Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2023 – 03:18 PM EDT

PDB ID	:	3ENZ
Title	:	Arsenolytic structure of Plasmodium falciparum purine nucleoside phosphorylase with hypoxanthine, ribose and arsenate ion
Authors	:	Chaikuad, A.; Brady, R.L.
Deposited on	:	2008-09-26
Resolution	:	2.03 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

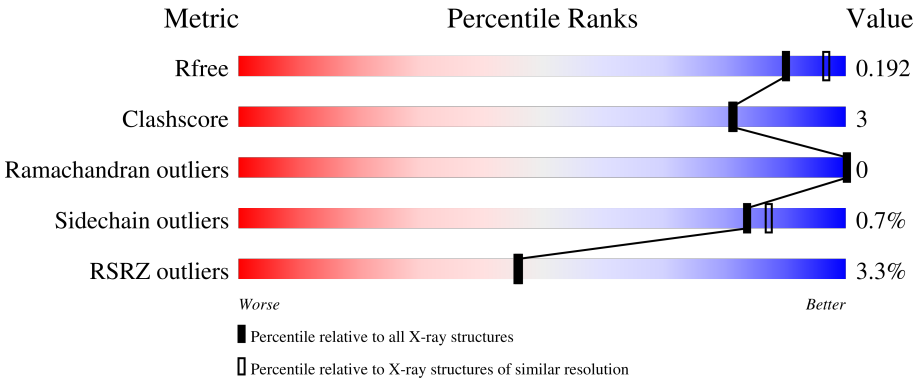
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.03 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



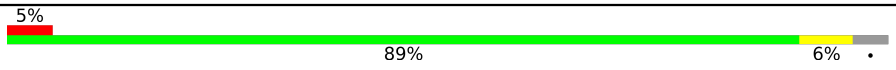
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	253	2% 91% 6% ·
1	B	253	2% 91% 5% ·
1	C	253	2% 92% 5% ·
1	D	253	4% 91% 6% ·
1	E	253	4% 91% 5% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	253	

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	ART	E	303	-	-	X	-
4	ART	F	303	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12047 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 Purine nucleoside phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	1	0
			1876	1190	322	348	16			
1	B	245	Total	C	N	O	S	0	1	0
			1885	1195	323	351	16			
1	C	246	Total	C	N	O	S	0	1	0
			1895	1201	326	352	16			
1	D	244	Total	C	N	O	S	0	1	0
			1876	1190	322	348	16			
1	E	243	Total	C	N	O	S	0	1	0
			1868	1184	321	347	16			
1	F	243	Total	C	N	O	S	0	1	0
			1868	1184	321	347	16			

There are 48 discrepancies between the modelled and reference sequences:

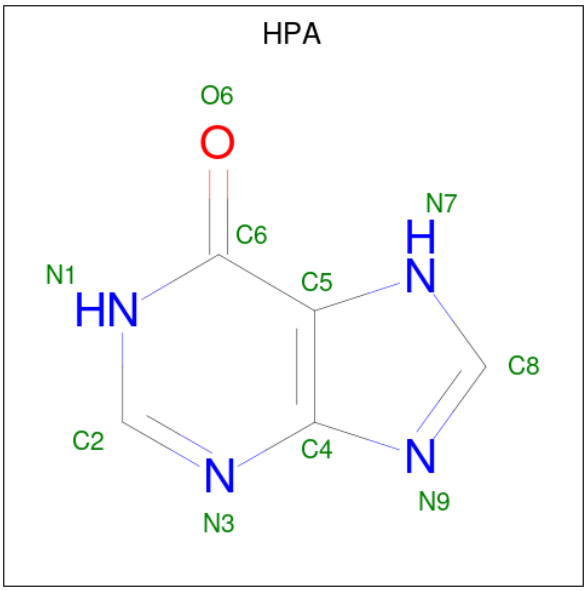
Chain	Residue	Modelled	Actual	Comment	Reference
A	246	LEU	-	expression tag	UNP Q8I3X4
A	247	GLU	-	expression tag	UNP Q8I3X4
A	248	HIS	-	expression tag	UNP Q8I3X4
A	249	HIS	-	expression tag	UNP Q8I3X4
A	250	HIS	-	expression tag	UNP Q8I3X4
A	251	HIS	-	expression tag	UNP Q8I3X4
A	252	HIS	-	expression tag	UNP Q8I3X4
A	253	HIS	-	expression tag	UNP Q8I3X4
B	246	LEU	-	expression tag	UNP Q8I3X4
B	247	GLU	-	expression tag	UNP Q8I3X4
B	248	HIS	-	expression tag	UNP Q8I3X4
B	249	HIS	-	expression tag	UNP Q8I3X4
B	250	HIS	-	expression tag	UNP Q8I3X4
B	251	HIS	-	expression tag	UNP Q8I3X4
B	252	HIS	-	expression tag	UNP Q8I3X4
B	253	HIS	-	expression tag	UNP Q8I3X4
C	246	LEU	-	expression tag	UNP Q8I3X4

Continued on next page...

Continued from previous page...

