wwPDB X-ray Structure Validation Summary Report (i)

Mar 7, 2026 – 02:35 AM UTC

PDB ID	:	4MGG / pdb_00004mgg
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

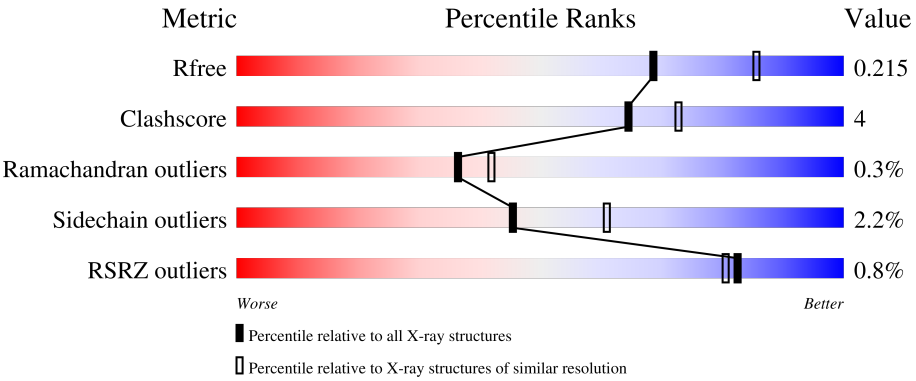
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	91% 8% •
1	B	369	90% 7% ••
1	C	369	91% 8% ••
1	D	369	3% 85% 11% ••

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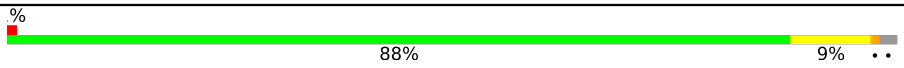
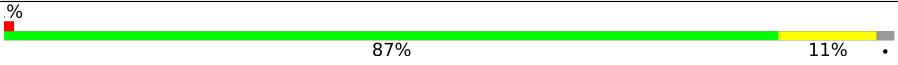
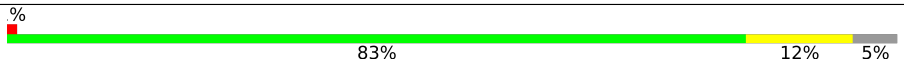
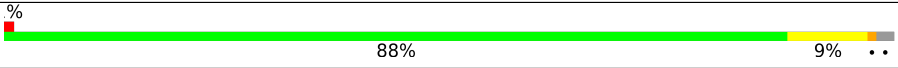
Mol	Chain	Length	Quality of chain
1	E	369	
1	F	369	
1	G	369	
1	H	369	

2 Entry composition (i)

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 (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

- Molecule 5 is water.

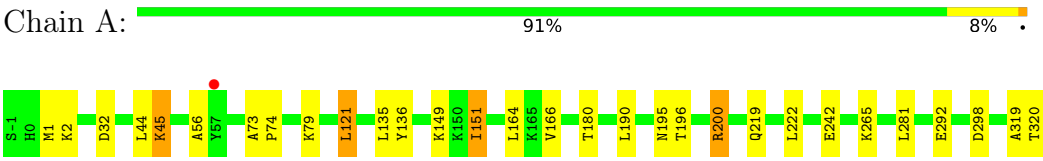
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	316	Total O 316 316	0	0
5	B	311	Total O 311 311	0	0
5	C	245	Total O 245 245	0	0
5	D	173	Total O 173 173	0	0
5	E	246	Total O 246 246	0	0
5	F	215	Total O 215 215	0	0
5	G	225	Total O 225 225	0	0
5	H	147	Total O 147 147	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

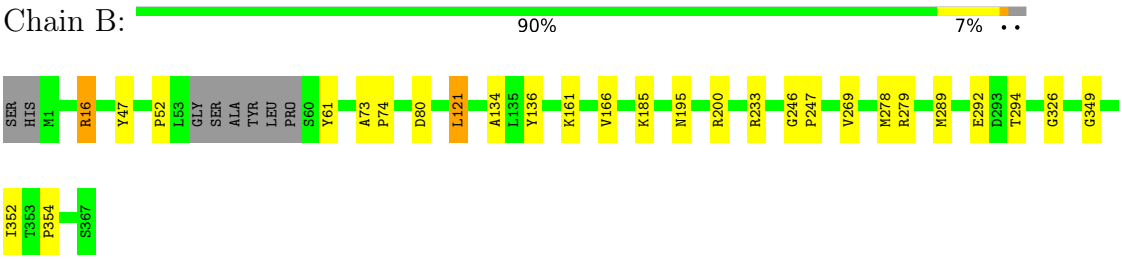
• Molecule 1: Muconate lactonizing enzyme

