Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:59 AM GMT

PDB ID	:	3GTS
Title	:	Crystal Structure of Dicamba Monooxygenase with Non-heme Iron and Dicamba
Authors	:	Rydel, T.J.; Sturman, E.J.; Moshiri, F.; Brown, G.R.; Qi, Y.
Deposited on	:	2009-03-28
Resolution	:	2.20 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

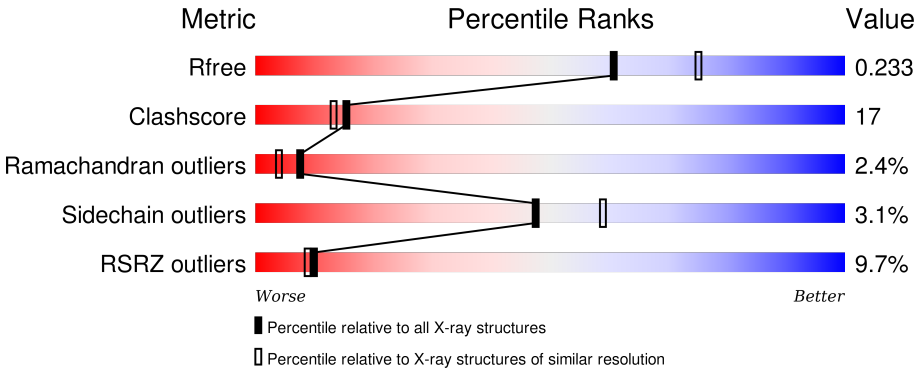
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	349	5% 70% 25%
1	B	349	13% 67% 29%
1	C	349	10% 65% 23% 5% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8329 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 DdmC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2641	1665	474	489	13			
1	B	341	Total	C	N	O	S	0	0	0
			2641	1665	474	489	13			
1	C	327	Total	C	N	O	S	0	0	0
			2524	1594	450	467	13			

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	2	ALA	-	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	2	ALA	-	EXPRESSION TAG	UNP Q5S3I3

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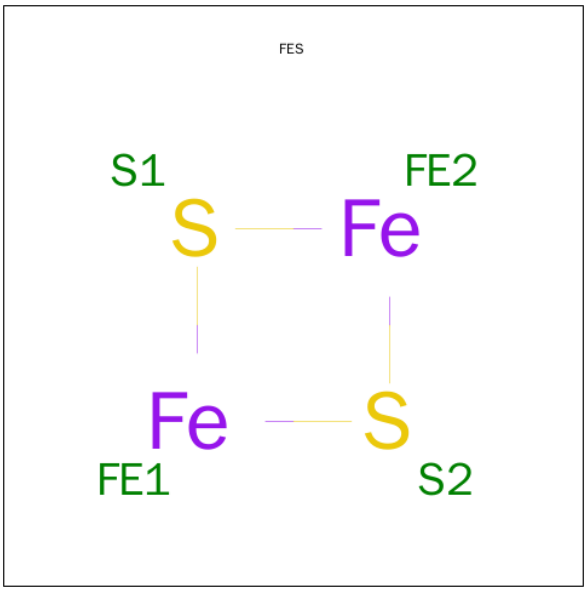
Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	MET	ENGINEERED	UNP Q5S3I3
C	341	ARG	-	EXPRESSION TAG	UNP Q5S3I3
C	342	LEU	-	EXPRESSION TAG	UNP Q5S3I3
C	343	GLU	-	EXPRESSION TAG	UNP Q5S3I3
C	344	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	345	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	346	HIS	-	EXPRESSION TAG	UNP 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_2S_2).



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 FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Fe 1 1	0	0

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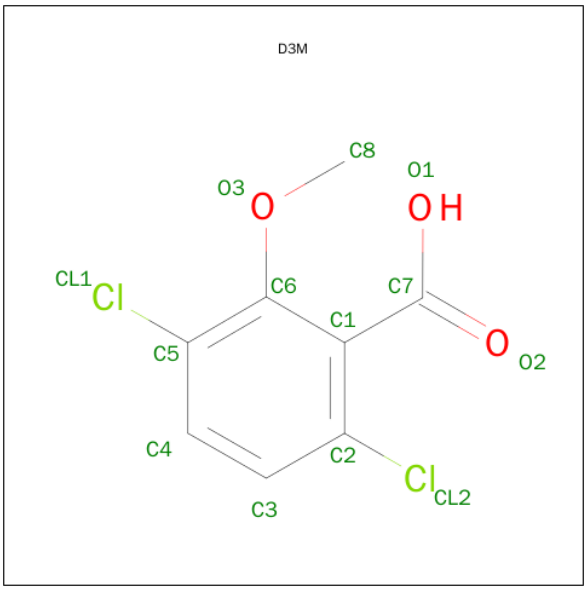
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe 1 1	0	0

- Molecule 4 is 3,6-DICHLORO-2-METHOXYBENZOIC ACID (three-letter code: D3M) (formula: $C_8H_6Cl_2O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Cl O 13 8 2 3	0	0
4	B	1	Total C Cl O 13 8 2 3	0	0

- Molecule 5 is water.

