Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:43 PM GMT

PDB ID	:	4MGG
Title	:	Crystal structure of an enolase (mandelate racemase subgroup) from labrenzia aggregata iam 12614 (target nysgrc-012903) with bound mg, space group p212121
Authors	:	Vetting, M.W.; Zhang, X.; Wasserman, S.R.; Morisco, L.L.; Sojitra, S.; Bonanno, J.B.; Gerlt, J.A.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2013-08-28
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:

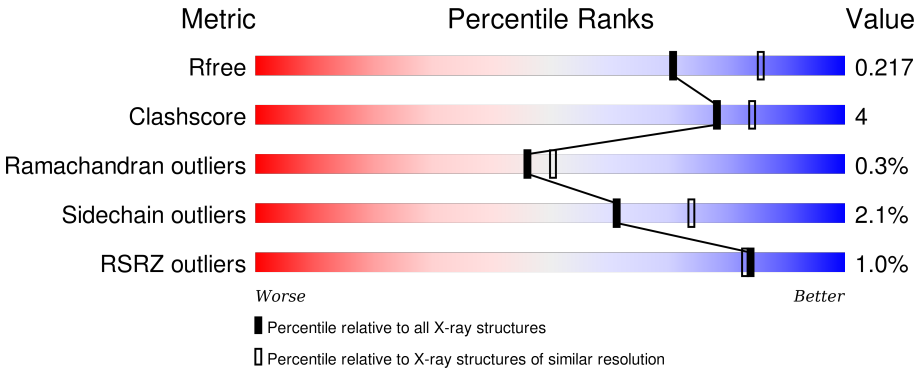
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	369	90% 9%
1	B	369	91% 7% •
1	C	369	92% 7% ••
1	D	369	4% 86% 11% ••
1	E	369	% 88% 9% ••

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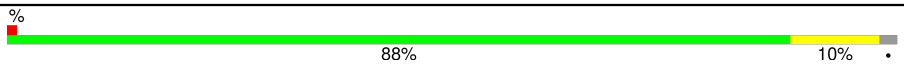
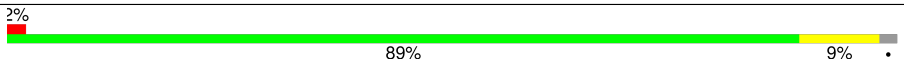
Mol	Chain	Length	Quality of chain
1	F	369	
1	G	369	
1	H	369	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	G	404	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 45845 atoms, of which 21959 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 Muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	369	Total	C	H	N	O	S	0	0	0
			5600	1768	2798	479	542	13			
1	B	361	Total	C	H	N	O	S	0	0	0
			5487	1731	2743	469	531	13			
1	C	367	Total	C	H	N	O	S	0	0	0
			5568	1759	2782	475	539	13			
1	D	361	Total	C	H	N	O	S	0	0	0
			5450	1722	2718	468	529	13			
1	E	361	Total	C	H	N	O	S	0	2	0
			5508	1738	2752	473	532	13			
1	F	362	Total	C	H	N	O	S	0	0	0
			5505	1737	2751	472	532	13			
1	G	351	Total	C	H	N	O	S	0	0	0
			5323	1675	2666	453	516	13			
1	H	362	Total	C	H	N	O	S	0	0	0
			5503	1737	2749	472	532	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP A0NXQ8
A	0	HIS	-	EXPRESSION TAG	UNP A0NXQ8
B	-1	SER	-	EXPRESSION TAG	UNP A0NXQ8
B	0	HIS	-	EXPRESSION TAG	UNP A0NXQ8
C	-1	SER	-	EXPRESSION TAG	UNP A0NXQ8
C	0	HIS	-	EXPRESSION TAG	UNP A0NXQ8
D	-1	SER	-	EXPRESSION TAG	UNP A0NXQ8
D	0	HIS	-	EXPRESSION TAG	UNP A0NXQ8
E	-1	SER	-	EXPRESSION TAG	UNP A0NXQ8
E	0	HIS	-	EXPRESSION TAG	UNP A0NXQ8
F	-1	SER	-	EXPRESSION TAG	UNP A0NXQ8
F	0	HIS	-	EXPRESSION TAG	UNP A0NXQ8
G	-1	SER	-	EXPRESSION TAG	UNP A0NXQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	EXPRESSION TAG	UNP A0NXQ8
H	-1	SER	-	EXPRESSION TAG	UNP A0NXQ8
H	0	HIS	-	EXPRESSION TAG	UNP A0NXQ8

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	3	Total Mg 3 3	0	0
4	D	2	Total Mg 2 2	0	0
4	E	2	Total Mg 2 2	0	0
4	H	2	Total Mg 2 2	0	0
4	B	2	Total Mg 2 2	0	0
4	C	2	Total Mg 2 2	0	0
4	A	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	2	Total Mg 2 2	0	0

- Molecule 5 is water.

