



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:01 AM GMT

PDB ID : 3GOB  
Title : Crystal Structure of Dicamba Monooxygenase with Non-heme Cobalt and DCSA  
Authors : Rydel, T.J.; Sturman, E.J.; Moshiri, F.; Brown, G.R.; Qi, Y.  
Deposited on : 2009-03-18  
Resolution : 2.05 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

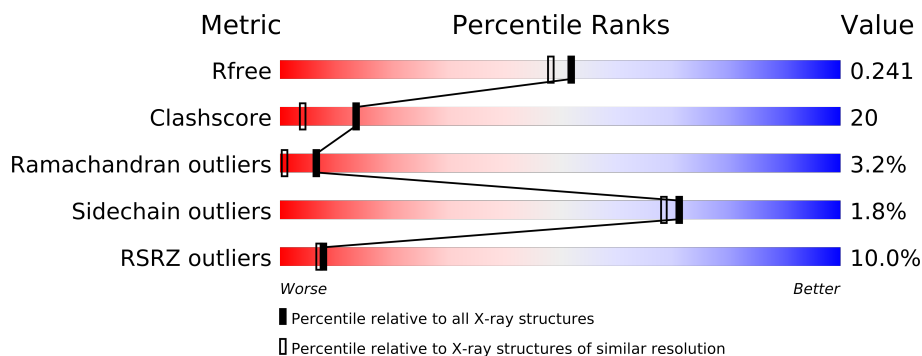
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.05 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))
$R_{free}$	66092	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	349	
1	B	349	
1	C	349	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CO	A	602	-	X
4	HXX	A	601	-	X
4	HXX	B	601	-	X
4	HXX	C	601	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8517 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DdmC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2649	1670	475	490	14			
1	B	341	Total	C	N	O	S	0	0	0
			2641	1665	474	489	13			
1	C	342	Total	C	N	O	S	0	0	0
			2649	1670	475	490	14			

There are 33 discrepancies between the modelled and reference sequences:

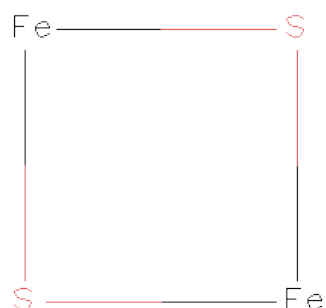
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q5S3I3
A	2	ALA	MET	ENGINEERED	UNP Q5S3I3
A	341	ARG	-	EXPRESSION TAG	UNP Q5S3I3
A	342	LEU	-	EXPRESSION TAG	UNP Q5S3I3
A	343	GLU	-	EXPRESSION TAG	UNP Q5S3I3
A	344	HIS	-	EXPRESSION TAG	UNP Q5S3I3
A	345	HIS	-	EXPRESSION TAG	UNP Q5S3I3
A	346	HIS	-	EXPRESSION TAG	UNP Q5S3I3
A	347	HIS	-	EXPRESSION TAG	UNP Q5S3I3
A	348	HIS	-	EXPRESSION TAG	UNP Q5S3I3
A	349	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	1	MET	-	EXPRESSION TAG	UNP Q5S3I3
B	2	ALA	MET	ENGINEERED	UNP Q5S3I3
B	341	ARG	-	EXPRESSION TAG	UNP Q5S3I3
B	342	LEU	-	EXPRESSION TAG	UNP Q5S3I3
B	343	GLU	-	EXPRESSION TAG	UNP Q5S3I3
B	344	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	345	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	346	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	347	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	348	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	349	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	1	MET	-	EXPRESSION TAG	UNP Q5S3I3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	MET	ENGINEERED	UNP Q5S3I3
C	341	ARG	-	EXPRESSION TAG	UNP Q5S3I3
C	342	LEU	-	EXPRESSION TAG	UNP Q5S3I3
C	343	GLU	-	EXPRESSION TAG	UNP Q5S3I3
C	344	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	345	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	346	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	347	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	348	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	349	HIS	-	EXPRESSION TAG	UNP Q5S3I3

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

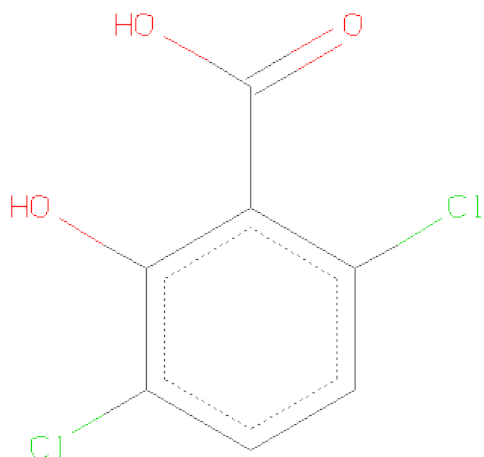
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Co 2 2	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Co 2	0	0
3	C	4	Total 4	Co 4	0	0

- Molecule 4 is 3,6-DICHLORO-2-HYDROXYBENZOICACID (three-letter code: HXX) (formula: C<sub>7</sub>H<sub>4</sub>Cl<sub>2</sub>O<sub>3</sub>).

