



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:10 AM GMT

PDB ID : 3HFU  
Title : Crystal structure of the ligand binding domain of E. coli CynR with its specific effector azide  
Authors : Singer, A.U.; Evdokimova, E.; Kagan, O.; Dong, A.; Edwards, A.M.; Savchenko, A.  
Deposited on : 2009-05-12  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

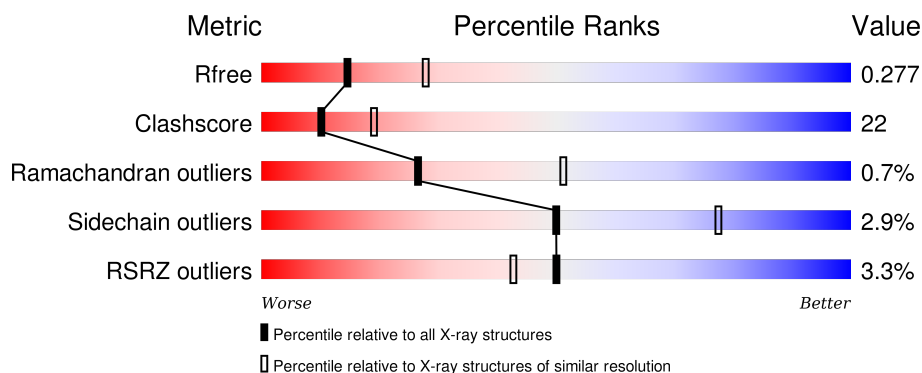
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	238	<div> <div>57%</div> <div>26%</div> <div>•</div> <div>15%</div> </div>
1	B	238	<div> <div>58%</div> <div>26%</div> <div>•</div> <div>14%</div> </div>
1	C	238	<div> <div>49%</div> <div>35%</div> <div>•</div> <div>15%</div> </div>
1	D	238	<div> <div>50%</div> <div>33%</div> <div>•</div> <div>15%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AZI	A	2102	-	-	-	X
2	AZI	B	2104	-	-	X	X
2	AZI	C	2103	-	-	-	X
2	AZI	D	2101	-	-	X	X
3	EDO	C	2002	-	-	-	X
3	EDO	D	2001	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6782 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.

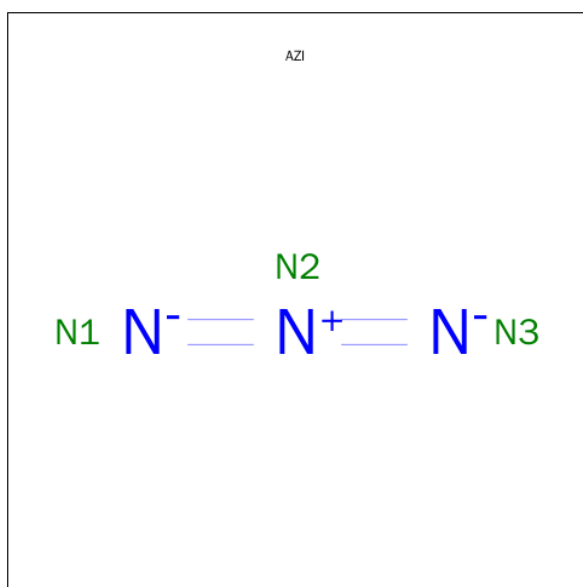
- Molecule 1 is a protein called HTH-type transcriptional regulator cynR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	Se	0	0	0
			1565	1001	269	288	3	4			
1	B	204	Total	C	N	O	S	Se	0	0	0
			1581	1010	274	290	3	4			
1	C	203	Total	C	N	O	S	Se	0	0	0
			1570	1004	270	289	3	4			
1	D	202	Total	C	N	O	S	Se	0	0	0
			1565	1001	269	288	3	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	GLY	-	EXPRESSION TAG	UNP P27111
B	62	GLY	-	EXPRESSION TAG	UNP P27111
C	62	GLY	-	EXPRESSION TAG	UNP P27111
D	62	GLY	-	EXPRESSION TAG	UNP P27111

- Molecule 2 is AZIDE ION (three-letter code: AZI) (formula: N<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total N 3 3	0	0
2	B	1	Total N 3 3	0	0
2	C	1	Total N 3 3	0	0
2	D	1	Total N 3 3	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

