Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 02:49 AM EDT

PDB ID	:	3JZE
Title	:	1.8 Angstrom resolution crystal structure of dihydroorotase (pyrC) from Salmonella enterica subsp. enterica serovar Typhimurium str. LT2
Authors	:	Minasov, G.; Halavaty, A.; Shuvalova, L.; Dubrovska, I.; Winsor, J.; Papazisi, L.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2009-09-23
Resolution	:	1.80 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 (i) 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 (i)) were used in the production of this report:

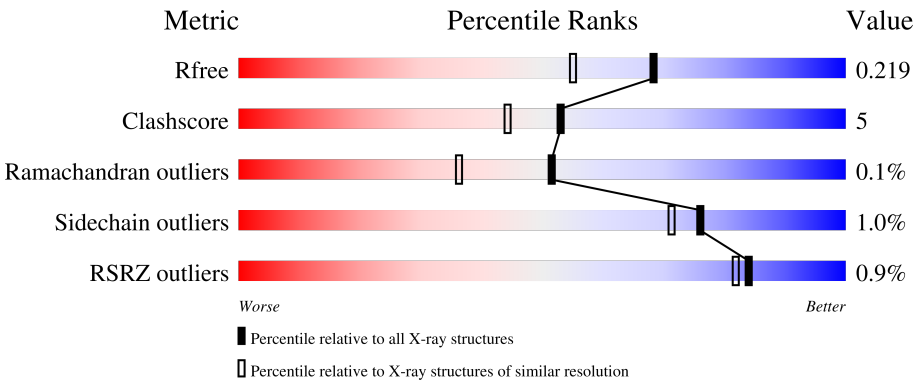
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	372	.% 81% 12% 8%
1	B	372	% 81% 10% • 8%
1	C	372	.% 84% 8% 8%
1	D	372	.% 81% 10% 8%

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
6	ACY	B	425	-	-	X	-
6	ACY	B	428	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12498 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 Dihydroorotase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	344	2759	1739	489	515	16	0	8	0
1	B	342	2770	1746	491	517	16	0	11	0
1	C	344	2753	1737	485	515	16	0	8	0
1	D	342	2754	1737	489	510	18	0	9	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP P06204
A	-22	HIS	-	expression tag	UNP P06204
A	-21	HIS	-	expression tag	UNP P06204
A	-20	HIS	-	expression tag	UNP P06204
A	-19	HIS	-	expression tag	UNP P06204
A	-18	HIS	-	expression tag	UNP P06204
A	-17	HIS	-	expression tag	UNP P06204
A	-16	SER	-	expression tag	UNP P06204
A	-15	SER	-	expression tag	UNP P06204
A	-14	GLY	-	expression tag	UNP P06204
A	-13	VAL	-	expression tag	UNP P06204
A	-12	ASP	-	expression tag	UNP P06204
A	-11	LEU	-	expression tag	UNP P06204
A	-10	GLY	-	expression tag	UNP P06204
A	-9	THR	-	expression tag	UNP P06204
A	-8	GLU	-	expression tag	UNP P06204
A	-7	ASN	-	expression tag	UNP P06204
A	-6	LEU	-	expression tag	UNP P06204
A	-5	TYR	-	expression tag	UNP P06204
A	-4	PHE	-	expression tag	UNP P06204
A	-3	GLN	-	expression tag	UNP P06204

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P06204
A	-1	ASN	-	expression tag	UNP P06204
A	0	ALA	-	expression tag	UNP P06204
B	-23	MET	-	expression tag	UNP P06204
B	-22	HIS	-	expression tag	UNP P06204
B	-21	HIS	-	expression tag	UNP P06204
B	-20	HIS	-	expression tag	UNP P06204
B	-19	HIS	-	expression tag	UNP P06204
B	-18	HIS	-	expression tag	UNP P06204
B	-17	HIS	-	expression tag	UNP P06204
B	-16	SER	-	expression tag	UNP P06204
B	-15	SER	-	expression tag	UNP P06204
B	-14	GLY	-	expression tag	UNP P06204
B	-13	VAL	-	expression tag	UNP P06204
B	-12	ASP	-	expression tag	UNP P06204
B	-11	LEU	-	expression tag	UNP P06204
B	-10	GLY	-	expression tag	UNP P06204
B	-9	THR	-	expression tag	UNP P06204
B	-8	GLU	-	expression tag	UNP P06204
B	-7	ASN	-	expression tag	UNP P06204
B	-6	LEU	-	expression tag	UNP P06204
B	-5	TYR	-	expression tag	UNP P06204
B	-4	PHE	-	expression tag	UNP P06204
B	-3	GLN	-	expression tag	UNP P06204
B	-2	SER	-	expression tag	UNP P06204
B	-1	ASN	-	expression tag	UNP P06204
B	0	ALA	-	expression tag	UNP P06204
C	-23	MET	-	expression tag	UNP P06204
C	-22	HIS	-	expression tag	UNP P06204
C	-21	HIS	-	expression tag	UNP P06204
C	-20	HIS	-	expression tag	UNP P06204
C	-19	HIS	-	expression tag	UNP P06204
C	-18	HIS	-	expression tag	UNP P06204
C	-17	HIS	-	expression tag	UNP P06204
C	-16	SER	-	expression tag	UNP P06204
C	-15	SER	-	expression tag	UNP P06204
C	-14	GLY	-	expression tag	UNP P06204
C	-13	VAL	-	expression tag	UNP P06204
C	-12	ASP	-	expression tag	UNP P06204
C	-11	LEU	-	expression tag	UNP P06204
C	-10	GLY	-	expression tag	UNP P06204
C	-9	THR	-	expression tag	UNP P06204