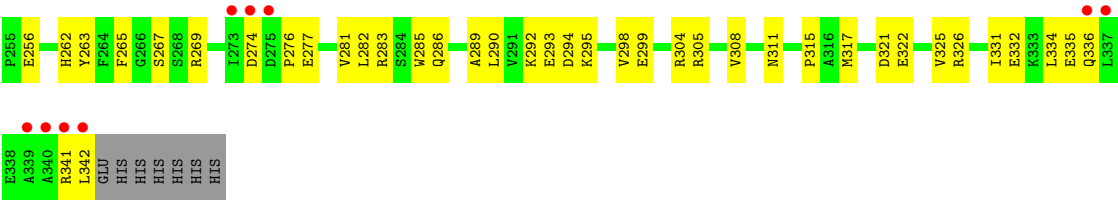


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 12	C 7	Cl 2	O 3	0	0
4	B	1	Total 12	C 7	Cl 2	O 3	0	0
4	C	1	Total 12	C 7	Cl 2	O 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	189	Total 189	O 189	0	0
5	B	173	Total 173	O 173	0	0
5	C	160	Total 160	O 160	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.01Å 81.01Å 161.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.05 42.63 – 2.05	Depositor EDS
% Data completeness (in resolution range)	81.8 (20.00-2.05) 82.2 (42.63-2.05)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.19 (at 2.05Å)	Xtriage
Refinement program	CNX2002	Depositor
R, $R_{free}$	0.232 , 0.267 0.211 , 0.241	Depositor DCC
$R_{free}$ test set	6147 reflections (11.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 59.1	EDS
Estimated twinning fraction	0.003 for -h,-k,l 0.039 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 60695 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8517	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HXX, CO, FES