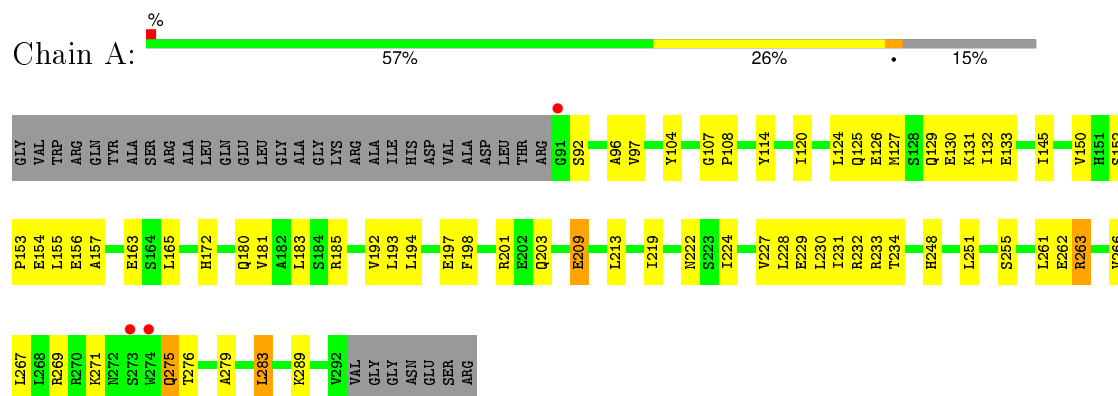
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total	O	0	0
			130	130		
4	B	88	Total	O	0	0
			88	88		
4	C	127	Total	O	0	0
			127	127		
4	D	136	Total	O	0	0
			136	136		

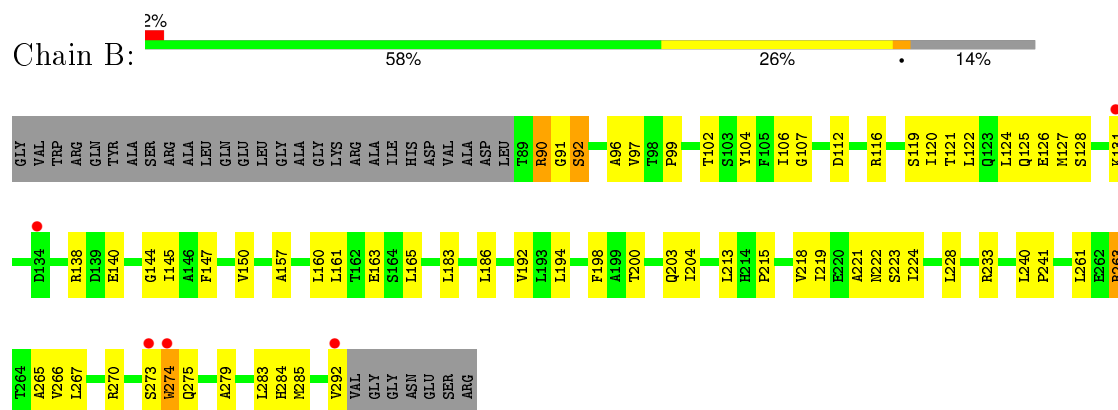
### 3 Residue-property plots

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.

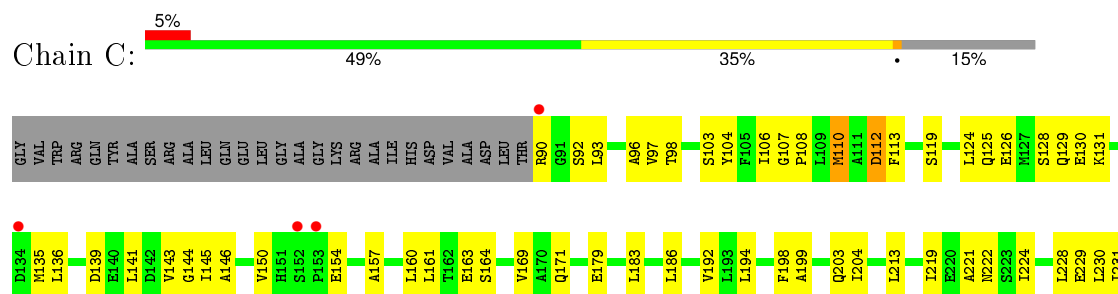
- Molecule 1: HTH-type transcriptional regulator cynR

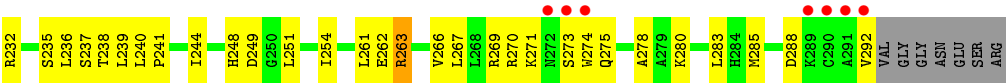


- Molecule 1: HTH-type transcriptional regulator cynR

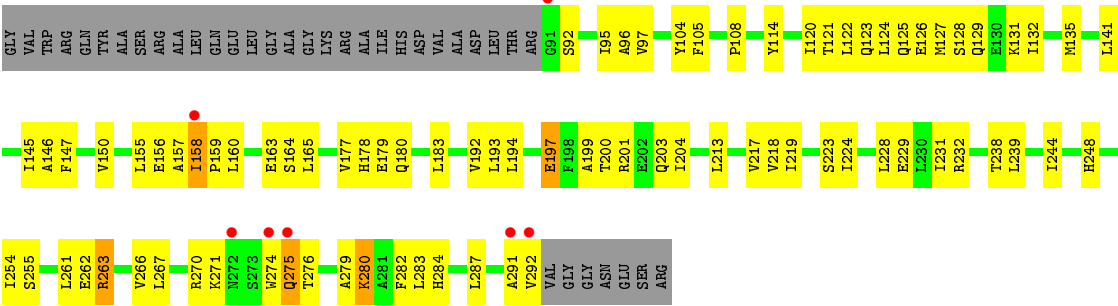


- Molecule 1: HTH-type transcriptional regulator cynR





● Molecule 1: HTH-type transcriptional regulator cynR





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.18Å 98.36Å 86.27Å 90.00° 103.77° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 28.25 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.60) 99.4 (28.25-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.223 , 0.274 0.227 , 0.277	Depositor DCC
$R_{free}$ test set	1531 reflections (4.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.4	Xtriage
Anisotropy	0.782	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 66.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 44500 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6782	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.34 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7911e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: AZI, EDO

