Full wwPDB X-ray Structure Validation Report (i)

Jul 27, 2016 – 03:47 PM EDT

PDB ID	:	5ITT
Title	:	Crystal Structure of Human NEIL1 bound to duplex DNA containing THF
Authors	:	Zhu, C.; Lu, L.; Zhang, J.; Yue, Z.; Song, J.; Zong, S.; Liu, M.; Stovicek, O.; Gao, Y.; Yi, C.
Deposited on	:	2016-03-17
Resolution	:	2.53 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:

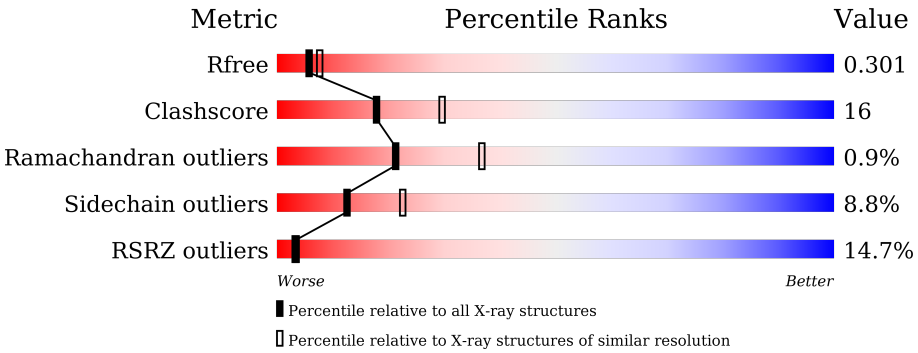
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.53 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	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (2.54-2.50)

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	400	5% 52% 12% 32%
1	B	400	5% 51% 12% 35%
1	C	400	19% 44% 17% 35%
2	D	26	8% 77% 23%
2	F	26	38% 31% 65%
3	E	26	8% 58% 38%

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
4	GOL	A	501	-	-	-	X
4	GOL	B	501	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8033 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 Endonuclease 8-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2143	1367	389	377	10			
1	B	261	Total	C	N	O	S	0	0	0
			2076	1327	381	358	10			
1	C	259	Total	C	N	O	S	0	0	0
			2074	1330	378	356	10			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	ARG	LYS	engineered mutation	UNP Q96FI4
A	391	ALA	-	expression tag	UNP Q96FI4
A	392	ALA	-	expression tag	UNP Q96FI4
A	393	LEU	-	expression tag	UNP Q96FI4
A	394	GLY	-	expression tag	UNP Q96FI4
A	395	HIS	-	expression tag	UNP Q96FI4
A	396	HIS	-	expression tag	UNP Q96FI4
A	397	HIS	-	expression tag	UNP Q96FI4
A	398	HIS	-	expression tag	UNP Q96FI4
A	399	HIS	-	expression tag	UNP Q96FI4
A	400	HIS	-	expression tag	UNP Q96FI4
B	242	ARG	LYS	engineered mutation	UNP Q96FI4
B	391	ALA	-	expression tag	UNP Q96FI4
B	392	ALA	-	expression tag	UNP Q96FI4
B	393	LEU	-	expression tag	UNP Q96FI4
B	394	GLY	-	expression tag	UNP Q96FI4
B	395	HIS	-	expression tag	UNP Q96FI4
B	396	HIS	-	expression tag	UNP Q96FI4
B	397	HIS	-	expression tag	UNP Q96FI4
B	398	HIS	-	expression tag	UNP Q96FI4
B	399	HIS	-	expression tag	UNP Q96FI4
B	400	HIS	-	expression tag	UNP Q96FI4
C	242	ARG	LYS	engineered mutation	UNP Q96FI4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	391	ALA	-	expression tag	UNP Q96FI4
C	392	ALA	-	expression tag	UNP Q96FI4
C	393	LEU	-	expression tag	UNP Q96FI4
C	394	GLY	-	expression tag	UNP Q96FI4
C	395	HIS	-	expression tag	UNP Q96FI4
C	396	HIS	-	expression tag	UNP Q96FI4
C	397	HIS	-	expression tag	UNP Q96FI4
C	398	HIS	-	expression tag	UNP Q96FI4
C	399	HIS	-	expression tag	UNP Q96FI4
C	400	HIS	-	expression tag	UNP Q96FI4

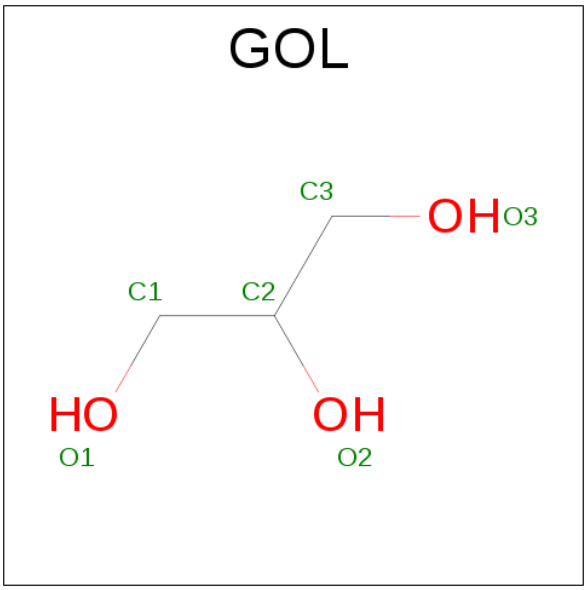
- Molecule 2 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	26	Total	C	N	O	P	0	0	0
			516	247	94	151	24			
2	F	26	Total	C	N	O	P	0	0	0
			516	247	94	151	24			

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	26	Total	C	N	O	P	0	0	0
			514	247	94	149	24			

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



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

- Molecule 5 is water.