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	0.30	0/2714	0.63	0/3695
1	B	0.29	0/2706	0.61	1/3685 (0.0%)
1	C	0.28	0/2714	0.62	0/3695
All	All	0.29	0/8134	0.62	1/11075 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	GLY	N-CA-C	5.01	125.62	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2649	0	2589	118	0
1	B	2641	0	2577	91	0
1	C	2649	0	2589	112	0
2	A	4	0	0	1	0
2	B	4	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	4	0	0	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	4	0	0	0	0
4	A	12	0	3	0	0
4	B	12	0	3	0	0
4	C	12	0	3	0	0
5	A	189	0	0	15	0
5	B	173	0	0	11	0
5	C	160	0	0	8	0
All	All	8517	0	7764	318	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (318) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:169:ALA:HB2	1:C:202:LEU:HD12	1.45	0.99
1:A:166:ARG:O	1:A:170:GLN:HB2	1.67	0.93
1:A:272:GLY:HA3	1:A:278:MET:HE1	1.56	0.87
1:A:175:ASP:HB3	1:A:177:LEU:HD11	1.57	0.84
1:C:171:THR:HG22	1:C:173:ALA:H	1.44	0.83
1:C:242:GLU:HG3	1:C:243:GLN:HE21	1.42	0.83
1:A:217:TRP:CH2	1:A:239:THR:HB	2.15	0.81
1:C:286:GLN:HA	1:C:290:LEU:HD23	1.62	0.81
1:A:206:PHE:HB2	1:A:245:ILE:HD13	1.61	0.81
1:A:215:ASP:HB2	1:A:239:THR:HG21	1.62	0.79
1:B:269:ARG:HG3	5:B:766:HOH:O	1.83	0.79
1:C:269:ARG:HD3	1:C:282:LEU:HD11	1.65	0.78
1:B:174:PHE:O	1:B:177:LEU:HG	1.82	0.78
1:A:240:PRO:O	1:A:241:LYS:HB2	1.84	0.78
1:C:194:ILE:HB	1:C:216:ALA:HB3	1.66	0.77
1:C:192:MET:HE3	1:C:194:ILE:HD11	1.68	0.76
1:C:207:LEU:HD11	1:C:234:VAL:HG21	1.70	0.72
1:A:269:ARG:HD3	1:A:282:LEU:HD11	1.70	0.72
1:A:156:MET:HE1	1:A:220:ILE:HD13	1.70	0.71
1:A:269:ARG:HG3	5:A:840:HOH:O	1.88	0.71
1:A:217:TRP:HH2	1:A:239:THR:HB	1.52	0.71
1:C:174:PHE:O	1:C:177:LEU:HG	1.91	0.71
1:B:162:GLN:OE1	1:B:170:GLN:HA	1.91	0.70
1:A:199:PRO:HB3	1:A:234:VAL:HG21	1.74	0.69
1:C:195:PRO:HB3	1:C:214:VAL:HA	1.74	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:195:PRO:CB	1:C:214:VAL:HA	2.23	0.68
1:B:171:THR:HG21	1:B:194:ILE:HG21	1.75	0.67
1:A:208:ARG:HG2	1:A:209:GLY:N	2.09	0.67
1:C:269:ARG:HH11	1:C:282:LEU:CD1	2.06	0.67
1:C:158:LEU:HD13	1:C:192:MET:HE2	1.75	0.67
1:B:86:HIS:ND1	5:B:865:HOH:O	2.27	0.67
1:B:193:LYS:HE2	1:B:217:TRP:HE1	1.60	0.66
1:B:171:THR:HG22	1:B:173:ALA:H	1.59	0.66
1:A:88:ASN:HD21	1:A:90:ALA:HB2	1.61	0.66
1:C:193:LYS:HB3	5:C:1089:HOH:O	1.96	0.66
1:A:269:ARG:HD3	1:A:282:LEU:CD1	2.26	0.66
1:C:269:ARG:HH11	1:C:282:LEU:HD12	1.60	0.65
1:A:10:TYR:CE2	1:A:225:VAL:HG11	2.31	0.65
1:B:177:LEU:CD2	1:B:194:ILE:HG12	2.27	0.65
1:A:156:MET:HE2	1:A:228:MET:SD	2.37	0.64
1:B:165:HIS:ND1	1:B:293:GLU:OE2	2.23	0.64
1:B:289:ALA:HA	1:B:293:GLU:OE2	1.98	0.64
1:B:295:LYS:O	1:B:299:GLU:HG3	1.98	0.64
1:A:233:ALA:HB2	1:A:246:HIS:HB3	1.79	0.64
1:A:270:ASN:HB3	5:A:1017:HOH:O	1.96	0.64
1:A:177:LEU:N	1:A:177:LEU:HD12	2.13	0.64
1:C:27:ILE:HD12	1:C:254:THR:HG21	1.80	0.63
1:C:295:LYS:O	1:C:299:GLU:HG3	1.98	0.63
1:C:1:MET:SD	1:C:6:ARG:NH1	2.71	0.63
1:C:237:GLU:C	1:C:239:THR:H	2.01	0.63
1:A:143:HIS:HE1	1:A:256:GLU:OE1	1.82	0.63
1:C:88:ASN:HD21	1:C:90:ALA:HB2	1.63	0.63
1:C:277:GLU:O	1:C:281:VAL:HG23	1.99	0.62
1:B:27:ILE:HD12	1:B:254:THR:HG21	1.80	0.62
1:C:160:HIS:HB2	1:C:164:VAL:HG23	1.82	0.62
1:A:4:PHE:HB3	1:A:28:LEU:HD13	1.81	0.62
1:B:4:PHE:HB3	1:B:28:LEU:HD13	1.82	0.62
1:B:236:PRO:HG2	1:B:239:THR:HG21	1.82	0.62
1:C:233:ALA:HB2	1:C:246:HIS:HB3	1.81	0.61
1:B:88:ASN:HD21	1:B:90:ALA:HB2	1.64	0.61
1:C:202:LEU:HD21	1:C:285:TRP:CE3	2.35	0.61
1:B:292:LYS:O	1:B:296:VAL:HG23	2.00	0.61
1:C:156:MET:HE1	1:C:220:ILE:HD13	1.82	0.61
1:C:119:ALA:O	1:C:120:ASP:HB3	2.00	0.61
1:B:282:LEU:O	1:B:286:GLN:HG3	2.01	0.60
1:C:198:THR:O	1:C:199:PRO:O	2.19	0.60