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	0.39	0/1592	0.64	0/2161
1	B	0.39	0/1608	0.65	0/2182
1	C	0.40	0/1597	0.65	0/2168
1	D	0.40	0/1592	0.65	0/2161
All	All	0.40	0/6389	0.65	0/8672

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	1565	0	1604	59	0
1	B	1581	0	1619	65	0
1	C	1570	0	1606	87	0
1	D	1565	0	1604	87	0
2	A	3	0	0	1	0
2	B	3	0	0	2	0
2	C	3	0	0	1	0
2	D	3	0	0	2	0
3	C	4	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	4	0	6	1	0
4	A	130	0	0	2	0
4	B	88	0	0	2	0
4	C	127	0	0	7	0
4	D	136	0	0	6	0
All	All	6782	0	6445	278	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 22.

All (278) 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:C:249:ASP:HB3	1:D:177:VAL:HG21	1.26	1.13
1:A:97:VAL:HG12	1:A:145:ILE:HB	1.30	1.08
1:B:157:ALA:HB1	1:B:266:VAL:HG21	1.42	1.01
1:A:157:ALA:HB1	1:A:266:VAL:HG21	1.43	1.00
1:C:97:VAL:HG12	1:C:145:ILE:HB	1.47	0.97
1:C:194:LEU:HD21	1:C:224:ILE:HD12	1.45	0.96
1:C:231:ILE:HD11	1:C:238:THR:HB	1.48	0.95
1:D:158:ILE:HG22	1:D:267:LEU:HB2	1.53	0.90
1:C:249:ASP:CB	1:D:177:VAL:HG21	2.02	0.88
1:C:157:ALA:HB1	1:C:266:VAL:HG21	1.56	0.88
1:B:163:GLU:HG3	1:B:241:PRO:HB3	1.54	0.86
1:A:92:SER:HB3	1:A:120:ILE:HG23	1.58	0.86
1:D:157:ALA:HB1	1:D:266:VAL:HG21	1.56	0.85
1:A:263:ARG:HB2	1:A:263:ARG:HH11	1.37	0.85
1:C:263:ARG:HG3	1:C:263:ARG:HH11	1.42	0.83
1:A:194:LEU:HD21	1:A:224:ILE:HD12	1.61	0.82
1:D:165:LEU:HD12	1:D:261:LEU:HB3	1.62	0.82
1:A:155:LEU:O	1:A:271:LYS:HE3	1.79	0.81
1:B:97:VAL:HG12	1:B:145:ILE:HD13	1.66	0.78
1:C:164:SER:HB3	1:C:262:GLU:HG3	1.65	0.78
1:D:194:LEU:HD21	1:D:224:ILE:HD12	1.67	0.77
1:C:224:ILE:HD13	3:C:2002:EDO:H11	1.65	0.77
1:C:163:GLU:HG3	1:C:241:PRO:HB3	1.67	0.76
1:D:127:MSE:HB2	1:D:131:LYS:HD2	1.66	0.76
1:C:183:LEU:HG	1:C:213:LEU:HD11	1.68	0.76
1:B:198:PHE:HB3	2:B:2104:AZI:N1	2.01	0.76
1:C:261:LEU:HD21	1:C:263:ARG:HD3	1.67	0.75
1:B:183:LEU:HG	1:B:213:LEU:HD11	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:THR:HG22	4:D:1980:HOH:O	1.87	0.74
1:D:231:ILE:HD11	1:D:238:THR:HB	1.70	0.74
1:D:275:GLN:NE2	1:D:280:LYS:HB2	2.03	0.74
1:C:103:SER:HB2	1:C:244:ILE:CD1	2.18	0.74
1:C:150:VAL:HG21	1:C:157:ALA:HB2	1.70	0.73
1:D:150:VAL:HG21	1:D:157:ALA:HB2	1.71	0.73
1:B:274:TRP:HA	1:B:274:TRP:CE3	2.22	0.72
1:D:263:ARG:HD3	4:D:1495:HOH:O	1.90	0.71
1:B:99:PRO:HD2	2:B:2104:AZI:N3	2.05	0.71
1:D:105:PHE:O	1:D:108:PRO:HD2	1.91	0.70
1:A:192:VAL:HG22	1:A:219:ILE:HB	1.74	0.70
1:A:263:ARG:CB	1:A:263:ARG:HH11	2.05	0.69
1:B:203:GLN:HB3	1:B:261:LEU:HD22	1.73	0.69
1:C:275:GLN:HB2	1:C:280:LYS:CD	2.22	0.69
1:C:203:GLN:HB3	1:C:261:LEU:HD22	1.72	0.69
1:D:203:GLN:HE22	1:D:263:ARG:CZ	2.05	0.69
1:A:269:ARG:HD2	1:A:275:GLN:OE1	1.92	0.69
1:D:158:ILE:CG2	1:D:267:LEU:HB2	2.23	0.68
1:D:275:GLN:HG2	1:D:280:LYS:NZ	2.08	0.68
1:C:288:ASP:HB3	4:C:1906:HOH:O	1.95	0.67
1:C:163:GLU:CG	1:C:241:PRO:HB3	2.25	0.66
1:B:144:GLY:C	1:B:145:ILE:HD12	2.15	0.66
1:D:218:VAL:HG23	1:D:219:ILE:HG13	1.76	0.66
1:D:180:GLN:HG3	1:D:255:SER:HB2	1.78	0.66
1:B:200:THR:O	1:B:204:ILE:HG12	1.95	0.66
1:C:270:ARG:HG3	1:C:273:SER:CB	2.26	0.65
1:D:199:ALA:N	2:D:2101:AZI:N1	2.45	0.65
1:C:192:VAL:HG22	1:C:219:ILE:HB	1.78	0.65
1:B:194:LEU:HD21	1:B:224:ILE:HD12	1.78	0.65
1:A:209:GLU:HB3	4:A:1832:HOH:O	1.97	0.65
1:A:153:PRO:HD2	1:A:154:GLU:OE1	1.97	0.64
1:B:186:LEU:O	1:B:215:PRO:HB3	1.96	0.64