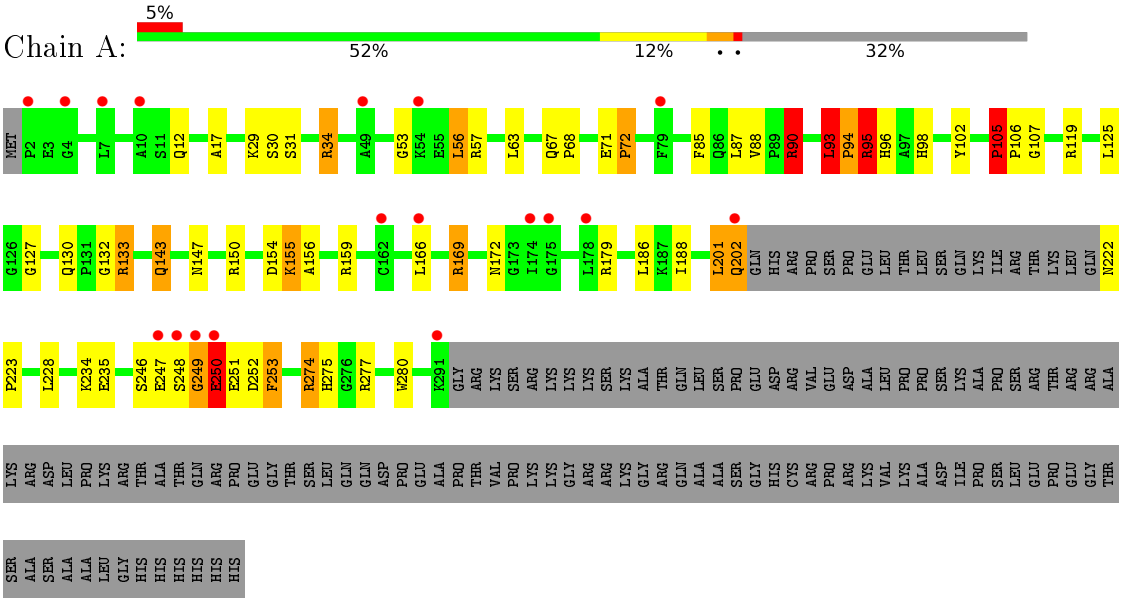
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	108	Total O 108 108	0	0
5	B	48	Total O 48 48	0	0
5	C	4	Total O 4 4	0	0
5	D	14	Total O 14 14	0	0
5	E	6	Total O 6 6	0	0
5	F	2	Total O 2 2	0	0

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.

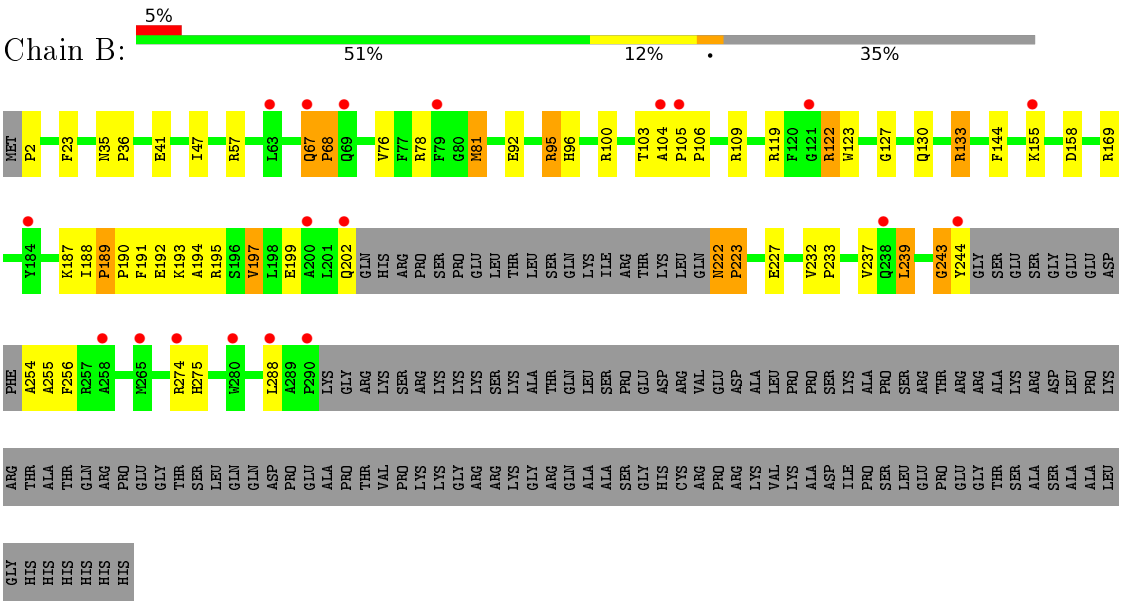
- Molecule 1: Endonuclease 8-like 1

Chain A:

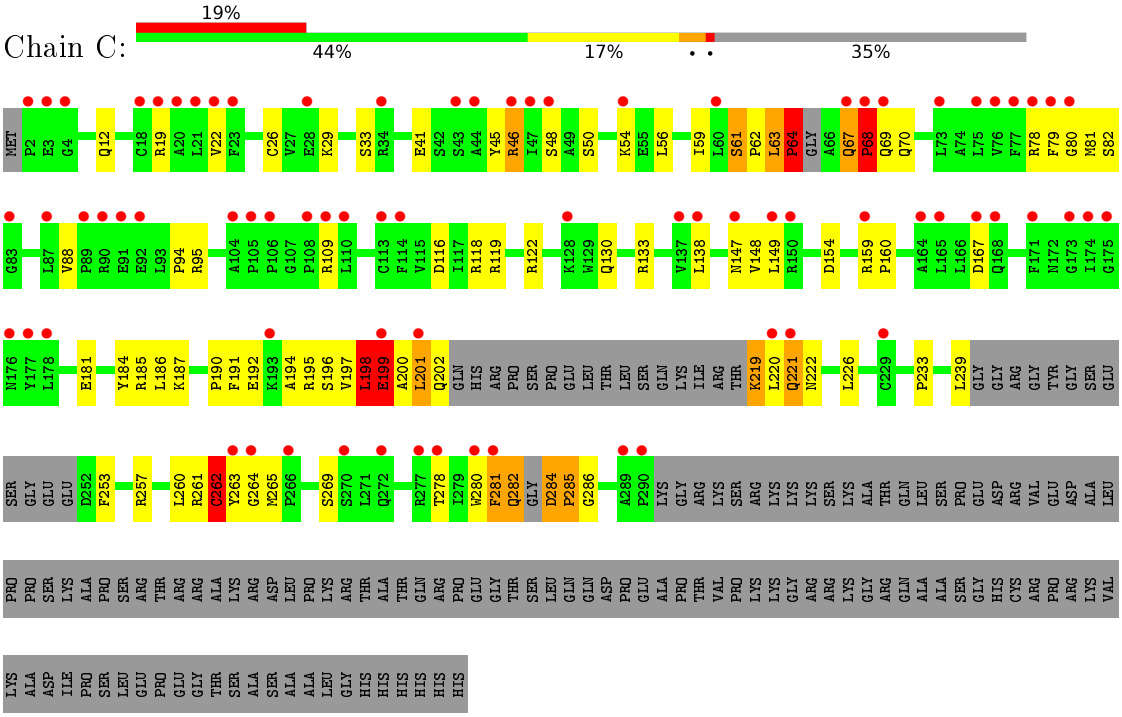


- Molecule 1: Endonuclease 8-like 1

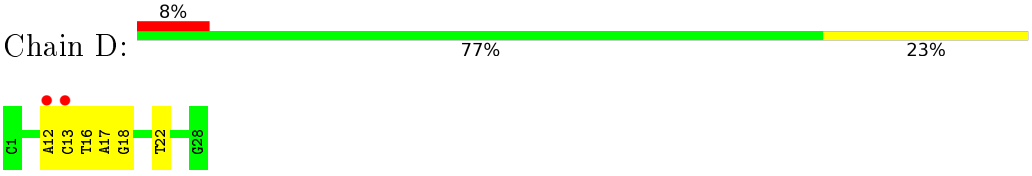
Chain B:



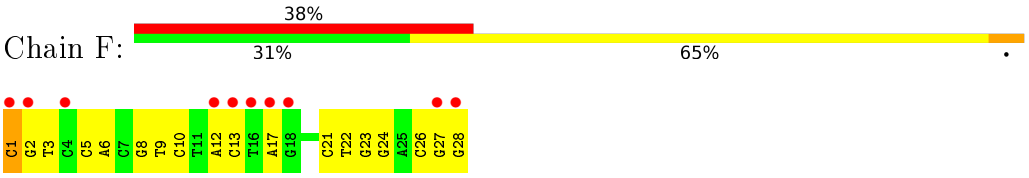
- Molecule 1: Endonuclease 8-like 1



• Molecule 2: DNA (26-MER)



• Molecule 2: DNA (26-MER)



• Molecule 3: DNA (26-MER)

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.86Å 108.75Å 171.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.81 – 2.53 32.54 – 2.53	Depositor EDS
% Data completeness (in resolution range)	97.9 (81.81-2.53) 97.9 (32.54-2.53)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.210 , 0.278 0.264 , 0.301	Depositor DCC
R_{free} test set	2319 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	56.2	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8033	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: GOL

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	1.10	2/2202 (0.1%)	1.11	16/2979 (0.5%)
1	B	0.94	1/2133 (0.0%)	1.05	10/2885 (0.3%)
1	C	0.57	2/2129 (0.1%)	0.78	4/2878 (0.1%)
2	D	0.55	0/577	0.91	1/886 (0.1%)
2	F	0.42	0/577	0.81	2/886 (0.2%)
3	E	0.61	0/575	0.99	1/882 (0.1%)
All	All	0.83	5/8193 (0.1%)	0.98	34/11396 (0.3%)

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	2
1	B	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	223	PRO	N-CD	5.52	1.55	1.47
1	A	280	TRP	CE3-CZ3	5.40	1.47	1.38
1	C	64	PRO	N-CD	5.29	1.55	1.47
1	C	68	PRO	N-CD	5.24	1.55	1.47
1	A	68	PRO	N-CD	5.05	1.54	1.47

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	133	ARG	NE-CZ-NH2	-11.66	114.47	120.30
1	A	133	ARG	NE-CZ-NH1	11.19	125.89	120.30
1	A	133	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	A	119	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	B	133	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	B	119	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	A	169	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	179	ARG	NE-CZ-NH2	-7.03	116.79	120.30
2	D	22	DT	O5'-P-OP2	-6.72	99.65	105.70
1	C	284	ASP	C-N-CD	6.42	141.88	128.40
1	A	93	LEU	C-N-CD	6.30	141.64	128.40
1	A	169	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	B	119	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	C	61	SER	C-N-CD	6.08	141.16	128.40
1	A	179	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	71	GLU	C-N-CD	5.83	140.65	128.40
1	A	90	ARG	NE-CZ-NH1	5.74	123.17	120.30
3	E	5	DC	C1'-O4'-C4'	-5.71	104.39	110.10
2	F	1	DC	C5'-C4'-O4'	5.70	120.12	109.30
1	A	250	GLU	C-N-CA	-5.66	107.56	121.70
1	B	68	PRO	N-CA-C	-5.55	97.68	112.10
1	A	105	PRO	N-CA-C	5.51	126.42	112.10
1	B	189	PRO	C-N-CD	5.47	139.88	128.40
1	A	277	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	95	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	122	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	119	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	C	63	LEU	C-N-CD	5.25	139.43	128.40
1	B	67	GLN	C-N-CD	-5.24	109.07	120.60
1	B	122	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	190	PRO	CA-N-CD	-5.09	104.37	111.50
1	A	67	GLN	C-N-CD	5.08	139.06	128.40
1	C	67	GLN	C-N-CD	5.04	138.99	128.40
2	F	1	DC	C5'-C4'-C3'	5.02	123.13	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	249	GLY	Peptide
1	A	94	PRO	Peptide
1	B	67	GLN	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	2143	0	2103	84	0
1	B	2076	0	2061	46	0
1	C	2074	0	2064	80	0
2	D	516	0	290	7	0
2	F	516	0	290	23	0
3	E	514	0	290	8	0
4	A	6	0	8	1	0
4	B	6	0	8	0	0
5	A	108	0	0	4	0
5	B	48	0	0	2	0
5	C	4	0	0	0	0
5	D	14	0	0	0	0
5	E	6	0	0	0	0
5	F	2	0	0	0	0
All	All	8033	0	7114	236	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 16.

