1.39	1.33
3	E	201	53I	C02-N01	3.99	1.44	1.34
5	D	204[B]	53J	C13-C14	4.02	1.53	1.47
3	D	201[A]	53I	C02-N01	4.12	1.44	1.34
3	B	202	53I	C02-N01	4.18	1.44	1.34
3	F	201	53I	C02-N01	4.26	1.44	1.34
3	G	201	53I	C02-N01	4.26	1.44	1.34
3	H	201	53I	C15-C16	4.35	1.54	1.48
3	F	201	53I	C15-C16	4.41	1.54	1.48
3	G	201	53I	C34-N35	4.43	1.43	1.34
3	C	202	53I	C02-N01	4.50	1.45	1.34
3	G	201	53I	C15-C16	4.53	1.55	1.48
5	D	204[B]	53J	C16-N17	4.56	1.44	1.35
3	E	201	53I	C15-C16	4.59	1.55	1.48
3	A	202	53I	C34-N35	4.62	1.43	1.34
3	F	201	53I	C34-N35	4.66	1.43	1.34
3	D	201[A]	53I	C34-N35	4.72	1.43	1.34
3	B	202	53I	C15-C16	4.75	1.55	1.48
3	D	201[A]	53I	C15-C16	4.77	1.55	1.48
3	E	201	53I	C34-N35	4.90	1.44	1.34
5	D	204[B]	53J	C34-N35	4.93	1.44	1.34
3	A	202	53I	C15-C16	4.95	1.55	1.48
3	C	202	53I	C34-N35	4.96	1.44	1.34
3	E	201	53I	C29-C24	4.96	1.46	1.39
3	B	202	53I	C34-N35	5.06	1.44	1.34
3	H	201	53I	C34-N35	5.08	1.44	1.34
3	G	201	53I	C29-C24	5.10	1.46	1.39
3	H	201	53I	C29-C24	5.12	1.46	1.39
3	F	201	53I	C29-C24	5.15	1.46	1.39
3	B	202	53I	C29-C24	5.18	1.46	1.39
3	C	202	53I	C15-C16	5.20	1.56	1.48
3	F	201	53I	C16-N17	5.25	1.46	1.35
3	D	201[A]	53I	C29-C24	5.36	1.47	1.39
3	A	202	53I	C29-C24	5.39	1.47	1.39
3	G	201	53I	C16-N17	5.47	1.46	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	201	53I	C16-N17	5.50	1.46	1.35
3	H	201	53I	C16-N17	5.54	1.46	1.35
3	C	202	53I	C29-C24	5.57	1.47	1.39
3	D	201[A]	53I	C16-N17	6.15	1.47	1.35
3	A	202	53I	C16-N17	6.32	1.48	1.35
3	B	202	53I	C16-N17	6.50	1.48	1.35
3	C	202	53I	C16-N17	6.57	1.48	1.35
5	D	204[B]	53J	C19-N18	10.55	1.41	1.29
3	H	201	53I	C19-N18	11.06	1.41	1.29
3	E	201	53I	C19-N18	11.17	1.41	1.29
3	G	201	53I	C19-N18	11.36	1.42	1.29
3	D	201[A]	53I	C19-N18	11.45	1.42	1.29
3	A	202	53I	C19-N18	11.62	1.42	1.29
3	C	202	53I	C19-N18	11.76	1.42	1.29
3	F	201	53I	C19-N18	11.77	1.42	1.29
3	B	202	53I	C19-N18	12.18	1.43	1.29

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	201	53I	C25-C19-N18	-6.61	117.48	125.69
3	A	202	53I	C25-C19-N18	-6.49	117.63	125.69
3	B	202	53I	C25-C19-N18	-6.39	117.76	125.69
3	F	201	53I	C25-C19-N18	-6.37	117.78	125.69
3	C	202	53I	C25-C19-N18	-6.04	118.20	125.69
5	D	204[B]	53J	C25-C19-N18	-5.87	118.40	125.69
3	D	201[A]	53I	C25-C19-N18	-5.73	118.58	125.69
3	E	201	53I	C25-C19-N18	-5.62	118.71	125.69
3	H	201	53I	C04-C03-C02	-5.54	115.13	122.21
3	H	201	53I	C25-C19-N18	-5.44	118.94	125.69
3	E	201	53I	C04-C03-C02	-5.27	115.47	122.21
3	B	202	53I	C04-C03-C02	-5.27	115.47	122.21
3	A	202	53I	C04-C03-C02	-5.18	115.59	122.21
3	G	201	53I	C04-C03-C02	-5.09	115.71	122.21
3	F	201	53I	C04-C03-C02	-5.07	115.73	122.21
3	E	201	53I	N33-C34-N36	-5.03	120.52	125.78
3	H	201	53I	N33-C34-N36	-5.00	120.56	125.78
3	B	202	53I	N33-C34-N36	-4.99	120.57	125.78
3	C	202	53I	C04-C03-C02	-4.94	115.90	122.21