1:C:263:ARG:HG3	1:C:263:ARG:NH1	2.13	0.64
1:C:224:ILE:HD13	3:C:2002:EDO:C1	2.29	0.63
1:D:183:LEU:HG	1:D:213:LEU:HD11	1.81	0.63
1:D:123:GLN:HG2	4:D:1558:HOH:O	1.98	0.63
1:B:165:LEU:HD13	1:B:204:ILE:CD1	2.29	0.63
1:C:232:ARG:HD3	4:C:1726:HOH:O	1.98	0.63
1:C:160:LEU:O	1:C:292:VAL:HG21	1.97	0.63
1:A:145:ILE:HG12	1:A:267:LEU:HD23	1.81	0.63
1:D:200:THR:HA	1:D:203:GLN:NE2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:SER:H	1:B:131:LYS:HE3	1.64	0.63
1:A:181:VAL:HB	1:A:185:ARG:HG3	1.81	0.62
1:D:129:GLN:NE2	1:D:146:ALA:HB1	2.15	0.62
1:A:230:LEU:HD21	1:C:110:MSE:HB3	1.82	0.62
1:B:124:LEU:C	1:B:124:LEU:HD13	2.20	0.62
1:B:124:LEU:HD13	1:B:125:GLN:N	2.14	0.62
1:C:267:LEU:HD13	1:C:283:LEU:HD22	1.81	0.61
1:C:103:SER:HB2	1:C:244:ILE:HD12	1.82	0.60
1:A:248:HIS:HB2	1:A:251:LEU:HD12	1.83	0.60
1:C:98:THR:HB	4:C:1882:HOH:O	2.01	0.60
1:B:219:ILE:HD12	1:D:122:LEU:HB2	1.83	0.60
1:A:203:GLN:HB3	1:A:261:LEU:HD22	1.82	0.60
1:D:197:GLU:N	1:D:197:GLU:OE1	2.36	0.59
1:C:231:ILE:HD11	1:C:238:THR:CB	2.28	0.59
1:A:192:VAL:HB	1:A:231:ILE:HD11	1.84	0.59
1:A:192:VAL:HG12	1:A:227:VAL:HG13	1.85	0.59
1:B:145:ILE:HD12	1:B:145:ILE:N	2.18	0.59
1:C:192:VAL:HA	1:C:219:ILE:O	2.03	0.59
1:A:92:SER:CB	1:A:120:ILE:HG23	2.32	0.58
1:B:122:LEU:HB2	1:D:219:ILE:HG23	1.84	0.58
1:B:263:ARG:HD3	4:B:2018:HOH:O	2.03	0.58
1:B:218:VAL:HG23	1:B:219:ILE:HG12	1.84	0.58
1:D:284:HIS:HB3	4:D:1802:HOH:O	2.02	0.58
1:B:92:SER:H	1:B:120:ILE:HG23	1.67	0.58
1:B:270:ARG:NH1	1:B:273:SER:HB2	2.18	0.57
1:B:165:LEU:HD13	1:B:204:ILE:HD11	1.86	0.57
1:D:280:LYS:HA	1:D:280:LYS:NZ	2.20	0.57
1:D:156:GLU:HB2	1:D:271:LYS:HG3	1.86	0.57
1:A:267:LEU:HD13	1:A:283:LEU:HD22	1.85	0.57
1:B:218:VAL:O	1:B:219:ILE:HD13	2.04	0.57
1:D:193:LEU:HD12	1:D:217:VAL:CG2	2.35	0.57
1:D:135:MSE:HE2	1:D:141:LEU:HG	1.87	0.57
1:B:274:TRP:HE3	1:B:274:TRP:HA	1.67	0.56
1:B:163:GLU:CG	1:B:241:PRO:HB3	2.32	0.56
1:B:275:GLN:HE22	1:B:283:LEU:HD11	1.69	0.56
1:B:147:PHE:CZ	1:B:263:ARG:NH1	2.74	0.56
1:C:204:ILE:HD13	1:C:239:LEU:HB2	1.87	0.56
1:A:263:ARG:CG	1:A:263:ARG:HH11	2.19	0.55
1:C:145:ILE:HG12	1:C:267:LEU:HD23	1.87	0.55
1:D:275:GLN:HG2	1:D:280:LYS:HZ3	1.72	0.55
1:A:180:GLN:HG3	1:A:255:SER:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:SER:OG	1:C:93:LEU:N	2.40	0.55
1:D:120:ILE:N	1:D:120:ILE:HD12	2.22	0.55
1:D:155:LEU:HD23	1:D:270:ARG:HA	1.88	0.55
1:B:127:MSE:HB2	1:B:131:LYS:HE3	1.87	0.55
1:C:249:ASP:CA	1:D:177:VAL:HG21	2.37	0.55
1:C:130:GLU:H	1:C:130:GLU:CD	2.11	0.55
1:A:97:VAL:HG12	1:A:145:ILE:CB	2.21	0.54
1:D:280:LYS:HZ1	1:D:280:LYS:HA	1.72	0.54
1:C:171:GLN:HE21	1:C:171:GLN:HA	1.73	0.54
1:C:128:SER:OG	1:C:131:LYS:HG3	2.08	0.54
1:B:150:VAL:HG21	1:B:157:ALA:HB2	1.90	0.54
1:D:105:PHE:CZ	1:D:160:LEU:HD21	2.43	0.53
1:C:269:ARG:NH2	4:C:1636:HOH:O	2.41	0.53
1:A:107:GLY:HA3	1:C:229:GLU:HG2	1.90	0.53
1:D:203:GLN:HE22	1:D:263:ARG:NH2	2.06	0.53
1:D:291:ALA:O	1:D:292:VAL:HB	2.08	0.53
1:C:112:ASP:HB3	1:C:285:MSE:HE1	1.91	0.52
1:C:171:GLN:HA	1:C:171:GLN:NE2	2.25	0.52
1:D:276:THR:HB	4:D:1789:HOH:O	2.09	0.52
1:A:130:GLU:HG3	4:A:1749:HOH:O	2.10	0.52
1:A:156:GLU:HB2	1:A:271:LYS:HG2	1.92	0.52
1:B:145:ILE:HG13	1:B:267:LEU:HD23	1.90	0.52
1:D:228:LEU:O	1:D:232:ARG:HG3	2.10	0.52
1:D:201:ARG:O	1:D:201:ARG:HD2	2.10	0.51
1:D:145:ILE:HG12	1:D:267:LEU:HD23	1.92	0.51
