Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:20 PM GMT

PDB ID	:	4EGF
Title	:	Crystal structure of a L-xylulose reductase from Mycobacterium smegmatis
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID); Arakaki, T.L.; Staker, B.L.; Fairman, J.
Deposited on	:	2012-03-30
Resolution	:	2.30 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:

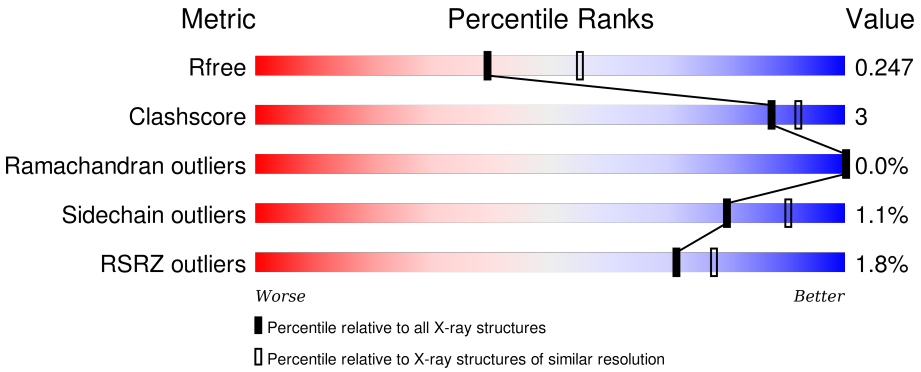
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	266	88% 8%
1	B	266	91% 5%
1	C	266	3% 91% 5%
1	D	266	4% 89% 6% 5%
1	E	266	2% 89% 7%

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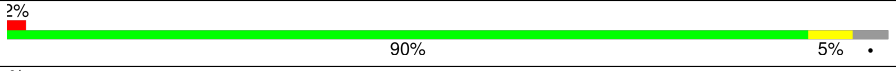
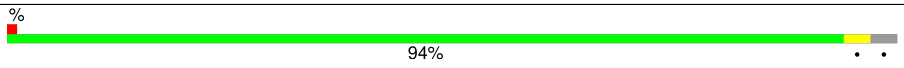
Mol	Chain	Length	Quality of chain
1	F	266	
1	G	266	
1	H	266	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15293 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 L-xylulose reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	1	0
			1825	1146	327	344	8			
1	B	257	Total	C	N	O	S	0	1	0
			1821	1145	329	339	8			
1	C	257	Total	C	N	O	S	0	0	0
			1784	1124	318	335	7			
1	D	253	Total	C	N	O	S	0	1	0
			1786	1125	319	334	8			
1	E	257	Total	C	N	O	S	0	1	0
			1804	1133	323	340	8			
1	F	257	Total	C	N	O	S	0	1	0
			1834	1151	331	344	8			
1	G	255	Total	C	N	O	S	0	0	0
			1793	1128	323	334	8			
1	H	257	Total	C	N	O	S	0	0	0
			1800	1131	324	338	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP A0QXD6
A	-2	PRO	-	EXPRESSION TAG	UNP A0QXD6
A	-1	GLY	-	EXPRESSION TAG	UNP A0QXD6
A	0	SER	-	EXPRESSION TAG	UNP A0QXD6
B	-3	GLY	-	EXPRESSION TAG	UNP A0QXD6
B	-2	PRO	-	EXPRESSION TAG	UNP A0QXD6
B	-1	GLY	-	EXPRESSION TAG	UNP A0QXD6
B	0	SER	-	EXPRESSION TAG	UNP A0QXD6
C	-3	GLY	-	EXPRESSION TAG	UNP A0QXD6
C	-2	PRO	-	EXPRESSION TAG	UNP A0QXD6
C	-1	GLY	-	EXPRESSION TAG	UNP A0QXD6
C	0	SER	-	EXPRESSION TAG	UNP A0QXD6
D	-3	GLY	-	EXPRESSION TAG	UNP A0QXD6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	PRO	-	EXPRESSION TAG	UNP A0QXD6
D	-1	GLY	-	EXPRESSION TAG	UNP A0QXD6
D	0	SER	-	EXPRESSION TAG	UNP A0QXD6
E	-3	GLY	-	EXPRESSION TAG	UNP A0QXD6
E	-2	PRO	-	EXPRESSION TAG	UNP A0QXD6
E	-1	GLY	-	EXPRESSION TAG	UNP A0QXD6
E	0	SER	-	EXPRESSION TAG	UNP A0QXD6
F	-3	GLY	-	EXPRESSION TAG	UNP A0QXD6
F	-2	PRO	-	EXPRESSION TAG	UNP A0QXD6
F	-1	GLY	-	EXPRESSION TAG	UNP A0QXD6
F	0	SER	-	EXPRESSION TAG	UNP A0QXD6
G	-3	GLY	-	EXPRESSION TAG	UNP A0QXD6
G	-2	PRO	-	EXPRESSION TAG	UNP A0QXD6
G	-1	GLY	-	EXPRESSION TAG	UNP A0QXD6
G	0	SER	-	EXPRESSION TAG	UNP A0QXD6
H	-3	GLY	-	EXPRESSION TAG	UNP A0QXD6
H	-2	PRO	-	EXPRESSION TAG	UNP A0QXD6
H	-1	GLY	-	EXPRESSION TAG	UNP A0QXD6
H	0	SER	-	EXPRESSION TAG	UNP A0QXD6