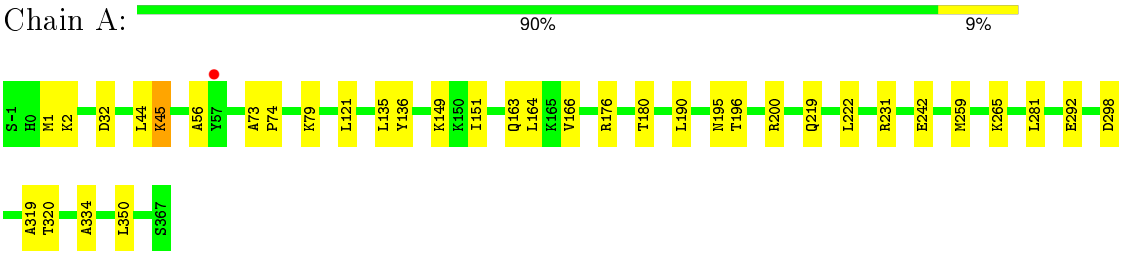
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	316	Total O 316 316	0	0
5	B	311	Total O 311 311	0	0
5	C	245	Total O 245 245	0	0
5	D	173	Total O 173 173	0	0
5	E	246	Total O 246 246	0	0
5	F	215	Total O 215 215	0	0
5	G	225	Total O 225 225	0	0
5	H	147	Total O 147 147	0	0

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.

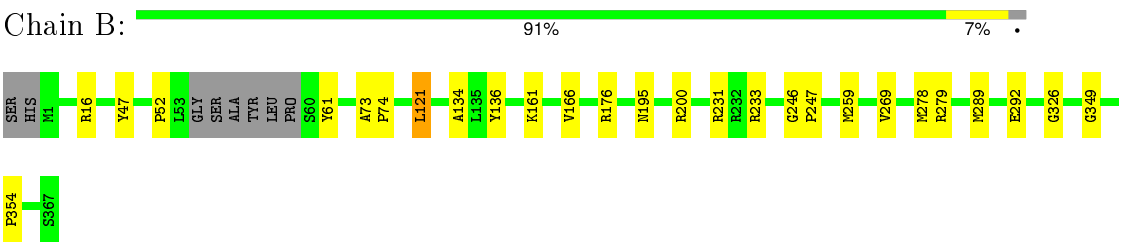
- Molecule 1: Muconate lactonizing enzyme

Chain A:



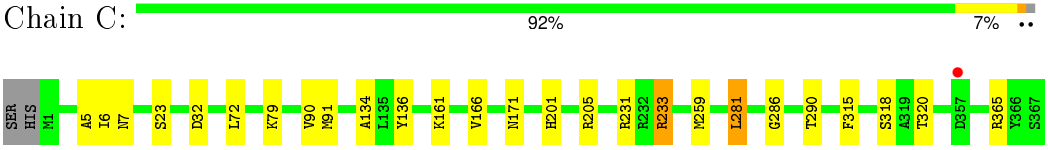
- Molecule 1: Muconate lactonizing enzyme

Chain B:



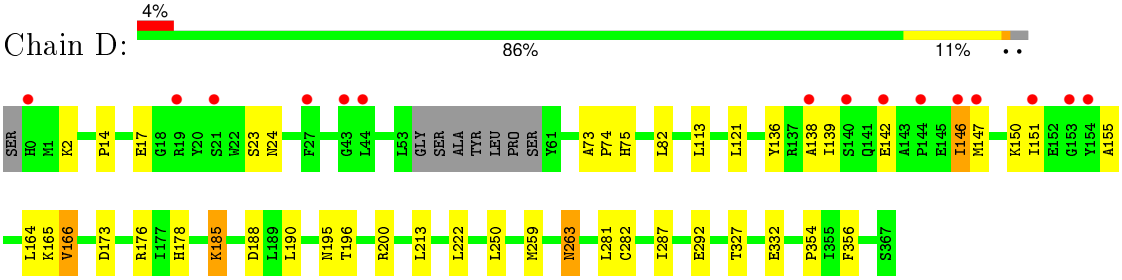
- Molecule 1: Muconate lactonizing enzyme