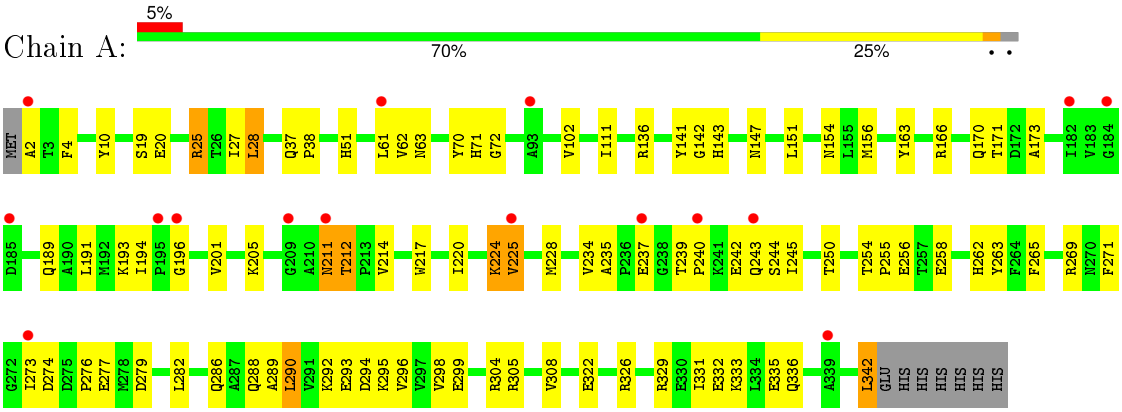
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	169	Total O 169 169	0	0
5	B	155	Total O 155 155	0	0
5	C	159	Total O 159 159	0	0

3 Residue-property plots (i)

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

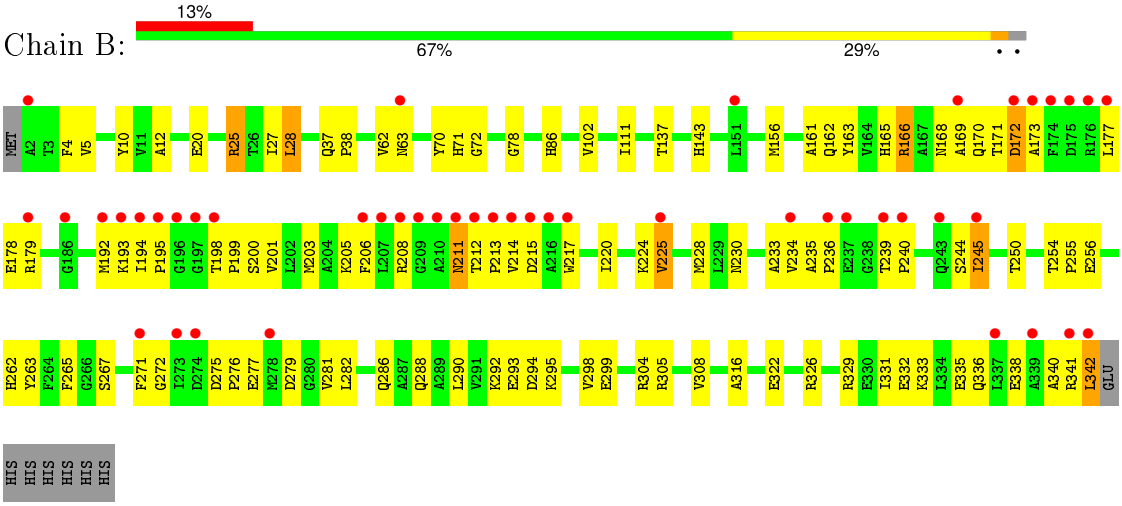
- Molecule 1: DdmC

Chain A:



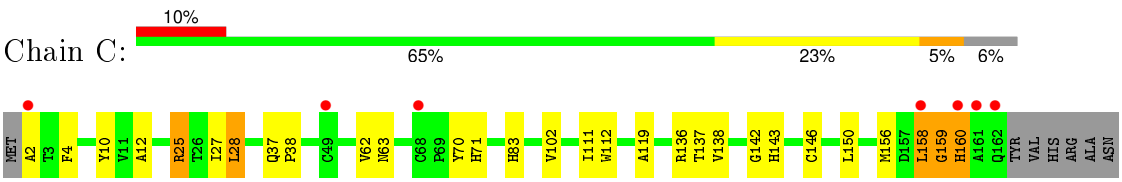
- Molecule 1: DdmC

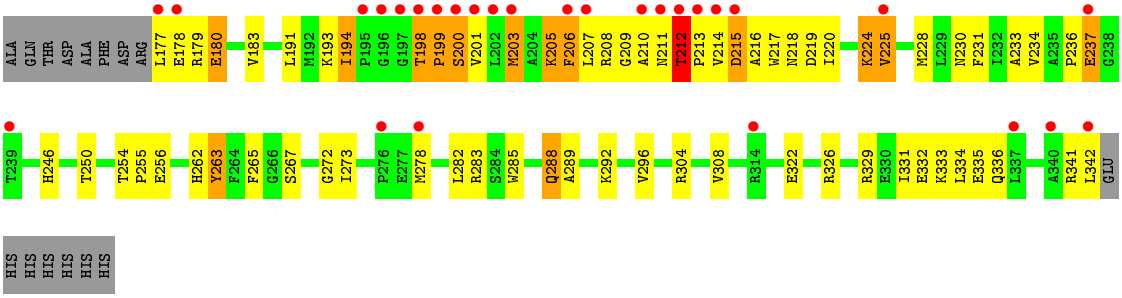
Chain B:



- Molecule 1: DdmC

Chain C:




ALA GLN THR ASP ALA PHE ASP ARG L177 E178 R179 E180 V183 L191 M192 K193 I194 P195 G196 G197 T198 P199 S200 V201 L202 M203 A204 K205 F206 L207 R208 G209 A210 N211 T212 P213 V214 D215 A216 W217 N218 D219 I220 K224 V225 M228 L229 N230 F231 I232 A233 V234 A235 P236 E237 G238
T239 H246 T250 T254 P255 E256 H262 Y263 F264 F265 G266 S267 G272 I273 P276 E277 M278 L282 R283 S284 W285 Q288 A289 K292 V296 R304 V308 R314 E322 R326 R329 E330 I331 E332 K333 L334 E335 Q336 L337 A340 R341 L342 GLU
HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	80.80Å 80.80Å 159.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.20 36.04 – 2.20	Depositor EDS
% Data completeness (in resolution range)	84.9 (20.00-2.20) 85.2 (36.04-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.07 (at 2.20Å)	Xtriage
Refinement program	CNX2002	Depositor
R, R_{free}	0.230 , 0.266 0.205 , 0.233	Depositor DCC
R_{free} test set	5057 reflections (11.20%)	DCC
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.4	EDS
Estimated twinning fraction	0.003 for -h,-k,l 0.046 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 50259 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8329	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D3M, FE, 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	0.31	0/2706	0.61	1/3685 (0.0%)
1	B	0.29	0/2706	0.61	1/3685 (0.0%)
1	C	0.31	0/2585	0.62	0/3519
All	All	0.30	0/7997	0.61	2/10889 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	GLY	N-CA-C	5.04	125.71	113.10
1	B	72	GLY	N-CA-C	5.04	125.71	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2641	0	2577	75	0
1	B	2641	0	2577	100	0
1	C	2524	0	2472	95	0
2	A	4	0	0	1	0
2	B	4	0	0	1	0
2	C	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	13	0	5	0	0
4	B	13	0	5	0	0
5	A	169	0	0	5	0
5	B	155	0	0	7	0
5	C	159	0	0	9	0
All	All	8329	0	7636	267	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 17.