1:D:275:GLN:HG2	1:D:280:LYS:HZ2	1.75	0.51
1:A:124:LEU:HD22	1:A:125:GLN:N	2.26	0.51
1:B:107:GLY:HA3	1:D:229:GLU:HG2	1.92	0.51
1:A:228:LEU:O	1:A:232:ARG:HG3	2.11	0.51
1:D:163:GLU:OE2	1:D:263:ARG:NH1	2.44	0.51
1:C:204:ILE:CD1	1:C:239:LEU:HB2	2.41	0.51
1:C:163:GLU:HG3	1:C:241:PRO:CB	2.39	0.50
1:C:96:ALA:HA	1:C:125:GLN:O	2.11	0.50
1:B:192:VAL:HG13	1:B:219:ILE:HB	1.92	0.50
1:C:270:ARG:HG3	1:C:273:SER:HB2	1.92	0.50
1:D:199:ALA:HB3	2:D:2101:AZI:N1	2.26	0.50
1:D:156:GLU:HB2	1:D:271:LYS:CG	2.41	0.50
1:A:183:LEU:HG	1:A:213:LEU:HD11	1.94	0.50
1:A:248:HIS:CB	1:A:251:LEU:HD12	2.42	0.50
1:A:126:GLU:HG2	1:C:222:ASN:OD1	2.11	0.50
1:D:177:VAL:HG13	1:D:178:HIS:ND1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ILE:HG12	1:C:124:LEU:HD21	1.93	0.50
1:C:169:VAL:HG12	1:C:237:SER:HB3	1.94	0.50
1:C:98:THR:CB	4:C:1882:HOH:O	2.58	0.49
1:C:136:LEU:HD23	1:C:141:LEU:HB2	1.94	0.49
1:B:223:SER:HB2	3:D:2001:EDO:H11	1.94	0.49
1:A:172:HIS:HE1	1:A:234:THR:O	1.96	0.49
1:B:203:GLN:HB3	1:B:261:LEU:CD2	2.41	0.49
1:B:91:GLY:HA2	1:B:120:ILE:HG12	1.94	0.48
1:C:161:LEU:HD12	1:C:161:LEU:C	2.33	0.48
1:D:96:ALA:HA	1:D:125:GLN:O	2.12	0.48
1:C:112:ASP:HB3	1:C:285:MSE:CE	2.42	0.48
1:C:135:MSE:HE2	1:C:141:LEU:HD21	1.95	0.48
1:D:193:LEU:HD12	1:D:217:VAL:HG22	1.95	0.48
1:A:222:ASN:OD1	1:C:125:GLN:HA	2.12	0.48
1:B:263:ARG:HB2	1:B:263:ARG:HH11	1.79	0.48
1:A:96:ALA:HA	1:A:125:GLN:O	2.12	0.48
1:B:284:HIS:HB3	4:B:1935:HOH:O	2.12	0.48
1:D:164:SER:HB3	1:D:262:GLU:HG2	1.94	0.48
1:C:93:LEU:HD22	1:C:278:ALA:HB1	1.95	0.48
1:C:186:LEU:HD12	1:C:213:LEU:HD13	1.96	0.48
1:C:228:LEU:HD11	1:C:244:ILE:CG2	2.44	0.48
1:C:139:ASP:OD1	1:C:270:ARG:HD3	2.13	0.48
1:D:279:ALA:O	1:D:283:LEU:HD12	2.14	0.48
1:B:219:ILE:HD11	1:D:114:TYR:CD1	2.49	0.47
1:D:158:ILE:HD13	1:D:159:PRO:N	2.29	0.47
1:B:128:SER:H	1:B:131:LYS:CE	2.28	0.47
1:A:180:GLN:HG3	1:A:255:SER:CB	2.44	0.47
1:B:292:VAL:O	1:B:292:VAL:HG13	2.15	0.47
1:B:161:LEU:HG	1:B:265:ALA:HB3	1.96	0.47
1:C:135:MSE:HE2	1:C:141:LEU:HG	1.97	0.47
1:B:116:ARG:HH11	1:B:285:MSE:SE	2.47	0.47
1:B:233:ARG:CZ	1:D:108:PRO:HG3	2.45	0.47
1:B:165:LEU:CD1	1:B:204:ILE:CD1	2.93	0.47
1:D:183:LEU:HG	1:D:213:LEU:CD1	2.45	0.47
1:B:275:GLN:HB3	1:B:279:ALA:HB3	1.97	0.47
1:A:275:GLN:HG2	1:A:279:ALA:HB1	1.98	0.46
1:C:113:PHE:N	1:C:285:MSE:HE1	2.29	0.46
1:D:127:MSE:HG3	1:D:132:ILE:HG13	1.97	0.46
1:C:154:GLU:O	1:C:271:LYS:HG2	2.16	0.46
1:B:275:GLN:HE22	1:B:283:LEU:CD1	2.27	0.46
1:D:158:ILE:HD12	1:D:287:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ASN:OD1	1:D:125:GLN:HA	2.15	0.46
1:C:240:LEU:HB3	1:C:241:PRO:HD2	1.98	0.46
1:A:114:TYR:CE2	1:C:236:LEU:HD11	2.51	0.46
1:D:179:GLU:HG3	4:D:1714:HOH:O	2.15	0.46
1:D:244:ILE:O	1:D:248:HIS:HD2	1.99	0.46
1:C:194:LEU:HD21	1:C:224:ILE:CD1	2.32	0.46
1:B:160:LEU:HD13	1:B:267:LEU:HD11	1.97	0.46
1:D:95:ILE:HD13	1:D:282:PHE:CZ	2.51	0.46
1:A:155:LEU:C	1:A:271:LYS:HE3	2.36	0.45
1:B:228:LEU:HD21	1:B:240:LEU:CD1	2.46	0.45
1:D:193:LEU:HD12	1:D:217:VAL:HG21	1.99	0.45
1:D:97:VAL:O	1:D:126:GLU:HA	2.17	0.45
1:A:193:LEU:HD13	1:A:201:ARG:HD3	1.99	0.45
1:C:275:GLN:HB2	1:C:280:LYS:HD3	1.95	0.45
1:A:201:ARG:O	1:A:201:ARG:HD2	2.17	0.45
1:C:199:ALA:O	1:C:203:GLN:HG2	2.17	0.45
1:C:124:LEU:C	1:C:124:LEU:HD13	2.36	0.45
1:B:92:SER:N	1:B:120:ILE:HG23	2.32	0.44
1:A:124:LEU:O	1:C:221:ALA:HA	2.17	0.44