Chain C:



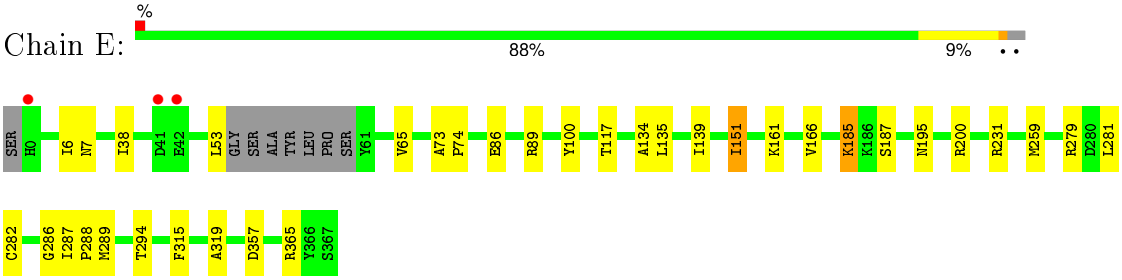
- Molecule 1: Muconate lactonizing enzyme

Chain D:



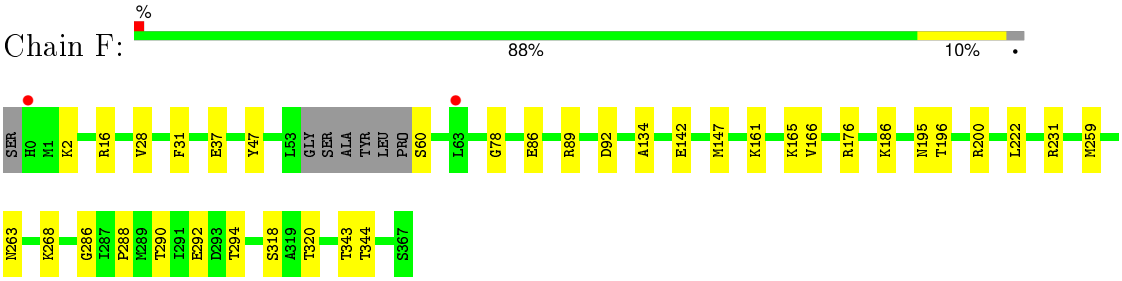
- Molecule 1: Muconate lactonizing enzyme

Chain E:



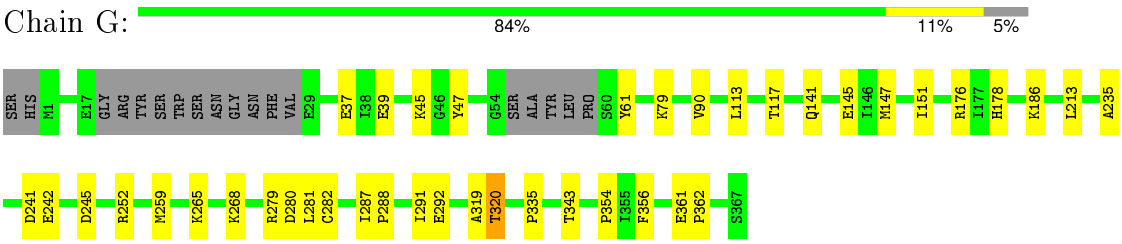
- Molecule 1: Muconate lactonizing enzyme

Chain F:



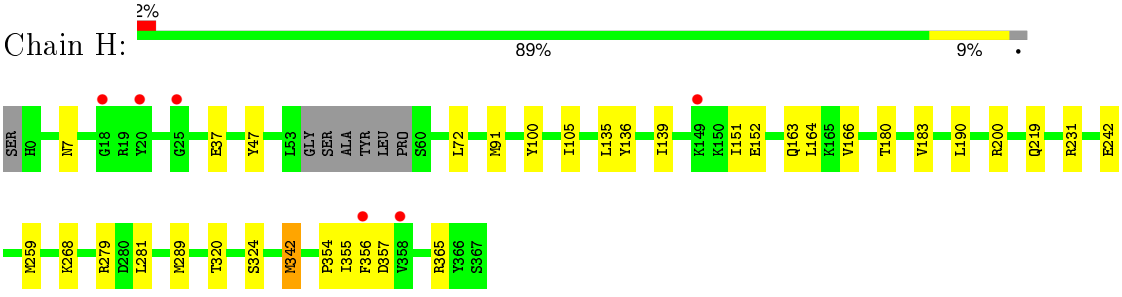
- Molecule 1: Muconate lactonizing enzyme