1:C:289:ALA:HA	1:C:293:GLU:OE2	2.01	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:4:PHE:HB3	1:C:28:LEU:HD13	1.81	0.60
1:A:215:ASP:CB	1:A:239:THR:HG21	2.32	0.60
1:A:330:GLU:HG3	5:A:1135:HOH:O	2.00	0.60
1:B:156:MET:HE2	1:B:220:ILE:HD13	1.84	0.60
1:A:27:ILE:HD12	1:A:254:THR:HG21	1.83	0.60
1:C:157:ASP:HB2	5:C:884:HOH:O	2.02	0.60
1:A:138:VAL:HG23	5:A:1152:HOH:O	2.01	0.59
1:C:290:LEU:HD22	1:C:290:LEU:H	1.66	0.59
1:A:37:GLN:HB3	1:A:38:PRO:HD2	1.84	0.59
1:C:217:TRP:CH2	1:C:241:LYS:HA	2.37	0.59
1:A:119:ALA:O	1:A:120:ASP:HB3	2.02	0.59
1:C:160:HIS:HB2	1:C:164:VAL:CG2	2.33	0.58
1:A:76:ASP:OD2	1:A:80:GLN:HB3	2.03	0.58
1:B:193:LYS:HG2	1:B:217:TRP:CD1	2.39	0.58
1:A:295:LYS:O	1:A:299:GLU:HG3	2.03	0.58
1:A:156:MET:CE	1:A:228:MET:SD	2.91	0.58
1:A:212:THR:HG23	1:A:213:PRO:HD2	1.86	0.57
1:A:2:ALA:O	1:A:3:THR:OG1	2.22	0.57
1:C:331:ILE:O	1:C:335:GLU:HG3	2.04	0.57
1:B:269:ARG:HH11	1:B:282:LEU:HD12	1.70	0.56
1:A:162:GLN:O	1:A:166:ARG:HA	2.06	0.56
1:C:198:THR:HG23	1:C:198:THR:O	2.06	0.56
5:A:820:HOH:O	1:B:320:CYS:HB3	2.05	0.56
1:C:212:THR:HG23	1:C:213:PRO:HD2	1.86	0.56
1:C:37:GLN:HB3	1:C:38:PRO:HD2	1.88	0.56
1:B:37:GLN:HB3	1:B:38:PRO:HD2	1.88	0.55
1:B:225:VAL:HG12	1:B:226:SER:N	2.22	0.55
1:C:332:GLU:O	1:C:336:GLN:HG3	2.07	0.55
1:A:176:ARG:HA	5:A:771:HOH:O	2.05	0.55
1:C:283:ARG:HG2	5:C:1068:HOH:O	2.06	0.55
1:C:308:VAL:O	1:C:311:ASN:O	2.25	0.55
1:B:143:HIS:HE1	1:B:256:GLU:OE1	1.89	0.55
1:C:171:THR:HG22	1:C:173:ALA:N	2.19	0.55
1:C:202:LEU:HD11	1:C:285:TRP:CZ3	2.42	0.55
1:A:237:GLU:HG3	1:A:238:GLY:N	2.22	0.54
1:C:274:ASP:O	1:C:276:PRO:HD3	2.07	0.54
1:C:136:ARG:HG2	1:C:269:ARG:NH2	2.22	0.54
1:C:290:LEU:N	1:C:290:LEU:HD22	2.23	0.54
1:A:175:ASP:HB3	1:A:177:LEU:CD1	2.32	0.54
1:A:240:PRO:O	1:A:241:LYS:CB	2.56	0.54
1:C:10:TYR:CE2	1:C:225:VAL:HG11	2.42	0.54
1:A:137:THR:HA	1:A:267:SER:O	2.07	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:76:ASP:OD2	1:C:80:GLN:HB3	2.08	0.53
1:A:288:GLN:NE2	1:A:292:LYS:HB2	2.23	0.53
1:A:159:GLY:HA3	5:A:1121:HOH:O	2.09	0.53
1:A:245:ILE:HA	5:A:1017:HOH:O	2.09	0.53
1:B:156:MET:HE3	1:B:228:MET:SD	2.48	0.53
1:B:55:PRO:HB3	1:C:304:ARG:CZ	2.39	0.53
1:A:269:ARG:CD	1:A:278:MET:HE3	2.39	0.53
1:B:190:ALA:HB2	1:B:323:ALA:CB	2.38	0.53
1:B:76:ASP:OD2	1:B:80:GLN:HB3	2.09	0.53
1:C:203:MET:HG2	1:C:207:LEU:HD12	1.90	0.52
1:C:203:MET:CE	1:C:234:VAL:HB	2.38	0.52
1:A:214:VAL:HG12	1:A:236:PRO:HA	1.91	0.52
1:A:2:ALA:O	1:A:258:GLU:OE1	2.26	0.52
1:A:304:ARG:CZ	1:C:55:PRO:HB3	2.39	0.52
1:B:193:LYS:HE2	1:B:217:TRP:NE1	2.23	0.52
1:C:156:MET:HE2	1:C:228:MET:SD	2.49	0.52
1:A:320:CYS:SG	5:A:1121:HOH:O	2.58	0.52
1:A:331:ILE:O	1:A:335:GLU:HG3	2.10	0.52
1:B:71:HIS:HB2	2:B:501:FES:S1	2.50	0.52
1:B:237:GLU:HA	5:B:1118:HOH:O	2.09	0.52
1:A:240:PRO:HG2	1:A:241:LYS:H	1.74	0.52
1:B:286:GLN:O	1:B:290:LEU:HB2	2.09	0.52
1:A:10:TYR:CZ	1:A:225:VAL:HG11	2.45	0.52
1:C:326:ARG:NE	5:C:1044:HOH:O	2.42	0.52
1:A:269:ARG:HH11	1:A:282:LEU:HD12	1.75	0.52
1:A:156:MET:HE3	1:A:228:MET:HG2	1.92	0.52
1:C:305:ARG:HA	1:C:308:VAL:HG22	1.92	0.51
1:A:274:ASP:O	1:A:276:PRO:HD3	2.10	0.51
1:B:217:TRP:CE2	1:B:241:LYS:HB3	2.45	0.51
1:C:225:VAL:HG12	1:C:226:SER:N	2.25	0.51
1:B:341:ARG:HG2	1:B:342:LEU:HD22	1.93	0.51
1:B:158:LEU:HB2	1:B:192:MET:SD	2.51	0.51
1:C:242:GLU:C	1:C:244:SER:H	2.13	0.51
1:B:331:ILE:O	1:B:335:GLU:HG3	2.11	0.50
1:C:282:LEU:O	1:C:286:GLN:HG3	2.10	0.50
1:A:233:ALA:CB	1:A:246:HIS:HB3	2.41	0.50
1:C:137:THR:HA	1:C:267:SER:O	2.10	0.50
1:C:269:ARG:CD	1:C:282:LEU:HD11	2.41	0.50
1:C:19:SER:HB2	5:C:1022:HOH:O	2.10	0.50
1:B:305:ARG:HA	1:B:308:VAL:HG22	1.94	0.50
1:A:235:ALA:O	1:A:239:THR:HG22	2.12	0.50
1:C:240:PRO:C	1:C:242:GLU:N	2.65	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:173:ALA:HB2	1:B:176:ARG:HH21	1.77	0.50