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLU	-	expression tag	UNP P06204
C	-7	ASN	-	expression tag	UNP P06204
C	-6	LEU	-	expression tag	UNP P06204
C	-5	TYR	-	expression tag	UNP P06204
C	-4	PHE	-	expression tag	UNP P06204
C	-3	GLN	-	expression tag	UNP P06204
C	-2	SER	-	expression tag	UNP P06204
C	-1	ASN	-	expression tag	UNP P06204
C	0	ALA	-	expression tag	UNP P06204
D	-23	MET	-	expression tag	UNP P06204
D	-22	HIS	-	expression tag	UNP P06204
D	-21	HIS	-	expression tag	UNP P06204
D	-20	HIS	-	expression tag	UNP P06204
D	-19	HIS	-	expression tag	UNP P06204
D	-18	HIS	-	expression tag	UNP P06204
D	-17	HIS	-	expression tag	UNP P06204
D	-16	SER	-	expression tag	UNP P06204
D	-15	SER	-	expression tag	UNP P06204
D	-14	GLY	-	expression tag	UNP P06204
D	-13	VAL	-	expression tag	UNP P06204
D	-12	ASP	-	expression tag	UNP P06204
D	-11	LEU	-	expression tag	UNP P06204
D	-10	GLY	-	expression tag	UNP P06204
D	-9	THR	-	expression tag	UNP P06204
D	-8	GLU	-	expression tag	UNP P06204
D	-7	ASN	-	expression tag	UNP P06204
D	-6	LEU	-	expression tag	UNP P06204
D	-5	TYR	-	expression tag	UNP P06204
D	-4	PHE	-	expression tag	UNP P06204
D	-3	GLN	-	expression tag	UNP P06204
D	-2	SER	-	expression tag	UNP P06204
D	-1	ASN	-	expression tag	UNP P06204
D	0	ALA	-	expression tag	UNP P06204

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0
			Total	Zn		
2	B	2	2	2	0	0
			Total	Zn		
2	C	2	2	2	0	0

Continued on next page...

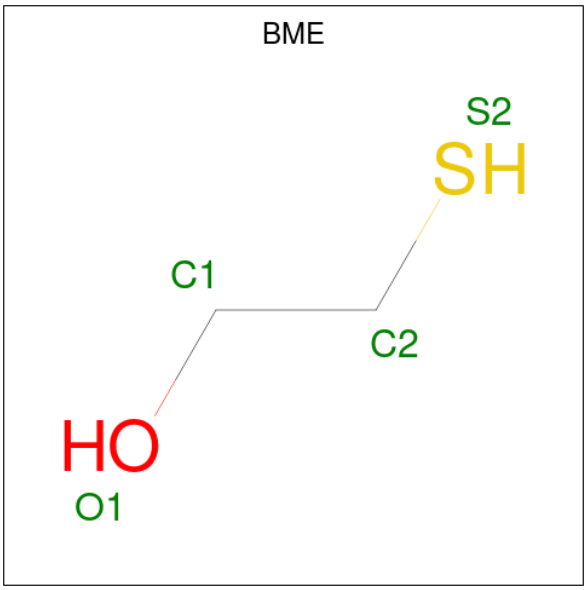
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	D	2	2	2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	1	1	1	0	0
			Total	Cl		
3	C	1	1	1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



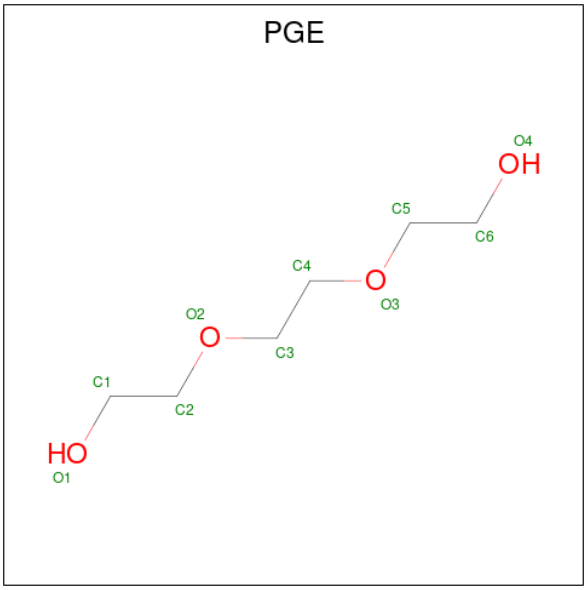
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
4	A	1	4	2	1	1	0	0
			Total	C	O	S		
4	A	1	4	2	1	1	0	0
			Total	C	O	S		
4	B	1	4	2	1	1	0	0
			Total	C	O	S		
4	B	1	4	2	1	1	0	0
			Total	C	O	S		
4	C	1	4	2	1	1	0	0
			Total	C	O	S		
4	C	1	4	2	1	1	0	0

Continued on next page...