Chain G:



- Molecule 1: Muconate lactonizing enzyme

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	110.31Å 154.90Å 181.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.81 – 2.20 40.81 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.81-2.20) 99.9 (40.81-2.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.150 , 0.216 0.161 , 0.217	Depositor DCC
R_{free} test set	7927 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 158071 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	45845	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: NI, MG, CL

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	0.66	0/2856	0.72	1/3881 (0.0%)
1	B	0.62	0/2794	0.74	2/3794 (0.1%)
1	C	0.60	0/2839	0.70	0/3858
1	D	0.58	0/2782	0.69	0/3779
1	E	0.60	0/2811	0.70	0/3817
1	F	0.59	0/2805	0.68	0/3809
1	G	0.58	0/2702	0.67	1/3667 (0.0%)
1	H	0.53	0/2805	0.66	1/3809 (0.0%)
All	All	0.60	0/22394	0.70	5/30414 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	176	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	G	245	ASP	CB-CG-OD1	5.75	123.48	118.30
1	B	176	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	176	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	H	342	MET	CG-SD-CE	5.40	108.85	100.20

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	2802	2798	2792	19	0
1	B	2744	2743	2739	13	0
1	C	2786	2782	2780	17	0
1	D	2732	2718	2714	27	0
1	E	2756	2752	2744	21	0
1	F	2754	2751	2746	20	0
1	G	2657	2666	2663	24	0
1	H	2754	2749	2746	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	G	1	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	3	0	0	0	0
4	H	2	0	0	0	0
5	A	316	0	0	2	0
5	B	311	0	0	0	0
5	C	245	0	0	3	0
5	D	173	0	0	3	0
5	E	246	0	0	5	0
5	F	215	0	0	3	0
5	G	225	0	0	1	0
5	H	147	0	0	0	0
All	All	23886	21959	21924	158	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 4.