Chain A:



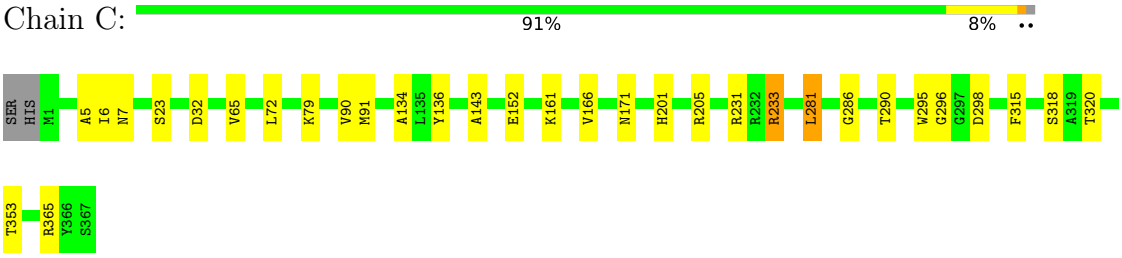
• Molecule 1: Muconate lactonizing enzyme

Chain B:



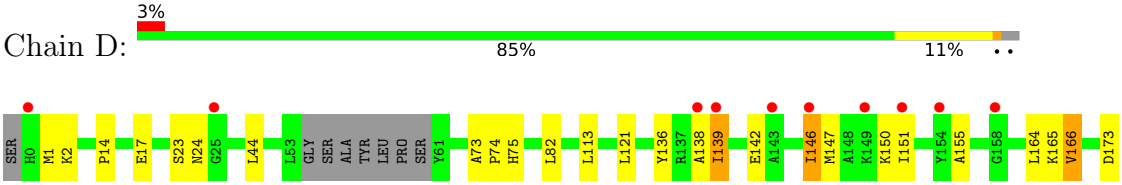
• Molecule 1: Muconate lactonizing enzyme

Chain C:



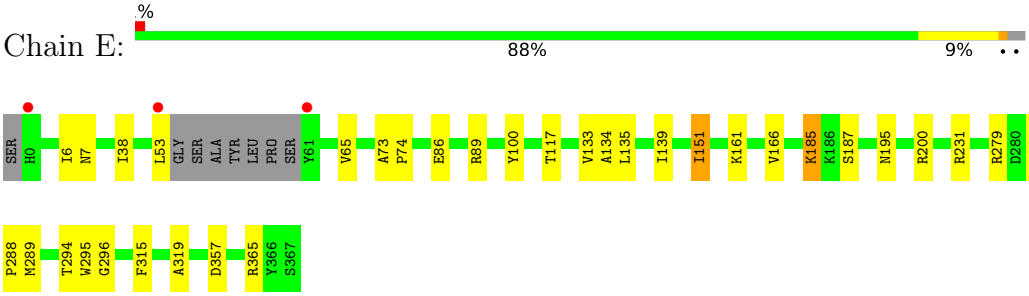
• Molecule 1: Muconate lactonizing enzyme

Chain D:



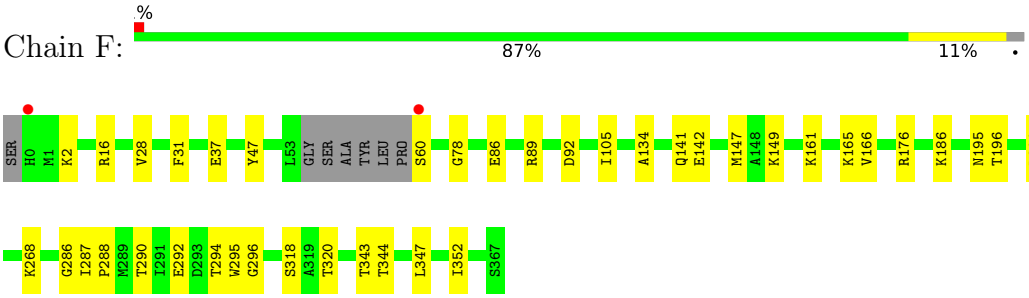
• Molecule 1: Muconate lactonizing enzyme