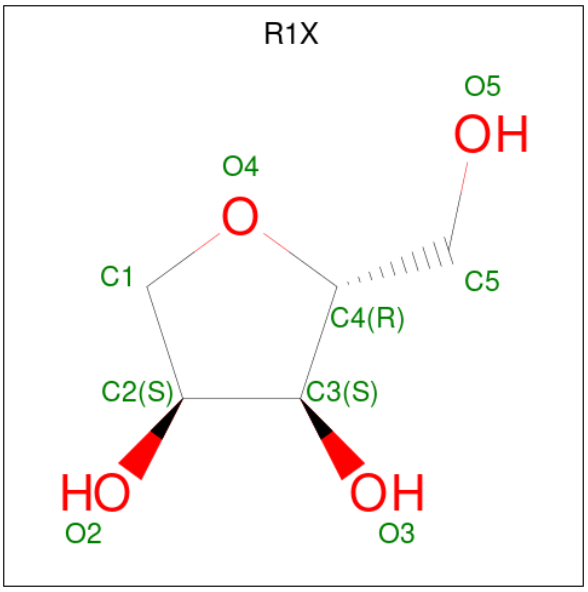
Chain	Residue	Modelled	Actual	Comment	Reference
C	247	GLU	-	expression tag	UNP Q8I3X4
C	248	HIS	-	expression tag	UNP Q8I3X4
C	249	HIS	-	expression tag	UNP Q8I3X4
C	250	HIS	-	expression tag	UNP Q8I3X4
C	251	HIS	-	expression tag	UNP Q8I3X4
C	252	HIS	-	expression tag	UNP Q8I3X4
C	253	HIS	-	expression tag	UNP Q8I3X4
D	246	LEU	-	expression tag	UNP Q8I3X4
D	247	GLU	-	expression tag	UNP Q8I3X4
D	248	HIS	-	expression tag	UNP Q8I3X4
D	249	HIS	-	expression tag	UNP Q8I3X4
D	250	HIS	-	expression tag	UNP Q8I3X4
D	251	HIS	-	expression tag	UNP Q8I3X4
D	252	HIS	-	expression tag	UNP Q8I3X4
D	253	HIS	-	expression tag	UNP Q8I3X4
E	246	LEU	-	expression tag	UNP Q8I3X4
E	247	GLU	-	expression tag	UNP Q8I3X4
E	248	HIS	-	expression tag	UNP Q8I3X4
E	249	HIS	-	expression tag	UNP Q8I3X4
E	250	HIS	-	expression tag	UNP Q8I3X4
E	251	HIS	-	expression tag	UNP Q8I3X4
E	252	HIS	-	expression tag	UNP Q8I3X4
E	253	HIS	-	expression tag	UNP Q8I3X4
F	246	LEU	-	expression tag	UNP Q8I3X4
F	247	GLU	-	expression tag	UNP Q8I3X4
F	248	HIS	-	expression tag	UNP Q8I3X4
F	249	HIS	-	expression tag	UNP Q8I3X4
F	250	HIS	-	expression tag	UNP Q8I3X4
F	251	HIS	-	expression tag	UNP Q8I3X4
F	252	HIS	-	expression tag	UNP Q8I3X4
F	253	HIS	-	expression tag	UNP Q8I3X4

- Molecule 2 is HYPOXANTHINE (three-letter code: HPA) (formula: $C_5H_4N_4O$).



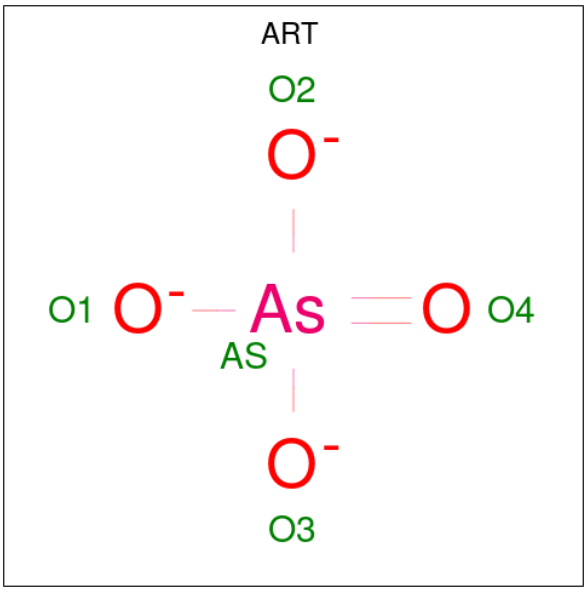
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 10 5 4 1	0	0
2	B	1	Total C N O 10 5 4 1	0	0
2	C	1	Total C N O 10 5 4 1	0	0
2	D	1	Total C N O 10 5 4 1	0	0
2	E	1	Total C N O 10 5 4 1	0	0
2	F	1	Total C N O 10 5 4 1	0	0

- Molecule 3 is 1,4-anhydro-D-ribitol (three-letter code: R1X) (formula: $C_5H_{10}O_4$).



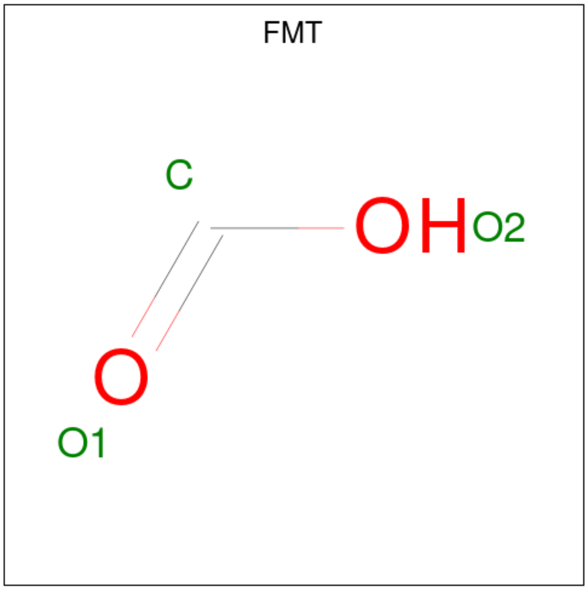
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 5 4	0	0
3	B	1	Total C O 9 5 4	0	0
3	C	1	Total C O 9 5 4	0	0
3	D	1	Total C O 9 5 4	0	0
3	E	1	Total C O 9 5 4	0	0
3	F	1	Total C O 9 5 4	0	0

