Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:19 AM GMT

PDB ID	:	3OPS
Title	:	Crystal structure of mandelate racemase/muconate lactonizing protein FROM GEOBACILLUS SP. Y412MC10 complexed with magnesium/tartrate
Authors	:	Malashkevich, V.N.; Patskovsky, Y.; Ramagopal, U.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2010-09-01
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:

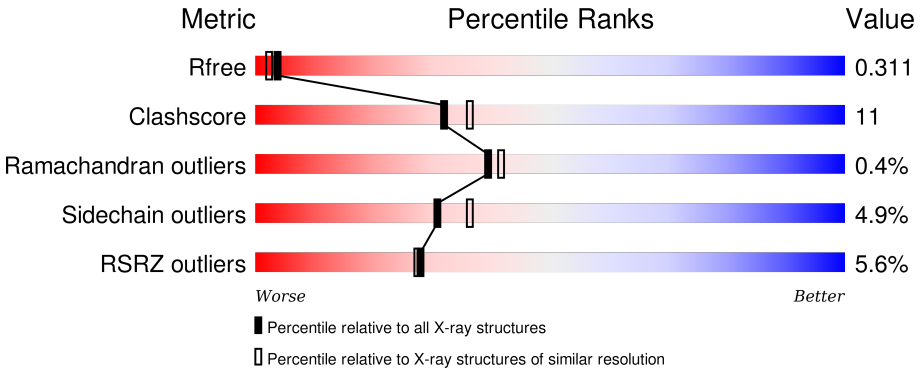
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	392	5% 76% 22%
1	B	392	4% 74% 22%
1	C	392	% 80% 17%
1	D	392	11% 67% 25%

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
3	TAR	A	503	X	-	-	X
3	TAR	A	504	X	-	-	X
3	TAR	B	503	X	-	X	-
3	TAR	C	503	X	-	-	-
3	TAR	D	503	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13128 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 Mandelate racemase/muconate lactonizing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	Se	0	3	0
			3060	1937	538	575	3	7			
1	B	386	Total	C	N	O	S	Se	0	1	0
			3050	1929	536	574	3	8			
1	C	386	Total	C	N	O	S	Se	0	3	0
			3060	1939	536	574	3	8			
1	D	376	Total	C	N	O	S	Se	0	0	0
			2965	1877	518	560	3	7			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP D3EID5
A	2	SER	-	expression tag	UNP D3EID5
A	3	LEU	-	expression tag	UNP D3EID5
A	385	GLU	-	expression tag	UNP D3EID5
A	386	GLY	-	expression tag	UNP D3EID5
A	387	HIS	-	expression tag	UNP D3EID5
A	388	HIS	-	expression tag	UNP D3EID5
A	389	HIS	-	expression tag	UNP D3EID5
A	390	HIS	-	expression tag	UNP D3EID5
A	391	HIS	-	expression tag	UNP D3EID5
A	392	HIS	-	expression tag	UNP D3EID5
B	1	MSE	-	expression tag	UNP D3EID5
B	2	SER	-	expression tag	UNP D3EID5
B	3	LEU	-	expression tag	UNP D3EID5
B	385	GLU	-	expression tag	UNP D3EID5
B	386	GLY	-	expression tag	UNP D3EID5
B	387	HIS	-	expression tag	UNP D3EID5
B	388	HIS	-	expression tag	UNP D3EID5
B	389	HIS	-	expression tag	UNP D3EID5
B	390	HIS	-	expression tag	UNP D3EID5
B	391	HIS	-	expression tag	UNP D3EID5

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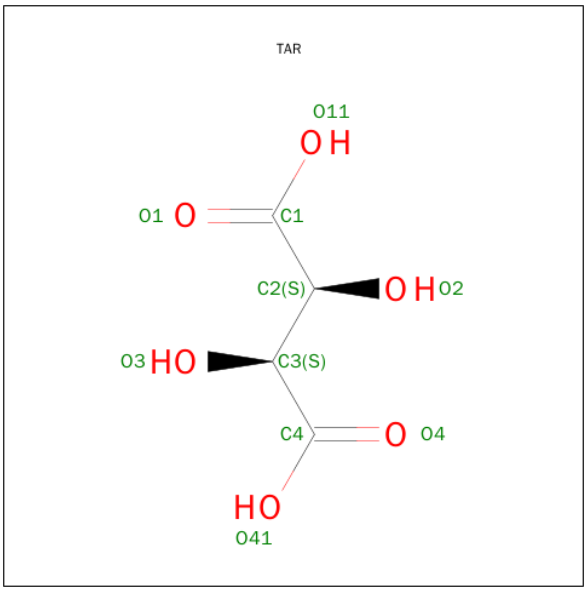
Chain	Residue	Modelled	Actual	Comment	Reference
B	392	HIS	-	expression tag	UNP D3EID5
C	1	MSE	-	expression tag	UNP D3EID5
C	2	SER	-	expression tag	UNP D3EID5
C	3	LEU	-	expression tag	UNP D3EID5
C	385	GLU	-	expression tag	UNP D3EID5
C	386	GLY	-	expression tag	UNP D3EID5
C	387	HIS	-	expression tag	UNP D3EID5
C	388	HIS	-	expression tag	UNP D3EID5
C	389	HIS	-	expression tag	UNP D3EID5
C	390	HIS	-	expression tag	UNP D3EID5
C	391	HIS	-	expression tag	UNP D3EID5
C	392	HIS	-	expression tag	UNP D3EID5
D	1	MSE	-	expression tag	UNP D3EID5
D	2	SER	-	expression tag	UNP D3EID5
D	3	LEU	-	expression tag	UNP D3EID5
D	385	GLU	-	expression tag	UNP D3EID5
D	386	GLY	-	expression tag	UNP D3EID5
D	387	HIS	-	expression tag	UNP D3EID5
D	388	HIS	-	expression tag	UNP D3EID5
D	389	HIS	-	expression tag	UNP D3EID5
D	390	HIS	-	expression tag	UNP D3EID5
D	391	HIS	-	expression tag	UNP D3EID5
D	392	HIS	-	expression tag	UNP D3EID5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 4 6	0	0
3	A	1	Total C O 10 4 6	0	0
3	B	1	Total C O 10 4 6	0	0
3	C	1	Total C O 10 4 6	0	0
3	D	1	Total C O 10 4 6	0	0

- Molecule 4 is water.