All (236) 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:199:GLU:OE1	1:B:202:GLN:NE2	1.57	1.35
1:A:250:GLU:HG3	1:A:253:PHE:HD1	1.03	1.16
1:A:250:GLU:HG3	1:A:253:PHE:CD1	1.85	1.11
1:A:250:GLU:HB2	1:A:253:PHE:HB3	1.08	1.08
1:C:282:GLN:OE1	1:C:284:ASP:N	1.88	1.07
1:A:250:GLU:HB2	1:A:253:PHE:CB	1.92	0.99
1:A:147:ASN:HD22	1:A:150:ARG:HH12	1.11	0.98
2:D:13:DC:H2"	2:F:1:DC:C6	2.00	0.97
1:B:189:PRO:HB2	1:B:192:GLU:CG	1.96	0.96
1:B:199:GLU:O	1:B:202:GLN:HG3	1.67	0.95
1:A:249:GLY:N	1:A:250:GLU:HB3	1.82	0.94
1:A:250:GLU:CB	1:A:253:PHE:HB3	1.99	0.93
1:A:95:ARG:HG3	1:A:96:HIS:HA	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ASN:HD22	1:A:150:ARG:NH1	1.65	0.91
1:A:186:LEU:HD21	1:A:228:LEU:HD11	1.55	0.87
1:B:78:ARG:NH1	3:E:10:DC:OP2	2.08	0.86
1:A:250:GLU:CG	1:A:253:PHE:HD1	1.87	0.85
1:B:199:GLU:O	1:B:202:GLN:CG	2.25	0.85
1:B:189:PRO:O	1:B:192:GLU:HG3	1.77	0.84
1:B:189:PRO:HB2	1:B:192:GLU:HG3	1.58	0.84
1:C:281:PHE:CE2	1:C:285:PRO:HB3	2.16	0.80
1:A:248:SER:HA	1:A:250:GLU:HB3	1.64	0.78
2:F:2:DG:H1	2:F:26:DC:H42	1.31	0.77
1:C:195:ARG:O	1:C:199:GLU:HB3	1.84	0.77
1:C:78:ARG:NH1	2:F:10:DC:OP1	2.17	0.77
1:C:41:GLU:O	1:C:70:GLN:OE1	2.04	0.76
1:A:250:GLU:O	1:A:251:GLU:C	2.16	0.75
1:A:34:ARG:HH11	1:A:34:ARG:HG2	1.52	0.75
1:C:62:PRO:HG2	1:C:70:GLN:O	1.86	0.74
1:C:88:VAL:HG21	1:C:94:PRO:HD3	1.71	0.73
1:A:249:GLY:N	1:A:250:GLU:OE1	2.20	0.72
1:A:143:GLN:NE2	5:A:601:HOH:O	2.21	0.72
1:B:239:LEU:HD23	1:B:239:LEU:N	2.04	0.71
1:A:147:ASN:ND2	1:A:150:ARG:NH1	2.39	0.70
1:A:95:ARG:CG	1:A:96:HIS:HA	2.21	0.70
1:C:186:LEU:O	1:C:187:LYS:C	2.29	0.69
1:B:57:ARG:NH1	1:B:127:GLY:O	2.25	0.69
1:A:248:SER:CA	1:A:250:GLU:HB3	2.23	0.69
1:A:250:GLU:CG	1:A:253:PHE:CD1	2.68	0.69
1:C:46:ARG:HG3	1:C:63:LEU:HD11	1.75	0.69
1:C:281:PHE:CZ	1:C:285:PRO:HB3	2.29	0.68
1:B:130:GLN:NE2	1:B:133:ARG:HD2	2.09	0.68
1:A:95:ARG:HH11	1:A:95:ARG:CG	2.08	0.67
1:C:149:LEU:HD21	1:C:201:LEU:HB3	1.76	0.67
1:C:149:LEU:HD21	1:C:201:LEU:CB	2.24	0.67
1:C:138:LEU:HD21	1:C:233:PRO:HB2	1.76	0.67
1:C:221:GLN:HE21	1:C:221:GLN:CA	2.05	0.66
1:B:158:ASP:HA	1:B:193:LYS:HE3	1.78	0.66
1:A:250:GLU:O	1:A:250:GLU:HG2	1.97	0.65
1:B:194:ALA:O	1:B:197:VAL:HG23	1.96	0.65
1:C:46:ARG:N	1:C:61:SER:O	2.26	0.64
1:A:147:ASN:ND2	1:A:150:ARG:HH12	1.89	0.64
2:F:2:DG:H1	2:F:26:DC:N4	1.94	0.64
1:B:222:ASN:N	1:B:222:ASN:OD1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLY:H	1:A:250:GLU:HB3	1.63	0.63
1:B:243:GLY:O	1:B:256:PHE:CD2	2.53	0.62
1:B:105:PRO:O	1:C:222:ASN:ND2	2.32	0.62
2:D:13:DC:C2'	2:F:1:DC:C6	2.80	0.62
2:F:26:DC:H2'	2:F:27:DG:C8	2.35	0.61
1:A:130:GLN:NE2	1:A:133:ARG:HD2	2.16	0.61
1:B:104:ALA:HB1	1:B:105:PRO:HD2	1.82	0.60
1:A:248:SER:C	1:A:250:GLU:HB3	2.20	0.60
1:A:248:SER:HA	1:A:250:GLU:CB	2.30	0.60
1:C:181:GLU:O	1:C:185:ARG:HG2	2.02	0.60
1:A:246:SER:OG	1:A:253:PHE:HA	2.02	0.59
1:B:189:PRO:HG2	1:B:192:GLU:CD	2.21	0.59
1:A:155:LYS:HD3	2:F:27:DG:OP1	2.01	0.59
1:A:30:SER:HB3	1:A:98:HIS:HA	1.85	0.59
1:A:132:GLY:O	1:A:169:ARG:HG2	2.03	0.59
1:A:72:PRO:HG3	5:A:660:HOH:O	2.02	0.59
1:A:30:SER:HB2	1:A:95:ARG:NH2	2.18	0.59
1:C:281:PHE:CE2	1:C:285:PRO:CB	2.86	0.59
1:C:269:SER:HB2	1:C:281:PHE:CE1	2.38	0.58
2:F:17:DA:OP2	2:F:17:DA:C8	2.56	0.58
1:A:250:GLU:HB2	1:A:253:PHE:CG	2.39	0.58
1:B:81:MET:SD	3:E:8:DG:H5"	2.43	0.58
1:C:196:SER:O	1:C:199:GLU:HG2	2.03	0.57
2:F:1:DC:H2'	2:F:1:DC:O2	2.03	0.57
1:A:90:ARG:O	1:A:93:LEU:HD13	2.04	0.57
1:C:198:LEU:C	1:C:200:ALA:H	2.08	0.57