- Molecule 4 is ARSENATE (three-letter code: ART) (formula: AsO_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	As	O	0	0
			5	1	4		
4	B	1	Total	As	O	0	0
			5	1	4		
4	C	1	Total	As	O	0	0
			5	1	4		
4	D	1	Total	As	O	0	0
			5	1	4		
4	E	1	Total	As	O	0	0
			5	1	4		
4	F	1	Total	As	O	0	0
			5	1	4		

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 3 1 2	0	0
5	A	1	Total C O 3 1 2	0	0
5	A	1	Total C O 3 1 2	0	0
5	A	1	Total C O 3 1 2	0	0
5	A	1	Total C O 3 1 2	0	0
5	A	1	Total C O 3 1 2	0	0
5	A	1	Total C O 3 1 2	0	0
5	B	1	Total C O 3 1 2	0	0
5	B	1	Total C O 3 1 2	0	0
5	C	1	Total C O 3 1 2	0	0
5	C	1	Total C O 3 1 2	0	0
5	C	1	Total C O 3 1 2	0	0
5	C	1	Total C O 3 1 2	0	0
5	C	1	Total C O 3 1 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 3 1 2	0	0
5	D	1	Total C O 3 1 2	0	0
5	D	1	Total C O 3 1 2	0	0
5	D	1	Total C O 3 1 2	0	0
5	D	1	Total C O 3 1 2	0	0
5	D	1	Total C O 3 1 2	0	0
5	E	1	Total C O 3 1 2	0	0
5	F	1	Total C O 3 1 2	0	0
5	F	1	Total C O 3 1 2	0	0
5	F	1	Total C O 3 1 2	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0
6	B	1	Total Na 1 1	0	0
6	C	1	Total Na 1 1	0	0
6	D	2	Total Na 2 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	106	Total O 106 106	0	0
7	B	94	Total O 94 94	0	0
7	C	115	Total O 115 115	0	0

Continued on next page...

Continued from previous page...

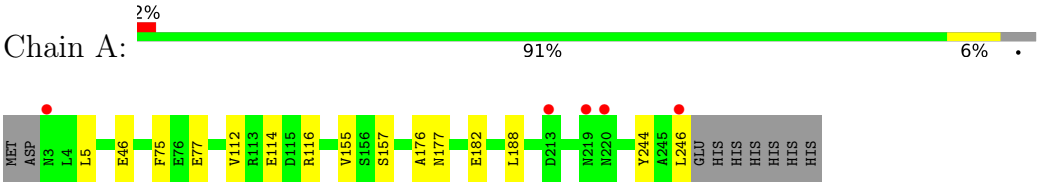
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	86	Total O 86 86	0	0
7	E	84	Total O 84 84	0	0
7	F	73	Total O 73 73	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

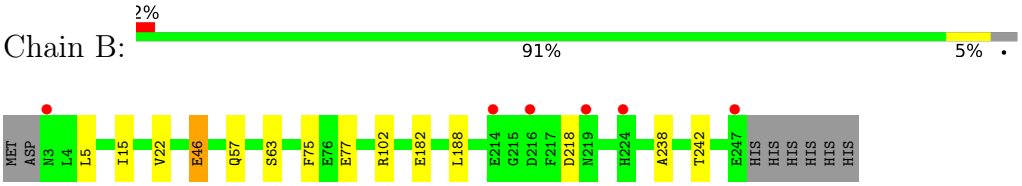
• Molecule 1: Purine nucleoside phosphorylase

Chain A:



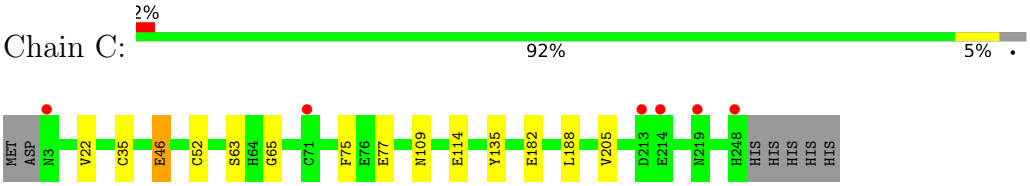
• Molecule 1: Purine nucleoside phosphorylase

Chain B:



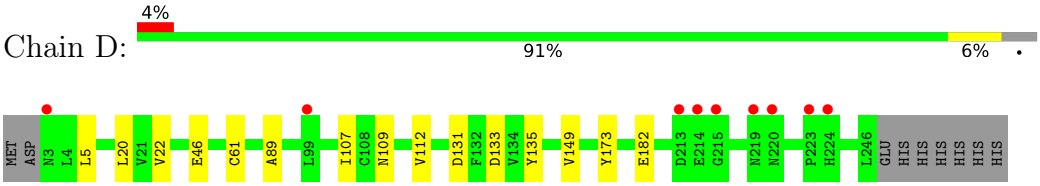
• Molecule 1: Purine nucleoside phosphorylase

Chain C:



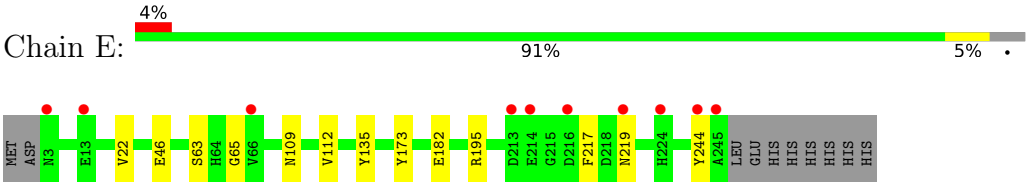
• Molecule 1: Purine nucleoside phosphorylase