Continued from previous page...

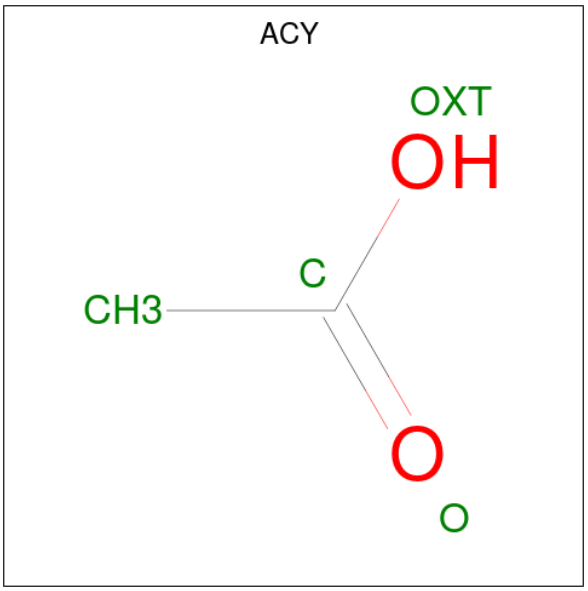
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
4	D	1	4	2	1	1	0	0
			Total	C	O	S		
4	D	1	4	2	1	1	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



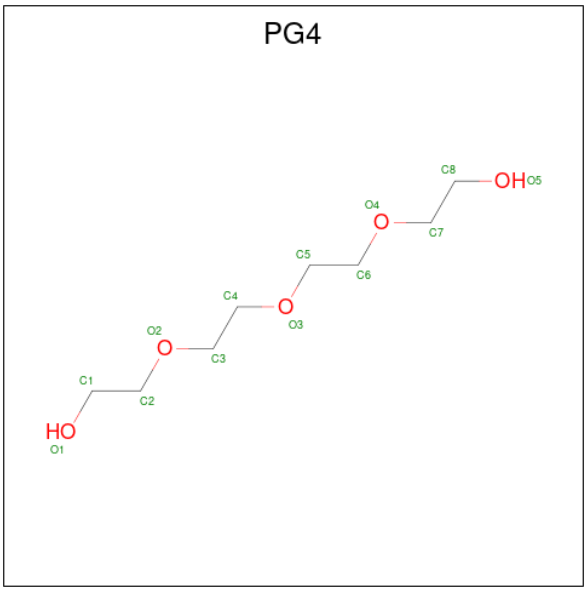
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	10	6	4	0	0
			Total	C	O		
5	C	1	10	6	4	0	0

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0
6	B	1	4	2	2	0	0
6	B	1	4	2	2	0	0
6	C	1	4	2	2	0	0
6	D	1	4	2	2	0	0
6	D	1	4	2	2	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	B	1	13	8	5	0	0
			Total	C	O		
7	D	1	13	8	5	0	0

- Molecule 8 is water.

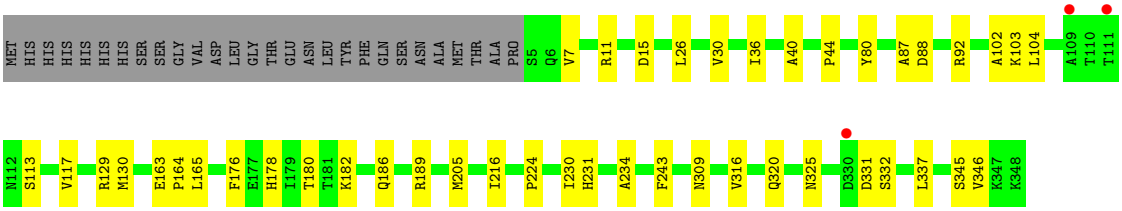
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	282	289	289	0	8
			Total	O		
8	B	360	362	362	0	2
			Total	O		
8	C	320	327	327	0	9
			Total	O		
8	D	366	372	372	0	7

3 Residue-property plots (i)

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.