All (267) 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:A:28:LEU:HD22	1:A:255:PRO:HG2	1.41	1.02
1:B:28:LEU:HD22	1:B:255:PRO:HG2	1.48	0.94
1:C:28:LEU:HD22	1:C:255:PRO:HG2	1.50	0.93
1:A:245:ILE:HD12	1:A:271:PHE:HB3	1.50	0.92
1:B:171:THR:HG22	1:B:173:ALA:H	1.37	0.88
1:B:286:GLN:HA	1:B:290:LEU:HD23	1.57	0.85
1:A:171:THR:HG22	1:A:173:ALA:H	1.39	0.84
1:C:342:LEU:H	1:C:342:LEU:HD23	1.44	0.82
1:B:171:THR:HG21	1:B:194:ILE:HG21	1.62	0.79
1:B:211:ASN:ND2	1:B:212:THR:H	1.81	0.78
1:A:286:GLN:HA	1:A:290:LEU:HD23	1.67	0.77
1:C:233:ALA:HB2	1:C:246:HIS:HB3	1.65	0.77
1:A:295:LYS:O	1:A:299:GLU:HG3	1.84	0.77
1:C:194:ILE:HG13	1:C:216:ALA:HB3	1.67	0.76
1:B:217:TRP:HB2	1:B:233:ALA:HB3	1.68	0.75
1:A:245:ILE:HG23	1:A:271:PHE:CD2	2.21	0.75
1:C:177:LEU:HD12	1:C:178:GLU:H	1.53	0.73
1:B:63:ASN:HB3	5:B:1001:HOH:O	1.88	0.73
1:A:290:LEU:HD22	1:A:290:LEU:H	1.53	0.72
1:A:342:LEU:H	1:A:342:LEU:HD23	1.54	0.72
1:A:143:HIS:HE1	1:A:256:GLU:OE1	1.72	0.72
1:A:191:LEU:N	1:A:191:LEU:HD12	2.05	0.71
1:A:214:VAL:HG21	1:A:234:VAL:HG22	1.72	0.71
1:B:342:LEU:H	1:B:342:LEU:HD23	1.57	0.70
1:B:341:ARG:HB3	1:B:342:LEU:HD23	1.73	0.70
1:B:214:VAL:HG21	1:B:234:VAL:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:GLN:HA	1:C:288:GLN:HE21	1.59	0.68
1:B:295:LYS:O	1:B:299:GLU:HG3	1.93	0.68
1:B:245:ILE:HG12	1:B:271:PHE:HB3	1.75	0.68
1:A:290:LEU:HD22	1:A:290:LEU:N	2.10	0.66
1:B:178:GLU:OE2	1:B:193:LYS:HE2	1.96	0.65
1:C:4:PHE:HB3	1:C:28:LEU:HD13	1.79	0.65
1:B:177:LEU:HD11	1:B:192:MET:SD	2.38	0.64
1:C:143:HIS:HE1	1:C:256:GLU:OE1	1.80	0.63
1:B:143:HIS:HE1	1:B:256:GLU:OE1	1.82	0.62
1:C:198:THR:H	1:C:199:PRO:HD2	1.64	0.62
1:C:193:LYS:HE3	1:C:217:TRP:HE1	1.65	0.62
1:B:331:ILE:O	1:B:335:GLU:HG3	2.00	0.62
1:B:245:ILE:HG23	1:B:271:PHE:CD2	2.35	0.61
1:C:212:THR:O	1:C:214:VAL:HG13	2.01	0.61
1:B:267:SER:OG	1:B:282:LEU:HD13	2.01	0.61
1:C:288:GLN:HB2	5:C:988:HOH:O	2.00	0.61
1:B:4:PHE:HB3	1:B:28:LEU:HD13	1.83	0.60
1:C:37:GLN:HB3	1:C:38:PRO:HD2	1.83	0.60
1:B:172:ASP:OD1	1:B:198:THR:HB	2.00	0.60
1:C:233:ALA:CB	1:C:246:HIS:HB3	2.32	0.60
1:B:208:ARG:HH22	1:B:272:GLY:HA2	1.67	0.60
1:B:71:HIS:HB2	2:B:501:FES:S1	2.43	0.59
1:C:331:ILE:O	1:C:335:GLU:HG3	2.02	0.59
1:A:19:SER:HB2	5:A:853:HOH:O	2.03	0.59
1:B:27:ILE:HD12	1:B:254:THR:HG21	1.85	0.59
1:B:162:GLN:HE22	1:B:171:THR:H	1.50	0.58
1:A:37:GLN:HB3	1:A:38:PRO:HD2	1.84	0.58
1:C:211:ASN:O	1:C:212:THR:HG22	2.03	0.58
1:A:331:ILE:O	1:A:335:GLU:HG3	2.03	0.58
1:B:37:GLN:HB3	1:B:38:PRO:HD2	1.85	0.57
1:C:272:GLY:HA3	1:C:278:MET:HE1	1.84	0.57
1:C:193:LYS:HG2	1:C:217:TRP:CD1	2.39	0.57
1:B:28:LEU:CD2	1:B:255:PRO:HG2	2.30	0.57
1:B:165:HIS:HA	1:B:293:GLU:OE2	2.04	0.57
1:C:265:PHE:CE2	1:C:285:TRP:HE3	2.23	0.56
1:C:137:THR:HA	1:C:267:SER:O	2.05	0.56
1:B:10:TYR:CE2	1:B:225:VAL:HG11	2.41	0.56
1:B:20:GLU:HB2	5:B:815:HOH:O	2.04	0.56
1:A:4:PHE:HB3	1:A:28:LEU:HD13	1.86	0.56
1:C:206:PHE:HE2	1:C:246:HIS:HA	1.71	0.56