Chain D:



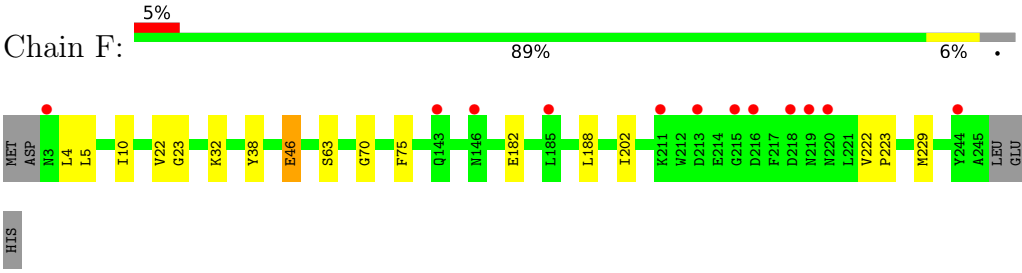
• Molecule 1: Purine nucleoside phosphorylase

Chain E:



• Molecule 1: Purine nucleoside phosphorylase

Chain F:


5%
89%
6%
MET
ASP
N3
L4
L5
I10
V22
G23
K32
Y38
E46
S63
G70
F75
Q143
N146
E182
L185
L188
I202
K211
W212
D213
E214
G215
D216
F217
D218
N219
N220
L221
V222
P223
M229
Y244
A245
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	177.82Å 177.82Å 253.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.86 – 2.03 30.94 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.4 (145.86-2.03) 99.4 (30.94-2.03)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.160 , 0.193 0.161 , 0.192	Depositor DCC
R_{free} test set	6502 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.009 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.007 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12047	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: ART, HPA, NA, FMT, R1X

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	0.82	1/1912 (0.1%)	0.68	1/2587 (0.0%)
1	B	0.84	1/1921 (0.1%)	0.69	0/2599
1	C	0.89	4/1932 (0.2%)	0.71	0/2614
1	D	0.80	0/1912	0.66	0/2587
1	E	0.78	0/1904	0.66	0/2576
1	F	0.80	1/1904 (0.1%)	0.69	0/2576
All	All	0.82	7/11485 (0.1%)	0.68	1/15539 (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	E	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	GLU	CD-OE1	-6.53	1.18	1.25
1	C	114	GLU	CD-OE2	-6.41	1.18	1.25
1	B	46	GLU	CD-OE1	-6.12	1.19	1.25
1	C	205	VAL	CB-CG2	-5.44	1.41	1.52
1	C	77	GLU	CD-OE2	-5.30	1.19	1.25
1	F	46	GLU	CD-OE2	-5.29	1.19	1.25
1	A	244	TYR	CD2-CE2	-5.08	1.31	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	116	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	244	TYR	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	1876	0	1900	6	0
1	B	1885	0	1905	8	0
1	C	1895	0	1913	7	0
1	D	1876	0	1900	8	0
1	E	1868	0	1889	8	0
1	F	1868	0	1889	9	0
2	A	10	0	4	2	0
2	B	10	0	4	1	0
2	C	10	0	4	1	0
2	D	10	0	4	1	0
2	E	10	0	4	2	0
2	F	10	0	4	1	0
3	A	9	0	0	2	0
3	B	9	0	0	2	0
3	C	9	0	0	2	0
3	D	9	0	0	2	0
3	E	9	0	0	3	0
3	F	9	0	0	3	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
4	C	5	0	0	1	0
4	D	5	0	0	1	0
4	E	5	0	0	2	0
4	F	5	0	0	3	0
5	A	21	0	7	1	0
5	B	6	0	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	18	0	6	0	0
5	D	15	0	5	0	0
5	E	3	0	1	1	0
5	F	9	0	3	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
7	A	106	0	0	2	0
7	B	94	0	0	0	0
7	C	115	0	0	0	0
7	D	86	0	0	0	0
7	E	84	0	0	1	0
7	F	73	0	0	1	0
All	All	12047	0	11444	60	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 3.