Chain E:



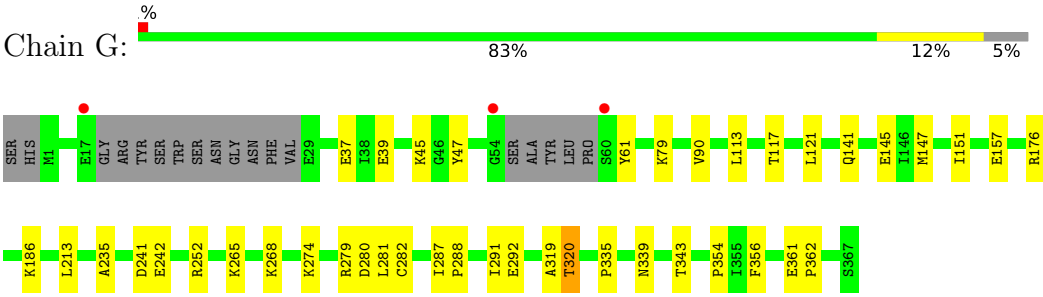
• Molecule 1: Muconate lactonizing enzyme

Chain F:



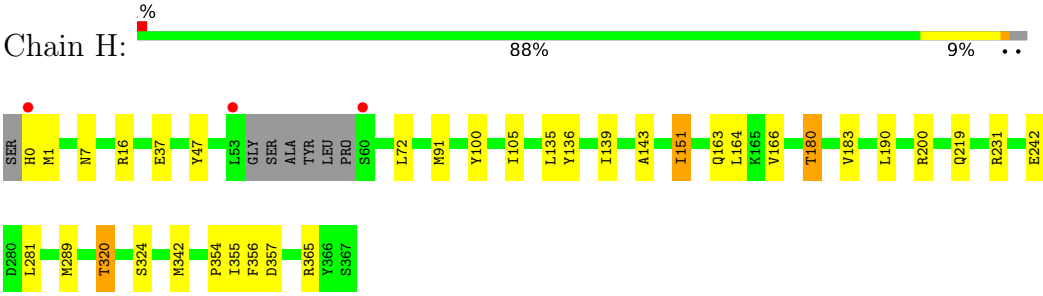
• Molecule 1: Muconate lactonizing enzyme

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 1.8.1_1168	Depositor
R, R_{free}	0.150 , 0.216 0.155 , 0.215	Depositor DCC
R_{free} test set	7927 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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: CL, MG, NI

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	0.85	0/2856	0.91	0/3881
1	B	0.82	0/2794	0.94	2/3794 (0.1%)
1	C	0.77	1/2839 (0.0%)	0.95	5/3858 (0.1%)
1	D	0.76	0/2782	0.93	1/3779 (0.0%)
1	E	0.77	0/2811	0.91	0/3817
1	F	0.77	0/2805	0.92	4/3809 (0.1%)
1	G	0.75	0/2702	0.89	1/3667 (0.0%)
1	H	0.69	0/2805	0.89	2/3809 (0.1%)
All	All	0.77	1/22394 (0.0%)	0.92	15/30414 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	65	VAL	CA-CB	5.70	1.61	1.54

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	80	ASP	CA-C-N	-6.95	112.54	120.04
1	B	80	ASP	C-N-CA	-6.95	112.54	120.04
1	C	353	THR	CA-C-N	-6.70	113.40	120.03
1	C	353	THR	C-N-CA	-6.70	113.40	120.03
1	C	298	ASP	N-CA-C	5.95	117.77	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2802	2798	2792	20	0
1	B	2744	2743	2739	14	0
1	C	2786	2782	2780	19	0
1	D	2732	2718	2714	28	0
1	E	2756	2752	2744	22	0
1	F	2754	2751	2746	23	0
1	G	2657	2666	2663	25	0
1	H	2754	2749	2746	25	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	170	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.