1:B:214:VAL:HG23	1:B:235:ALA:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:PHE:HD1	1:C:206:PHE:H	1.54	0.55
1:B:208:ARG:HH22	1:B:272:GLY:CA	2.20	0.55
1:B:276:PRO:O	1:B:279:ASP:HB2	2.06	0.55
1:C:177:LEU:O	1:C:193:LYS:HB2	2.06	0.55
1:A:147:ASN:ND2	5:A:890:HOH:O	2.40	0.55
1:C:199:PRO:HG2	1:C:200:SER:H	1.72	0.55
1:C:71:HIS:HB2	2:C:501:FES:S1	2.47	0.54
1:A:71:HIS:HB2	2:A:501:FES:S1	2.47	0.54
1:C:207:LEU:C	1:C:209:GLY:H	2.11	0.54
1:A:211:ASN:O	1:A:212:THR:HB	2.07	0.54
1:B:235:ALA:HB1	1:B:239:THR:OG1	2.08	0.54
1:B:201:VAL:HG22	1:B:205:LYS:HE3	1.88	0.54
1:B:177:LEU:HD11	1:B:192:MET:CG	2.37	0.54
1:C:233:ALA:HB2	1:C:246:HIS:CB	2.36	0.54
1:B:236:PRO:O	1:B:239:THR:HG23	2.08	0.54
1:C:272:GLY:HA3	1:C:278:MET:CE	2.38	0.54
1:A:102:VAL:HB	1:A:111:ILE:HD13	1.89	0.54
1:B:342:LEU:HD23	1:B:342:LEU:N	2.22	0.54
1:B:25:ARG:HD2	1:B:262:HIS:CE1	2.43	0.53
1:C:283:ARG:HG2	5:C:1164:HOH:O	2.06	0.53
1:A:240:PRO:HG2	1:A:243:GLN:HB2	1.90	0.53
1:A:239:THR:HB	1:A:240:PRO:HD2	1.91	0.53
1:B:193:LYS:HG2	1:B:195:PRO:HD3	1.90	0.53
1:C:207:LEU:O	1:C:209:GLY:N	2.41	0.53
1:A:25:ARG:HD2	1:A:262:HIS:CE1	2.44	0.52
1:A:282:LEU:O	1:A:286:GLN:HG3	2.09	0.52
1:B:322:GLU:HG2	1:B:326:ARG:NH1	2.25	0.52
1:A:240:PRO:HG3	1:A:243:GLN:OE1	2.10	0.52
1:A:62:VAL:HG12	1:A:63:ASN:ND2	2.25	0.52
1:C:156:MET:HE3	1:C:228:MET:SD	2.49	0.52
1:B:203:MET:O	1:B:206:PHE:HB2	2.09	0.52
1:A:269:ARG:HD3	1:A:282:LEU:HD11	1.91	0.52
1:A:290:LEU:CD2	1:A:290:LEU:H	2.20	0.52
1:A:224:LYS:HB2	5:A:894:HOH:O	2.09	0.52
1:C:179:ARG:O	1:C:180:GLU:HB2	2.09	0.52
1:C:214:VAL:HG12	1:C:236:PRO:HA	1.92	0.52
1:A:294:ASP:O	1:A:298:VAL:HG22	2.10	0.52
1:C:178:GLU:HG3	1:C:179:ARG:H	1.76	0.52
1:B:277:GLU:O	1:B:281:VAL:HG23	2.10	0.51
1:B:28:LEU:HD23	1:B:28:LEU:N	2.25	0.51
1:C:213:PRO:O	1:C:236:PRO:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:HB2	1:A:170:GLN:HE21	1.76	0.51
1:B:288:GLN:HE22	1:B:292:LYS:HD2	1.75	0.50
1:B:163:TYR:O	1:B:166:ARG:HB2	2.12	0.50
1:C:25:ARG:HD3	5:C:1152:HOH:O	2.09	0.50
1:A:326:ARG:HG3	1:A:326:ARG:HH11	1.76	0.50
1:A:245:ILE:HD12	1:A:271:PHE:CB	2.32	0.50
1:A:242:GLU:CD	1:A:242:GLU:H	2.15	0.50
1:B:71:HIS:HD2	1:C:160:HIS:CD2	2.30	0.50
1:C:206:PHE:N	1:C:206:PHE:CD1	2.79	0.50
1:A:289:ALA:HB3	1:A:290:LEU:HD22	1.94	0.50
1:C:156:MET:CE	1:C:228:MET:SD	2.99	0.50
1:A:191:LEU:CD1	1:A:191:LEU:N	2.74	0.50
1:A:10:TYR:CZ	1:A:225:VAL:HG11	2.47	0.50
1:B:179:ARG:HB3	5:B:1027:HOH:O	2.12	0.50
1:B:201:VAL:O	1:B:205:LYS:HG3	2.11	0.50
1:C:236:PRO:O	1:C:237:GLU:C	2.51	0.49
1:A:322:GLU:HG2	1:A:326:ARG:NH1	2.27	0.49
1:C:288:GLN:NE2	5:C:988:HOH:O	2.46	0.49
1:B:137:THR:HA	1:B:267:SER:O	2.12	0.49
1:C:62:VAL:HG12	1:C:63:ASN:ND2	2.26	0.49
1:A:304:ARG:HG3	1:A:304:ARG:HH11	1.77	0.49
1:C:28:LEU:N	1:C:28:LEU:HD23	2.27	0.49
1:B:173:ALA:HB3	1:B:194:ILE:CG2	2.43	0.49
1:B:10:TYR:CZ	1:B:225:VAL:HG11	2.47	0.49
1:B:102:VAL:HB	1:B:111:ILE:HD13	1.93	0.49
1:B:20:GLU:HG3	5:B:997:HOH:O	2.12	0.49
1:B:214:VAL:HG22	1:B:215:ASP:N	2.28	0.49
1:A:274:ASP:HB3	5:A:710:HOH:O	2.12	0.49