2:D:16:DT:H5"	2:F:28:DG:O3'	2.05	0.57
2:D:17:DA:H2"	2:D:18:DG:H5"	1.87	0.56
1:C:194:ALA:O	1:C:198:LEU:HD12	2.06	0.56
1:C:281:PHE:CE2	1:C:285:PRO:CA	2.88	0.56
1:C:285:PRO:HD2	1:C:286:GLY:H	1.69	0.56
1:B:199:GLU:O	1:B:202:GLN:HG2	2.03	0.56
1:A:275:HIS:HB3	5:A:680:HOH:O	2.06	0.56
2:F:9:DT:H2"	2:F:10:DC:OP1	2.05	0.56
1:C:63:LEU:HB3	1:C:64:PRO:CD	2.36	0.56
2:F:27:DG:H2'	2:F:28:DG:C8	2.40	0.56
1:C:45:TYR:HB2	1:C:61:SER:O	2.06	0.56
1:B:95:ARG:NH1	3:E:23:DG:OP1	2.39	0.56
1:C:281:PHE:N	1:C:281:PHE:CD1	2.72	0.56
1:A:247:GLU:O	1:A:250:GLU:HA	2.07	0.55
1:A:96:HIS:CD2	1:A:96:HIS:N	2.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ASN:N	1:B:223:PRO:HD3	2.22	0.55
1:B:188:ILE:HG21	1:B:197:VAL:HG11	1.89	0.54
1:A:34:ARG:HG2	1:A:34:ARG:NH1	2.21	0.54
1:A:246:SER:OG	1:A:253:PHE:CA	2.56	0.54
1:C:260:LEU:HB2	1:C:265:MET:HE2	1.87	0.54
1:A:94:PRO:O	1:A:95:ARG:HD2	2.08	0.54
1:C:79:PHE:O	1:C:80:GLY:C	2.46	0.54
1:C:221:GLN:HE21	1:C:221:GLN:HA	1.72	0.53
1:B:191:PHE:O	1:B:288:LEU:HB2	2.08	0.53
1:B:130:GLN:HE21	1:B:133:ARG:HD2	1.71	0.53
1:C:149:LEU:CD2	1:C:201:LEU:CB	2.87	0.53
1:B:189:PRO:HB2	1:B:192:GLU:HG2	1.86	0.53
1:C:154:ASP:O	1:C:195:ARG:NH2	2.43	0.52
1:B:35:ASN:HB2	1:B:123:TRP:CZ2	2.44	0.52
1:C:190:PRO:HD2	1:C:285:PRO:HA	1.92	0.52
1:C:221:GLN:NE2	1:C:221:GLN:HA	2.25	0.52
1:C:191:PHE:N	1:C:285:PRO:O	2.33	0.52
1:A:130:GLN:HE22	1:A:133:ARG:HH11	1.57	0.52
1:A:250:GLU:O	1:A:252:ASP:N	2.42	0.51
1:C:116:ASP:OD2	1:C:119:ARG:HA	2.10	0.51
1:C:278:THR:CG2	1:C:280:TRP:NE1	2.73	0.51
1:C:281:PHE:H	1:C:281:PHE:HD1	1.58	0.51
1:C:109:ARG:NE	1:C:109:ARG:HA	2.25	0.51
1:C:184:TYR:CE2	1:C:261:ARG:O	2.64	0.51
1:A:247:GLU:O	1:A:250:GLU:CA	2.59	0.51
1:B:199:GLU:OE1	1:B:199:GLU:HA	2.11	0.51
1:A:95:ARG:HH11	1:A:95:ARG:HG2	1.75	0.50
1:B:223:PRO:HA	1:B:227:GLU:OE2	2.11	0.50
1:C:281:PHE:CE2	1:C:285:PRO:HA	2.47	0.50
1:C:48:SER:OG	1:C:59:ILE:HB	2.12	0.50
1:A:247:GLU:O	1:A:250:GLU:CB	2.60	0.50
1:C:221:GLN:NE2	1:C:221:GLN:CA	2.73	0.50
1:C:221:GLN:HE21	1:C:221:GLN:C	2.15	0.50
1:C:149:LEU:CD2	1:C:201:LEU:HB2	2.42	0.50
1:B:232:VAL:HB	1:B:233:PRO:CD	2.43	0.49
1:C:19:ARG:O	1:C:46:ARG:NH1	2.45	0.49
1:A:130:GLN:HE21	1:A:133:ARG:HD2	1.78	0.49
1:A:17:ALA:HB1	1:A:87:LEU:HD22	1.93	0.49
1:A:249:GLY:CA	1:A:250:GLU:OE1	2.60	0.49
1:A:95:ARG:NH1	1:A:95:ARG:CG	2.72	0.49
1:A:53:GLY:HA3	1:A:172:ASN:CG	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:PRO:N	1:B:106:PRO:HD2	2.28	0.48
1:C:201:LEU:HD12	1:C:226:LEU:HD12	1.93	0.48
3:E:1:DC:O2	3:E:1:DC:O4'	2.31	0.48
1:A:154:ASP:OD1	1:A:155:LYS:HE2	2.13	0.48
1:B:35:ASN:HB3	1:B:36:PRO:CD	2.42	0.48
1:C:196:SER:C	1:C:199:GLU:HG2	2.33	0.48
1:A:130:GLN:NE2	1:A:133:ARG:HH11	2.12	0.48
1:B:233:PRO:O	1:B:237:VAL:HG23	2.14	0.48
1:C:159:ARG:HB3	1:C:160:PRO:HD2	1.96	0.48
1:C:269:SER:CB	1:C:281:PHE:CE1	2.96	0.48
1:C:41:GLU:H	1:C:70:GLN:HE22	1.61	0.48
1:A:105:PRO:O	1:A:106:PRO:C	2.48	0.48
1:A:56:LEU:C	1:A:56:LEU:HD23	2.34	0.48
3:E:17:DA:H2"	3:E:18:DG:OP2	2.14	0.47
1:A:105:PRO:O	1:A:107:GLY:N	2.47	0.47
1:B:76:VAL:O	1:B:123:TRP:HA	2.14	0.47
1:B:243:GLY:O	1:B:244:TYR:HB2	2.13	0.47
1:A:90:ARG:HD3	1:A:102:TYR:CD1	2.50	0.47
1:C:148:VAL:CG1	1:C:198:LEU:HD22	2.45	0.47
1:B:193:LYS:HA	1:B:288:LEU:CD1	2.45	0.47
1:C:190:PRO:HG3	1:C:281:PHE:CG	2.49	0.47
1:C:281:PHE:N	1:C:281:PHE:HD1	2.11	0.47
3:E:1:DC:H2"	3:E:2:DG:H5'	1.97	0.47
3:E:21:DC:H2'	3:E:22:DT:C6	2.50	0.47
1:C:281:PHE:HE2	1:C:285:PRO:CA	2.28	0.47
1:A:201:LEU:O	1:A:202:GLN:HB2	2.15	0.46