All (158) 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:F:142:GLU:H	1:F:147:MET:HE2	1.34	0.89
1:E:185:LYS:HD2	1:E:187:SER:OG	1.73	0.86
1:E:200:ARG:NH2	5:E:913:HOH:O	2.03	0.84
1:H:72:LEU:HD13	1:H:91:MET:HE2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:GLU:OE1	1:F:89:ARG:NH1	2.14	0.80
1:B:246:GLY:HA2	1:B:278:MET:HE1	1.65	0.76
1:E:7:ASN:OD1	1:E:365:ARG:HG2	1.87	0.75
1:F:142:GLU:N	1:F:147:MET:HE2	2.05	0.72
1:F:28:VAL:HG11	1:F:31:PHE:CZ	2.26	0.70
1:B:247:PRO:HD3	1:B:278:MET:HE2	1.74	0.69
1:H:72:LEU:HD13	1:H:91:MET:CE	2.22	0.69
1:C:171:ASN:OD1	1:G:186:LYS:NZ	2.25	0.69
1:D:173:ASP:OD1	1:D:176:ARG:NH1	2.27	0.67
1:G:292:GLU:HB3	1:G:320:THR:HG23	1.77	0.67
1:H:164:LEU:HD21	1:H:180:THR:HG21	1.80	0.64
1:D:155:ALA:HB3	5:D:509:HOH:O	1.97	0.64
1:C:72:LEU:HD13	1:C:91:MET:HE2	1.81	0.63
1:A:1:MET:HE1	1:A:44:LEU:HD12	1.81	0.62
1:G:61:TYR:OH	5:G:718:HOH:O	2.14	0.62
1:H:91:MET:HE1	1:H:105:ILE:HG13	1.82	0.61
1:G:147:MET:O	1:G:151:ILE:HG12	2.01	0.59
1:D:139:ILE:CB	1:D:151:ILE:HD11	2.34	0.58
1:E:286:GLY:O	1:E:288:PRO:HD3	2.04	0.58
1:H:139:ILE:HG13	1:H:151:ILE:HD11	1.86	0.58
1:A:1:MET:CE	1:A:44:LEU:HD12	2.34	0.58
1:C:7:ASN:OD1	1:C:365:ARG:HG2	2.04	0.58
1:H:139:ILE:HG13	1:H:151:ILE:CD1	2.35	0.57
1:G:279:ARG:NH2	1:G:280:ASP:OD1	2.33	0.57
1:F:37:GLU:HG3	1:F:47:TYR:CE1	2.40	0.57
1:B:246:GLY:HA2	1:B:278:MET:CE	2.34	0.56
1:D:14:PRO:HG2	1:D:327:THR:OG1	2.05	0.56
1:A:265:LYS:NZ	1:A:292:GLU:OE2	2.38	0.56
1:F:92:ASP:OD2	5:F:561:HOH:O	2.16	0.56
1:F:142:GLU:O	1:F:147:MET:HE3	2.05	0.56
1:B:16:ARG:HD2	1:B:326:GLY:O	2.06	0.55
1:H:72:LEU:CD1	1:H:91:MET:HE2	2.34	0.55
1:A:121:LEU:HD22	1:A:350:LEU:HD23	1.88	0.55
1:D:196:THR:HB	1:D:222:LEU:HA	1.88	0.55
1:D:147:MET:O	1:D:151:ILE:HG12	2.07	0.54
1:C:72:LEU:HD13	1:C:91:MET:CE	2.38	0.54
1:G:241:ASP:HB3	1:G:242:GLU:OE1	2.08	0.54
1:E:86:GLU:OE1	1:E:89:ARG:NH1	2.40	0.54
1:B:134:ALA:HB1	1:B:161:LYS:HE2	1.90	0.54
1:G:242:GLU:HA	1:G:268:LYS:HE3	1.91	0.53
1:D:185:LYS:HG3	1:D:188:ASP:OD2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:292:GLU:OE1	1:G:320:THR:HG21	2.08	0.53
1:H:164:LEU:HG	1:H:190:LEU:HD11	1.90	0.53
1:D:17:GLU:OE2	1:D:150:LYS:HD3	2.09	0.53
1:H:139:ILE:HG13	1:H:151:ILE:HG12	1.91	0.52
1:D:82:LEU:HD22	1:D:113:LEU:HA	1.91	0.52
1:G:141:GLN:HG3	1:G:176:ARG:CZ	2.41	0.51
1:B:47:TYR:CE1	1:B:354:PRO:HG3	2.45	0.51
1:E:200:ARG:NE	5:E:913:HOH:O	2.44	0.51
1:B:52:PRO:HG2	1:B:61:TYR:HB3	1.93	0.51
1:C:136:TYR:HA	1:C:161:LYS:O	2.11	0.51
1:H:91:MET:CE	1:H:105:ILE:HG13	2.42	0.50
1:A:2:LYS:HE3	5:A:785:HOH:O	2.11	0.50
1:F:268:LYS:HE2	5:F:705:HOH:O	2.12	0.50
1:H:135:LEU:HD21	1:H:342:MET:HG3	1.94	0.49
1:E:200:ARG:CZ	5:E:913:HOH:O	2.52	0.49