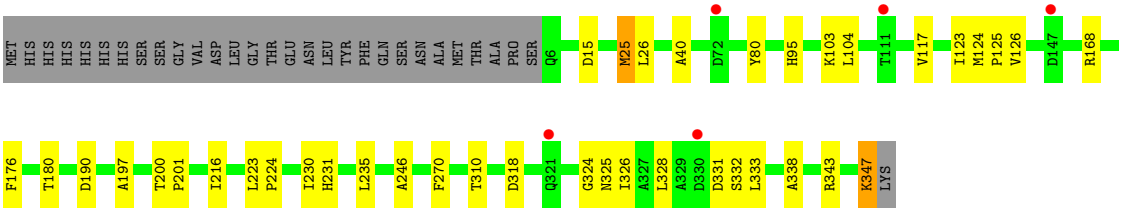
• Molecule 1: Dihydroorotase

Chain A:



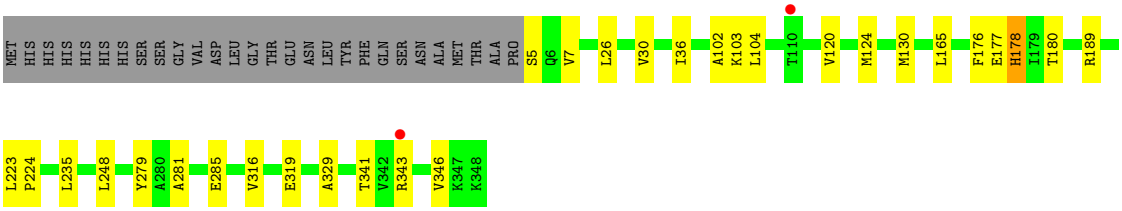
• Molecule 1: Dihydroorotase

Chain B:



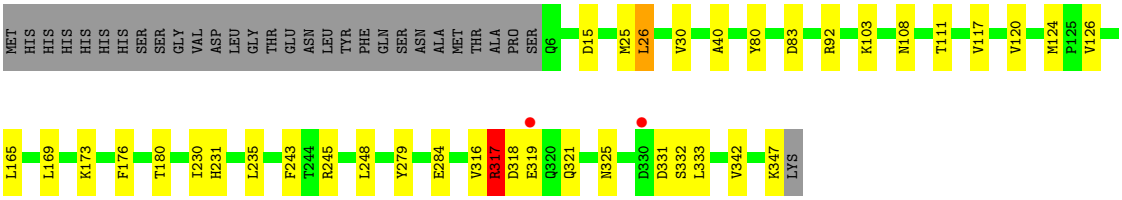
• Molecule 1: Dihydroorotase

Chain C:



• Molecule 1: Dihydroorotase

Chain D:


MET
HIS
HIS
HIS
HIS
HIS
HIS
SER
SER
GLY
VAL
ASP
LEU
GLY
THR
GLU
ASN
LEU
TYR
PHE
GLN
SER
ASN
ALA
MET
THR
ALA
PRO
SER
Q6
D15
M25
L26
V30
A40
Y80
D83
R92
K103
N108
T111
V117
V120
M124
P125
V126

L165
L169
K173
F176
T180
I230
H231
L235
F243
T244
R245
L248
Y279
E284
V316
R317
D318
E319
Q320
Q321
N325
D330
D331
S332
L333
V342
K347
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.44Å 79.49Å 180.61Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	29.83 – 1.80 29.83 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.83-1.80) 96.9 (29.83-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.163 , 0.203 0.181 , 0.219	Depositor DCC
R_{free} test set	6557 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 27.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.397 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12498	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BME, PGE, CL, PG4, KCX, ACY, ZN

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	0.51	0/2809	0.71	0/3818
1	B	0.58	0/2821	0.74	0/3838
1	C	0.52	0/2803	0.71	0/3812
1	D	0.59	0/2805	0.74	0/3814
All	All	0.55	0/11238	0.72	0/15282

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2759	0	2699	38	0
1	B	2770	0	2700	28	0
1	C	2753	0	2694	22	0
1	D	2754	0	2692	29	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	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	C	1	0	0	0	0
4	A	8	0	10	0	0
4	B	8	0	10	0	0
4	C	8	0	10	0	0
4	D	8	0	10	0	0
5	A	10	0	14	0	0
5	C	10	0	14	0	0
6	A	4	0	3	0	0
6	B	8	0	6	4	0
6	C	4	0	3	0	0
6	D	8	0	6	0	0
7	B	13	0	18	0	0
7	D	13	0	18	1	0
8	A	289	0	0	0	0
8	B	362	0	0	7	0
8	C	327	0	0	3	0
8	D	372	0	0	3	0
All	All	12498	0	10907	120	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 5.