1:B:127:MSE:SE	1:B:131:LYS:HB3	2.67	0.44
1:A:165:LEU:HD11	1:A:261:LEU:HD23	1.98	0.44
1:C:135:MSE:HE2	1:C:141:LEU:CD2	2.47	0.44
1:C:198:PHE:HB3	2:C:2103:AZI:N1	2.33	0.44
1:A:127:MSE:HG3	1:A:132:ILE:HG13	1.98	0.44
1:D:128:SER:OG	1:D:131:LYS:HG3	2.18	0.44
1:D:197:GLU:CD	1:D:197:GLU:H	2.20	0.44
1:D:231:ILE:HD11	1:D:238:THR:CB	2.45	0.44
1:C:219:ILE:HG21	1:C:230:LEU:HD13	1.99	0.44
1:B:292:VAL:O	1:B:292:VAL:HG22	2.18	0.43
1:C:254:ILE:N	1:C:254:ILE:HD12	2.32	0.43
1:B:219:ILE:HD12	1:D:122:LEU:HD12	1.99	0.43
1:A:127:MSE:SE	1:A:131:LYS:HB3	2.69	0.43
1:D:120:ILE:N	1:D:120:ILE:CD1	2.81	0.43
1:B:112:ASP:CB	1:B:285:MSE:HE1	2.47	0.43
1:C:275:GLN:HB2	1:C:280:LYS:HD2	2.00	0.43
1:A:197:GLU:H	1:A:197:GLU:HG3	1.52	0.43
1:D:192:VAL:HG22	1:D:219:ILE:HB	2.01	0.43
1:D:129:GLN:HE22	1:D:147:PHE:H	1.67	0.43
1:A:261:LEU:HD12	1:A:262:GLU:N	2.33	0.43
1:C:129:GLN:NE2	1:C:146:ALA:HB1	2.34	0.43
1:D:177:VAL:O	1:D:177:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:HIS:O	1:D:254:ILE:HD12	2.18	0.43
1:B:157:ALA:HB1	1:B:266:VAL:CG2	2.30	0.43
1:C:103:SER:CB	1:C:244:ILE:HD12	2.47	0.43
1:C:248:HIS:HB2	1:C:251:LEU:HD12	1.99	0.43
1:D:180:GLN:CG	1:D:255:SER:HB2	2.47	0.43
1:A:275:GLN:HG2	1:A:279:ALA:CB	2.49	0.43
1:B:219:ILE:HD11	1:D:114:TYR:HD1	1.84	0.42
1:B:221:ALA:HA	1:D:124:LEU:O	2.19	0.42
1:A:163:GLU:CG	1:A:263:ARG:HH12	2.32	0.42
1:A:152:SER:HA	1:A:153:PRO:HD3	1.84	0.42
1:C:135:MSE:HB3	1:C:141:LEU:HG	2.00	0.42
1:A:150:VAL:HG21	1:A:157:ALA:HB2	2.01	0.42
1:A:233:ARG:CZ	1:C:108:PRO:HG3	2.49	0.42
1:A:129:GLN:O	1:A:133:GLU:HG3	2.19	0.42
1:B:97:VAL:O	1:B:126:GLU:HA	2.19	0.42
1:D:194:LEU:HD11	1:D:224:ILE:HD11	2.02	0.42
1:A:219:ILE:HG21	1:A:230:LEU:HD13	2.02	0.42
1:B:102:THR:HA	1:B:106:ILE:HG22	2.02	0.42
1:A:108:PRO:HB2	1:A:289:LYS:NZ	2.35	0.42
1:C:97:VAL:O	1:C:126:GLU:HA	2.19	0.42
1:A:194:LEU:HD21	1:A:224:ILE:CD1	2.40	0.42
1:D:164:SER:CB	1:D:262:GLU:HG2	2.50	0.42
1:B:138:ARG:HB2	1:B:140:GLU:HG3	2.02	0.42
1:C:143:VAL:HG12	1:C:144:GLY:N	2.35	0.42
1:D:275:GLN:CD	1:D:280:LYS:HD2	2.41	0.42
1:D:274:TRP:HA	1:D:274:TRP:CE3	2.55	0.41
1:A:198:PHE:HB3	2:A:2102:AZI:N3	2.35	0.41
1:D:203:GLN:HB3	1:D:261:LEU:HD22	2.00	0.41
1:A:229:GLU:HG2	1:C:107:GLY:HA3	2.01	0.41
1:D:158:ILE:HG23	1:D:158:ILE:O	2.19	0.41
1:B:96:ALA:O	1:B:144:GLY:HA2	2.20	0.41
1:D:129:GLN:HB2	1:D:129:GLN:HE21	1.61	0.41
1:A:163:GLU:O	1:A:163:GLU:HG3	2.20	0.41
1:B:165:LEU:CD1	1:B:204:ILE:HD13	2.51	0.41
1:C:131:LYS:NZ	4:C:1536:HOH:O	2.54	0.41
1:C:90:ARG:HA	1:C:119:SER:O	2.20	0.41
1:D:231:ILE:CD1	1:D:238:THR:HB	2.45	0.41
1:C:274:TRP:HE3	1:C:274:TRP:HA	1.86	0.41
1:D:92:SER:HA	1:D:121:THR:O	2.21	0.41
1:D:204:ILE:CD1	1:D:239:LEU:HB2	2.51	0.40
1:C:236:LEU:HA	4:C:1813:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ALA:HB3	1:C:141:LEU:HD13	2.02	0.40
1:A:224:ILE:HD12	1:A:224:ILE:N	2.37	0.40
1:C:274:TRP:CE3	1:C:274:TRP:HA	2.57	0.40
1:D:204:ILE:HD13	1:D:239:LEU:HB2	2.03	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	200/238 (84%)	194 (97%)	5 (2%)	1 (0%)	34	60
1	B	202/238 (85%)	192 (95%)	7 (4%)	3 (2%)	13	26
1	C	201/238 (84%)	195 (97%)	5 (2%)	1 (0%)	34	60
1	D	200/238 (84%)	195 (98%)	4 (2%)	1 (0%)	34	60
All	All	803/952 (84%)	776 (97%)	21 (3%)	6 (1%)	26	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	ARG
1	A	104	TYR
1	B	92	SER
1	C	104	TYR
1	D	104	TYR
1	B	104	TYR