1:B:121:LEU:HD13	1:B:349:GLY:HA2	1.93	0.49
1:D:200:ARG:NH2	5:D:516:HOH:O	2.11	0.49
1:H:354:PRO:HG2	1:H:356:PHE:CE2	2.47	0.49
1:F:134:ALA:HB1	1:F:161:LYS:HE2	1.93	0.49
1:C:5:ALA:O	1:C:6:ILE:HD13	2.13	0.49
1:D:73:ALA:N	1:D:74:PRO:HD2	2.28	0.49
1:C:201:HIS:CD2	1:G:288:PRO:HG2	2.48	0.49
1:A:200:ARG:HG2	5:E:814:HOH:O	2.13	0.48
1:H:355:ILE:C	1:H:357:ASP:H	2.16	0.48
1:E:89:ARG:NH2	5:E:999:HOH:O	2.32	0.48
1:C:281:LEU:HD11	1:H:281:LEU:HD21	1.95	0.48
1:A:73:ALA:HB3	1:A:74:PRO:HD3	1.96	0.48
1:G:335:PRO:HB3	1:G:343:THR:O	2.12	0.48
1:F:290:THR:HA	1:F:318:SER:O	2.12	0.48
1:F:196:THR:HB	1:F:222:LEU:HA	1.96	0.48
1:C:205:ARG:HD3	5:C:582:HOH:O	2.13	0.47
1:G:113:LEU:O	1:G:117:THR:HG23	2.13	0.47
1:C:32:ASP:OD2	5:C:584:HOH:O	2.20	0.47
1:A:136:TYR:CE2	1:A:320:THR:HB	2.49	0.47
1:G:361:GLU:HG3	1:G:362:PRO:HD2	1.96	0.47
1:D:142:GLU:CD	1:D:146:ILE:HD11	2.35	0.47
1:E:282:CYS:HB3	1:E:287:ILE:O	2.15	0.47
1:B:269:VAL:HB	1:B:278:MET:CE	2.45	0.47
1:A:79:LYS:HE3	5:A:706:HOH:O	2.15	0.47
1:H:72:LEU:HD22	1:H:91:MET:HE2	1.96	0.47
1:E:53:LEU:HD11	1:E:294:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ASP:HB2	1:A:56:ALA:HA	1.97	0.47
1:E:134:ALA:HB1	1:E:161:LYS:HE2	1.97	0.47
1:H:139:ILE:HG13	1:H:151:ILE:CG1	2.45	0.47
1:F:2:LYS:HE3	1:F:78:GLY:HA2	1.96	0.46
1:F:147:MET:HE1	1:F:176:ARG:HD3	1.98	0.46
1:D:165:LYS:HD3	1:D:195:ASN:HD21	1.80	0.46
1:G:282:CYS:HB3	1:G:287:ILE:O	2.16	0.46
1:D:75:HIS:HE1	5:D:583:HOH:O	1.98	0.46
1:C:134:ALA:HB1	1:C:161:LYS:HE2	1.98	0.46
1:A:196:THR:HB	1:A:222:LEU:HA	1.97	0.46
1:D:185:LYS:HE3	1:D:188:ASP:OD1	2.15	0.46
1:A:149:LYS:HB3	1:A:149:LYS:HE2	1.80	0.46
1:E:281:LEU:HD21	1:G:281:LEU:HD21	1.98	0.46
1:C:290:THR:HA	1:C:318:SER:O	2.16	0.45
1:D:73:ALA:N	1:D:74:PRO:CD	2.79	0.45
1:D:164:LEU:HG	1:D:190:LEU:HD11	1.99	0.45
1:A:298:ASP:HB3	1:A:334:ALA:HB2	1.98	0.45
1:D:136:TYR:CE2	1:D:138:ALA:HB2	2.52	0.45
1:A:219:GLN:HG2	1:A:242:GLU:OE1	2.17	0.45
1:E:6:ILE:HD12	1:E:38:ILE:HG12	1.98	0.45
1:G:291:ILE:O	1:G:319:ALA:HA	2.16	0.44
1:H:219:GLN:HG2	1:H:242:GLU:OE1	2.17	0.44
1:C:233:ARG:HG2	1:G:235:ALA:HA	1.98	0.44
1:D:263:ASN:ND2	1:D:292:GLU:OE2	2.47	0.44
1:H:100:TYR:OH	1:H:268:LYS:HD2	2.17	0.44
1:C:136:TYR:CE2	1:C:320:THR:HB	2.52	0.44
1:H:136:TYR:CE2	1:H:320:THR:HB	2.53	0.44
1:F:147:MET:HE3	1:F:176:ARG:HE	1.82	0.44
1:E:286:GLY:HA2	1:E:315:PHE:CE1	2.53	0.44
1:F:263:ASN:OD1	1:F:292:GLU:OE2	2.35	0.44
1:E:117:THR:HB	1:G:117:THR:HB	2.00	0.43
1:D:136:TYR:HE2	1:D:138:ALA:HB2	1.83	0.43
1:A:164:LEU:HG	1:A:190:LEU:HD11	1.99	0.43
1:D:178:HIS:CD2	1:D:213:LEU:HD11	2.54	0.43
1:H:279:ARG:HG2	1:H:289:MET:SD	2.58	0.43
1:A:135:LEU:HA	1:A:319:ALA:O	2.18	0.43