All (120) 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)
6:B:425:ACY:H1	6:B:428:ACY:H2	1.33	1.08
1:A:11[B]:ARG:HH11	1:A:11[B]:ARG:HG2	1.23	1.03
1:A:11[B]:ARG:HH11	1:A:11[B]:ARG:CG	1.79	0.94
1:D:317:ARG:HH11	1:D:317:ARG:HG3	1.34	0.92
6:B:425:ACY:H3	8:B:575:HOH:O	1.80	0.82
6:B:425:ACY:H1	6:B:428:ACY:CH3	2.13	0.79
1:A:11[B]:ARG:HG2	1:A:11[B]:ARG:NH1	1.99	0.73
1:D:230:ILE:HD12	1:D:231:HIS:N	2.06	0.70
1:A:230:ILE:HD12	1:A:231:HIS:N	2.07	0.70
1:C:281:ALA:HB1	1:C:343:ARG:NH2	2.11	0.66
1:C:36:ILE:HD12	1:C:346:VAL:HG11	1.78	0.65
1:A:26:LEU:C	1:A:26:LEU:HD23	2.18	0.65
1:D:25[B]:MET:SD	1:D:333:LEU:HD11	2.37	0.65
1:A:36:ILE:HD12	1:A:346:VAL:HG11	1.80	0.64
1:B:95[A]:HIS:ND1	8:B:998:HOH:O	2.30	0.63
1:A:11[B]:ARG:HH11	1:A:11[B]:ARG:CB	2.11	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25[B]:MET:HE1	1:D:333:LEU:HD21	1.81	0.62
1:C:120:VAL:HG12	1:C:124:MET:CE	2.29	0.61
1:B:310[B]:THR:HG23	8:B:1009:HOH:O	1.99	0.61
1:D:26:LEU:C	1:D:26:LEU:HD23	2.21	0.61
1:B:25:MET:CE	1:B:333:LEU:HD21	2.32	0.60
6:B:425:ACY:CH3	6:B:428:ACY:H2	2.20	0.60
1:A:165:LEU:C	1:A:165:LEU:HD23	2.23	0.59
1:C:26:LEU:C	1:C:26:LEU:HD23	2.23	0.59
1:B:347:LYS:HE3	1:B:347:LYS:HA	1.85	0.59
1:A:230:ILE:HD11	1:A:231:HIS:CD2	2.38	0.58
1:B:230:ILE:HD12	1:B:231:HIS:N	2.19	0.58
1:C:26:LEU:O	1:C:30:VAL:HG23	2.03	0.57
1:A:325:ASN:OD1	1:A:332:SER:HB2	2.04	0.56
1:A:178:HIS:CE1	1:A:224:PRO:HD3	2.40	0.56
1:B:26:LEU:C	1:B:26:LEU:HD23	2.26	0.56
1:D:317:ARG:HG3	1:D:317:ARG:NH1	2.09	0.55
1:A:104:LEU:CD1	1:A:117:VAL:HG21	2.36	0.55
1:C:120:VAL:HG12	1:C:124:MET:HE2	1.89	0.53
1:A:7:VAL:HG22	1:A:316[A]:VAL:HG12	1.89	0.53
1:D:126:VAL:HG23	8:D:631:HOH:O	2.09	0.53
1:A:180:THR:HG21	1:A:224:PRO:HB2	1.91	0.52
1:A:102:ALA:HB3	1:A:130:MET:CE	2.39	0.52
1:B:104:LEU:HD11	1:B:117:VAL:HG21	1.90	0.52
1:A:11[B]:ARG:CG	1:A:11[B]:ARG:NH1	2.51	0.52
1:A:331[B]:ASP:N	1:A:331[B]:ASP:OD1	2.43	0.52
1:B:117:VAL:HG11	1:B:123:ILE:HD13	1.92	0.52
1:A:230:ILE:HD11	1:A:231:HIS:NE2	2.24	0.52
1:C:165:LEU:HD23	1:C:165:LEU:C	2.31	0.51
1:C:223:LEU:HD11	8:D:588:HOH:O	2.09	0.51
1:B:25:MET:HE2	1:B:333:LEU:HD21	1.93	0.51
1:A:11[B]:ARG:HD2	1:A:309:ASN:O	2.10	0.51
1:A:11[B]:ARG:NH1	1:A:11[B]:ARG:CB	2.75	0.50
1:A:11[B]:ARG:NH1	1:A:11[B]:ARG:HB2	2.26	0.49
1:A:163:GLU:HB3	1:A:164:PRO:HD3	1.94	0.49
1:B:343:ARG:HD2	8:B:454:HOH:O	2.12	0.49
1:B:270:PHE:HE2	1:B:326:ILE:HD12	1.78	0.49
1:A:87:ALA:HB1	1:A:129:ARG:HG3	1.94	0.49
1:A:165:LEU:HD23	1:A:165:LEU:O	2.13	0.48
1:C:285:GLU:OE2	1:C:343:ARG:NH2	2.47	0.48
1:D:165:LEU:HD11	1:D:169:LEU:HD12	1.95	0.48
1:C:7:VAL:HG22	1:C:316[A]:VAL:HG12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:VAL:HG11	1:D:347:LYS:HD3	1.95	0.47
1:D:173:LYS:HE2	7:D:422:PG4:H32	1.97	0.47
1:C:180:THR:HA	1:C:235:LEU:HD11	1.96	0.47
1:D:248:LEU:HG	1:D:279:TYR:CE2	2.51	0.46
1:D:120:VAL:HG11	1:D:165:LEU:HD13	1.97	0.46
1:D:319:GLU:HA	1:D:342:VAL:O	2.15	0.46