The worst 5 of 170 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: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:B:269:VAL:HB	1:B:278:MET:HE1	1.58	0.84
1:H:72:LEU:HD13	1:H:91:MET:HE2	1.62	0.80
1:F:86:GLU:OE1	1:F:89:ARG:NH1	2.14	0.80

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%)	36	42
1	B	357/369 (97%)	351 (98%)	5 (1%)	1 (0%)	36	42
1	C	365/369 (99%)	356 (98%)	7 (2%)	2 (0%)	24	27
1	D	357/369 (97%)	344 (96%)	12 (3%)	1 (0%)	36	42
1	E	359/369 (97%)	350 (98%)	8 (2%)	1 (0%)	36	42
1	F	358/369 (97%)	344 (96%)	13 (4%)	1 (0%)	36	42
1	G	345/369 (94%)	340 (99%)	5 (1%)	0	100	100
1	H	358/369 (97%)	347 (97%)	10 (3%)	1 (0%)	36	42
All	All	2866/2952 (97%)	2791 (97%)	67 (2%)	8 (0%)	36	42

5 of 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

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%)	48	64
1	B	291/297 (98%)	284 (98%)	7 (2%)	43	58
1	C	295/297 (99%)	291 (99%)	4 (1%)	59	75
1	D	288/297 (97%)	282 (98%)	6 (2%)	47	63
1	E	292/297 (98%)	286 (98%)	6 (2%)	47	63
1	F	292/297 (98%)	284 (97%)	8 (3%)	39	53
1	G	282/297 (95%)	277 (98%)	5 (2%)	51	68
1	H	292/297 (98%)	282 (97%)	10 (3%)	32	44
All	All	2329/2376 (98%)	2277 (98%)	52 (2%)	45	61

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	357	ASP
1	F	294	THR
1	H	231	ARG
1	F	16	ARG
1	F	186	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	195	ASN
1	F	178	HIS
1	E	306	HIS
1	D	195	ASN
1	F	75	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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 (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	369/369 (100%)	-0.98	1 (0%) 90 88	10, 17, 35, 70	0
1	B	361/369 (97%)	-0.93	0 100 100	10, 20, 36, 71	0
1	C	367/369 (99%)	-0.72	0 100 100	11, 26, 49, 72	0
1	D	361/369 (97%)	-0.37	10 (2%) 55 52	13, 33, 72, 90	0
1	E	361/369 (97%)	-0.67	3 (0%) 82 80	12, 28, 50, 96	1 (0%)
1	F	362/369 (98%)	-0.67	2 (0%) 85 83	13, 29, 48, 91	0
1	G	351/369 (95%)	-0.72	3 (0%) 81 79	13, 26, 54, 89	0
1	H	362/369 (98%)	-0.38	3 (0%) 82 80	17, 36, 63, 88	0
All	All	2894/2952 (98%)	-0.68	22 (0%) 82 80	10, 26, 56, 96	1 (0%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	54	GLY	4.4
1	D	151	ILE	4.2
1	E	0	HIS	3.9
1	D	154	TYR	3.8
1	F	0	HIS	3.6

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

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

6.3 Carbohydrates

There are no oligosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	CL	B	403	1/1	0.92	0.21	52,52,52,52	0
2	CL	G	404	1/1	0.93	0.19	55,55,55,55	0
4	MG	D	403	1/1	0.96	0.04	48,48,48,48	0
4	MG	H	401	1/1	0.96	0.03	31,31,31,31	0
4	MG	G	402	1/1	0.97	0.04	31,31,31,31	0
4	MG	G	403	1/1	0.97	0.04	27,27,27,27	0
2	CL	A	401	1/1	0.97	0.05	27,27,27,27	0
4	MG	H	402	1/1	0.97	0.03	28,28,28,28	0
4	MG	C	402	1/1	0.98	0.03	19,19,19,19	0
4	MG	B	401	1/1	0.98	0.04	21,21,21,21	0
4	MG	F	402	1/1	0.98	0.03	18,18,18,18	0
4	MG	G	401	1/1	0.98	0.02	38,38,38,38	0
4	MG	E	402	1/1	0.99	0.02	26,26,26,26	0
4	MG	F	401	1/1	0.99	0.02	16,16,16,16	0
4	MG	B	402	1/1	0.99	0.02	21,21,21,21	0
4	MG	A	404	1/1	0.99	0.03	18,18,18,18	0
4	MG	C	403	1/1	0.99	0.01	22,22,22,22	0
4	MG	D	402	1/1	0.99	0.03	25,25,25,25	0
4	MG	A	403	1/1	0.99	0.06	19,19,19,19	0
4	MG	E	401	1/1	0.99	0.05	20,20,20,20	0
3	NI	D	401	1/1	1.00	0.01	28,28,28,28	0
3	NI	A	402	1/1	1.00	0.01	18,18,18,18	0
3	NI	C	401	1/1	1.00	0.04	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.