1:C:54:LYS:HB2	1:C:133:ARG:NH2	2.30	0.46
1:A:186:LEU:CD2	1:A:228:LEU:HD11	2.37	0.46
1:C:264:GLY:O	1:C:265:MET:SD	2.73	0.46
1:C:278:THR:HG22	1:C:280:TRP:NE1	2.30	0.46
1:A:88:VAL:HG21	1:A:94:PRO:HD3	1.98	0.46
1:C:186:LEU:O	1:C:187:LYS:O	2.34	0.46
1:B:222:ASN:N	1:B:223:PRO:CD	2.79	0.46
1:C:56:LEU:HD23	1:C:56:LEU:C	2.36	0.45
1:A:186:LEU:HB2	1:A:188:ILE:HG13	1.99	0.45
1:A:250:GLU:CB	1:A:253:PHE:CD1	3.00	0.45
1:C:29:LYS:NZ	1:C:33:SER:O	2.44	0.45
1:B:23:PHE:HA	1:B:103:THR:HA	1.96	0.45
1:A:222:ASN:N	1:A:223:PRO:CD	2.80	0.45
1:A:95:ARG:HD2	1:A:95:ARG:HA	1.63	0.45
1:A:156:ALA:O	1:A:159:ARG:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2:DG:H2"	2:F:3:DT:O5'	2.16	0.44
1:C:149:LEU:CD2	1:C:201:LEU:HB3	2.42	0.44
1:B:95:ARG:O	1:B:96:HIS:HB2	2.18	0.44
1:C:185:ARG:NH1	1:C:261:ARG:NH2	2.65	0.44
1:C:219:LYS:HA	1:C:219:LYS:HE3	1.99	0.44
2:F:8:DG:H2"	2:F:9:DT:O5'	2.18	0.44
1:A:159:ARG:NH2	1:A:274:ARG:NE	2.66	0.44
2:F:23:DG:H1'	2:F:24:DG:C8	2.53	0.44
1:A:30:SER:HB2	1:A:95:ARG:HH22	1.82	0.44
1:B:169:ARG:NH1	5:B:606:HOH:O	2.49	0.44
1:A:274:ARG:HG3	1:A:275:HIS:CD2	2.53	0.44
1:B:23:PHE:CD1	1:B:47:ILE:HG13	2.53	0.44
2:F:5:DC:H2"	2:F:6:DA:H5'	1.99	0.43
1:C:198:LEU:C	1:C:200:ALA:N	2.70	0.43
1:B:254:ALA:O	1:B:255:ALA:HB3	2.18	0.43
1:C:263:TYR:O	1:C:265:MET:HG2	2.18	0.43
1:C:63:LEU:HD23	1:C:63:LEU:HA	1.80	0.43
2:F:12:DA:H1'	2:F:13:DC:O5'	2.18	0.43
1:C:46:ARG:HG3	1:C:63:LEU:CD1	2.47	0.43
2:F:8:DG:H1'	2:F:9:DT:C6	2.54	0.43
2:D:12:DA:H2"	2:D:13:DC:OP2	2.18	0.43
3:E:5:DC:H2"	3:E:6:DA:C8	2.54	0.43
1:C:67:GLN:HA	1:C:68:PRO:HA	1.69	0.43
1:A:90:ARG:NH1	1:A:102:TYR:HB3	2.33	0.43
1:C:149:LEU:HD13	1:C:202:GLN:HB3	2.00	0.43
1:A:250:GLU:HB2	1:A:253:PHE:CD1	2.53	0.43
1:B:275:HIS:HB3	5:B:636:HOH:O	2.18	0.43
1:A:159:ARG:NH2	1:A:274:ARG:CZ	2.82	0.43
1:A:63:LEU:HD23	5:A:636:HOH:O	2.19	0.42
2:F:21:DC:H2'	2:F:22:DT:C6	2.54	0.42
1:A:155:LYS:CD	2:F:27:DG:OP1	2.67	0.42
1:A:249:GLY:N	1:A:250:GLU:CB	2.68	0.42
1:A:246:SER:HB2	1:A:252:ASP:CG	2.39	0.42
1:A:29:LYS:HG2	1:A:30:SER:O	2.20	0.42
1:C:278:THR:HG21	1:C:280:TRP:NE1	2.34	0.42
1:A:166:LEU:HA	1:A:166:LEU:HD23	1.84	0.42
1:A:95:ARG:HH11	1:A:95:ARG:HG3	1.85	0.42
1:B:195:ARG:O	1:B:199:GLU:HG2	2.20	0.42
1:B:243:GLY:O	1:B:256:PHE:CG	2.73	0.42
1:C:262:CYS:O	1:C:265:MET:HG2	2.20	0.42
2:D:16:DT:C5'	2:F:28:DG:O3'	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LEU:O	1:C:200:ALA:N	2.53	0.42
1:B:194:ALA:O	1:B:197:VAL:N	2.47	0.42
1:C:148:VAL:HG11	1:C:198:LEU:HD22	2.01	0.42
1:A:57:ARG:NH1	1:A:127:GLY:O	2.43	0.41
1:C:285:PRO:HD2	1:C:286:GLY:N	2.35	0.41
1:A:274:ARG:HG3	1:A:275:HIS:HD2	1.85	0.41
1:C:81:MET:CE	2:F:6:DA:H2'	2.50	0.41
1:C:197:VAL:C	1:C:199:GLU:N	2.73	0.41
1:A:250:GLU:C	1:A:252:ASP:N	2.72	0.41
1:B:189:PRO:HG2	1:B:192:GLU:OE1	2.21	0.41
1:A:85:PHE:O	4:A:501:GOL:H31	2.20	0.41
1:C:118:ARG:O	1:C:119:ARG:HB2	2.21	0.41
1:C:285:PRO:CD	1:C:286:GLY:H	2.33	0.41
1:A:222:ASN:N	1:A:223:PRO:HD2	2.36	0.40
1:A:234:LYS:O	1:A:235:GLU:C	2.59	0.40
1:C:197:VAL:O	1:C:199:GLU:N	2.55	0.40
2:D:17:DA:H2"	2:D:18:DG:C5'	2.50	0.40
2:F:26:DC:C2'	2:F:27:DG:O5'	2.69	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	267/400 (67%)	254 (95%)	13 (5%)	0	100 100
1	B	255/400 (64%)	228 (89%)	25 (10%)	2 (1%)	24 40
1	C	249/400 (62%)	215 (86%)	29 (12%)	5 (2%)	9 14
All	All	771/1200 (64%)	697 (90%)	67 (9%)	7 (1%)	21 37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	PRO
1	C	199	GLU
1	C	167	ASP
1	C	198	LEU
1	C	262	CYS
1	C	285	PRO
1	B	243	GLY