1:D:180:THR:HA	1:D:235:LEU:HD11	1.98	0.46
1:D:124[A]:MET:HE1	1:D:169:LEU:HD11	1.96	0.46
1:B:230:ILE:HD12	1:B:230:ILE:C	2.36	0.46
1:C:329:ALA:HB3	8:C:918:HOH:O	2.16	0.46
1:B:126:VAL:HG23	8:B:508[A]:HOH:O	2.16	0.46
1:C:189[B]:ARG:CZ	8:C:563:HOH:O	2.63	0.46
1:D:284:GLU:OE2	1:D:317:ARG:NH2	2.45	0.46
1:A:26:LEU:O	1:A:30:VAL:HG23	2.16	0.46
1:B:168[A]:ARG:CZ	1:B:168[A]:ARG:HB2	2.45	0.45
1:C:248:LEU:HG	1:C:279:TYR:CE2	2.51	0.45
1:B:200:THR:HB	1:B:201:PRO:HD2	1.97	0.45
1:C:281:ALA:HB1	1:C:343:ARG:HH21	1.82	0.45
1:B:318[A]:ASP:C	1:B:318[A]:ASP:OD1	2.53	0.45
1:D:243:PHE:CZ	1:D:245:ARG:HB2	2.52	0.45
1:A:320[B]:GLN:CD	1:A:345[B]:SER:CB	2.85	0.45
1:B:331:ASP:CG	1:B:332:SER:H	2.20	0.45
1:B:124:MET:N	1:B:125:PRO:CD	2.80	0.44
1:D:230:ILE:HD12	1:D:231:HIS:H	1.79	0.44
1:D:15:ASP:O	1:D:40:ALA:HA	2.18	0.44
1:A:216:ILE:HD11	1:B:216:ILE:HD11	2.00	0.43
1:C:5:SER:N	8:C:567:HOH:O	2.50	0.43
1:C:102:ALA:HB3	1:C:130:MET:CE	2.47	0.43
1:B:15:ASP:O	1:B:40:ALA:HA	2.18	0.43
1:C:26:LEU:HD23	1:C:26:LEU:O	2.18	0.43
1:C:319[A]:GLU:OE1	1:C:341:THR:HG21	2.18	0.43
1:B:25:MET:HE2	1:B:328:LEU:HD11	2.00	0.43
1:D:25[B]:MET:CE	1:D:333:LEU:HD21	2.48	0.43
1:C:177:GLU:O	1:C:178:HIS:C	2.57	0.43
1:B:190:ASP:OD2	8:B:1211:HOH:O	2.22	0.43
1:A:230:ILE:HD12	1:A:230:ILE:C	2.40	0.42
1:A:26:LEU:C	1:A:26:LEU:CD2	2.87	0.42
1:A:80:TYR:OH	1:A:113:SER:HA	2.19	0.42
1:C:104:LEU:C	1:C:104:LEU:HD23	2.40	0.42
1:C:178:HIS:CE1	1:C:224:PRO:HD3	2.55	0.42
1:D:321:GLN:NE2	8:D:1232:HOH:O	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ASP:CG	1:D:332:SER:H	2.22	0.42
1:D:317:ARG:NH1	1:D:317:ARG:CG	2.79	0.41
1:A:88:ASP:O	1:A:92:ARG:HG2	2.21	0.41
1:A:182:LYS:HG3	1:A:234:ALA:CB	2.51	0.41
1:B:223:LEU:HA	1:B:224:PRO:C	2.40	0.41
1:D:92[A]:ARG:CZ	1:D:92[A]:ARG:HB2	2.50	0.41
1:A:15:ASP:O	1:A:40:ALA:HA	2.20	0.41
1:D:83:ASP:OD1	1:D:117:VAL:HA	2.21	0.41
1:B:197:ALA:O	1:B:246:ALA:HA	2.21	0.41
1:D:124[A]:MET:CE	1:D:169:LEU:HD11	2.50	0.41
1:A:230:ILE:CD1	1:A:231:HIS:CD2	3.03	0.41
1:B:168[A]:ARG:NH2	8:B:1025:HOH:O	2.31	0.41
1:D:108:ASN:O	1:D:111:THR:HG22	2.21	0.41
1:A:189[A]:ARG:HA	1:A:243:PHE:CE1	2.56	0.40
1:B:180:THR:HG21	1:B:224:PRO:HB2	2.03	0.40
1:D:26:LEU:O	1:D:30:VAL:HG23	2.21	0.40
1:A:205:MET:CE	1:A:337:LEU:HD11	2.51	0.40
1:A:44:PRO:HB2	1:A:80:TYR:HB2	2.03	0.40
1:A:182:LYS:NZ	1:A:186:GLN:OE1	2.53	0.40
1:B:180:THR:HA	1:B:235:LEU:HD11	2.03	0.40
1:D:316:VAL:C	1:D:318:ASP:H	2.25	0.40
1:B:324:GLY:HA2	1:B:338:ALA:HB1	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	349/372 (94%)	334 (96%)	15 (4%)	0	100	100
1	B	350/372 (94%)	343 (98%)	7 (2%)	0	100	100
1	C	349/372 (94%)	336 (96%)	12 (3%)	1 (0%)	41	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	348/372 (94%)	338 (97%)	9 (3%)	1 (0%)	41	27
All	All	1396/1488 (94%)	1351 (97%)	43 (3%)	2 (0%)	51	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	317	ARG
1	C	178	HIS