1:B:2:ALA:HB1	1:B:258:GLU:OE1	2.12	0.50
1:B:332:GLU:O	1:B:336:GLN:HG3	2.12	0.49
1:B:202:LEU:HD22	1:B:285:TRP:CE3	2.48	0.49
1:A:193:LYS:HD3	1:A:217:TRP:HE1	1.77	0.49
1:C:191:LEU:HA	1:C:219:ASP:OD1	2.12	0.49
1:A:308:VAL:O	1:A:311:ASN:O	2.31	0.49
1:C:269:ARG:NH1	1:C:282:LEU:HD12	2.25	0.49
1:C:192:MET:N	1:C:219:ASP:OD1	2.38	0.49
1:A:235:ALA:HB2	1:A:244:SER:CB	2.43	0.49
1:C:71:HIS:HB2	2:C:501:FES:S1	2.53	0.49
1:A:208:ARG:HG2	1:A:209:GLY:H	1.77	0.48
1:B:177:LEU:HD22	1:B:194:ILE:HG12	1.95	0.48
1:A:263:TYR:CD1	1:A:290:LEU:HD13	2.48	0.48
1:A:167:ALA:HA	1:A:170:GLN:HB2	1.95	0.48
1:A:162:GLN:HG3	1:A:170:GLN:HG3	1.94	0.48
1:C:158:LEU:HG	1:C:179:ARG:CZ	2.43	0.48
1:B:194:ILE:HB	1:B:216:ALA:HB3	1.94	0.48
1:B:308:VAL:O	1:B:311:ASN:O	2.30	0.48
1:C:315:PRO:HB2	1:C:317:MET:CE	2.44	0.48
1:B:126:ASP:HA	5:B:762:HOH:O	2.13	0.48
1:A:269:ARG:NE	1:A:278:MET:HE3	2.28	0.48
1:A:237:GLU:CG	1:A:238:GLY:H	2.26	0.48
1:A:225:VAL:HG12	1:A:226:SER:N	2.28	0.48
1:B:190:ALA:HB2	1:B:323:ALA:HB2	1.96	0.48
1:C:198:THR:O	1:C:198:THR:CG2	2.61	0.48
1:C:289:ALA:O	1:C:293:GLU:HB2	2.13	0.47
1:C:199:PRO:HG3	1:C:203:MET:SD	2.55	0.47
1:A:305:ARG:HA	1:A:308:VAL:HG22	1.95	0.47
1:A:332:GLU:O	1:A:336:GLN:HG3	2.14	0.47
1:A:88:ASN:ND2	1:A:90:ALA:HB2	2.28	0.47
1:A:25:ARG:HD2	1:A:262:HIS:CE1	2.50	0.47
1:A:294:ASP:O	1:A:298:VAL:HG22	2.14	0.47
1:A:165:HIS:HB2	1:A:169:ALA:HB3	1.96	0.47
1:B:162:GLN:HG3	1:B:174:PHE:CD1	2.50	0.47
1:B:174:PHE:CE1	1:B:177:LEU:HD11	2.50	0.47
1:C:10:TYR:CZ	1:C:225:VAL:HG11	2.50	0.47
1:B:289:ALA:O	1:B:293:GLU:HB2	2.14	0.47
1:C:88:ASN:ND2	1:C:90:ALA:HB2	2.29	0.47
1:B:341:ARG:HD3	5:B:1069:HOH:O	2.14	0.47
1:B:277:GLU:O	1:B:281:VAL:HG23	2.14	0.47
1:A:195:PRO:HA	1:A:215:ASP:OD2	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:237:GLU:O	1:A:239:THR:N	2.38	0.46
1:C:237:GLU:O	1:C:239:THR:N	2.48	0.46
1:C:178:GLU:O	1:C:192:MET:HG3	2.16	0.46
1:A:135:TYR:HA	1:A:269:ARG:O	2.16	0.46
1:C:214:VAL:HG13	1:C:214:VAL:O	2.16	0.46
1:C:25:ARG:HD2	1:C:262:HIS:CE1	2.51	0.46
1:B:294:ASP:O	1:B:298:VAL:HG22	2.16	0.45
1:C:294:ASP:O	1:C:298:VAL:HG22	2.16	0.45
1:A:234:VAL:O	1:A:244:SER:HB2	2.16	0.45
1:C:242:GLU:C	1:C:244:SER:N	2.69	0.45
1:A:237:GLU:O	1:A:239:THR:HG23	2.16	0.45
1:A:71:HIS:HB2	2:A:501:FES:S1	2.56	0.45
1:C:237:GLU:C	1:C:239:THR:N	2.68	0.45
1:C:220:ILE:HA	1:C:230:ASN:HA	1.98	0.45
1:B:291:VAL:O	1:B:291:VAL:HG12	2.17	0.45
1:B:196:GLY:N	1:B:215:ASP:OD2	2.49	0.45
1:C:240:PRO:C	1:C:242:GLU:H	2.18	0.45
1:B:88:ASN:ND2	1:B:90:ALA:HB2	2.31	0.45
1:B:10:TYR:CZ	1:B:225:VAL:HG11	2.51	0.45
1:A:315:PRO:HB2	1:A:317:MET:CE	2.46	0.45
1:C:1:MET:SD	1:C:6:ARG:HD2	2.57	0.45
1:C:143:HIS:HE1	1:C:256:GLU:OE1	2.00	0.45
1:A:224:LYS:O	1:A:225:VAL:HB	2.17	0.45
1:A:212:THR:CG2	1:A:213:PRO:HD2	2.46	0.45
1:A:171:THR:HG22	1:A:173:ALA:H	1.82	0.45
1:B:305:ARG:O	1:B:308:VAL:HG22	2.17	0.45
1:B:36:ARG:NH1	5:B:1213:HOH:O	2.49	0.45
1:A:305:ARG:O	1:A:308:VAL:HG22	2.16	0.44
1:B:163:TYR:O	1:B:166:ARG:HB2	2.17	0.44
1:C:213:PRO:O	1:C:214:VAL:HB	2.17	0.44
1:A:171:THR:CG2	1:A:173:ALA:HB3	2.47	0.44
1:C:210:ALA:O	1:C:211:ASN:ND2	2.49	0.44
1:B:10:TYR:CE2	1:B:225:VAL:HG11	2.52	0.44
1:B:276:PRO:O	1:B:279:ASP:HB2	2.17	0.44
1:A:215:ASP:H	1:A:239:THR:HG21	1.82	0.44
1:B:289:ALA:HA	1:B:293:GLU:HB2	2.00	0.44
1:A:119:ALA:O	1:A:120:ASP:CB	2.65	0.44
1:B:217:TRP:CZ2	1:B:241:LYS:HB3	2.52	0.44
1:C:156:MET:HE1	1:C:220:ILE:CD1	2.47	0.44
1:B:208:ARG:HG2	1:B:208:ARG:HH11	1.83	0.44
1:C:212:THR:HG22	1:C:214:VAL:HG12	2.00	0.44
1:C:342:LEU:C	1:C:342:LEU:HD23	2.38	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:223:ASN:ND2	5:C:736:HOH:O	2.46	0.44
1:A:237:GLU:CG	1:A:238:GLY:N	2.80	0.43