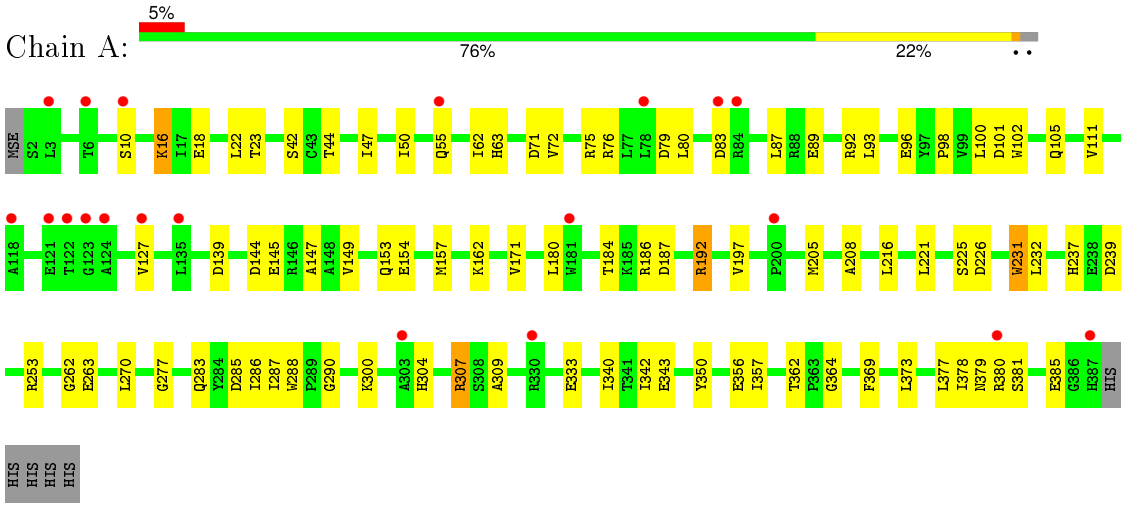
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	253	Total O 253 253	0	0
4	B	235	Total O 235 235	0	0
4	C	324	Total O 324 324	0	0
4	D	123	Total O 123 123	0	0

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.

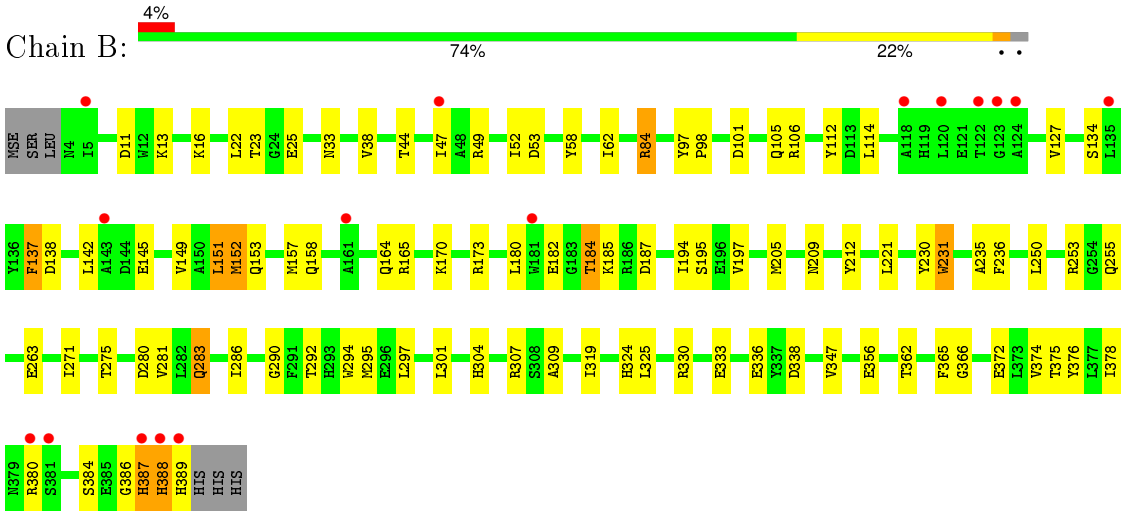
- Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain A:



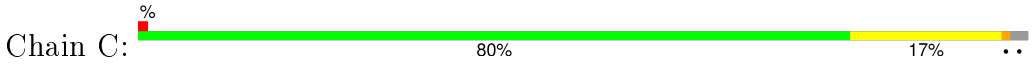
- Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain B:



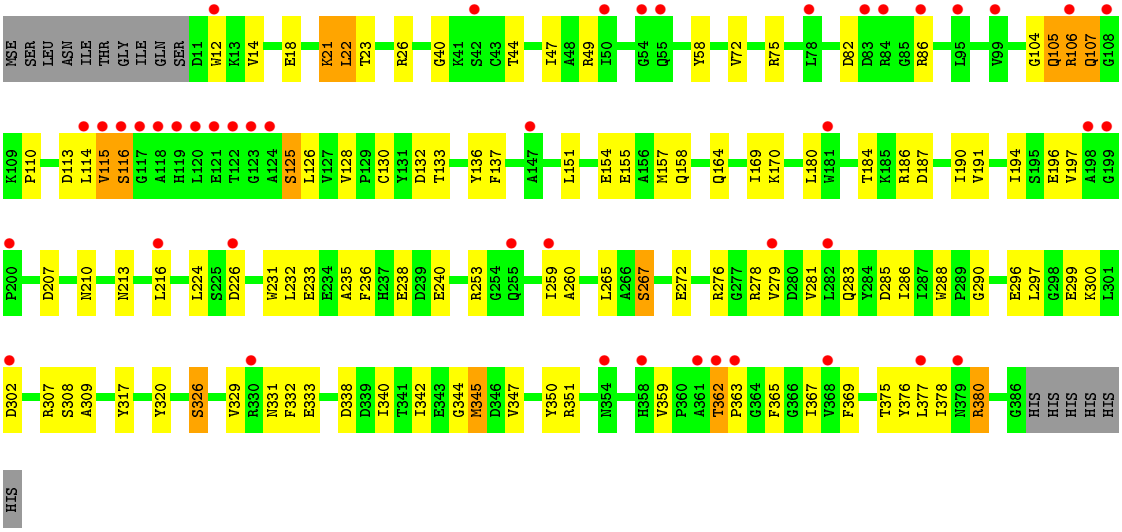
- Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain C:



• Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	159.99Å 66.38Å 154.85Å 90.00° 96.59° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	82.5 (20.00-2.20) 82.5 (20.00-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.228 , 0.311 0.228 , 0.311	Depositor DCC
R_{free} test set	3428 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 67849 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13128	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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 57.23 % 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 2.4399e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: MG, TAR

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	0.44	0/3133	0.62	0/4234
1	B	0.47	0/3119	0.65	0/4216
1	C	0.51	0/3135	0.67	2/4238 (0.0%)
1	D	0.41	0/3028	0.62	1/4093 (0.0%)
All	All	0.46	0/12415	0.64	3/16781 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	282[A]	LEU	CA-CB-CG	-5.69	102.21	115.30
1	C	282[B]	LEU	CA-CB-CG	-5.69	102.21	115.30
1	D	151	LEU	CA-CB-CG	5.49	127.93	115.30

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	3060	0	2967	61	0
1	B	3050	0	2937	68	0
1	C	3060	0	2959	53	0
1	D	2965	0	2856	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	20	0	8	3	0
3	B	10	0	4	6	0
3	C	10	0	3	0	0
3	D	10	0	4	0	0
4	A	253	0	0	13	0
4	B	235	0	0	9	0
4	C	324	0	0	7	0
4	D	123	0	0	6	0
All	All	13128	0	11738	254	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 11.