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	295/311 (95%)	294 (100%)	1 (0%)	92	91
1	B	296/311 (95%)	291 (98%)	5 (2%)	60	51
1	C	295/311 (95%)	294 (100%)	1 (0%)	92	91
1	D	294/311 (94%)	289 (98%)	5 (2%)	60	51
All	All	1180/1244 (95%)	1168 (99%)	12 (1%)	76	71

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	PHE
1	B	25	MET
1	B	80	TYR
1	B	176	PHE
1	B	325	ASN
1	B	347	LYS
1	C	176	PHE
1	D	26	LEU
1	D	80	TYR
1	D	176	PHE
1	D	317	ARG
1	D	325	ASN

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

Mol	Chain	Res	Type
1	B	115	HIS
1	D	325	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	KCX	A	103	2,1	9,11,12	1.37	2 (22%)	5,12,14	2.37	1 (20%)
1	KCX	D	103	2,1	9,11,12	1.46	2 (22%)	5,12,14	1.87	1 (20%)
1	KCX	C	103	2,1	9,11,12	1.18	1 (11%)	5,12,14	2.60	1 (20%)
1	KCX	B	103	2,1	9,11,12	1.38	2 (22%)	5,12,14	0.91	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
1	KCX	A	103	2,1	-	0/9/10/12	-
1	KCX	D	103	2,1	-	0/9/10/12	-
1	KCX	C	103	2,1	-	0/9/10/12	-
1	KCX	B	103	2,1	-	0/9/10/12	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	103	KCX	OQ1-CX	3.20	1.27	1.21
1	B	103	KCX	OQ1-CX	2.90	1.27	1.21
1	A	103	KCX	CE-NZ	2.71	1.52	1.46
1	C	103	KCX	CE-NZ	2.39	1.51	1.46
1	B	103	KCX	CE-NZ	2.35	1.51	1.46
1	D	103	KCX	CE-NZ	2.31	1.51	1.46
1	A	103	KCX	OQ1-CX	2.11	1.25	1.21