All (60) 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)
3:E:302:R1X:C1	4:E:303:ART:O1	2.08	1.01
3:B:302:R1X:C1	4:B:303:ART:O1	2.34	0.75
3:D:302:R1X:C1	4:D:303:ART:O1	2.35	0.73
2:A:301:HPA:N9	3:A:302:R1X:C1	2.53	0.71
3:F:302:R1X:C1	4:F:303:ART:O1	2.39	0.71
1:C:46:GLU:HB3	1:E:46:GLU:HB3	1.73	0.69
1:A:176:ALA:O	1:A:177:ASN:HB2	1.93	0.67
1:C:109:ASN:HB3	1:C:135:TYR:CD1	2.31	0.66
2:B:301:HPA:N9	3:B:302:R1X:C1	2.59	0.66
3:C:302:R1X:C1	4:C:303:ART:O1	2.44	0.65
3:A:302:R1X:C1	4:A:303:ART:O1	2.46	0.64
1:E:195:ARG:HE	5:E:304:FMT:C	2.16	0.58
1:D:46:GLU:HB3	1:F:46:GLU:HB3	1.87	0.57
2:F:301:HPA:N9	3:F:302:R1X:C1	2.68	0.57
1:B:238:ALA:O	1:B:242:THR:HG23	2.06	0.55
2:E:301:HPA:H2	7:E:393:HOH:O	2.06	0.55
2:D:301:HPA:N9	3:D:302:R1X:C1	2.71	0.54
2:C:301:HPA:N9	3:C:302:R1X:C1	2.70	0.53
2:E:301:HPA:N9	3:E:302:R1X:C1	2.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLU:HB3	1:B:46:GLU:HB3	1.92	0.52
1:B:102:ARG:HE	1:B:218:ASP:HB3	1.75	0.51
1:B:5:LEU:HD11	1:B:15:ILE:HD11	1.91	0.51
1:E:109:ASN:HB3	1:E:135:TYR:CE1	2.47	0.50
2:A:301:HPA:H2	7:A:325:HOH:O	2.12	0.50
1:E:109:ASN:HB3	1:E:135:TYR:CD1	2.48	0.49
1:D:109:ASN:HB3	1:D:135:TYR:CE1	2.48	0.48
1:A:114:GLU:HB3	1:A:157:SER:HA	1.96	0.48
1:F:202:ILE:HG12	1:F:229:MET:HG3	1.94	0.47
5:A:308:FMT:H	7:A:392:HOH:O	2.14	0.47
1:F:32:LYS:HE3	1:F:38:TYR:CE1	2.49	0.47
1:E:22:VAL:O	1:E:63:SER:HA	2.13	0.47
1:E:46:GLU:HG3	1:E:65:GLY:HA3	1.95	0.47
1:D:131:ASP:OD1	1:D:133:ASP:HB2	2.15	0.46
3:F:302:R1X:O3	4:F:303:ART:O3	2.33	0.45
1:F:22:VAL:O	1:F:63:SER:HA	2.17	0.45
1:B:22:VAL:O	1:B:63:SER:HA	2.17	0.45
1:D:107:ILE:HD12	1:D:149:VAL:HG21	1.99	0.45
1:F:5:LEU:HG	1:F:10:ILE:O	2.17	0.44
1:C:109:ASN:HB3	1:C:135:TYR:CE1	2.52	0.44
1:F:70:GLY:HA3	7:F:379:HOH:O	2.18	0.44
1:C:46:GLU:HG3	1:C:65:GLY:HA3	2.00	0.44
1:E:217:PHE:CZ	1:E:219:ASN:HB3	2.53	0.43
1:F:75:PHE:CE1	1:F:188:LEU:HB2	2.53	0.43
1:D:22:VAL:HG12	1:D:89:ALA:O	2.17	0.43
1:D:20:LEU:O	1:D:61:CYS:HA	2.18	0.43
1:B:5:LEU:HD13	1:B:77:GLU:HB3	2.00	0.43
1:D:109:ASN:HB3	1:D:135:TYR:CD1	2.54	0.42
1:A:112:VAL:HB	1:A:155:VAL:HA	2.00	0.42
1:C:35:CYS:SG	1:C:52:CYS:HB3	2.59	0.42
1:B:75:PHE:CE1	1:B:188:LEU:HB2	2.54	0.42
1:F:222:VAL:HA	1:F:223:PRO:HD3	1.88	0.42
1:A:75:PHE:CE1	1:A:188:LEU:HB2	2.55	0.41
1:A:5:LEU:HD13	1:A:77:GLU:HB3	2.02	0.41
3:E:302:R1X:O3	4:E:303:ART:O3	2.39	0.41
1:E:112:VAL:HG11	1:E:173:TYR:CZ	2.55	0.41
1:B:57:GLN:CD	1:B:242:THR:HG22	2.40	0.41
1:C:22:VAL:O	1:C:63:SER:HA	2.21	0.40
1:D:112:VAL:HG11	1:D:173:TYR:CZ	2.56	0.40
1:F:23:GLY:HA3	4:F:303:ART:O3	2.21	0.40
1:C:75:PHE:CE1	1:C:188:LEU:HB2	2.57	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	243/253 (96%)	236 (97%)	7 (3%)	0	100	100
1	B	244/253 (96%)	238 (98%)	6 (2%)	0	100	100
1	C	245/253 (97%)	237 (97%)	8 (3%)	0	100	100
1	D	243/253 (96%)	236 (97%)	7 (3%)	0	100	100
1	E	242/253 (96%)	236 (98%)	6 (2%)	0	100	100
1	F	242/253 (96%)	236 (98%)	6 (2%)	0	100	100
All	All	1459/1518 (96%)	1419 (97%)	40 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	208/216 (96%)	206 (99%)	2 (1%)	76	80
1	B	209/216 (97%)	208 (100%)	1 (0%)	88	91
1	C	210/216 (97%)	209 (100%)	1 (0%)	88	91
1	D	208/216 (96%)	206 (99%)	2 (1%)	76	80
1	E	207/216 (96%)	206 (100%)	1 (0%)	88	91
1	F	207/216 (96%)	205 (99%)	2 (1%)	76	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1249/1296 (96%)	1240 (99%)	9 (1%)	84 87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	GLU
1	A	246	LEU
1	B	182	GLU
1	C	182	GLU
1	D	5	LEU
1	D	182	GLU
1	E	182	GLU
1	F	4	LEU
1	F	182	GLU