All (254) 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:B:347:VAL:HG22	4:B:906:HOH:O	1.55	1.05
1:D:132:ASP:HB2	1:D:164:GLN:HG2	1.36	1.02
1:A:237:HIS:HD2	3:A:503:TAR:H2	1.27	0.99
1:B:292:THR:HA	1:B:295:MSE:HE2	1.46	0.98
1:A:237:HIS:CD2	3:A:503:TAR:H2	1.99	0.97
1:B:292:THR:HA	1:B:295:MSE:CE	1.98	0.94
1:B:170:LYS:HZ2	3:B:503:TAR:H2	1.32	0.94
1:D:115:VAL:HG23	1:D:116:SER:H	1.35	0.89
1:A:225:SER:HB2	4:A:1534:HOH:O	1.76	0.85
1:C:154:GLU:HA	1:C:157[B]:MSE:HE3	1.60	0.84
1:C:152:MSE:HG3	1:C:190:ILE:HD13	1.58	0.84
1:D:170:LYS:HE2	1:D:207:ASP:HB3	1.61	0.82
1:B:84:ARG:HG2	1:B:84:ARG:HH11	1.45	0.81
1:D:155:GLU:HA	1:D:158:GLN:HE21	1.45	0.81
1:B:112:TYR:H	1:B:324:HIS:HD2	1.30	0.78
1:A:154:GLU:HB3	4:A:636:HOH:O	1.84	0.76
1:B:319:ILE:HG13	4:B:883:HOH:O	1.84	0.76
1:A:197:VAL:HG13	4:A:1389:HOH:O	1.89	0.73
1:B:170:LYS:NZ	3:B:503:TAR:H2	2.03	0.72
1:D:317:TYR:HD2	4:D:1761:HOH:O	1.73	0.71
1:D:106:ARG:HB2	1:D:106:ARG:HH11	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:TYR:CE1	1:D:347:VAL:HG11	2.26	0.70
1:B:221:LEU:HD13	1:B:250:LEU:HD21	1.74	0.70
1:D:180:LEU:HD11	1:D:216:LEU:HD11	1.75	0.69
1:B:23:THR:HG22	1:B:44:THR:HG22	1.74	0.68
1:B:84:ARG:HG2	1:B:84:ARG:NH1	2.08	0.67
1:C:387:HIS:O	1:C:388:HIS:HB2	1.94	0.67
1:D:317:TYR:CD2	4:D:1761:HOH:O	2.46	0.67
1:D:286:ILE:O	1:D:290:GLY:HA2	1.96	0.65
1:D:132:ASP:HB2	1:D:164:GLN:CG	2.22	0.65
1:C:192:ARG:NH2	1:C:223:ALA:O	2.28	0.65
1:B:53:ASP:OD2	1:B:106:ARG:NH1	2.27	0.64
1:C:173:ARG:HD3	1:C:186:ARG:HG2	1.79	0.64
1:D:347:VAL:O	1:D:347:VAL:HG12	1.97	0.63
1:C:206:ILE:HG12	1:C:229:LEU:HD21	1.80	0.63
1:D:197:VAL:HG13	4:D:1346:HOH:O	1.99	0.62
1:D:362:THR:HG22	1:D:363:PRO:HD2	1.81	0.62
1:B:97:TYR:HD1	1:B:365:PHE:CZ	2.16	0.62
1:D:285:ASP:HB3	1:D:288:TRP:O	1.99	0.61
1:A:377:LEU:HD22	1:A:380:ARG:HH12	1.64	0.61
1:C:205:MSE:HG2	1:C:231:TRP:CE2	2.35	0.61
1:A:22:LEU:HD12	1:A:377:LEU:HD12	1.83	0.61
1:B:386:GLY:O	1:B:387:HIS:HB3	2.01	0.60
1:C:221:LEU:HD13	1:C:250:LEU:HD21	1.84	0.59
1:C:101:ASP:O	1:C:105:GLN:HG2	2.01	0.59
1:B:145:GLU:O	1:B:149:VAL:HG23	2.02	0.59
1:B:112:TYR:N	1:B:324:HIS:HD2	1.99	0.59
1:C:157[A]:MSE:SE	1:C:197:VAL:HG22	2.53	0.59
1:C:186:ARG:O	1:C:190:ILE:HG13	2.04	0.58
1:A:286:ILE:O	1:A:290:GLY:HA2	2.02	0.58
1:B:309:ALA:HB2	1:B:333:GLU:HB2	1.86	0.58
1:D:272:GLU:HG2	1:D:276:ARG:NH2	2.18	0.58
1:A:285:ASP:HB3	1:A:288:TRP:O	2.03	0.58
1:D:350:TYR:CE2	1:D:359:VAL:HG22	2.38	0.57
1:B:195:SER:HB2	4:B:1195:HOH:O	2.04	0.57
1:D:155:GLU:HA	1:D:158:GLN:NE2	2.18	0.57
1:B:271:ILE:O	1:B:275:THR:HG23	2.05	0.57
1:C:18:GLU:O	1:C:48:ALA:HA	2.05	0.57
1:B:286:ILE:O	1:B:290:GLY:HA2	2.05	0.56
1:D:169:ILE:HD11	1:D:194:ILE:HB	1.88	0.56
1:D:115:VAL:HG23	1:D:116:SER:N	2.14	0.56
1:A:47[B]:ILE:HD13	1:A:369:PHE:HE1	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LYS:HG2	1:A:385:GLU:O	2.07	0.55
1:D:184:THR:O	1:D:187:ASP:HB2	2.07	0.55
1:D:283:GLN:HG2	1:D:309:ALA:O	2.07	0.55
1:A:72:VAL:HA	1:A:75:ARG:HD2	1.89	0.55
1:B:153:GLN:O	1:B:157[B]:MSE:HG3	2.07	0.54
1:A:18:GLU:HB3	1:A:378:ILE:HD13	1.89	0.54
1:D:232:LEU:HD21	1:D:235:ALA:HB2	1.87	0.54
1:C:286:ILE:HG23	1:C:287:ILE:HG12	1.88	0.54
1:B:101:ASP:O	1:B:105:GLN:HG2	2.08	0.54
1:B:281:VAL:HG22	1:B:307:ARG:HB2	1.91	0.53
1:C:38:VAL:HG23	4:C:767:HOH:O	2.07	0.53
1:D:18:GLU:HB2	1:D:49:ARG:HB3	1.89	0.53
1:B:84:ARG:CG	1:B:84:ARG:HH11	2.20	0.53
1:D:345:MSE:SE	4:D:1761:HOH:O	2.77	0.53
1:D:238:GLU:HG3	1:D:267:SER:HB3	1.91	0.53
1:A:237:HIS:CD2	3:A:503:TAR:C2	2.85	0.53
1:A:96:GLU:O	1:A:100:LEU:HG	2.08	0.53
1:B:275:THR:HG22	1:B:304:HIS:CD2	2.43	0.53
1:A:63:HIS:HD2	1:A:93:LEU:HD12	1.73	0.53
1:B:158:GLN:NE2	4:B:950:HOH:O	2.41	0.52
1:D:365:PHE:O	1:D:367:ILE:HG13	2.08	0.52
1:C:131:TYR:HD2	1:C:334:PHE:HB3	1.74	0.52
1:D:82:ASP:N	1:D:86:ARG:O	2.37	0.52
1:D:240:GLU:HG3	1:D:278:ARG:HG2	1.92	0.52