- Molecule 2 is water.

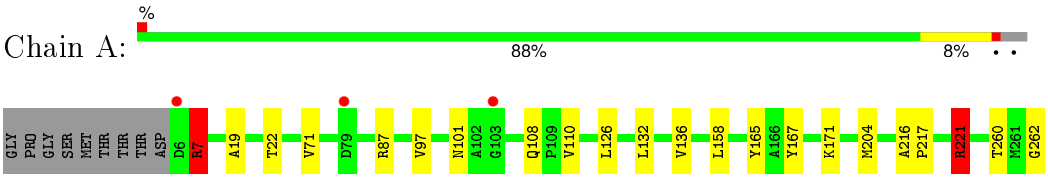
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	84	Total O 84 84	0	0
2	B	138	Total O 138 138	0	0
2	C	86	Total O 86 86	0	0
2	D	99	Total O 99 99	0	0
2	E	111	Total O 111 111	0	0
2	F	120	Total O 120 120	0	0
2	G	99	Total O 99 99	0	0
2	H	109	Total O 109 109	0	0

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.

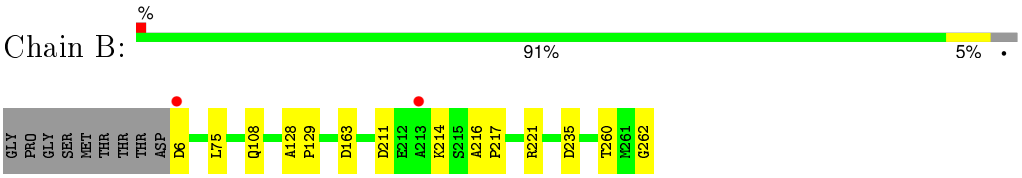
- Molecule 1: L-xylulose reductase

Chain A:



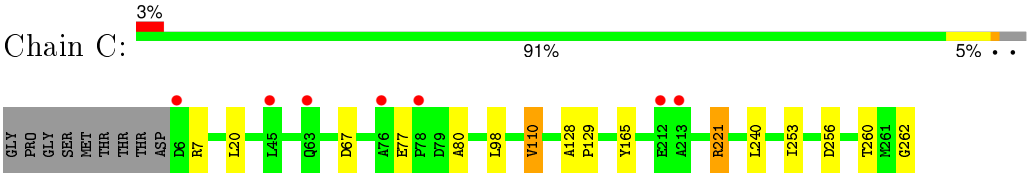
- Molecule 1: L-xylulose reductase

Chain B:



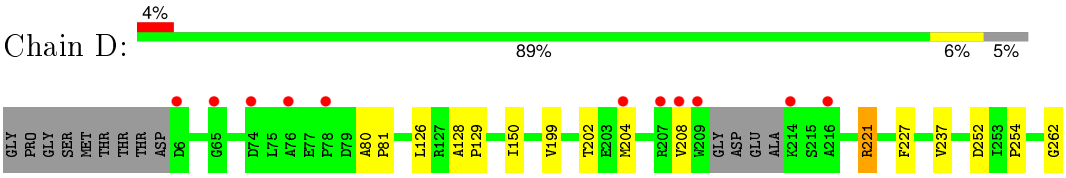
- Molecule 1: L-xylulose reductase

Chain C:



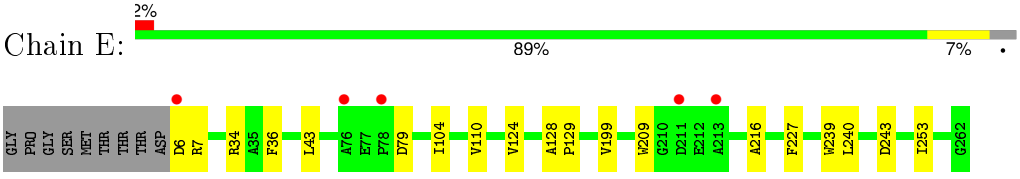
- Molecule 1: L-xylulose reductase

Chain D:



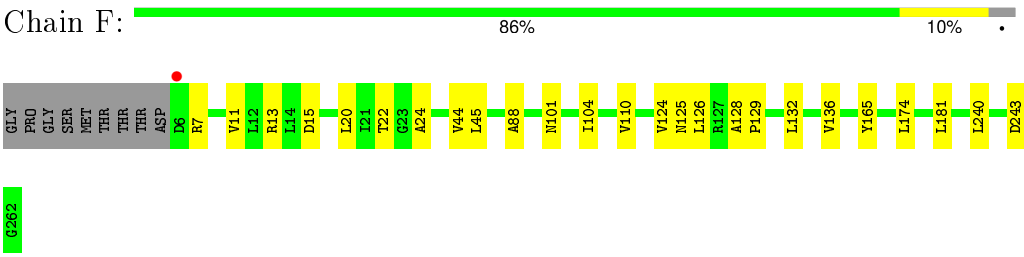
- Molecule 1: L-xylulose reductase

Chain E:



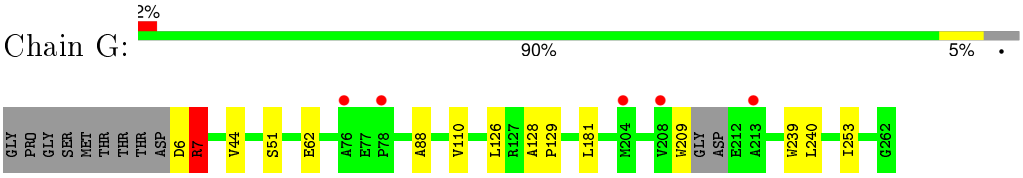
- Molecule 1: L-xylulose reductase

Chain F:



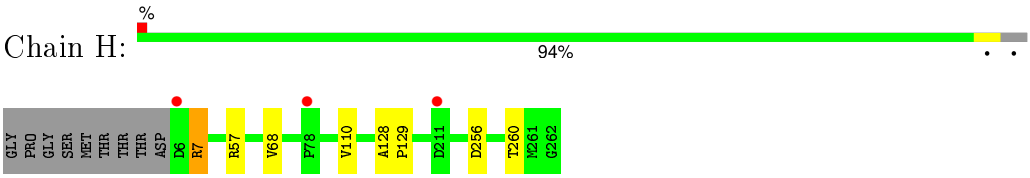
• Molecule 1: L-xylulose reductase

Chain G:



• Molecule 1: L-xylulose reductase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.80Å 130.75Å 114.97Å 90.00° 103.74° 90.00°	Depositor
Resolution (Å)	19.88 – 2.30 19.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.88-2.30) 99.8 (19.86-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.187 , 0.247 0.191 , 0.247	Depositor DCC
R_{free} test set	4693 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 93607 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15293	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.78% 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