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	222/335 (66%)	205 (92%)	17 (8%)	16 29
1	B	217/335 (65%)	202 (93%)	15 (7%)	19 34
1	C	219/335 (65%)	193 (88%)	26 (12%)	6 11
All	All	658/1005 (66%)	600 (91%)	58 (9%)	12 22

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	31	SER
1	A	34	ARG
1	A	56	LEU
1	A	72	PRO
1	A	90	ARG
1	A	93	LEU
1	A	95	ARG
1	A	105	PRO
1	A	125	LEU
1	A	143	GLN
1	A	155	LYS
1	A	201	LEU
1	A	202	GLN
1	A	250	GLU
1	A	253	PHE

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Mol	Chain	Res	Type
1	A	274	ARG
1	B	2	PRO
1	B	41	GLU
1	B	81	MET
1	B	92	GLU
1	B	95	ARG
1	B	100	ARG
1	B	109	ARG
1	B	122	ARG
1	B	144	PHE
1	B	155	LYS
1	B	187	LYS
1	B	197	VAL
1	B	222	ASN
1	B	239	LEU
1	B	274	ARG
1	C	12	GLN
1	C	22	VAL
1	C	26	CYS
1	C	46	ARG
1	C	50	SER
1	C	64	PRO
1	C	68	PRO
1	C	69	GLN
1	C	82	SER
1	C	95	ARG
1	C	122	ARG
1	C	130	GLN
1	C	147	ASN
1	C	192	GLU
1	C	198	LEU
1	C	199	GLU
1	C	201	LEU
1	C	219	LYS
1	C	220	LEU
1	C	221	GLN
1	C	239	LEU
1	C	253	PHE
1	C	257	ARG
1	C	262	CYS
1	C	281	PHE
1	C	282	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	96	HIS
1	A	130	GLN
1	A	143	GLN
1	A	147	ASN
1	A	275	HIS
1	B	130	GLN
1	B	143	GLN
1	B	222	ASN
1	C	69	GLN
1	C	70	GLN
1	C	221	GLN
1	C	222	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