### 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	170/192 (88%)	165 (97%)	5 (3%)	50	77
1	B	171/192 (89%)	167 (98%)	4 (2%)	58	83
1	C	170/192 (88%)	165 (97%)	5 (3%)	50	77
1	D	170/192 (88%)	164 (96%)	6 (4%)	43	71
All	All	681/768 (89%)	661 (97%)	20 (3%)	50	77

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	GLU
1	A	263	ARG
1	A	275	GLN
1	A	276	THR
1	A	283	LEU
1	B	90	ARG
1	B	119	SER
1	B	263	ARG
1	B	274	TRP
1	C	110	MSE
1	C	112	ASP
1	C	179	GLU
1	C	235	SER
1	C	263	ARG
1	D	158	ILE
1	D	197	GLU
1	D	223	SER
1	D	263	ARG
1	D	275	GLN
1	D	280	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	A	172	HIS
1	A	216	GLN

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Mol	Chain	Res	Type
1	B	129	GLN
1	B	216	GLN
1	B	275	GLN
1	C	129	GLN
1	C	171	GLN
1	C	216	GLN
1	D	123	GLN
1	D	129	GLN
1	D	171	GLN
1	D	203	GLN
1	D	216	GLN
1	D	248	HIS
1	D	275	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	AZI	A	2102	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	AZI	B	2104	-	0,2,2	0.00	-	0,1,1	0.00	-
3	EDO	C	2002	-	3,3,3	0.62	0	2,2,2	0.21	0
2	AZI	C	2103	-	0,2,2	0.00	-	0,1,1	0.00	-
3	EDO	D	2001	-	3,3,3	0.52	0	2,2,2	0.37	0
2	AZI	D	2101	-	0,2,2	0.00	-	0,1,1	0.00	-