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	0.75	1/1859 (0.1%)	0.75	2/2537 (0.1%)
1	B	0.80	0/1855	0.73	0/2532
1	C	0.69	0/1814	0.70	1/2482 (0.0%)
1	D	0.73	0/1819	0.72	0/2484
1	E	0.79	2/1838 (0.1%)	0.72	1/2512 (0.0%)
1	F	0.77	0/1868	0.73	0/2548
1	G	0.77	2/1822 (0.1%)	0.73	0/2487
1	H	0.70	1/1830 (0.1%)	0.71	0/2501
All	All	0.75	6/14705 (0.0%)	0.73	4/20083 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	209	TRP	CD2-CE2	5.95	1.48	1.41
1	E	239	TRP	CD2-CE2	5.71	1.48	1.41
1	H	7	ARG	N-CA	5.27	1.56	1.46
1	A	7	ARG	N-CA	5.11	1.56	1.46
1	E	209	TRP	CD2-CE2	5.04	1.47	1.41
1	G	239	TRP	CD2-CE2	5.01	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	221	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	221	ARG	NE-CZ-NH1	5.66	123.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	34	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	C	221	ARG	NE-CZ-NH2	-5.34	117.63	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	7	ARG	Peptide

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	1825	0	1832	13	0
1	B	1821	0	1831	8	0
1	C	1784	0	1761	10	0
1	D	1786	0	1789	10	0
1	E	1804	0	1793	10	0
1	F	1834	0	1846	19	0
1	G	1793	0	1790	10	1
1	H	1800	0	1788	5	0
2	A	84	0	0	0	0
2	B	138	0	0	1	2
2	C	86	0	0	0	0
2	D	99	0	0	0	0
2	E	111	0	0	4	1
2	F	120	0	0	4	0
2	G	99	0	0	0	0
2	H	109	0	0	0	0
All	All	15293	0	14430	76	2

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 3.