1:A:102:VAL:HB	1:A:111:ILE:CD1	2.43	0.48
1:B:203:MET:CE	1:B:234:VAL:HB	2.43	0.48
1:A:2:ALA:N	1:A:258:GLU:OE1	2.47	0.48
1:A:288:GLN:HE21	1:A:293:GLU:HG3	1.78	0.48
1:A:201:VAL:HG12	1:A:205:LYS:HE2	1.95	0.48
1:A:214:VAL:CG2	1:A:234:VAL:HG22	2.43	0.48
1:B:201:VAL:CG2	1:B:205:LYS:HE3	2.43	0.48
1:A:292:LYS:O	1:A:296:VAL:HG23	2.14	0.48
1:C:292:LYS:O	1:C:296:VAL:HG23	2.14	0.48
1:C:332:GLU:O	1:C:336:GLN:HG3	2.14	0.48
1:C:207:LEU:HD23	1:C:207:LEU:C	2.34	0.48
1:A:276:PRO:O	1:A:279:ASP:HB2	2.13	0.48
1:B:282:LEU:O	1:B:286:GLN:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ILE:HG22	1:A:28:LEU:HD23	1.96	0.48
1:A:342:LEU:H	1:A:342:LEU:CD2	2.25	0.48
1:B:214:VAL:CG2	1:B:234:VAL:HG22	2.43	0.48
1:C:206:PHE:CE2	1:C:246:HIS:HA	2.49	0.48
1:C:288:GLN:CA	1:C:288:GLN:HE21	2.22	0.48
1:B:62:VAL:HG12	1:B:63:ASN:ND2	2.28	0.47
1:A:193:LYS:HD2	1:A:217:TRP:HE1	1.79	0.47
1:B:304:ARG:HG3	1:B:304:ARG:HH11	1.79	0.47
1:B:192:MET:HE3	1:B:194:ILE:HD11	1.97	0.47
1:A:163:TYR:HB3	1:A:166:ARG:HH21	1.79	0.47
1:C:178:GLU:HG3	1:C:179:ARG:N	2.29	0.47
1:C:198:THR:HB	1:C:199:PRO:HD3	1.96	0.47
1:B:5:VAL:HG13	1:B:338:GLU:OE2	2.14	0.47
1:A:51:HIS:HD2	1:B:316:ALA:O	1.98	0.47
1:C:156:MET:HE2	1:C:220:ILE:HD13	1.96	0.47
1:A:235:ALA:HB2	1:A:244:SER:OG	2.14	0.47
1:B:326:ARG:HH11	1:B:326:ARG:HG3	1.80	0.47
1:B:78:GLY:HA3	5:B:872:HOH:O	2.14	0.47
1:C:10:TYR:CZ	1:C:225:VAL:HG11	2.50	0.47
1:B:173:ALA:HB3	1:B:194:ILE:HG22	1.97	0.47
1:C:288:GLN:HG2	5:C:802:HOH:O	2.15	0.47
1:C:205:LYS:H	1:C:205:LYS:HD3	1.80	0.47
1:C:102:VAL:HB	1:C:111:ILE:HD13	1.96	0.47
1:C:322:GLU:HG2	1:C:326:ARG:NH1	2.29	0.47
1:B:168:ASN:O	1:B:200:SER:HB2	2.14	0.47
1:A:156:MET:HE2	1:A:220:ILE:HD13	1.96	0.47
1:C:224:LYS:HG3	1:C:334:LEU:HD11	1.96	0.47
1:A:304:ARG:O	1:A:308:VAL:HG13	2.15	0.46
1:B:156:MET:HE3	1:B:228:MET:SD	2.55	0.46
1:A:211:ASN:N	1:A:211:ASN:HD22	2.13	0.46
1:C:304:ARG:O	1:C:308:VAL:HG13	2.15	0.46
1:C:12:ALA:HB2	1:C:111:ILE:HG13	1.98	0.46
1:B:275:ASP:OD1	1:B:277:GLU:HB2	2.16	0.46
1:C:10:TYR:CE2	1:C:225:VAL:HG11	2.50	0.46
1:B:290:LEU:H	1:B:290:LEU:HD22	1.80	0.46
1:B:168:ASN:HA	1:B:201:VAL:CG1	2.46	0.46
1:A:201:VAL:O	1:A:205:LYS:HG3	2.16	0.46
1:C:158:LEU:O	1:C:160:HIS:N	2.49	0.46
1:B:288:GLN:NE2	1:B:292:LYS:HD2	2.31	0.46
1:A:28:LEU:N	1:A:28:LEU:HD23	2.31	0.45
1:B:102:VAL:HB	1:B:111:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:VAL:CG2	1:C:326:ARG:HD3	2.46	0.45
1:B:290:LEU:HD22	1:B:290:LEU:N	2.32	0.45
1:A:154:ASN:HA	5:C:703:HOH:O	2.17	0.45
1:B:211:ASN:ND2	1:B:212:THR:N	2.57	0.45
1:C:206:PHE:HD2	1:C:234:VAL:HG12	1.82	0.45
1:C:142:GLY:HA3	1:C:285:TRP:CZ3	2.51	0.45
1:B:304:ARG:O	1:B:308:VAL:HG13	2.17	0.45
1:C:218:ASN:HA	1:C:231:PHE:O	2.18	0.45
1:C:83:HIS:HD2	5:C:952:HOH:O	1.99	0.44
1:A:342:LEU:O	1:A:342:LEU:HG	2.16	0.44
1:C:191:LEU:CD2	1:C:219:ASP:HB3	2.48	0.44
1:B:250:THR:O	1:B:265:PHE:HA	2.17	0.44
1:A:189:GLN:HG3	5:A:892:HOH:O	2.16	0.44
1:A:28:LEU:CD2	1:A:255:PRO:HG2	2.29	0.44