3	A	202	53I	N33-C34-N36	-4.92	120.64	125.78
3	F	201	53I	N33-C34-N36	-4.83	120.74	125.78
3	C	202	53I	N33-C34-N36	-4.66	120.92	125.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	201	53I	N33-C34-N36	-4.65	120.92	125.78
3	H	201	53I	C14-C15-C16	-4.52	114.14	120.79
5	D	204[B]	53J	N33-C34-N36	-4.35	121.24	125.78
3	D	201[A]	53I	N33-C34-N36	-4.32	121.27	125.78
3	F	201	53I	C13-C14-C15	-3.86	119.19	126.87
3	H	201	53I	C13-C31-C05	-3.75	118.28	122.29
3	G	201	53I	C14-C15-C16	-3.66	115.41	120.79
3	H	201	53I	C13-C14-C15	-3.64	119.62	126.87
5	D	204[B]	53J	C04-C03-C02	-3.60	117.61	122.21
3	D	201[A]	53I	C13-C14-C15	-3.48	119.93	126.87
3	D	201[A]	53I	C04-C03-C02	-3.40	117.86	122.21
3	E	201	53I	C13-C31-C05	-3.38	118.68	122.29
3	H	201	53I	C03-C32-N33	-3.31	118.11	123.86
3	G	201	53I	C13-C14-C15	-3.30	120.30	126.87
3	A	202	53I	O08-C07-C06	-3.27	118.62	124.21
3	G	201	53I	C13-C31-C05	-3.19	118.88	122.29
3	E	201	53I	C13-C14-C15	-3.18	120.53	126.87
3	A	202	53I	C03-C32-N33	-3.15	118.39	123.86
3	E	201	53I	C03-C32-N33	-3.14	118.41	123.86
3	F	201	53I	C14-C15-C16	-3.10	116.22	120.79
3	D	201[A]	53I	O08-C07-C06	-3.05	119.00	124.21
3	F	201	53I	C13-C31-C05	-3.03	119.05	122.29
5	D	204[B]	53J	O08-C07-C06	-3.02	119.06	124.21
3	B	202	53I	O08-C07-C06	-2.98	119.11	124.21
5	D	204[B]	53J	C03-C32-N33	-2.92	118.78	123.86
3	D	201[A]	53I	C03-C32-N33	-2.91	118.81	123.86
3	B	202	53I	C03-C32-N33	-2.86	118.89	123.86
3	C	202	53I	C03-C32-N33	-2.83	118.95	123.86
3	F	201	53I	C03-C32-N33	-2.58	119.38	123.86
3	G	201	53I	C03-C32-N33	-2.48	119.56	123.86
5	D	204[B]	53J	C13-C14-C15	-2.44	122.01	126.87
3	A	202	53I	C13-C14-C15	-2.30	122.28	126.87
3	D	201[A]	53I	C13-C31-C05	-2.30	119.83	122.29
3	A	202	53I	C13-C31-C05	-2.19	119.95	122.29
3	C	202	53I	C13-C14-C15	-2.17	122.54	126.87
3	B	202	53I	C13-C14-C15	-2.15	122.59	126.87
5	D	204[B]	53J	C13-C31-C05	-2.12	120.02	122.29
3	E	201	53I	C14-C15-C16	-2.12	117.68	120.79
3	E	201	53I	C03-C02-N01	-2.12	119.15	122.25
3	B	202	53I	O30-C16-C15	-2.03	118.20	122.15
3	C	202	53I	C03-C02-N01	-2.02	119.29	122.25
3	A	202	53I	N01-C02-N36	2.03	119.89	116.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	201	53I	C24-C25-C19	2.04	119.58	117.68
3	C	202	53I	C32-C03-C02	2.07	118.69	115.72
3	C	202	53I	C12-O11-C10	2.07	120.26	114.82
3	B	202	53I	O11-C10-C13	2.10	122.77	118.97
3	E	201	53I	O08-C07-C10	2.14	119.13	115.26
3	D	201[A]	53I	C32-C03-C02	2.18	118.84	115.72
5	D	204[B]	53J	C24-C25-C19	2.20	119.73	117.68
5	D	204[B]	53J	C32-C03-C02	2.23	118.92	115.72
3	G	201	53I	C12-O11-C10	2.31	120.90	114.82
3	G	201	53I	N01-C02-N36	2.37	120.39	116.95
3	F	201	53I	C15-C16-N17	2.48	120.34	117.67
3	A	202	53I	C12-O11-C10	2.48	121.35	114.82
3	C	202	53I	C04-C03-C32	2.48	125.40	121.72
3	H	201	53I	C15-C16-N17	2.57	120.44	117.67
3	F	201	53I	N01-C02-N36	2.58	120.69	116.95