1:F:286:GLY:O	1:F:288:PRO:HD3	2.18	0.43
1:B:136:TYR:OH	1:B:292:GLU:OE1	2.22	0.43
1:E:73:ALA:HB3	1:E:74:PRO:HD3	2.00	0.43
1:C:205:ARG:NH1	5:C:582:HOH:O	2.42	0.42
1:B:73:ALA:HB3	1:B:74:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:178:HIS:CD2	1:G:213:LEU:HD11	2.54	0.42
1:G:265:LYS:NZ	1:G:292:GLU:OE2	2.52	0.42
1:H:7:ASN:OD1	1:H:365:ARG:HG2	2.19	0.42
1:B:269:VAL:HB	1:B:278:MET:HE1	2.01	0.42
1:G:39:GLU:OE2	1:G:45:LYS:HE3	2.20	0.42
1:E:135:LEU:HA	1:E:319:ALA:O	2.20	0.42
1:B:279:ARG:HG2	1:B:289:MET:SD	2.60	0.42
1:F:268:LYS:CE	5:F:705:HOH:O	2.67	0.42
1:E:53:LEU:HD12	1:E:53:LEU:N	2.34	0.42
1:A:45:LYS:HB2	1:A:45:LYS:HE2	1.83	0.42
1:D:121:LEU:HD23	1:D:121:LEU:HA	1.92	0.41
1:D:354:PRO:HG2	1:D:356:PHE:CZ	2.54	0.41
1:D:282:CYS:HB3	1:D:287:ILE:O	2.20	0.41
1:C:286:GLY:HA2	1:C:315:PHE:CE1	2.55	0.41
1:F:165:LYS:HA	1:F:165:LYS:HD3	1.92	0.41
1:F:343:THR:OG1	1:F:344:THR:N	2.53	0.41
1:G:79:LYS:HE2	1:G:90:VAL:HG21	2.02	0.41
1:H:37:GLU:HG3	1:H:47:TYR:CE1	2.55	0.41
1:A:151:ILE:HD12	1:A:180:THR:HB	2.02	0.41
1:G:37:GLU:HG3	1:G:47:TYR:CE1	2.55	0.41
1:G:354:PRO:HG2	1:G:356:PHE:CZ	2.56	0.41
1:D:166:VAL:HG12	1:D:176:ARG:HD2	2.01	0.41
1:H:135:LEU:HD11	1:H:342:MET:HG3	2.03	0.41
1:E:279:ARG:HA	1:E:289:MET:SD	2.61	0.41
1:E:65:VAL:HG22	1:E:100:TYR:HB3	2.02	0.41
1:D:250:LEU:HD23	1:D:281:LEU:HD23	2.03	0.41
1:C:79:LYS:HE2	1:C:90:VAL:HG21	2.03	0.41
1:F:147:MET:HE3	1:F:176:ARG:NE	2.36	0.40
1:E:139:ILE:HG13	1:E:151:ILE:HG13	2.04	0.40
1:A:298:ASP:HB3	1:A:334:ALA:CB	2.51	0.40
1:D:23:SER:O	1:D:24:ASN:HB2	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	367/369 (100%)	359 (98%)	7 (2%)	1 (0%)	46	50
1	B	357/369 (97%)	351 (98%)	5 (1%)	1 (0%)	46	50
1	C	365/369 (99%)	356 (98%)	7 (2%)	2 (0%)	34	35
1	D	357/369 (97%)	344 (96%)	12 (3%)	1 (0%)	46	50
1	E	359/369 (97%)	350 (98%)	8 (2%)	1 (0%)	46	50
1	F	358/369 (97%)	344 (96%)	13 (4%)	1 (0%)	46	50
1	G	345/369 (94%)	340 (99%)	5 (1%)	0	100	100
1	H	358/369 (97%)	347 (97%)	10 (3%)	1 (0%)	46	50
All	All	2866/2952 (97%)	2791 (97%)	67 (2%)	8 (0%)	46	50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	23	SER
1	E	166	VAL
1	A	166	VAL
1	C	166	VAL
1	B	166	VAL
1	D	166	VAL
1	F	166	VAL
1	H	166	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	297/297 (100%)	291 (98%)	6 (2%)	63	76
1	B	291/297 (98%)	285 (98%)	6 (2%)	61	74
1	C	295/297 (99%)	291 (99%)	4 (1%)	74	85
1	D	288/297 (97%)	282 (98%)	6 (2%)	61	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	292/297 (98%)	286 (98%)	6 (2%)	61 74
1	F	292/297 (98%)	283 (97%)	9 (3%)	47 59
1	G	282/297 (95%)	278 (99%)	4 (1%)	74 85
1	H	292/297 (98%)	285 (98%)	7 (2%)	57 69
All	All	2329/2376 (98%)	2281 (98%)	48 (2%)	61 74