1:C:326:ARG:HG3	1:C:326:ARG:HH11	1.82	0.44
1:C:138:VAL:HG21	1:C:282:LEU:HB2	1.98	0.44
1:C:250:THR:O	1:C:265:PHE:HA	2.18	0.44
1:C:304:ARG:HH11	1:C:304:ARG:HG3	1.83	0.44
1:C:28:LEU:CD2	1:C:255:PRO:HG2	2.34	0.44
1:C:206:PHE:CD2	1:C:234:VAL:HG12	2.52	0.44
1:A:10:TYR:CE2	1:A:225:VAL:HG11	2.53	0.44
1:B:332:GLU:O	1:B:336:GLN:HG3	2.18	0.44
1:B:288:GLN:O	1:B:292:LYS:HB3	2.18	0.43
1:B:244:SER:HA	5:B:1056:HOH:O	2.17	0.43
1:C:205:LYS:HB2	1:C:205:LYS:HE2	1.80	0.43
1:C:25:ARG:HD2	1:C:262:HIS:CE1	2.53	0.43
1:C:146:CYS:HB2	1:C:150:LEU:HD12	2.01	0.43
1:A:27:ILE:HD12	1:A:254:THR:HG21	1.99	0.43
1:C:27:ILE:HD12	1:C:254:THR:HG21	2.00	0.43
1:B:156:MET:CE	1:B:228:MET:SD	3.06	0.43
1:C:201:VAL:C	1:C:203:MET:H	2.20	0.43
1:B:166:ARG:O	1:B:170:GLN:HB2	2.19	0.43
1:A:329:ARG:O	1:A:333:LYS:HG3	2.19	0.43
1:A:171:THR:HG21	1:A:194:ILE:HG21	2.00	0.43
1:A:305:ARG:O	1:A:308:VAL:HG22	2.19	0.43
1:A:156:MET:HE3	1:A:228:MET:SD	2.59	0.43
1:C:136:ARG:HB2	1:C:273:ILE:HG23	2.01	0.42
1:B:203:MET:HE1	1:B:234:VAL:HB	2.00	0.42
1:C:158:LEU:HB3	1:C:218:ASN:HD21	1.84	0.42
1:C:112:TRP:CD1	1:C:119:ALA:HB2	2.54	0.42
1:A:332:GLU:O	1:A:336:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ALA:O	1:B:341:ARG:C	2.57	0.42
1:A:141:TYR:CG	1:A:142:GLY:N	2.87	0.42
1:A:250:THR:O	1:A:265:PHE:HA	2.19	0.42
1:B:211:ASN:HD22	1:B:212:THR:H	1.61	0.42
1:B:166:ARG:HB2	1:B:166:ARG:HE	1.74	0.42
1:C:288:GLN:HA	1:C:288:GLN:NE2	2.29	0.42
1:C:191:LEU:HD23	1:C:219:ASP:HB3	2.02	0.42
1:C:2:ALA:HA	5:C:1045:HOH:O	2.20	0.42
1:B:329:ARG:O	1:B:333:LYS:HG3	2.19	0.42
1:B:239:THR:HB	1:B:240:PRO:CD	2.50	0.42
1:C:112:TRP:CG	1:C:119:ALA:HB2	2.55	0.42
1:C:212:THR:HG23	1:C:213:PRO:N	2.33	0.42
1:A:20:GLU:O	1:A:61:LEU:HD13	2.20	0.42
1:B:282:LEU:HD23	1:B:282:LEU:HA	1.94	0.41
1:B:161:ALA:HB1	1:B:169:ALA:HB3	2.02	0.41
1:B:170:GLN:NE2	1:B:170:GLN:HA	2.35	0.41
1:B:12:ALA:HB2	1:B:111:ILE:HG13	2.01	0.41
1:A:136:ARG:HB2	1:A:273:ILE:HG23	2.01	0.41
1:B:220:ILE:HA	1:B:230:ASN:HA	2.02	0.41
1:B:199:PRO:HB3	1:B:214:VAL:HG11	2.03	0.41
1:A:288:GLN:HE21	1:A:293:GLU:CG	2.34	0.41
1:C:215:ASP:O	1:C:234:VAL:HA	2.21	0.41
1:B:86:HIS:HE1	1:C:160:HIS:CE1	2.38	0.41
1:B:225:VAL:HB	5:B:736:HOH:O	2.20	0.41
1:C:220:ILE:HA	1:C:230:ASN:HA	2.03	0.41
1:C:183:VAL:HG21	1:C:326:ARG:HD3	2.02	0.41
1:B:294:ASP:O	1:B:298:VAL:HG22	2.20	0.41
1:C:263:TYR:CE1	1:C:289:ALA:HB1	2.55	0.41
1:C:158:LEU:O	1:C:159:GLY:C	2.59	0.41
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.78	0.41
1:C:329:ARG:O	1:C:333:LYS:HG3	2.21	0.40
1:C:199:PRO:HG2	1:C:200:SER:N	2.35	0.40
1:C:341:ARG:NH1	5:C:1166:HOH:O	2.55	0.40
1:B:161:ALA:HA	1:B:165:HIS:CD2	2.57	0.40
1:B:304:ARG:HG3	1:B:304:ARG:NH1	2.37	0.40
1:B:305:ARG:O	1:B:308:VAL:HG22	2.21	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	339/349 (97%)	316 (93%)	17 (5%)	6 (2%)	11 7
1	B	339/349 (97%)	310 (91%)	25 (7%)	4 (1%)	16 12
1	C	323/349 (93%)	285 (88%)	24 (7%)	14 (4%)	3 1
All	All	1001/1047 (96%)	911 (91%)	66 (7%)	24 (2%)	7 4