1:A:47[B]:ILE:HD13	1:A:369:PHE:CE1	2.45	0.51
1:A:263:GLU:HG2	4:A:731:HOH:O	2.09	0.51
1:D:259:ILE:HG22	1:D:279:VAL:HG13	1.93	0.51
1:D:350:TYR:HE2	1:D:359:VAL:HG22	1.75	0.51
1:A:205:MSE:HG2	1:A:231:TRP:CG	2.45	0.51
1:C:111:VAL:HB	1:C:324:HIS:CD2	2.45	0.51
1:B:157[A]:MSE:SE	1:B:197:VAL:HG13	2.61	0.51
1:A:205:MSE:HG2	1:A:231:TRP:CD1	2.45	0.51
1:B:180:LEU:O	1:B:184:THR:OG1	2.26	0.51
1:D:210:ASN:HA	1:D:236:PHE:HA	1.92	0.51
1:D:296:GLU:O	1:D:299:GLU:HB2	2.11	0.51
1:B:127:VAL:HG12	1:B:356:GLU:HB3	1.93	0.50
1:D:154:GLU:HA	1:D:157:MSE:HE2	1.93	0.50
1:B:22:LEU:HD21	1:B:374:VAL:HG22	1.93	0.50
1:B:182:GLU:HB3	4:B:908:HOH:O	2.11	0.50
1:A:300:LYS:HD3	1:A:304:HIS:CE1	2.47	0.50
1:C:112:TYR:N	1:C:324:HIS:HD2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:VAL:HA	1:D:75:ARG:HD3	1.94	0.49
1:A:101:ASP:O	1:A:105:GLN:HG2	2.13	0.49
1:B:297:LEU:O	1:B:301:LEU:HG	2.13	0.49
1:D:281:VAL:HG22	1:D:307:ARG:HB2	1.93	0.49
1:C:285:ASP:HA	1:C:311:HIS:HB3	1.94	0.49
1:C:285:ASP:HB3	1:C:288:TRP:O	2.12	0.49
1:B:152:MSE:HB3	1:B:194:ILE:HD11	1.93	0.49
1:C:95:LEU:O	1:C:99:VAL:HG23	2.13	0.49
1:B:16:LYS:NZ	1:B:384:SER:OG	2.43	0.49
1:B:112:TYR:H	1:B:324:HIS:CD2	2.20	0.49
1:D:186:ARG:O	1:D:190:ILE:HG12	2.12	0.48
1:B:151:LEU:HB3	1:B:152:MSE:HE3	1.94	0.48
1:B:231:TRP:C	1:B:231:TRP:CD1	2.87	0.48
1:A:23:THR:HG22	1:A:44:THR:HG22	1.95	0.48
1:A:62:ILE:HG13	1:A:93:LEU:HB3	1.96	0.48
1:D:302:ASP:HA	1:D:331:ASN:HD22	1.79	0.48
1:A:139:ASP:OD2	1:A:186:ARG:HD2	2.14	0.48
1:C:345:MSE:HG3	1:C:369:PHE:CE1	2.49	0.47
1:B:25:GLU:HG2	4:B:728:HOH:O	2.14	0.47
1:D:125:SER:HB3	4:D:624:HOH:O	2.14	0.47
1:A:153:GLN:HB3	1:A:197:VAL:HG21	1.97	0.47
1:D:233:GLU:HG3	1:D:283:GLN:HE22	1.79	0.47
1:D:376:TYR:CE1	1:D:380:ARG:HD3	2.50	0.47
1:A:157:MSE:HG2	4:A:1389:HOH:O	2.15	0.47
1:D:104:GLY:O	1:D:363:PRO:HB3	2.14	0.47
1:B:137:PHE:CE2	1:B:173:ARG:HA	2.50	0.47
1:C:388:HIS:O	1:C:389:HIS:CD2	2.68	0.47
1:A:377:LEU:CD2	1:A:380:ARG:HH12	2.27	0.47
1:A:340:ILE:HG22	1:A:342:ILE:HD12	1.97	0.47
1:D:344:GLY:O	1:D:369:PHE:HA	2.15	0.47
1:B:292:THR:HA	1:B:295:MSE:HE3	1.90	0.47
1:B:319:ILE:HD11	1:B:338:ASP:H	1.79	0.47
1:A:180:LEU:HD11	1:A:216:LEU:HD11	1.97	0.47
1:D:49:ARG:HD3	1:D:58:TYR:CZ	2.49	0.46
1:B:142:LEU:HD11	1:B:151:LEU:HD12	1.96	0.46
1:C:16:LYS:HE3	1:C:387:HIS:HA	1.97	0.46
1:A:144:ASP:OD1	1:A:147:ALA:N	2.44	0.46
1:C:253:ARG:NH2	1:C:255:GLN:OE1	2.48	0.46
1:C:356:GLU:OE1	4:C:688:HOH:O	2.21	0.46
1:C:112:TYR:H	1:C:324:HIS:HD2	1.62	0.46
1:A:127:VAL:HG12	1:A:356:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:MSE:HG3	1:B:230:TYR:HB3	1.96	0.46
1:D:169:ILE:HD13	1:D:191:VAL:HA	1.98	0.46
1:C:53:ASP:OD2	1:C:106:ARG:NH1	2.45	0.46
1:A:350:TYR:HB3	1:A:357:ILE:HD11	1.97	0.46
1:D:82:ASP:HB2	1:D:86:ARG:HB2	1.97	0.46
1:C:22:LEU:HD22	1:C:47[B]:ILE:HG13	1.98	0.46
1:D:26:ARG:NH1	1:D:40:GLY:O	2.44	0.46
1:A:192[B]:ARG:HD2	4:A:1168:HOH:O	2.16	0.46
1:C:131:TYR:CE1	1:C:168:LYS:HE3	2.51	0.45
1:C:278:ARG:NH1	4:C:677:HOH:O	2.48	0.45
1:B:347:VAL:O	1:B:347:VAL:HG23	2.15	0.45
1:C:67:GLU:H	1:C:67:GLU:CD	2.19	0.45
1:A:79:ASP:OD2	4:A:1198:HOH:O	2.21	0.45
1:D:309:ALA:HB2	1:D:333:GLU:HB2	1.98	0.45
1:A:221:LEU:HD11	1:A:232:LEU:HD22	1.99	0.45
1:B:212:TYR:HB2	1:B:235:ALA:O	2.17	0.45
1:C:168:LYS:HE2	1:C:233:GLU:OE1	2.17	0.45
1:C:283:GLN:O	1:C:311:HIS:HB2	2.17	0.45
1:A:55:GLN:HB3	1:A:102:TRP:HE1	1.81	0.45
1:C:86:ARG:HA	4:C:626:HOH:O	2.17	0.45
1:A:55:GLN:HB3	1:A:102:TRP:NE1	2.32	0.45
1:A:10:SER:HB2	1:A:76:ARG:HH21	1.82	0.44
1:A:379:ASN:HA	4:A:715:HOH:O	2.18	0.44
1:D:213:ASN:HB2	4:D:1637:HOH:O	2.18	0.44
1:C:192:ARG:NH1	4:C:717:HOH:O	2.51	0.44
1:C:16:LYS:HE3	1:C:388:HIS:H	1.82	0.44
1:C:387:HIS:O	1:C:388:HIS:CB	2.65	0.44
1:D:329:VAL:HG23	1:D:332:PHE:HB2	2.00	0.44
1:A:63:HIS:CD2	1:A:93:LEU:HD12	2.51	0.43
1:D:22:LEU:HB3	1:D:342:ILE:CG2	2.48	0.43
1:A:171:VAL:O	1:A:208:ALA:HA	2.18	0.43