1:C:217:TRP:CZ2	1:C:241:LYS:HA	2.52	0.43
1:B:212:THR:HG22	1:B:213:PRO:HD2	1.99	0.43
1:A:175:ASP:CG	1:A:176:ARG:H	2.21	0.43
1:B:36:ARG:NE	5:B:769:HOH:O	2.38	0.43
1:B:179:ARG:HA	1:B:191:LEU:O	2.17	0.43
1:B:224:LYS:O	1:B:225:VAL:HB	2.18	0.43
1:B:212:THR:CG2	1:B:213:PRO:HD2	2.47	0.43
1:B:118:LEU:O	1:B:119:ALA:C	2.57	0.43
1:A:237:GLU:C	1:A:239:THR:H	2.18	0.43
1:A:191:LEU:HB3	5:A:1099:HOH:O	2.17	0.43
1:C:286:GLN:HA	1:C:290:LEU:CD2	2.40	0.43
1:C:211:ASN:HA	1:C:211:ASN:HD22	1.62	0.43
1:C:250:THR:O	1:C:265:PHE:HA	2.18	0.43
1:A:167:ALA:O	1:A:170:GLN:N	2.52	0.43
1:A:220:ILE:HA	1:A:230:ASN:HA	2.01	0.43
1:A:167:ALA:HA	1:A:170:GLN:CB	2.49	0.43
1:A:213:PRO:O	1:A:236:PRO:HA	2.19	0.43
1:C:135:TYR:HA	1:C:269:ARG:O	2.19	0.43
1:B:220:ILE:HA	1:B:230:ASN:HA	2.01	0.43
1:B:49:CYS:HA	1:B:50:PRO:HD3	1.86	0.43
1:A:269:ARG:NE	1:A:278:MET:CE	2.82	0.43
1:A:214:VAL:HG12	1:A:236:PRO:CA	2.49	0.43
1:A:49:CYS:HA	1:A:50:PRO:HD3	1.85	0.43
1:B:326:ARG:NE	5:B:890:HOH:O	2.51	0.43
1:C:292:LYS:HD2	5:C:1205:HOH:O	2.19	0.42
1:B:223:ASN:ND2	5:B:721:HOH:O	2.51	0.42
1:A:176:ARG:N	1:A:177:LEU:HD12	2.34	0.42
1:B:27:ILE:HD12	1:B:254:THR:CG2	2.48	0.42
1:A:235:ALA:HB2	1:A:244:SER:HB3	2.02	0.42
1:C:224:LYS:O	1:C:225:VAL:HB	2.19	0.42
1:A:263:TYR:HD1	1:A:290:LEU:HD13	1.83	0.42
1:B:36:ARG:NH2	5:B:769:HOH:O	2.50	0.42
1:B:214:VAL:HG21	1:B:234:VAL:HG22	2.02	0.42
1:A:166:ARG:NE	5:A:1085:HOH:O	2.53	0.42
1:A:171:THR:HG22	1:A:173:ALA:N	2.35	0.42
1:B:322:GLU:OE2	1:B:326:ARG:CZ	2.68	0.42
1:B:25:ARG:HD2	1:B:262:HIS:CE1	2.55	0.42
1:C:341:ARG:HD3	5:C:1144:HOH:O	2.19	0.42
1:A:225:VAL:HB	5:A:925:HOH:O	2.19	0.42
1:C:1:MET:HE3	1:C:6:ARG:HD2	2.00	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:272:GLY:HA3	1:A:278:MET:CE	2.39	0.42
1:C:233:ALA:CB	1:C:246:HIS:HB3	2.47	0.42
1:B:36:ARG:NH1	1:B:36:ARG:HB2	2.35	0.42
1:A:156:MET:HE3	1:A:228:MET:SD	2.60	0.42
1:A:330:GLU:CG	5:A:1135:HOH:O	2.65	0.42
1:A:276:PRO:O	1:A:279:ASP:HB2	2.20	0.42
1:A:205:LYS:O	1:A:205:LYS:HG3	2.19	0.42
1:A:28:LEU:HD23	1:A:28:LEU:N	2.34	0.41
1:B:282:LEU:HD13	5:B:766:HOH:O	2.20	0.41
1:B:236:PRO:O	1:B:239:THR:HG23	2.20	0.41
1:B:151:LEU:HA	1:B:151:LEU:HD23	1.87	0.41
1:C:321:ASP:O	1:C:325:VAL:HG23	2.20	0.41
1:C:207:LEU:HG	1:C:234:VAL:HG11	2.02	0.41
1:B:166:ARG:HB2	1:B:166:ARG:HE	1.70	0.41
1:B:112:TRP:CD2	1:B:119:ALA:HA	2.56	0.41
1:A:36:ARG:NH1	5:A:832:HOH:O	2.53	0.41
1:A:224:LYS:HE3	1:A:334:LEU:HD22	2.03	0.41
1:B:342:LEU:H	1:B:342:LEU:HD23	1.83	0.41
1:B:342:LEU:HD23	1:B:342:LEU:N	2.35	0.41
1:A:237:GLU:HG3	1:A:238:GLY:H	1.81	0.41
1:A:283:ARG:HH11	1:A:283:ARG:HG2	1.86	0.41
1:A:304:ARG:NH2	1:C:55:PRO:HB3	2.36	0.41
1:A:166:ARG:O	1:A:170:GLN:CB	2.55	0.41
1:C:305:ARG:O	1:C:308:VAL:HG22	2.19	0.41
1:A:136:ARG:NH2	1:A:279:ASP:OD1	2.50	0.41
1:A:198:THR:HG22	1:A:198:THR:O	2.21	0.41
1:B:137:THR:HA	1:B:267:SER:O	2.21	0.41
1:C:28:LEU:N	1:C:28:LEU:HD23	2.36	0.41
1:A:283:ARG:NH2	5:A:806:HOH:O	2.54	0.41
1:C:242:GLU:HG3	1:C:243:GLN:NE2	2.22	0.40
1:C:224:LYS:HE3	1:C:334:LEU:HD22	2.03	0.40
1:A:171:THR:C	1:A:173:ALA:N	2.72	0.40
1:C:165:HIS:O	1:C:166:ARG:C	2.58	0.40
1:C:285:TRP:CZ3	1:C:289:ALA:HB2	2.57	0.40
1:C:156:MET:HE3	1:C:228:MET:HG2	2.02	0.40
1:B:315:PRO:HB2	1:B:317:MET:CE	2.51	0.40
1:C:194:ILE:HB	1:C:216:ALA:CB	2.46	0.40
1:C:304:ARG:HH11	1:C:304:ARG:HG3	1.86	0.40
1:C:322:GLU:OE2	1:C:326:ARG:CZ	2.70	0.40
1:B:329:ARG:O	1:B:333:LYS:HG3	2.21	0.40
1:B:239:THR:HA	1:B:240:PRO:HD3	1.92	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	340/349 (97%)	308 (91%)	19 (6%)	13 (4%)	5	0
1	B	339/349 (97%)	314 (93%)	21 (6%)	4 (1%)	19	7
1	C	340/349 (97%)	298 (88%)	26 (8%)	16 (5%)	4	0
All	All	1019/1047 (97%)	920 (90%)	66 (6%)	33 (3%)	6	1