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

Mol	Chain	Res	Type
1	A	151	ASN
1	F	151	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 47 ligands modelled in this entry, 5 are monoatomic - leaving 42 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	$\#\|Z\| > 2$
5	FMT	D	306	-	2,2,2	1.13	0	1,1,1	0.19	0
4	ART	C	303	-	0,4,4	-	-	0,6,6	-	-
5	FMT	F	305	-	2,2,2	0.67	0	1,1,1	0.14	0
5	FMT	A	305	-	2,2,2	0.68	0	1,1,1	0.13	0
5	FMT	F	306	-	2,2,2	0.67	0	1,1,1	0.20	0
3	R1X	C	302	-	9,9,9	1.42	3 (33%)	10,12,12	2.00	4 (40%)
5	FMT	D	305	6	2,2,2	0.70	0	1,1,1	0.12	0
3	R1X	E	302	-	9,9,9	1.19	1 (11%)	10,12,12	1.99	4 (40%)
5	FMT	C	306	-	2,2,2	0.67	0	1,1,1	0.18	0
2	HPA	A	301	-	8,11,11	2.76	4 (50%)	5,15,15	3.62	2 (40%)
5	FMT	D	307	-	2,2,2	0.50	0	1,1,1	0.07	0
5	FMT	A	308	-	2,2,2	0.54	0	1,1,1	0.05	0
5	FMT	A	304	-	2,2,2	0.71	0	1,1,1	0.25	0
4	ART	A	303	-	0,4,4	-	-	0,6,6	-	-
5	FMT	C	309	-	2,2,2	0.56	0	1,1,1	0.03	0
5	FMT	D	308	-	2,2,2	0.58	0	1,1,1	0.05	0
5	FMT	B	304	-	2,2,2	1.14	0	1,1,1	0.21	0
4	ART	B	303	-	0,4,4	-	-	0,6,6	-	-
3	R1X	B	302	-	9,9,9	1.50	3 (33%)	10,12,12	2.56	6 (60%)
5	FMT	C	308	-	2,2,2	0.52	0	1,1,1	0.07	0
3	R1X	F	302	-	9,9,9	1.06	0	10,12,12	1.81	3 (30%)
5	FMT	C	307	-	2,2,2	0.69	0	1,1,1	0.24	0
5	FMT	A	309	-	2,2,2	0.69	0	1,1,1	0.19	0
3	R1X	A	302	-	9,9,9	1.50	3 (33%)	10,12,12	2.55	6 (60%)
4	ART	F	303	-	0,4,4	-	-	0,6,6	-	-
2	HPA	C	301	-	8,11,11	2.17	4 (50%)	5,15,15	3.80	4 (80%)
4	ART	E	303	-	0,4,4	-	-	0,6,6	-	-
5	FMT	F	304	-	2,2,2	0.61	0	1,1,1	0.21	0
2	HPA	F	301	-	8,11,11	2.23	4 (50%)	5,15,15	2.76	2 (40%)
2	HPA	E	301	-	8,11,11	2.37	3 (37%)	5,15,15	3.61	3 (60%)
5	FMT	A	307	-	2,2,2	0.66	0	1,1,1	0.32	0
5	FMT	C	304	-	2,2,2	0.69	0	1,1,1	0.07	0
5	FMT	A	306	-	2,2,2	0.67	0	1,1,1	0.54	0
5	FMT	B	305	-	2,2,2	0.66	0	1,1,1	0.14	0
5	FMT	E	304	-	2,2,2	1.06	0	1,1,1	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HPA	D	301	-	8,11,11	2.29	4 (50%)	5,15,15	3.23	3 (60%)
2	HPA	B	301	-	8,11,11	2.39	4 (50%)	5,15,15	2.84	2 (40%)
4	ART	D	303	-	0,4,4	-	-	0,6,6	-	-
3	R1X	D	302	-	9,9,9	1.20	1 (11%)	10,12,12	2.00	4 (40%)
5	FMT	D	304	6	2,2,2	0.97	0	1,1,1	0.33	0
5	FMT	A	310	-	2,2,2	0.64	0	1,1,1	0.10	0
5	FMT	C	305	-	2,2,2	0.49	0	1,1,1	0.01	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
2	HPA	A	301	-	-	-	0/2/2/2
3	R1X	B	302	-	-	0/2/15/15	0/1/1/1
3	R1X	F	302	-	-	2/2/15/15	0/1/1/1
2	HPA	D	301	-	-	-	0/2/2/2
2	HPA	B	301	-	-	-	0/2/2/2
3	R1X	A	302	-	-	0/2/15/15	0/1/1/1
2	HPA	C	301	-	-	-	0/2/2/2
3	R1X	D	302	-	-	0/2/15/15	0/1/1/1
3	R1X	C	302	-	-	0/2/15/15	0/1/1/1
2	HPA	F	301	-	-	-	0/2/2/2
3	R1X	E	302	-	-	0/2/15/15	0/1/1/1
2	HPA	E	301	-	-	-	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	HPA	C2-N3	4.83	1.39	1.32
2	E	301	HPA	C2-N3	4.12	1.38	1.32
2	E	301	HPA	C6-N1	4.12	1.40	1.33
2	D	301	HPA	C6-N1	3.99	1.40	1.33
2	A	301	HPA	C6-N1	3.90	1.39	1.33
2	B	301	HPA	C2-N3	3.89	1.38	1.32
2	A	301	HPA	C5-C6	-3.63	1.35	1.41
2	F	301	HPA	C2-N3	3.63	1.37	1.32
2	B	301	HPA	C6-N1	3.59	1.39	1.33
2	B	301	HPA	C2-N1	3.54	1.40	1.33
2	D	301	HPA	C2-N3	3.49	1.37	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	HPA	C6-N1	3.35	1.38	1.33
2	F	301	HPA	C6-N1	3.32	1.38	1.33
2	C	301	HPA	C2-N1	3.23	1.39	1.33
2	F	301	HPA	C2-N1	3.07	1.39	1.33
2	A	301	HPA	C2-N1	2.97	1.39	1.33
2	C	301	HPA	C2-N3	2.86	1.36	1.32
2	C	301	HPA	C5-C6	-2.73	1.36	1.41
2	D	301	HPA	C2-N1	2.61	1.38	1.33
3	A	302	R1X	C2-C3	2.47	1.57	1.53
3	A	302	R1X	C1-C2	2.46	1.55	1.51
3	B	302	R1X	C1-C2	2.46	1.55	1.51
2	E	301	HPA	C5-C6	-2.45	1.37	1.41
3	B	302	R1X	C2-C3	2.44	1.57	1.53
3	B	302	R1X	O3-C3	2.42	1.48	1.43
2	F	301	HPA	C5-C6	-2.40	1.37	1.41
3	A	302	R1X	O3-C3	2.38	1.48	1.43
3	C	302	R1X	O3-C3	2.33	1.48	1.43
2	D	301	HPA	C5-C6	-2.31	1.37	1.41
3	D	302	R1X	C2-C3	2.28	1.57	1.53
3	E	302	R1X	C2-C3	2.27	1.57	1.53
2	B	301	HPA	C5-C6	-2.09	1.37	1.41
3	C	302	R1X	C2-C3	2.06	1.57	1.53
3	C	302	R1X	O4-C1	2.02	1.48	1.43