1:A:162:LYS:HE3	4:A:640:HOH:O	2.18	0.43
1:D:345:MSE:O	1:D:347:VAL:HG23	2.18	0.43
1:C:67:GLU:N	1:C:67:GLU:CD	2.71	0.43
1:C:282[B]:LEU:HD22	1:C:301:LEU:HD21	2.00	0.43
1:B:209:ASN:HD21	3:B:503:TAR:C2	2.31	0.43
1:C:18:GLU:HB2	1:C:49:ARG:HB3	2.00	0.43
1:A:262:GLY:HA2	1:A:270:LEU:CD2	2.47	0.43
1:D:320:TYR:CZ	1:D:347:VAL:HG11	2.52	0.43
1:D:154:GLU:O	1:D:157:MSE:HB3	2.18	0.43
1:C:154:GLU:CA	1:C:157[B]:MSE:HE3	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:ASP:O	1:D:191:VAL:HG23	2.19	0.43
1:B:11:ASP:N	1:B:11:ASP:OD1	2.50	0.43
1:A:307:ARG:HG2	1:A:333:GLU:OE2	2.19	0.43
1:C:77:LEU:HD12	1:C:80:LEU:HD12	2.01	0.43
1:B:253:ARG:NH2	1:B:255:GLN:OE1	2.51	0.43
1:D:133:THR:O	1:D:136:TYR:HE1	2.01	0.43
1:D:110:PRO:HB3	1:D:362:THR:O	2.19	0.43
1:A:87:LEU:HD22	1:A:96:GLU:HA	1.99	0.43
1:B:97:TYR:N	1:B:98:PRO:HD2	2.34	0.43
1:C:18:GLU:CD	1:C:49:ARG:HH11	2.21	0.42
1:D:22:LEU:HD12	1:D:377:LEU:HD13	2.01	0.42
1:C:350:TYR:OH	1:C:365:PHE:O	2.23	0.42
1:B:33:ASN:ND2	3:B:503:TAR:O1	2.51	0.42
1:C:16:LYS:HB3	4:C:703:HOH:O	2.19	0.42
1:B:372:GLU:CD	1:B:372:GLU:H	2.22	0.42
1:B:376:TYR:CE2	1:B:380:ARG:HD3	2.54	0.42
1:A:153:GLN:O	1:A:157:MSE:HG3	2.19	0.42
1:B:283:GLN:HB3	1:B:309:ALA:O	2.19	0.42
1:B:49:ARG:HD3	1:B:58:TYR:CE1	2.54	0.42
1:B:173:ARG:HD2	1:B:187:ASP:OD1	2.20	0.42
1:A:111:VAL:HG23	1:A:364:GLY:C	2.39	0.42
1:B:38:VAL:HG23	4:B:1711:HOH:O	2.20	0.42
1:D:105:GLN:HA	1:D:105:GLN:OE1	2.19	0.42
1:B:294:TRP:HB3	1:B:325:LEU:HD11	2.02	0.42
1:C:337:TYR:CE2	1:C:352:ILE:HD11	2.54	0.42
1:B:336:GLU:OE2	3:B:503:TAR:O4	2.38	0.42
1:D:47:ILE:O	1:D:47:ILE:HG13	2.20	0.42
1:C:205:MSE:HG2	1:C:231:TRP:CD2	2.54	0.42
1:A:277:GLY:HA2	4:A:1189:HOH:O	2.18	0.42
1:A:184:THR:O	1:A:187:ASP:HB2	2.19	0.42
1:B:263:GLU:OE1	3:B:503:TAR:O2	2.32	0.41
1:A:239:ASP:C	1:A:239:ASP:OD1	2.58	0.41
1:C:173:ARG:CZ	1:C:190:ILE:HD12	2.49	0.41
1:B:388:HIS:HB3	1:B:389:HIS:H	1.64	0.41
1:D:338:ASP:O	1:D:340:ILE:HG12	2.20	0.41
1:D:137:PHE:CD1	1:D:137:PHE:N	2.87	0.41
1:C:296:GLU:HG3	4:C:1305:HOH:O	2.19	0.41
1:A:50:ILE:HG22	1:A:98:PRO:HB2	2.02	0.41
1:D:233:GLU:HA	1:D:260:ALA:O	2.20	0.41
1:C:112:TYR:O	1:C:116:SER:HB3	2.20	0.41
1:C:351:ARG:NH1	1:C:353:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:THR:HA	1:D:378:ILE:HD12	2.02	0.41
1:A:89:GLU:HA	1:A:92:ARG:CD	2.50	0.41
1:D:21:LYS:HE2	1:D:44:THR:HG21	2.01	0.41
1:D:308:SER:O	1:D:333:GLU:N	2.49	0.41
1:B:375:THR:HA	1:B:378:ILE:HD12	2.02	0.41
1:C:231:TRP:CD1	1:C:231:TRP:C	2.94	0.41
1:B:362:THR:OG1	1:B:366:GLY:HA2	2.21	0.41
1:B:280:ASP:HB3	4:B:698:HOH:O	2.19	0.41
1:D:107:GLN:HG3	1:D:107:GLN:H	1.77	0.41
1:A:285:ASP:HB2	4:A:629:HOH:O	2.20	0.41
1:B:184:THR:O	1:B:187:ASP:HB2	2.20	0.41
1:D:297:LEU:C	1:D:299:GLU:H	2.24	0.41
1:A:216:LEU:HA	1:A:216:LEU:HD23	1.93	0.41
1:A:76:ARG:O	1:A:79:ASP:HB2	2.21	0.41
1:A:283:GLN:HA	1:A:309:ALA:O	2.21	0.41
1:A:343:GLU:HB2	4:A:717:HOH:O	2.21	0.41
1:D:23:THR:HG22	1:D:44:THR:HG22	2.02	0.41
1:D:170:LYS:HA	1:D:170:LYS:HD3	1.86	0.40
1:A:226:ASP:N	1:A:226:ASP:OD1	2.53	0.40
1:A:145:GLU:O	1:A:149:VAL:HG23	2.21	0.40
1:B:134:SER:HB2	4:B:1334:HOH:O	2.22	0.40
1:B:164:GLN:O	1:B:165:ARG:NH1	2.54	0.40
1:D:362:THR:HG22	1:D:363:PRO:CD	2.50	0.40
1:B:138:ASP:HB2	1:B:152:MSE:CE	2.51	0.40
1:D:326:SER:HB2	1:D:332:PHE:CD1	2.56	0.40
1:A:373:LEU:HA	4:A:1566:HOH:O	2.21	0.40
1:C:62:ILE:HG13	1:C:93:LEU:HB3	2.03	0.40
1:B:13:LYS:O	1:B:52:ILE:HG23	2.22	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	387/392 (99%)	372 (96%)	15 (4%)	0	100	100
1	B	385/392 (98%)	361 (94%)	22 (6%)	2 (0%)	34	35
1	C	387/392 (99%)	372 (96%)	14 (4%)	1 (0%)	46	50
1	D	374/392 (95%)	345 (92%)	26 (7%)	3 (1%)	24	22
All	All	1533/1568 (98%)	1450 (95%)	77 (5%)	6 (0%)	39	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	388	HIS
1	D	115	VAL
1	B	387	HIS
1	B	137	PHE
1	D	116	SER
1	D	14	VAL