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ALA
1	A	166	ARG
1	A	225	VAL
1	B	196	GLY
1	B	225	VAL
1	C	119	ALA
1	C	199	PRO
1	C	214	VAL
1	C	225	VAL
1	C	237	GLU
1	A	210	ALA
1	A	240	PRO
1	A	241	LYS
1	C	236	PRO
1	A	224	LYS
1	A	237	GLU
1	B	224	LYS
1	B	237	GLU
1	C	2	ALA
1	C	195	PRO
1	C	200	SER
1	C	216	ALA
1	C	224	LYS
1	A	120	ASP
1	A	211	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	120	ASP
1	C	166	ARG
1	C	202	LEU
1	A	178	GLU
1	A	208	ARG
1	C	168	ASN
1	A	239	THR
1	C	238	GLY

### 5.3.2 Protein sidechains ⓘ

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	277/284 (98%)	272 (98%)	5 (2%)	71	68
1	B	276/284 (97%)	272 (99%)	4 (1%)	78	77
1	C	277/284 (98%)	271 (98%)	6 (2%)	64	60
All	All	830/852 (97%)	815 (98%)	15 (2%)	71	68

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	28	LEU
1	A	70	TYR
1	A	177	LEU
1	A	263	TYR
1	B	25	ARG
1	B	28	LEU
1	B	70	TYR
1	B	263	TYR
1	C	25	ARG
1	C	28	LEU
1	C	70	TYR
1	C	174	PHE
1	C	199	PRO
1	C	263	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	143	HIS
1	A	170	GLN
1	A	211	ASN
1	A	223	ASN
1	B	143	HIS
1	B	168	ASN
1	B	211	ASN
1	B	223	ASN
1	C	143	HIS
1	C	168	ASN
1	C	170	GLN
1	C	211	ASN
1	C	223	ASN
1	C	243	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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
2	FES	A	501	1	0,4,4	0.00	-	0,4,4	0.00	-
4	HXX	A	601	-	12,12,12	2.80	7 (58%)	17,17,17	1.23	2 (11%)
2	FES	B	501	1	0,4,4	0.00	-	0,4,4	0.00	-
4	HXX	B	601	-	12,12,12	2.74	7 (58%)	17,17,17	1.24	2 (11%)
2	FES	C	501	1	0,4,4	0.00	-	0,4,4	0.00	-
4	HXX	C	601	-	12,12,12	2.72	7 (58%)	17,17,17	1.25	2 (11%)