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LYS
1	A	163	GLN
1	A	195	ASN
1	A	231	ARG
1	A	259	MET
1	A	281	LEU
1	B	121	LEU
1	B	195	ASN
1	B	200	ARG
1	B	231	ARG
1	B	233	ARG
1	B	259	MET
1	C	231	ARG
1	C	233	ARG
1	C	259	MET
1	C	281	LEU
1	D	2	LYS
1	D	146	ILE
1	D	185	LYS
1	D	259	MET
1	D	263	ASN
1	D	332	GLU
1	E	151	ILE
1	E	185	LYS
1	E	195	ASN
1	E	231	ARG
1	E	259	MET
1	E	357	ASP
1	F	16	ARG
1	F	60	SER
1	F	186	LYS
1	F	195	ASN

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Mol	Chain	Res	Type
1	F	200	ARG
1	F	231	ARG
1	F	259	MET
1	F	294	THR
1	F	320	THR
1	G	145	GLU
1	G	252	ARG
1	G	259	MET
1	G	320	THR
1	H	152	GLU
1	H	163	GLN
1	H	183	VAL
1	H	200	ARG
1	H	231	ARG
1	H	259	MET
1	H	324	SER

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

Mol	Chain	Res	Type
1	A	0	HIS
1	F	178	HIS

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 23 ligands modelled in this entry, 23 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	369/369 (100%)	-0.78	1 (0%) 94 94	9, 16, 30, 65	0
1	B	361/369 (97%)	-0.82	0 100 100	10, 19, 33, 60	0
1	C	367/369 (99%)	-0.64	1 (0%) 94 94	11, 24, 45, 68	0
1	D	361/369 (97%)	-0.27	15 (4%) 40 39	12, 30, 66, 81	0
1	E	361/369 (97%)	-0.55	3 (0%) 87 87	12, 26, 44, 88	0
1	F	362/369 (98%)	-0.65	2 (0%) 90 90	12, 27, 45, 83	0
1	G	351/369 (95%)	-0.53	0 100 100	12, 24, 49, 83	0
1	H	362/369 (98%)	-0.21	6 (1%) 73 72	16, 33, 57, 77	0
All	All	2894/2952 (98%)	-0.56	28 (0%) 84 83	9, 24, 51, 88	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	151	ILE	5.2
1	D	138	ALA	3.7
1	D	146	ILE	3.3
1	A	57	TYR	3.2
1	H	149	LYS	3.0
1	D	27	PHE	2.8
1	D	0	HIS	2.7
1	D	153	GLY	2.6
1	H	25	GLY	2.6
1	E	0	HIS	2.6
1	D	142	GLU	2.5
1	H	356	PHE	2.5
1	D	147	MET	2.4
1	D	144	PRO	2.4
1	C	357	ASP	2.4
1	F	0	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	18	GLY	2.3
1	F	63	LEU	2.2
1	D	21	SER	2.2
1	E	42	GLU	2.2
1	H	358	VAL	2.1
1	D	19	ARG	2.1
1	D	43	GLY	2.1
1	D	44	LEU	2.1
1	D	154	TYR	2.1
1	H	20	TYR	2.1
1	D	140	SER	2.1
1	E	41	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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
2	CL	G	404	1/1	0.93	0.15	2.88	55,55,55,55	0
4	MG	B	401	1/1	0.97	0.12	1.44	21,21,21,21	0
4	MG	A	404	1/1	0.97	0.10	0.57	18,18,18,18	0
4	MG	C	402	1/1	0.97	0.10	0.38	19,19,19,19	0
4	MG	A	403	1/1	0.98	0.08	0.33	19,19,19,19	0
4	MG	E	401	1/1	0.99	0.08	0.04	20,20,20,20	0
3	NI	A	402	1/1	1.00	0.08	-0.22	18,18,18,18	0
4	MG	G	402	1/1	0.98	0.08	-0.49	31,31,31,31	0
4	MG	H	401	1/1	0.89	0.10	-0.63	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	MG	H	402	1/1	0.96	0.04	-1.08	28,28,28,28	0
3	NI	D	401	1/1	0.99	0.07	-1.22	28,28,28,28	0
4	MG	F	401	1/1	0.99	0.06	-1.37	16,16,16,16	0
2	CL	A	401	1/1	0.97	0.07	-1.47	27,27,27,27	0
4	MG	D	402	1/1	0.97	0.03	-1.56	25,25,25,25	0
4	MG	D	403	1/1	0.75	0.07	-1.62	48,48,48,48	0
4	MG	C	403	1/1	0.99	0.07	-1.67	22,22,22,22	0
4	MG	G	401	1/1	0.98	0.04	-2.21	38,38,38,38	0
4	MG	E	402	1/1	0.98	0.04	-2.24	26,26,26,26	0
4	MG	G	403	1/1	0.94	0.06	-2.76	27,27,27,27	0
4	MG	F	402	1/1	0.98	0.05	-3.31	18,18,18,18	0
4	MG	B	402	1/1	0.97	0.04	-3.37	21,21,21,21	0
3	NI	C	401	1/1	0.99	0.04	-3.42	28,28,28,28	0
2	CL	B	403	1/1	0.96	0.14	-	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.