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	313/308 (102%)	299 (96%)	14 (4%)	34	41
1	B	311/308 (101%)	298 (96%)	13 (4%)	36	44
1	C	313/308 (102%)	302 (96%)	11 (4%)	43	53
1	D	301/308 (98%)	276 (92%)	25 (8%)	14	13
All	All	1238/1232 (100%)	1175 (95%)	63 (5%)	31	34

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	42	SER
1	A	71	ASP
1	A	80	LEU
1	A	83	ASP

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Mol	Chain	Res	Type
1	A	192[A]	ARG
1	A	192[B]	ARG
1	A	231	TRP
1	A	253[A]	ARG
1	A	253[B]	ARG
1	A	287	ILE
1	A	307	ARG
1	A	362	THR
1	A	381	SER
1	B	47	ILE
1	B	62	ILE
1	B	84	ARG
1	B	114	LEU
1	B	151	LEU
1	B	152	MSE
1	B	184	THR
1	B	185	LYS
1	B	231	TRP
1	B	236	PHE
1	B	283	GLN
1	B	330	ARG
1	B	388	HIS
1	C	23	THR
1	C	83	ASP
1	C	146	ARG
1	C	197	VAL
1	C	205	MSE
1	C	226	ASP
1	C	229	LEU
1	C	231	TRP
1	C	282[A]	LEU
1	C	282[B]	LEU
1	C	373	LEU
1	D	12	TRP
1	D	21	LYS
1	D	22	LEU
1	D	105	GLN
1	D	106	ARG
1	D	107	GLN
1	D	113	ASP
1	D	114	LEU
1	D	125	SER

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Mol	Chain	Res	Type
1	D	126	LEU
1	D	128	VAL
1	D	130	CYS
1	D	196	GLU
1	D	224	LEU
1	D	226	ASP
1	D	231	TRP
1	D	253	ARG
1	D	265	LEU
1	D	267	SER
1	D	300	LYS
1	D	326	SER
1	D	345	MSE
1	D	351	ARG
1	D	362	THR
1	D	380	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	237	HIS
1	A	324	HIS
1	B	304	HIS
1	B	324	HIS
1	B	389	HIS
1	C	324	HIS
1	C	389	HIS
1	D	107	GLN
1	D	158	GLN
1	D	164	GLN
1	D	283	GLN
1	D	331	ASN

5.3.3 RNA

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)