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	FES	A	501	1	-	0/0/4/4	0/0/1/1
4	HXX	A	601	-	-	0/4/4/4	0/1/1/1
2	FES	B	501	1	-	0/0/4/4	0/0/1/1
4	HXX	B	601	-	-	0/4/4/4	0/1/1/1
2	FES	C	501	1	-	0/0/4/4	0/0/1/1
4	HXX	C	601	-	-	0/4/4/4	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	HXX	C1-C6	5.76	1.49	1.39
4	C	601	HXX	C1-C6	5.64	1.48	1.39
4	B	601	HXX	C1-C6	5.23	1.48	1.39
4	B	601	HXX	C2-C3	4.77	1.48	1.39
4	A	601	HXX	C2-C3	4.63	1.47	1.39
4	C	601	HXX	C2-C3	4.36	1.47	1.39
4	B	601	HXX	C1-C2	3.28	1.48	1.41
4	A	601	HXX	C1-C2	3.23	1.48	1.41
4	C	601	HXX	C1-C2	3.22	1.48	1.41
4	B	601	HXX	O2-C2	2.80	1.43	1.37
4	A	601	HXX	C4-C3	2.67	1.45	1.38
4	B	601	HXX	C4-C3	2.67	1.45	1.38
4	A	601	HXX	O2-C2	2.65	1.43	1.37
4	C	601	HXX	C4-C3	2.63	1.44	1.38
4	C	601	HXX	O2-C2	2.48	1.43	1.37
4	B	601	HXX	C5-C6	2.33	1.44	1.38
4	A	601	HXX	C5-C6	2.31	1.44	1.38
4	C	601	HXX	C4-C5	2.30	1.43	1.38
4	A	601	HXX	C4-C5	2.26	1.43	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	HXX	C4-C5	2.21	1.43	1.38
4	C	601	HXX	C5-C6	2.18	1.43	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	HXX	C1-C6-CL2	2.71	123.50	119.66
4	A	601	HXX	C1-C6-CL2	2.64	123.40	119.66
4	B	601	HXX	C2-C3-CL1	2.47	122.48	118.78
4	B	601	HXX	C1-C6-CL2	2.44	123.11	119.66
4	A	601	HXX	C2-C3-CL1	2.40	122.38	118.78
4	C	601	HXX	C2-C3-CL1	2.39	122.36	118.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	342/349 (97%)	0.46	31 (9%) 9 8	25, 39, 80, 90	0
1	B	341/349 (97%)	0.35	28 (8%) 12 11	26, 40, 74, 86	0
1	C	342/349 (97%)	0.83	45 (13%) 4 3	26, 43, 85, 90	0
All	All	1025/1047 (97%)	0.54	104 (10%) 8 7	25, 41, 81, 90	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	ALA	13.3
1	C	209	GLY	11.7
1	C	214	VAL	11.2
1	C	213	PRO	10.3
1	A	211	ASN	9.6
1	A	239	THR	9.4
1	C	176	ARG	9.2
1	C	210	ALA	9.1
1	A	342	LEU	8.1
1	C	212	THR	7.9
1	C	1	MET	7.9
1	A	1	MET	7.4
1	C	342	LEU	7.3
1	A	177	LEU	7.1
1	C	340	ALA	6.0
1	B	291	VAL	5.7
1	A	212	THR	5.7
1	A	173	ALA	5.7
1	A	209	GLY	5.7
1	A	238	GLY	5.6
1	C	174	PHE	5.5
1	A	174	PHE	5.4
1	C	211	ASN	5.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	169	ALA	5.3
1	C	167	ALA	5.1
1	A	172	ASP	5.0
1	A	169	ALA	4.7
1	A	170	GLN	4.5
1	C	208	ARG	4.5
1	C	238	GLY	4.3
1	C	274	ASP	4.2
1	B	177	LEU	4.1
1	C	337	LEU	4.0
1	C	198	THR	4.0
1	C	237	GLU	3.9
1	A	341	ARG	3.8
1	B	195	PRO	3.7
1	B	2	ALA	3.7
1	C	206	PHE	3.7
1	C	175	ASP	3.6
1	B	342	LEU	3.6
1	C	240	PRO	3.5
1	B	211	ASN	3.5
1	A	237	GLU	3.3
1	A	197	GLY	3.2
1	C	243	GLN	3.2
1	B	174	PHE	3.2
1	B	242	GLU	3.2
1	C	170	GLN	3.2
1	A	312	GLY	3.1
1	C	207	LEU	3.0
1	B	237	GLU	3.0
1	B	182	ILE	3.0
1	C	341	ARG	3.0
1	C	2	ALA	3.0
1	C	200	SER	3.0
1	A	175	ASP	2.9
1	C	203	MET	2.9
1	B	167	ALA	2.9
1	A	214	VAL	2.8
1	B	200	SER	2.8
1	B	175	ASP	2.8
1	B	213	PRO	2.8
1	B	281	VAL	2.8
1	B	225	VAL	2.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	239	THR	2.7
1	B	341	ARG	2.7
1	B	180	GLU	2.6
1	C	241	LYS	2.6
1	A	207	LEU	2.6
1	A	339	ALA	2.6
1	C	177	LEU	2.6
1	C	201	VAL	2.5
1	B	210	ALA	2.5
1	C	236	PRO	2.5
1	A	176	ARG	2.4
1	C	225	VAL	2.4
1	C	336	GLN	2.4
1	C	202	LEU	2.4
1	C	172	ASP	2.4
1	A	88	ASN	2.3
1	C	273	ILE	2.3
1	B	179	ARG	2.3
1	C	245	ILE	2.3
1	B	243	GLN	2.2
1	B	209	GLY	2.2
1	B	245	ILE	2.2
1	B	192	MET	2.2
1	A	168	ASN	2.2
1	B	88	ASN	2.2
1	B	234	VAL	2.1
1	C	275	ASP	2.1
1	A	340	ALA	2.1
1	C	339	ALA	2.1
1	A	178	GLU	2.1
1	A	2	ALA	2.1
1	B	277	GLU	2.1
1	B	270	ASN	2.1
1	A	240	PRO	2.1
1	C	199	PRO	2.1
1	C	193	LYS	2.1
1	A	171	THR	2.1
1	A	167	ALA	2.0
1	C	171	THR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	HXX	A	601	12/12	0.68	6.96	87,89,89,89	0
4	HXX	B	601	12/12	0.31	5.50	47,52,53,54	0
4	HXX	C	601	12/12	0.33	2.64	73,75,76,77	0
3	CO	A	602	1/1	0.15	2.35	55,55,55,55	0
3	CO	C	502	1/1	0.16	1.69	54,54,54,54	0
3	CO	B	502	1/1	0.12	1.31	41,41,41,41	0
2	FES	C	501	4/4	0.13	0.26	28,28,29,29	0
3	CO	C	603	1/1	0.14	0.23	70,70,70,70	0
2	FES	A	501	4/4	0.12	-0.04	28,29,30,31	0
3	CO	A	502	1/1	0.11	-0.28	36,36,36,36	0
3	CO	C	602	1/1	0.13	-0.74	59,59,59,59	0
3	CO	B	602	1/1	0.11	-1.01	64,64,64,64	0
2	FES	B	501	4/4	0.09	-1.06	33,35,35,37	0
3	CO	C	604	1/1	0.05	-1.33	76,76,76,76	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.