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	AZI	A	2102	-	-	0/0/0/0	0/0/0/0
2	AZI	B	2104	-	-	0/0/0/0	0/0/0/0
3	EDO	C	2002	-	-	0/1/1/1	0/0/0/0
2	AZI	C	2103	-	-	0/0/0/0	0/0/0/0
3	EDO	D	2001	-	-	0/1/1/1	0/0/0/0
2	AZI	D	2101	-	-	0/0/0/0	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.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2102	AZI	1	0
2	B	2104	AZI	2	0
3	C	2002	EDO	2	0
2	C	2103	AZI	1	0
3	D	2001	EDO	1	0
2	D	2101	AZI	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	198/238 (83%)	-0.19	3 (1%) 76 71	16, 35, 80, 119	0
1	B	200/238 (84%)	-0.14	5 (2%) 61 54	14, 33, 75, 116	0
1	C	199/238 (83%)	-0.01	11 (5%) 29 21	11, 36, 84, 110	0
1	D	198/238 (83%)	-0.08	7 (3%) 48 40	13, 35, 78, 118	0
All	All	795/952 (83%)	-0.11	26 (3%) 50 43	11, 35, 80, 119	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	292	VAL	7.7
1	D	274	TRP	6.5
1	C	274	TRP	6.1
1	D	292	VAL	5.5
1	D	272	ASN	4.5
1	D	91	GLY	4.1
1	D	275	GLN	3.6
1	C	153	PRO	3.5
1	A	91	GLY	3.1
1	B	131	LYS	2.9
1	C	290	CYS	2.8
1	B	292	VAL	2.8
1	C	289	LYS	2.7
1	A	274	TRP	2.7
1	B	273	SER	2.5
1	D	291	ALA	2.5
1	C	152	SER	2.5
1	C	291	ALA	2.4
1	B	134	ASP	2.4
1	C	272	ASN	2.4
1	A	273	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	158	ILE	2.3
1	B	274	TRP	2.2
1	C	273	SER	2.1
1	C	90	ARG	2.1
1	C	134	ASP	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	EDO	D	2001	4/4	0.83	0.48	11.67	57,57,57,57	0
3	EDO	C	2002	4/4	0.54	0.57	7.51	58,58,58,58	0
2	AZI	C	2103	3/3	0.97	0.25	3.06	17,17,17,17	0
2	AZI	D	2101	3/3	0.93	0.22	2.71	17,17,17,17	0
2	AZI	A	2102	3/3	0.95	0.25	2.66	30,30,30,30	0
2	AZI	B	2104	3/3	0.94	0.21	2.17	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.