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	103	KCX	OQ1-CX-NZ	-5.66	116.19	124.96
1	A	103	KCX	OQ1-CX-NZ	-5.21	116.88	124.96
1	D	103	KCX	OQ1-CX-NZ	-3.73	119.18	124.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 10 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
4	BME	C	412	1	3,3,3	0.46	0	1,2,2	0.37	0
4	BME	D	414	1	3,3,3	0.58	0	1,2,2	0.08	0
4	BME	B	413	1	3,3,3	0.36	0	1,2,2	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	PG4	D	422	-	12,12,12	0.44	0	11,11,11	0.24	0
5	PGE	A	420	-	9,9,9	0.41	0	8,8,8	0.16	0
4	BME	D	418	1	3,3,3	0.31	0	1,2,2	0.53	0
5	PGE	C	421	-	9,9,9	0.45	0	8,8,8	0.33	0
7	PG4	B	419	-	12,12,12	0.42	0	11,11,11	0.30	0
4	BME	A	415	1	3,3,3	0.37	0	1,2,2	0.32	0
6	ACY	D	427	2	3,3,3	0.79	0	3,3,3	0.71	0
4	BME	B	417	1	3,3,3	0.30	0	1,2,2	0.58	0
6	ACY	B	425	-	3,3,3	0.70	0	3,3,3	1.07	0
4	BME	C	416	1	3,3,3	0.37	0	1,2,2	0.26	0
6	ACY	C	424	-	3,3,3	0.67	0	3,3,3	0.84	0
6	ACY	A	423	-	3,3,3	0.79	0	3,3,3	0.66	0
6	ACY	D	426	-	3,3,3	0.72	0	3,3,3	0.96	0
6	ACY	B	428	2	3,3,3	0.87	0	3,3,3	0.74	0
4	BME	A	411	1	3,3,3	0.41	0	1,2,2	0.19	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	BME	C	412	1	-	0/1/1/1	-
4	BME	D	414	1	-	1/1/1/1	-
4	BME	B	413	1	-	1/1/1/1	-
5	PGE	A	420	-	-	3/7/7/7	-
4	BME	D	418	1	-	1/1/1/1	-
5	PGE	C	421	-	-	3/7/7/7	-
7	PG4	B	419	-	-	6/10/10/10	-
4	BME	A	415	1	-	1/1/1/1	-
4	BME	B	417	1	-	1/1/1/1	-
4	BME	C	416	1	-	0/1/1/1	-
7	PG4	D	422	-	-	5/10/10/10	-
4	BME	A	411	1	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	415	BME	O1-C1-C2-S2
4	B	417	BME	O1-C1-C2-S2
5	A	420	PGE	O1-C1-C2-O2
5	A	420	PGE	O2-C3-C4-O3
7	D	422	PG4	O3-C5-C6-O4
7	B	419	PG4	O4-C7-C8-O5
7	D	422	PG4	O1-C1-C2-O2
7	B	419	PG4	O2-C3-C4-O3
4	D	414	BME	O1-C1-C2-S2
4	D	418	BME	O1-C1-C2-S2
7	B	419	PG4	O3-C5-C6-O4
7	D	422	PG4	O4-C7-C8-O5
5	C	421	PGE	O1-C1-C2-O2
5	A	420	PGE	C6-C5-O3-C4
7	D	422	PG4	O2-C3-C4-O3
7	B	419	PG4	C8-C7-O4-C6
7	B	419	PG4	C4-C3-O2-C2
5	C	421	PGE	C1-C2-O2-C3
4	B	413	BME	O1-C1-C2-S2
7	D	422	PG4	C6-C5-O3-C4
5	C	421	PGE	C3-C4-O3-C5
7	B	419	PG4	C6-C5-O3-C4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	422	PG4	1	0
6	B	425	ACY	4	0
6	B	428	ACY	3	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	343/372 (92%)	0.07	3 (0%)	84	82	10, 20, 29, 48	0
1	B	341/372 (91%)	-0.01	5 (1%)	73	70	11, 18, 27, 34	0
1	C	343/372 (92%)	0.06	2 (0%)	89	87	14, 20, 31, 47	0
1	D	341/372 (91%)	-0.02	2 (0%)	89	87	12, 18, 27, 39	0
All	All	1368/1488 (91%)	0.02	12 (0%)	84	82	10, 19, 29, 48	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	330[A]	ASP	4.0
1	A	109	ALA	3.3
1	B	111[A]	THR	2.9
1	B	321	GLN	2.5
1	A	330[A]	ASP	2.5
1	D	330	ASP	2.5
1	C	343	ARG	2.4
1	C	110	THR	2.2
1	A	111	THR	2.2
1	D	319	GLU	2.2
1	B	72[A]	ASP	2.1
1	B	147	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KCX	D	103	12/13	0.84	0.12	15,18,25,26	0
1	KCX	C	103	12/13	0.85	0.12	18,21,28,29	0
1	KCX	A	103	12/13	0.85	0.14	16,17,27,28	0
1	KCX	B	103	12/13	0.91	0.11	14,16,24,25	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PG4	D	422	13/13	0.78	0.19	45,47,53,54	13
6	ACY	D	426	4/4	0.81	0.16	37,39,39,39	0
5	PGE	A	420	10/10	0.82	0.23	45,47,53,55	10
6	ACY	D	427	4/4	0.86	0.29	31,32,33,33	4
7	PG4	B	419	13/13	0.87	0.16	42,44,50,52	13
5	PGE	C	421	10/10	0.87	0.20	47,49,51,51	10
4	BME	D	414	4/4	0.88	0.13	25,26,27,31	4
6	ACY	B	428	4/4	0.88	0.15	28,31,32,32	4
3	CL	C	409	1/1	0.89	0.16	63,63,63,63	0
4	BME	C	412	4/4	0.92	0.12	24,27,30,32	4
3	CL	A	410	1/1	0.93	0.18	63,63,63,63	0
6	ACY	C	424	4/4	0.93	0.12	37,37,38,39	0
4	BME	B	413	4/4	0.94	0.11	28,30,31,35	4
4	BME	D	418	4/4	0.94	0.23	28,33,34,36	4
4	BME	B	417	4/4	0.94	0.25	23,25,28,32	4
4	BME	A	415	4/4	0.94	0.24	27,27,29,31	4
4	BME	C	416	4/4	0.94	0.26	25,29,30,34	4
6	ACY	A	423	4/4	0.95	0.12	34,36,37,38	1
2	ZN	D	408	1/1	0.96	0.08	27,27,27,27	1
4	BME	A	411	4/4	0.96	0.10	26,30,32,35	4
2	ZN	A	402	1/1	0.97	0.05	30,30,30,30	1
6	ACY	B	425	4/4	0.97	0.17	37,39,40,41	0
2	ZN	D	407	1/1	0.98	0.07	23,23,23,23	1
2	ZN	C	406	1/1	0.98	0.04	29,29,29,29	1
2	ZN	C	405	1/1	0.99	0.07	24,24,24,24	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	401	1/1	0.99	0.04	27,27,27,27	1
2	ZN	B	403	1/1	0.99	0.04	23,23,23,23	1
2	ZN	B	404	1/1	0.99	0.04	26,26,26,26	1

6.5 Other polymers (i)

There are no such residues in this entry.