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	HPA	N3-C2-N1	-6.64	118.30	128.68
2	A	301	HPA	N3-C2-N1	-6.31	118.82	128.68
2	E	301	HPA	N3-C2-N1	-6.23	118.94	128.68
2	D	301	HPA	N3-C2-N1	-5.76	119.68	128.68
2	B	301	HPA	N3-C2-N1	-5.18	120.59	128.68
2	F	301	HPA	N3-C2-N1	-4.87	121.06	128.68
3	B	302	R1X	C1-C2-C3	4.61	108.65	101.63
3	A	302	R1X	C1-C2-C3	4.60	108.64	101.63
2	A	301	HPA	C2-N1-C6	4.37	123.19	115.88
2	E	301	HPA	C2-N1-C6	4.25	123.00	115.88
2	C	301	HPA	C2-N1-C6	4.00	122.58	115.88
3	D	302	R1X	O2-C2-C3	3.66	118.19	111.27
3	E	302	R1X	O2-C2-C3	3.65	118.17	111.27
3	F	302	R1X	C1-C2-C3	3.61	107.13	101.63
3	C	302	R1X	O2-C2-C3	3.59	118.06	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	HPA	C2-N1-C6	3.45	121.65	115.88
2	D	301	HPA	C2-N1-C6	3.45	121.65	115.88
3	C	302	R1X	C1-C2-C3	3.31	106.67	101.63
3	B	302	R1X	O4-C4-C3	3.15	107.49	104.70
3	B	302	R1X	O2-C2-C3	3.15	117.23	111.27
3	A	302	R1X	O4-C4-C3	3.15	107.49	104.70
3	A	302	R1X	C1-O4-C4	3.14	115.48	108.16
3	A	302	R1X	O2-C2-C3	3.13	117.20	111.27
3	B	302	R1X	C1-O4-C4	3.13	115.47	108.16
2	B	301	HPA	C2-N1-C6	3.12	121.11	115.88
3	D	302	R1X	C1-C2-C3	2.79	105.88	101.63
3	E	302	R1X	C1-C2-C3	2.79	105.88	101.63
3	F	302	R1X	C1-O4-C4	2.71	114.48	108.16
3	A	302	R1X	O3-C3-C2	2.67	118.48	112.04
3	B	302	R1X	O3-C3-C2	2.67	118.47	112.04
3	C	302	R1X	C1-O4-C4	2.63	114.30	108.16
3	D	302	R1X	C1-O4-C4	2.54	114.09	108.16
3	E	302	R1X	C1-O4-C4	2.53	114.06	108.16
2	C	301	HPA	C2-N3-C4	2.50	119.31	113.45
3	A	302	R1X	O4-C1-C2	-2.36	101.42	105.99
3	B	302	R1X	O4-C1-C2	-2.36	101.42	105.99
2	D	301	HPA	C2-N3-C4	2.35	118.95	113.45
3	C	302	R1X	O4-C1-C2	-2.30	101.55	105.99
3	F	302	R1X	O4-C4-C3	2.18	106.63	104.70
2	E	301	HPA	C2-N3-C4	2.15	118.48	113.45
2	C	301	HPA	C4-C5-C6	-2.04	118.85	120.80
3	E	302	R1X	O3-C3-C2	2.03	116.94	112.04
3	D	302	R1X	O3-C3-C2	2.01	116.90	112.04

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	302	R1X	O4-C4-C5-O5
3	F	302	R1X	C3-C4-C5-O5

There are no ring outliers.