All (76) 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:G:128:ALA:HB3	1:G:129:PRO:HD3	1.58	0.86
1:F:243:ASP:HB3	2:F:340:HOH:O	1.81	0.80
1:C:128:ALA:HB3	1:C:129:PRO:HD3	1.71	0.72
1:A:126:LEU:C	1:A:126:LEU:HD23	2.10	0.71
1:A:262:GLY:OXT	1:B:221:ARG:NH2	2.24	0.69
1:C:221:ARG:NH2	1:D:262:GLY:OXT	2.27	0.67
1:A:221:ARG:HH22	1:B:262:GLY:C	2.00	0.65
1:D:126:LEU:C	1:D:126:LEU:HD23	2.17	0.65
2:F:341:HOH:O	1:H:110:VAL:HG12	1.98	0.64
1:C:256:ASP:OD2	1:C:260:THR:HG23	2.00	0.61
1:F:132:LEU:O	1:F:136:VAL:HG23	2.02	0.60
1:E:240:LEU:HD11	1:E:253:ILE:HD12	1.84	0.59
1:F:11:VAL:HB	1:G:7:ARG:H	1.69	0.58
1:E:243:ASP:HB3	2:E:366:HOH:O	2.03	0.58
1:G:126:LEU:C	1:G:126:LEU:HD23	2.24	0.58
1:C:110:VAL:HG23	1:C:165:TYR:CG	2.39	0.58
1:A:110:VAL:HG23	1:A:165:TYR:CG	2.40	0.57
1:D:128:ALA:HB3	1:D:129:PRO:HD3	1.87	0.56
1:H:57:ARG:HG3	1:H:68:VAL:HB	1.87	0.56
1:F:13:ARG:NH2	1:F:15:ASP:OD1	2.37	0.56
1:A:71:VAL:HG13	1:A:87:ARG:CZ	2.36	0.56
1:F:128:ALA:HB3	1:F:129:PRO:HD3	1.88	0.56
1:D:199:VAL:HB	1:D:227:PHE:CD1	2.41	0.55
1:H:256:ASP:OD2	1:H:260:THR:HG23	2.05	0.55
1:F:126:LEU:C	1:F:126:LEU:HD23	2.26	0.55
1:G:240:LEU:HD11	1:G:253:ILE:HD12	1.90	0.54
1:F:22:THR:O	1:F:101:ASN:HB3	2.08	0.53
1:B:216:ALA:HB3	1:B:217:PRO:HD3	1.89	0.53
1:F:181:LEU:HD23	1:H:110:VAL:HG21	1.90	0.53
1:B:260:THR:HA	2:B:425:HOH:O	2.08	0.52
1:A:216:ALA:HB3	1:A:217:PRO:HD3	1.92	0.52
1:E:110:VAL:HG21	1:G:181:LEU:HD23	1.92	0.51
1:D:150:ILE:HG21	1:D:237:VAL:HG13	1.92	0.50
1:D:80:ALA:HB3	1:D:81:PRO:HD3	1.94	0.49
1:F:240:LEU:HD21	1:F:253:ILE:CD1	2.43	0.49
1:D:252:ASP:O	1:D:254:PRO:HD3	2.12	0.49
1:G:128:ALA:HB3	1:G:129:PRO:CD	2.34	0.49
1:E:6:ASP:CB	2:E:346:HOH:O	2.61	0.48
1:F:125:ASN:O	1:F:174:LEU:HD22	2.13	0.48
1:B:211:ASP:OD2	1:B:214:LYS:N	2.45	0.48
1:C:262:GLY:C	1:D:221:ARG:HH22	2.17	0.48
1:E:110:VAL:HG21	1:G:181:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:LEU:HD21	1:F:253:ILE:HD11	1.96	0.47
1:F:24:ALA:HB1	1:F:45:LEU:HD22	1.97	0.47
1:F:259:TYR:OH	2:F:400:HOH:O	2.11	0.47
1:A:126:LEU:C	1:A:126:LEU:CD2	2.82	0.47
1:E:128:ALA:HB3	1:E:129:PRO:HD3	1.96	0.46
1:A:7:ARG:HB2	1:A:7:ARG:HH11	1.80	0.46
1:F:110:VAL:HG23	1:F:165:TYR:CG	2.51	0.46
1:E:199:VAL:HB	1:E:227:PHE:CD1	2.52	0.45
1:E:36:PHE:HB3	1:E:43:LEU:HD21	1.97	0.45
1:F:20:LEU:HA	1:F:44:VAL:O	2.18	0.44
1:C:240:LEU:HD11	1:C:253:ILE:HD12	1.98	0.44
1:H:128:ALA:HB3	1:H:129:PRO:HD3	1.99	0.44
1:B:108:GLN:O	1:B:163:ASP:HA	2.17	0.44
1:G:44:VAL:HG11	1:G:88:ALA:HA	2.00	0.44
1:D:126:LEU:C	1:D:126:LEU:CD2	2.86	0.44
1:C:77:GLU:HB2	1:C:80:ALA:HB2	1.99	0.44
1:B:6:ASP:CB	1:B:235:ASP:OD1	2.67	0.43
1:F:243:ASP:CB	2:F:340:HOH:O	2.55	0.43
1:F:104:ILE:HG23	1:F:124:VAL:HG11	2.01	0.42
2:E:349:HOH:O	1:G:110:VAL:HG12	2.19	0.42
1:A:19:ALA:HA	1:A:97:VAL:O	2.19	0.42
1:B:128:ALA:HB3	1:B:129:PRO:HD3	2.00	0.42
1:C:128:ALA:HB3	1:C:129:PRO:CD	2.47	0.42
1:C:20:LEU:HD23	1:C:98:LEU:HD13	2.02	0.42
1:A:22:THR:O	1:A:101:ASN:HB3	2.18	0.42
1:E:216:ALA:HA	2:E:375:HOH:O	2.20	0.42
1:F:11:VAL:HG21	1:G:6:ASP:HA	2.03	0.41
1:F:44:VAL:HG11	1:F:88:ALA:HA	2.02	0.41
1:A:158:LEU:HD12	1:A:260:THR:HG21	2.00	0.41
1:D:204:MET:O	1:D:208:VAL:HG23	2.19	0.41
1:A:167:TYR:CE1	1:A:171:LYS:HE3	2.56	0.41
1:E:104:ILE:HG23	1:E:124:VAL:HG11	2.02	0.41
1:C:110:VAL:HG23	1:C:165:TYR:CD1	2.56	0.40
1:A:132:LEU:O	1:A:136:VAL:HG23	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:HOH:O	2:E:338:HOH:O[1_554]	1.92	0.28
1:G:62:GLU:OE2	2:B:415:HOH:O[2_656]	2.17	0.03