3	D	201[A]	53I	N35-C34-N33	2.61	119.75	117.39
3	C	202	53I	C09-O08-C07	2.67	121.59	117.54
3	B	202	53I	N01-C02-N36	2.67	120.82	116.95
3	E	201	53I	N01-C02-N36	2.71	120.88	116.95
3	D	201[A]	53I	N01-C02-N36	2.73	120.90	116.95
5	D	204[B]	53J	N35-C34-N33	2.73	119.86	117.39
3	G	201	53I	C15-C16-N17	2.75	120.64	117.67
3	B	202	53I	O08-C07-C10	2.76	120.24	115.26
3	H	201	53I	C09-O08-C07	2.83	121.83	117.54
3	E	201	53I	C03-C04-C05	2.85	120.74	114.04
3	F	201	53I	C04-C03-C32	2.86	125.95	121.72
3	E	201	53I	C04-C03-C32	2.89	126.00	121.72
5	D	204[B]	53J	N01-C02-N36	2.91	121.16	116.95
3	G	201	53I	C03-C04-C05	2.92	120.90	114.04
3	C	202	53I	N01-C02-N36	2.97	121.25	116.95
3	B	202	53I	C04-C03-C32	3.05	126.23	121.72
3	H	201	53I	C04-C03-C32	3.08	126.28	121.72
3	G	201	53I	C09-O08-C07	3.09	122.22	117.54
3	H	201	53I	C24-C25-C19	3.10	120.56	117.68
3	E	201	53I	C24-C25-C19	3.12	120.58	117.68
5	D	204[B]	53J	O08-C07-C10	3.13	120.91	115.26
3	A	202	53I	C04-C03-C32	3.15	126.38	121.72
3	G	201	53I	C32-N33-C34	3.16	120.41	116.05
3	C	202	53I	C32-N33-C34	3.17	120.43	116.05
3	H	201	53I	C03-C04-C05	3.19	121.55	114.04
3	G	201	53I	C04-C03-C32	3.19	126.44	121.72
3	D	201[A]	53I	O08-C07-C10	3.29	121.21	115.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	204[B]	53J	C34-N36-C02	3.32	120.82	117.04
3	F	201	53I	C32-N33-C34	3.34	120.66	116.05
3	H	201	53I	C34-N36-C02	3.35	120.85	117.04
3	E	201	53I	C34-N36-C02	3.35	120.85	117.04
3	D	201[A]	53I	C34-N36-C02	3.38	120.88	117.04
3	F	201	53I	C03-C04-C05	3.40	122.05	114.04
3	D	201[A]	53I	C32-N33-C34	3.49	120.87	116.05
5	D	204[B]	53J	C32-N33-C34	3.51	120.90	116.05
3	D	201[A]	53I	C15-C16-N17	3.57	121.52	117.67
3	A	202	53I	O08-C07-C10	3.58	121.72	115.26
3	B	202	53I	C32-N33-C34	3.60	121.02	116.05
3	A	202	53I	C34-N36-C02	3.68	121.22	117.04
3	F	201	53I	C09-O08-C07	3.68	123.13	117.54
3	A	202	53I	C15-C16-N17	3.70	121.66	117.67
3	A	202	53I	C32-N33-C34	3.80	121.30	116.05
3	G	201	53I	C34-N36-C02	3.83	121.40	117.04
3	B	202	53I	C34-N36-C02	3.94	121.52	117.04
3	F	201	53I	C34-N36-C02	3.94	121.52	117.04
3	F	201	53I	N35-C34-N33	3.94	120.94	117.39
3	C	202	53I	C34-N36-C02	3.96	121.54	117.04
3	H	201	53I	C32-N33-C34	4.00	121.58	116.05
3	E	201	53I	C32-N33-C34	4.10	121.71	116.05
3	E	201	53I	N35-C34-N33	4.11	121.10	117.39
3	C	202	53I	C15-C16-N17	4.30	122.32	117.67
3	G	201	53I	N35-C34-N33	4.42	121.37	117.39
3	B	202	53I	N35-C34-N33	4.60	121.54	117.39
3	C	202	53I	N35-C34-N33	4.69	121.62	117.39
3	B	202	53I	C15-C16-N17	4.91	122.97	117.67
3	H	201	53I	N35-C34-N33	5.27	122.14	117.39
3	A	202	53I	N35-C34-N33	5.47	122.32	117.39

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	201[A]	53I	C20-C21-C22-C37
5	D	204[B]	53J	C20-C21-C22-C37
3	A	202	53I	C20-C21-C22-C37
5	D	204[B]	53J	C20-C21-C22-C23

There are no ring outliers.