20 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	303	ART	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302	R1X	2	0
3	E	302	R1X	3	0
2	A	301	HPA	2	0
5	A	308	FMT	1	0
4	A	303	ART	1	0
4	B	303	ART	1	0
3	B	302	R1X	2	0
3	F	302	R1X	3	0
3	A	302	R1X	2	0
4	F	303	ART	3	0
2	C	301	HPA	1	0
4	E	303	ART	2	0
2	F	301	HPA	1	0
2	E	301	HPA	2	0
5	E	304	FMT	1	0
2	D	301	HPA	1	0
2	B	301	HPA	1	0
4	D	303	ART	1	0
3	D	302	R1X	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	244/253 (96%)	-0.21	5 (2%)	65	64	6, 14, 24, 34	3 (1%)
1	B	245/253 (96%)	-0.18	6 (2%)	59	58	6, 13, 23, 35	2 (0%)
1	C	246/253 (97%)	-0.18	6 (2%)	59	58	7, 12, 23, 36	2 (0%)
1	D	244/253 (96%)	-0.23	9 (3%)	41	41	7, 14, 25, 38	4 (1%)
1	E	243/253 (96%)	-0.10	10 (4%)	37	37	10, 18, 29, 40	3 (1%)
1	F	243/253 (96%)	-0.04	12 (4%)	29	29	11, 18, 28, 37	1 (0%)
All	All	1465/1518 (96%)	-0.16	48 (3%)	46	46	6, 15, 26, 40	15 (1%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	245	ALA	6.1
1	C	3	ASN	6.1
1	E	3	ASN	5.8
1	D	3	ASN	5.6
1	B	3	ASN	5.2
1	A	3	ASN	4.7
1	F	3	ASN	4.2
1	F	216	ASP	3.3
1	D	214	GLU	3.3
1	F	219	ASN	3.3
1	F	215	GLY	3.2
1	B	247	GLU	3.2
1	A	246	LEU	3.1
1	B	214	GLU	3.0
1	E	214	GLU	3.0
1	B	219	ASN	2.9
1	A	219	ASN	2.9
1	C	219	ASN	2.8
1	F	211	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	213	ASP	2.7
1	B	224[A]	HIS	2.6
1	F	213	ASP	2.6
1	D	224[A]	HIS	2.6
1	E	13	GLU	2.6
1	F	244	TYR	2.6
1	F	146	ASN	2.6
1	E	213	ASP	2.5
1	E	224[A]	HIS	2.5
1	D	220	ASN	2.5
1	E	219	ASN	2.4
1	C	248	HIS	2.4
1	F	185	LEU	2.4
1	D	215	GLY	2.4
1	E	66	VAL	2.4
1	A	220	ASN	2.4
1	A	213	ASP	2.4
1	B	216	ASP	2.4
1	D	213	ASP	2.4
1	F	143	GLN	2.3
1	F	218	ASP	2.3
1	E	244	TYR	2.2
1	F	220	ASN	2.2
1	D	223	PRO	2.2
1	D	99	LEU	2.2
1	C	214	GLU	2.2
1	E	216	ASP	2.1
1	C	71	CYS	2.1
1	D	219	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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	R1X	F	302	9/9	0.69	0.30	21,27,28,29	9
3	R1X	D	302	9/9	0.70	0.25	20,28,30,30	9
3	R1X	E	302	9/9	0.73	0.28	20,28,30,30	9
5	FMT	A	310	3/3	0.75	0.32	60,60,60,61	0
3	R1X	C	302	9/9	0.77	0.20	17,23,25,25	9
3	R1X	A	302	9/9	0.78	0.23	16,22,27,27	9
5	FMT	C	309	3/3	0.78	0.23	46,46,46,47	0
5	FMT	B	305	3/3	0.79	0.20	52,52,53,54	0
5	FMT	C	305	3/3	0.82	0.22	40,40,41,42	0
3	R1X	B	302	9/9	0.82	0.19	16,22,27,27	9
5	FMT	F	306	3/3	0.85	0.15	56,56,57,57	0
5	FMT	C	308	3/3	0.86	0.16	38,38,41,43	0
5	FMT	D	305	3/3	0.87	0.18	46,46,46,47	0
5	FMT	D	307	3/3	0.89	0.19	34,34,38,42	0
5	FMT	A	306	3/3	0.89	0.24	47,47,49,50	0
6	NA	B	306	1/1	0.89	0.14	54,54,54,54	0
5	FMT	A	309	3/3	0.90	0.17	50,50,51,51	0
5	FMT	A	305	3/3	0.90	0.15	58,58,59,59	0
6	NA	D	310	1/1	0.90	0.09	46,46,46,46	0
5	FMT	D	306	3/3	0.91	0.30	36,36,37,37	0
5	FMT	B	304	3/3	0.91	0.25	39,39,39,39	0
5	FMT	D	308	3/3	0.91	0.19	49,49,49,49	0
5	FMT	E	304	3/3	0.92	0.27	33,33,33,34	0
5	FMT	A	308	3/3	0.92	0.12	42,42,44,45	0
5	FMT	D	304	3/3	0.94	0.09	35,35,37,40	0
5	FMT	C	304	3/3	0.94	0.17	35,35,37,38	0
5	FMT	C	307	3/3	0.94	0.22	44,44,45,45	0
2	HPA	C	301	10/10	0.95	0.09	20,23,24,24	0
2	HPA	D	301	10/10	0.95	0.09	20,24,25,26	0
5	FMT	F	305	3/3	0.95	0.26	34,34,36,37	0
5	FMT	C	306	3/3	0.95	0.24	56,56,57,57	0
5	FMT	A	307	3/3	0.95	0.36	45,45,45,45	0
2	HPA	E	301	10/10	0.95	0.09	15,20,23,23	0
2	HPA	F	301	10/10	0.96	0.07	24,26,28,28	0
5	FMT	F	304	3/3	0.96	0.22	35,35,38,40	0
2	HPA	A	301	10/10	0.96	0.07	18,21,22,22	0
2	HPA	B	301	10/10	0.97	0.06	17,20,24,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FMT	A	304	3/3	0.98	0.24	30,30,30,31	0
6	NA	A	311	1/1	0.99	0.06	12,12,12,12	0
4	ART	B	303	5/5	0.99	0.07	20,20,25,27	0
6	NA	C	310	1/1	0.99	0.04	12,12,12,12	0
6	NA	D	309	1/1	0.99	0.07	12,12,12,12	0
4	ART	F	303	5/5	0.99	0.10	31,34,36,36	5
4	ART	D	303	5/5	1.00	0.09	27,28,30,31	0
4	ART	E	303	5/5	1.00	0.06	23,24,26,26	0
4	ART	A	303	5/5	1.00	0.07	22,23,26,27	0
4	ART	C	303	5/5	1.00	0.06	21,23,24,25	0

6.5 Other polymers (i)

There are no such residues in this entry.