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	256/266 (96%)	245 (96%)	11 (4%)	0	100	100
1	B	256/266 (96%)	248 (97%)	8 (3%)	0	100	100
1	C	255/266 (96%)	245 (96%)	10 (4%)	0	100	100
1	D	250/266 (94%)	241 (96%)	8 (3%)	1 (0%)	39	48
1	E	256/266 (96%)	246 (96%)	10 (4%)	0	100	100
1	F	256/266 (96%)	247 (96%)	9 (4%)	0	100	100
1	G	251/266 (94%)	242 (96%)	9 (4%)	0	100	100
1	H	255/266 (96%)	247 (97%)	8 (3%)	0	100	100
All	All	2035/2128 (96%)	1961 (96%)	73 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	202	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	176/188 (94%)	172 (98%)	4 (2%)	58	75
1	B	174/188 (93%)	173 (99%)	1 (1%)	90	96
1	C	165/188 (88%)	162 (98%)	3 (2%)	66	82
1	D	171/188 (91%)	170 (99%)	1 (1%)	90	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	171/188 (91%)	169 (99%)	2 (1%)	78 89
1	F	177/188 (94%)	176 (99%)	1 (1%)	90 96
1	G	169/188 (90%)	167 (99%)	2 (1%)	78 89
1	H	169/188 (90%)	168 (99%)	1 (1%)	90 96
All	All	1372/1504 (91%)	1357 (99%)	15 (1%)	80 90

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

Mol	Chain	Res	Type
1	A	7	ARG
1	A	108	GLN
1	A	204	MET
1	A	221	ARG
1	B	75	LEU
1	C	7	ARG
1	C	67	ASP
1	C	110	VAL
1	D	221	ARG
1	E	7	ARG
1	E	79	ASP
1	F	7	ARG
1	G	7	ARG
1	G	51	SER
1	H	7	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	257/266 (96%)	-0.20	3 (1%) 81 85	22, 29, 47, 60	0
1	B	257/266 (96%)	-0.19	2 (0%) 87 90	22, 26, 50, 80	0
1	C	257/266 (96%)	-0.06	7 (2%) 58 67	22, 31, 66, 88	0
1	D	253/266 (95%)	-0.08	11 (4%) 39 48	22, 27, 62, 100	0
1	E	257/266 (96%)	-0.13	5 (1%) 70 76	22, 25, 51, 74	0
1	F	257/266 (96%)	-0.23	1 (0%) 93 95	22, 27, 38, 43	0
1	G	255/266 (95%)	-0.07	5 (1%) 68 75	23, 27, 60, 99	0
1	H	257/266 (96%)	-0.11	3 (1%) 81 85	23, 29, 64, 83	0
All	All	2050/2128 (96%)	-0.13	37 (1%) 71 78	22, 28, 57, 100	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	213	ALA	5.4
1	E	6	ASP	4.5
1	E	78	PRO	4.3
1	F	6	ASP	3.4
1	D	78	PRO	3.4
1	H	6	ASP	3.3
1	E	211	ASP	3.3
1	H	78	PRO	3.2
1	A	6	ASP	3.2
1	D	76	ALA	3.2
1	D	6	ASP	3.1
1	D	209	TRP	3.0
1	C	63	GLN	2.9
1	D	74	ASP	2.9
1	E	213	ALA	2.9
1	B	6	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	78	PRO	2.7
1	C	212	GLU	2.7
1	C	6	ASP	2.6
1	C	213	ALA	2.6
1	G	204	MET	2.6
1	D	216	ALA	2.5
1	D	204	MET	2.5
1	D	208	VAL	2.5
1	D	65	GLY	2.5
1	C	45	LEU	2.4
1	E	76	ALA	2.4
1	G	208	VAL	2.3
1	B	213	ALA	2.3
1	A	79	ASP	2.3
1	C	78	PRO	2.2
1	G	76	ALA	2.2
1	C	76	ALA	2.1
1	H	211	ASP	2.1
1	A	103	GLY	2.1
1	D	214	LYS	2.0
1	D	207	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.