8 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202	53I	7	0
3	B	202	53I	1	0
3	C	202	53I	4	0
3	D	201[A]	53I	9	0
5	D	204[B]	53J	5	0
3	E	201	53I	1	0
3	F	201	53I	4	0
3	H	201	53I	5	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	166/166 (100%)	-0.34	0 100 100	17, 30, 57, 69	0
1	B	166/166 (100%)	-0.38	0 100 100	19, 29, 52, 68	0
1	C	166/166 (100%)	-0.34	0 100 100	20, 30, 52, 64	0
1	D	166/166 (100%)	-0.19	2 (1%) 81 85	19, 36, 67, 78	0
1	E	166/166 (100%)	-0.30	0 100 100	21, 36, 63, 76	0
1	F	166/166 (100%)	-0.40	1 (0%) 90 92	19, 30, 52, 64	0
1	G	166/166 (100%)	-0.32	0 100 100	17, 32, 55, 78	0
1	H	166/166 (100%)	-0.03	6 (3%) 46 55	18, 36, 72, 93	0
All	All	1328/1328 (100%)	-0.29	9 (0%) 89 91	17, 32, 62, 93	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	89	ASN	7.1
1	D	55	LEU	5.2
1	H	73	GLY	3.3
1	H	72	GLU	2.9
1	H	70	HIS	2.8
1	H	68	GLY	2.5
1	H	98	GLY	2.4
1	D	57	GLY	2.2
1	F	55	LEU	2.2

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

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
3	53I	A	202	37/37	0.89	0.18	3.06	12,47,69,79	0
3	53I	C	202	37/37	0.89	0.18	2.73	20,45,63,67	0
3	53I	B	202	37/37	0.89	0.14	1.84	18,36,47,56	0
2	CA	D	202	1/1	0.99	0.12	1.07	30,30,30,30	0
3	53I	E	201	37/37	0.92	0.14	1.03	17,42,52,55	0
3	53I	D	201[A]	37/37	0.86	0.18	0.65	17,43,56,57	37
5	53J	D	204[B]	37/37	0.90	0.17	0.61	17,46,56,58	37
4	CL	C	203	1/1	1.00	0.13	0.56	30,30,30,30	0
3	53I	H	201	37/37	0.93	0.14	0.56	15,39,70,73	0
3	53I	G	201	37/37	0.94	0.12	0.56	16,32,46,51	0
3	53I	F	201	37/37	0.92	0.13	0.55	18,37,56,60	0
2	CA	B	201	1/1	0.98	0.11	0.43	29,29,29,29	0
2	CA	F	202	1/1	0.96	0.11	0.39	36,36,36,36	0
2	CA	C	201	1/1	0.99	0.10	-0.09	26,26,26,26	0
4	CL	F	203	1/1	0.99	0.11	-0.36	34,34,34,34	0
4	CL	G	203	1/1	0.99	0.10	-0.51	36,36,36,36	0
2	CA	G	202	1/1	0.99	0.09	-0.63	28,28,28,28	0
2	CA	E	202	1/1	0.99	0.08	-0.91	33,33,33,33	0
4	CL	D	203	1/1	0.98	0.09	-1.00	39,39,39,39	0
4	CL	H	203	1/1	0.96	0.10	-1.00	42,42,42,42	0
4	CL	A	203	1/1	0.99	0.10	-1.01	30,30,30,30	0
4	CL	E	203	1/1	0.98	0.09	-1.06	41,41,41,41	0
2	CA	H	202	1/1	0.98	0.07	-1.89	45,45,45,45	0
4	CL	B	203	1/1	0.99	0.09	-1.94	34,34,34,34	0
2	CA	A	201	1/1	0.93	0.09	-2.72	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.