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	VAL
1	C	158	LEU
1	C	208	ARG
1	C	225	VAL
1	A	211	ASN
1	B	166	ARG
1	B	225	VAL
1	C	159	GLY
1	C	160	HIS
1	C	237	GLU
1	A	224	LYS
1	A	237	GLU
1	B	224	LYS
1	C	180	GLU
1	C	198	THR
1	C	199	PRO
1	C	210	ALA
1	C	224	LYS
1	B	213	PRO
1	C	200	SER
1	C	203	MET
1	C	212	THR
1	A	196	GLY
1	A	212	THR

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	276/284 (97%)	269 (98%)	7 (2%)	55 67
1	B	276/284 (97%)	268 (97%)	8 (3%)	50 62
1	C	265/284 (93%)	255 (96%)	10 (4%)	40 49
All	All	817/852 (96%)	792 (97%)	25 (3%)	47 59

All (25) 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	263	TYR
1	A	277	GLU
1	A	290	LEU
1	A	342	LEU
1	B	25	ARG
1	B	28	LEU
1	B	70	TYR
1	B	172	ASP
1	B	211	ASN
1	B	245	ILE
1	B	263	TYR
1	B	342	LEU
1	C	25	ARG
1	C	28	LEU
1	C	70	TYR
1	C	194	ILE
1	C	205	LYS
1	C	206	PHE
1	C	212	THR
1	C	215	ASP
1	C	263	TYR
1	C	288	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	143	HIS
1	A	168	ASN
1	A	170	GLN
1	A	211	ASN
1	A	288	GLN
1	B	63	ASN
1	B	143	HIS
1	B	162	GLN
1	B	170	GLN
1	B	211	ASN
1	B	288	GLN
1	C	63	ASN
1	C	83	HIS
1	C	143	HIS
1	C	160	HIS
1	C	243	GLN
1	C	286	GLN
1	C	288	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	D3M	A	601	-	10,13,13	1.96	1 (10%)	11,18,18	1.31	1 (9%)
2	FES	B	501	1	0,4,4	0.00	-	0,4,4	0.00	-
4	D3M	B	601	-	10,13,13	2.12	3 (30%)	11,18,18	1.39	2 (18%)
2	FES	C	501	1	0,4,4	0.00	-	0,4,4	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	FES	A	501	1	-	0/0/4/4	0/1/1/1
4	D3M	A	601	-	-	0/2/6/6	0/1/1/1
2	FES	B	501	1	-	0/0/4/4	0/1/1/1
4	D3M	B	601	-	-	0/2/6/6	0/1/1/1
2	FES	C	501	1	-	0/0/4/4	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	D3M	C1-C6	2.01	1.45	1.40
4	B	601	D3M	O3-C6	2.34	1.42	1.38
4	A	601	D3M	C1-C2	4.44	1.44	1.40
4	B	601	D3M	C1-C2	4.73	1.45	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	D3M	C3-C2-C1	-2.07	120.30	122.41
4	A	601	D3M	C6-C5-CL1	2.89	121.98	118.43
4	B	601	D3M	C6-C5-CL1	3.20	122.36	118.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FES	1	0
2	B	501	FES	1	0
2	C	501	FES	1	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	341/349 (97%)	0.21	16 (4%) 35 34	26, 43, 68, 89	0
1	B	341/349 (97%)	0.65	47 (13%) 4 3	29, 45, 85, 90	0
1	C	327/349 (93%)	0.50	35 (10%) 8 7	27, 42, 85, 90	0
All	All	1009/1047 (96%)	0.46	98 (9%) 10 9	26, 43, 82, 90	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	200	SER	10.2
1	B	236	PRO	8.5
1	B	342	LEU	8.3
1	C	199	PRO	8.2
1	C	177	LEU	8.1
1	B	209	GLY	7.6
1	C	198	THR	7.1
1	C	212	THR	7.0
1	B	211	ASN	6.9
1	B	212	THR	6.9
1	B	210	ALA	6.7
1	C	197	GLY	6.6
1	B	194	ILE	6.5
1	C	202	LEU	6.3
1	C	211	ASN	6.0
1	C	340	ALA	5.7
1	C	2	ALA	5.3
1	C	210	ALA	5.3
1	B	341	ARG	4.9
1	C	162	GLN	4.9
1	B	213	PRO	4.8
1	A	209	GLY	4.4
1	B	2	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	193	LYS	4.1
1	A	237	GLU	4.0
1	C	201	VAL	4.0
1	B	215	ASP	3.9
1	C	342	LEU	3.9
1	B	175	ASP	3.9
1	B	172	ASP	3.9
1	B	177	LEU	3.9
1	B	240	PRO	3.8
1	B	176	ARG	3.8
1	B	208	ARG	3.8
1	B	339	ALA	3.8
1	B	207	LEU	3.7
1	C	206	PHE	3.7
1	A	211	ASN	3.6
1	B	174	PHE	3.6
1	C	160	HIS	3.5
1	B	197	GLY	3.5
1	C	237	GLU	3.5
1	B	196	GLY	3.5
1	C	161	ALA	3.5
1	A	243	GLN	3.4
1	B	243	GLN	3.3
1	B	245	ILE	3.1
1	B	239	THR	3.1
1	A	195	PRO	3.1
1	B	274	ASP	3.1
1	C	178	GLU	3.1
1	C	239	THR	3.1
1	B	198	THR	3.0
1	C	196	GLY	3.0
1	C	158	LEU	3.0
1	B	173	ALA	3.0
1	B	192	MET	2.9
1	C	203	MET	2.9
1	B	278	MET	2.8
1	B	225	VAL	2.8
1	C	207	LEU	2.8
1	A	225	VAL	2.7
1	A	240	PRO	2.7
1	A	185	ASP	2.7
1	B	337	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	213	PRO	2.7
1	B	186	GLY	2.7
1	C	215	ASP	2.6
1	B	214	VAL	2.5
1	B	217	TRP	2.4
1	A	182	ILE	2.4
1	C	195	PRO	2.4
1	A	196	GLY	2.4
1	C	276	PRO	2.4
1	B	169	ALA	2.4
1	B	195	PRO	2.4
1	C	314	ARG	2.4
1	B	179	ARG	2.3
1	A	339	ALA	2.3
1	C	214	VAL	2.3
1	C	337	LEU	2.3
1	B	63	ASN	2.3
1	C	49	CYS	2.3
1	A	273	ILE	2.3
1	A	61	LEU	2.3
1	C	278	MET	2.3
1	B	151	LEU	2.2
1	B	234	VAL	2.2
1	B	237	GLU	2.2
1	A	184	GLY	2.2
1	B	273	ILE	2.1
1	A	2	ALA	2.1
1	C	225	VAL	2.1
1	B	271	PHE	2.1
1	B	206	PHE	2.1
1	A	93	ALA	2.1
1	C	68	CYS	2.1
1	B	216	ALA	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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	FE	A	502	1/1	1.00	0.15	0.01	39,39,39,39	0
4	D3M	B	601	13/13	0.85	0.16	-0.28	45,49,50,51	0
2	FES	B	501	4/4	0.99	0.12	-0.35	29,30,30,31	0
4	D3M	A	601	13/13	0.92	0.12	-0.60	29,37,41,41	0
2	FES	A	501	4/4	0.98	0.10	-0.93	37,40,40,41	0
3	FE	B	502	1/1	0.97	0.07	-1.80	54,54,54,54	0
2	FES	C	501	4/4	0.99	0.14	-2.31	28,29,29,31	0

6.5 Other polymers

There are no such residues in this entry.