2 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	$\#\|Z\|>2$
4	GOL	A	501	-	5,5,5	0.92	0	5,5,5	1.02	0
4	GOL	B	501	-	5,5,5	0.49	0	5,5,5	0.53	0

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
4	GOL	A	501	-	-	0/4/4/4	0/0/0/0
4	GOL	B	501	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	GOL	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	271/400 (67%)	0.43	18 (6%) 22 24	2, 2, 17, 39	0
1	B	261/400 (65%)	0.76	19 (7%) 18 20	2, 12, 29, 42	0
1	C	259/400 (64%)	1.56	77 (29%) 1 0	29, 54, 74, 93	0
2	D	26/26 (100%)	0.55	2 (7%) 16 18	4, 25, 48, 53	0
2	F	26/26 (100%)	1.53	10 (38%) 0 0	30, 55, 64, 68	0
3	E	26/26 (100%)	0.57	2 (7%) 16 18	8, 26, 36, 39	0
All	All	869/1278 (67%)	0.90	128 (14%) 3 3	2, 15, 65, 93	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	264	GLY	8.6
1	C	44	ALA	7.2
1	C	20	ALA	6.4
1	C	280	TRP	5.7
1	C	46	ARG	4.9
1	C	109	ARG	4.6
2	F	13	DC	4.6
1	C	69	GLN	4.6
1	C	105	PRO	4.6
1	C	106	PRO	4.6
1	C	92	GLU	4.5
1	C	18	CYS	4.4
1	C	272	GLN	4.4
1	A	248	SER	4.4
1	C	68	PRO	4.3
1	C	43	SER	4.3
1	C	175	GLY	4.2
1	C	22	VAL	4.2
2	D	13	DC	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	110	LEU	4.2
1	C	67	GLN	4.2
1	C	159	ARG	4.2
1	C	270	SER	4.1
1	C	263	TYR	4.0
1	C	78	ARG	3.8
1	B	288	LEU	3.5
1	A	291	LYS	3.5
1	C	173	GLY	3.5
1	C	174	ILE	3.3
1	A	175	GLY	3.3
3	E	1	DC	3.3
1	C	79	PHE	3.2
1	C	164	ALA	3.2
2	F	2	DG	3.2
1	C	91	GLU	3.2
1	C	80	GLY	3.2
1	C	48	SER	3.1
2	F	1	DC	3.1
1	C	277	ARG	3.1
2	F	28	DG	3.1
1	C	266	PRO	3.1
1	C	73	LEU	3.1
2	D	12	DA	3.0
1	A	249	GLY	3.0
1	C	178	LEU	3.0
1	B	69	GLN	3.0
1	C	19	ARG	3.0
1	C	147	ASN	3.0
1	C	89	PRO	2.9
1	C	220	LEU	2.9
1	C	281	PHE	2.9
1	C	76	VAL	2.9
1	C	23	PHE	2.8
1	A	7	LEU	2.8
1	C	75	LEU	2.8
1	C	221	GLN	2.8
1	C	21	LEU	2.8
1	B	280	TRP	2.7
1	C	138	LEU	2.7
1	B	104	ALA	2.7
1	C	83	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	165	LEU	2.7
1	B	184	TYR	2.7
1	C	2	PRO	2.6
1	C	108	PRO	2.6
1	A	202	GLN	2.6
1	C	77	PHE	2.6
1	B	265	MET	2.6
1	C	290	PRO	2.6
2	F	12	DA	2.6
1	A	178	LEU	2.6
1	B	79	PHE	2.6
1	C	90	ARG	2.6
1	C	278	THR	2.6
3	E	13	DC	2.6
1	B	238	GLN	2.6
1	C	87	LEU	2.5
2	F	18	DG	2.5
1	C	34	ARG	2.5
1	A	4	GLY	2.5
1	C	4	GLY	2.5
1	B	274	ARG	2.4
1	C	201	LEU	2.4
2	F	17	DA	2.4
1	A	174	ILE	2.4
1	C	177	TYR	2.4
1	A	2	PRO	2.4
1	C	3	GLU	2.4
1	C	137	VAL	2.4
1	C	60	LEU	2.3
1	C	113	CYS	2.3
1	C	171	PHE	2.3
1	C	128	LYS	2.3
1	A	166	LEU	2.3
1	C	114	PHE	2.3
1	C	149	LEU	2.3
1	B	200	ALA	2.3
1	C	168	GLN	2.3
2	F	27	DG	2.3
2	F	16	DT	2.3
1	C	28	GLU	2.3
1	B	67	GLN	2.2
1	A	49	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	150	ARG	2.2
1	C	193	LYS	2.2
1	C	199	GLU	2.2
1	C	104	ALA	2.2
1	C	289	ALA	2.2
1	B	63	LEU	2.2
1	C	54	LYS	2.2
1	B	105	PRO	2.2
1	B	202	GLN	2.2
1	A	10	ALA	2.2
1	B	121	GLY	2.2
1	B	290	PRO	2.2
2	F	4	DC	2.2
1	C	229	CYS	2.1
1	B	155	LYS	2.1
1	C	47	ILE	2.1
1	A	79	PHE	2.1
1	A	54	LYS	2.1
1	B	244	TYR	2.1
1	A	247	GLU	2.1
1	C	167	ASP	2.0
1	A	250	GLU	2.0
1	C	176	ASN	2.0
1	B	258	ALA	2.0
1	A	162	CYS	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
4	GOL	B	501	6/6	0.80	0.48	11.42	64,73,79,79	0
4	GOL	A	501	6/6	0.72	0.52	5.77	58,61,63,78	0

6.5 Other polymers (i)

There are no such residues in this entry.