Of 13 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
3	TAR	A	503	2	3,9,9	0.65	0	6,12,12	0.74	0
3	TAR	A	504	2	3,9,9	0.43	0	6,12,12	0.80	0
3	TAR	B	503	2	3,9,9	0.39	0	6,12,12	1.68	1 (16%)
3	TAR	C	503	2	3,9,9	0.61	0	6,12,12	1.55	1 (16%)
3	TAR	D	503	2	3,9,9	0.45	0	6,12,12	1.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TAR	A	503	2	1/1/4/4	0/4/12/12	0/0/0/0
3	TAR	A	504	2	1/1/4/4	0/4/12/12	0/0/0/0
3	TAR	B	503	2	1/1/4/4	0/4/12/12	0/0/0/0
3	TAR	C	503	2	1/1/4/4	0/4/12/12	0/0/0/0
3	TAR	D	503	2	1/1/4/4	0/4/12/12	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	503	TAR	C1-C2-C3	-2.75	107.71	113.35
3	C	503	TAR	O2-C2-C3	2.81	116.53	108.61

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	503	TAR	C2
3	D	503	TAR	C2
3	B	503	TAR	C2
3	A	504	TAR	C2
3	A	503	TAR	C2

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	TAR	3	0
3	B	503	TAR	6	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	379/392 (96%)	0.23	20 (5%) 30 29	20, 36, 59, 68	0
1	B	379/392 (96%)	0.27	16 (4%) 40 39	22, 35, 51, 69	0
1	C	379/392 (96%)	0.02	3 (0%) 87 87	16, 29, 43, 68	0
1	D	369/392 (94%)	0.83	45 (12%) 5 5	30, 49, 70, 84	0
All	All	1506/1568 (96%)	0.34	84 (5%) 28 27	16, 36, 61, 84	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	117	GLY	8.4
1	D	118	ALA	7.9
1	C	389	HIS	6.7
1	C	388	HIS	6.3
1	A	118	ALA	5.4
1	B	143	ALA	5.1
1	B	389	HIS	4.9
1	B	123	GLY	4.7
1	D	282	LEU	4.4
1	A	122	THR	4.2
1	B	181	TRP	4.0
1	C	387	HIS	4.0
1	D	123	GLY	3.9
1	A	3	LEU	3.8
1	D	119	HIS	3.8
1	A	387	HIS	3.8
1	A	10	SER	3.7
1	D	120	LEU	3.6
1	D	124	ALA	3.5
1	B	120	LEU	3.5
1	D	122	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	84	ARG	3.4
1	D	147	ALA	3.4
1	B	122	THR	3.3
1	A	83	ASP	3.3
1	D	199	GLY	3.2
1	D	361	ALA	3.2
1	A	181	TRP	3.2
1	D	368	VAL	3.2
1	B	388	HIS	3.1
1	D	121	GLU	3.1
1	D	377	LEU	3.0
1	B	118	ALA	3.0
1	D	108	GLY	2.9
1	D	114	LEU	2.9
1	A	121	GLU	2.9
1	A	135	LEU	2.8
1	D	83	ASP	2.8
1	A	123	GLY	2.8
1	A	200	PRO	2.7
1	D	54	GLY	2.7
1	B	124	ALA	2.7
1	D	106	ARG	2.7
1	D	279	VAL	2.6
1	D	362	THR	2.6
1	D	78	LEU	2.6
1	D	42	SER	2.5
1	D	200	PRO	2.5
1	D	115	VAL	2.5
1	D	226	ASP	2.5
1	B	387	HIS	2.5
1	A	303	ALA	2.5
1	D	86	ARG	2.4
1	D	198	ALA	2.4
1	D	50	ILE	2.3
1	A	78	LEU	2.3
1	D	302	ASP	2.3
1	D	181	TRP	2.3
1	B	135	LEU	2.3
1	D	379	ASN	2.3
1	D	354	ASN	2.2
1	D	255	GLN	2.2
1	D	55	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	127	VAL	2.2
1	D	99	VAL	2.2
1	B	161	ALA	2.2
1	D	363	PRO	2.2
1	D	95	LEU	2.1
1	A	124	ALA	2.1
1	B	380	ARG	2.1
1	B	381	SER	2.1
1	A	6	THR	2.1
1	B	5	ILE	2.1
1	A	84	ARG	2.1
1	D	216	LEU	2.1
1	D	259	ILE	2.1
1	A	55	GLN	2.1
1	D	12	TRP	2.1
1	D	116	SER	2.1
1	B	47	ILE	2.1
1	A	380	ARG	2.0
1	A	330	ARG	2.0
1	D	358	HIS	2.0
1	D	330	ARG	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^{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	TAR	A	503	10/10	0.84	0.22	5.67	39,41,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	TAR	A	504	10/10	0.94	0.19	2.39	38,38,40,40	0
3	TAR	D	503	10/10	0.85	0.23	1.90	47,48,55,55	0
3	TAR	B	503	10/10	0.89	0.18	1.12	29,31,37,37	0
2	MG	B	501	1/1	0.99	0.12	-0.59	26,26,26,26	0
3	TAR	C	503	10/10	0.96	0.11	-0.81	18,20,35,35	0
2	MG	A	501	1/1	0.98	0.08	-1.48	23,23,23,23	0
2	MG	C	501	1/1	0.95	0.09	-1.96	39,39,39,39	0
2	MG	D	501	1/1	0.92	0.08	-2.04	59,59,59,59	0
2	MG	A	500	1/1	0.98	0.06	-2.59	21,21,21,21	0
2	MG	B	500	1/1	0.94	0.08	-3.14	30,30,30,30	0
2	MG	D	500	1/1	0.98	0.05	-3.49	31,31,31,31	0
2	MG	C	500	1/1	0.95	0.04	-6.15	21,21,21,21	0

6.5 Other polymers

There are no such residues in this entry.