Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 12:01 PM GMT

PDB ID	:	3QQW
Title	:	Crystal structure of a putative lyase (Reut_B4148) from Ralstonia eutropha JMP134 at 2.44 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2011-02-16
Resolution	:	2.44 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:

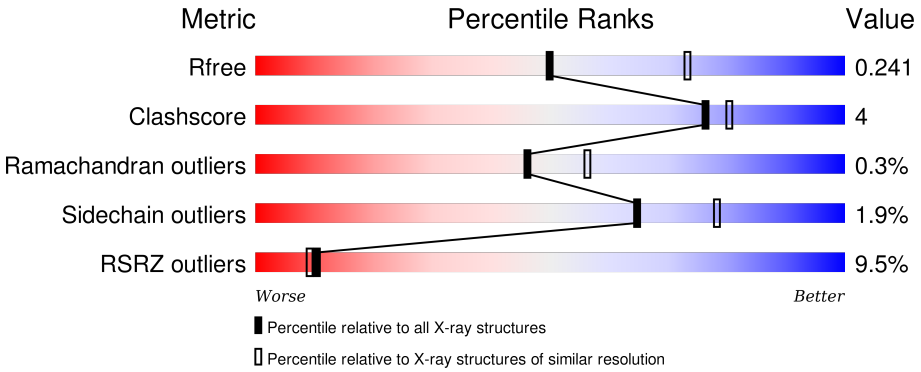
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.44 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	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

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	332	8% 79% 6% • 14%
1	B	332	8% 80% 8% • 11%
1	C	332	7% 83% 6% • 10%
1	D	332	9% 77% 7% 15%
1	E	332	5% 81% 8% • 10%

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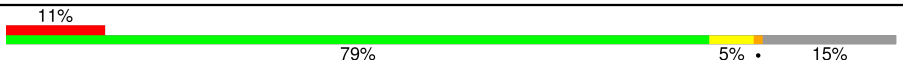
Mol	Chain	Length	Quality of chain
1	F	332	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13240 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 Putative citrate lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	Se	0	4	0
			2119	1334	384	386	5	10			
1	B	294	Total	C	N	O	S	Se	0	3	0
			2181	1376	389	401	5	10			
1	C	298	Total	C	N	O	S	Se	0	3	0
			2209	1387	396	412	5	9			
1	D	281	Total	C	N	O	S	Se	0	1	0
			2071	1302	372	382	5	10			
1	E	299	Total	C	N	O	S	Se	0	4	0
			2259	1427	403	414	5	10			
1	F	283	Total	C	N	O	S	Se	0	0	0
			2097	1321	378	384	5	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP Q46TN2
B	0	GLY	-	EXPRESSION TAG	UNP Q46TN2
C	0	GLY	-	EXPRESSION TAG	UNP Q46TN2
D	0	GLY	-	EXPRESSION TAG	UNP Q46TN2
E	0	GLY	-	EXPRESSION TAG	UNP Q46TN2
F	0	GLY	-	EXPRESSION TAG	UNP Q46TN2

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Cl	0	0
			1	1		
2	E	2	Total	Cl	0	0
			2	2		
2	B	2	Total	Cl	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	2	Total Cl 2 2	0	0
2	A	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0

- Molecule 3 is water.

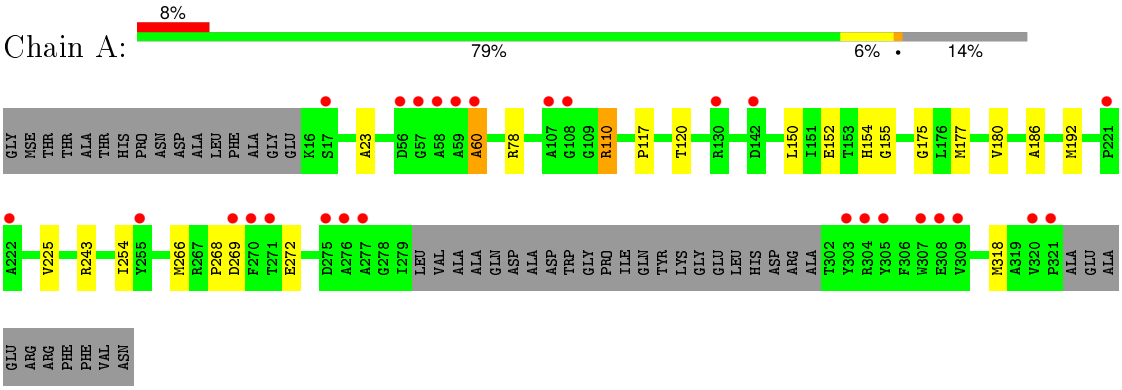
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	41	Total O 41 41	0	0
3	B	34	Total O 34 34	0	0
3	C	60	Total O 60 60	0	0
3	D	41	Total O 41 41	0	1
3	E	81	Total O 82 82	0	2
3	F	37	Total O 37 37	0	0

3 Residue-property plots

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.

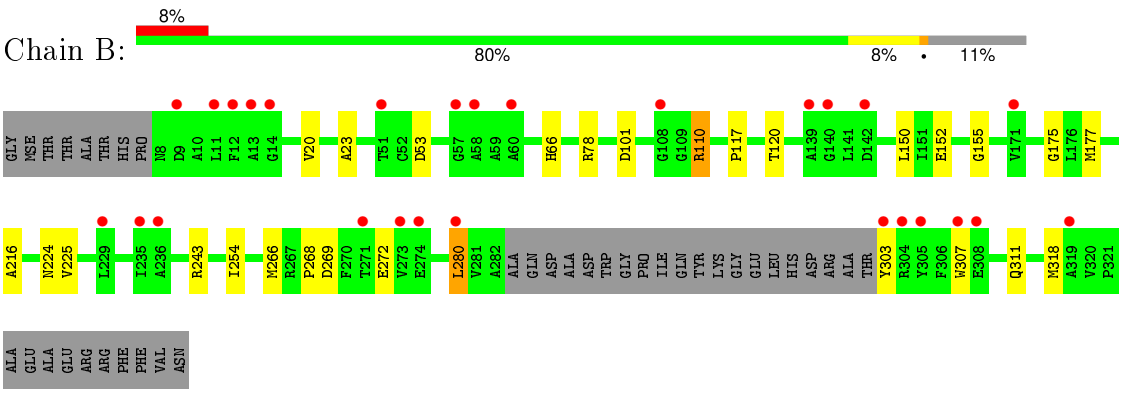
- Molecule 1: Putative citrate lyase

Chain A:



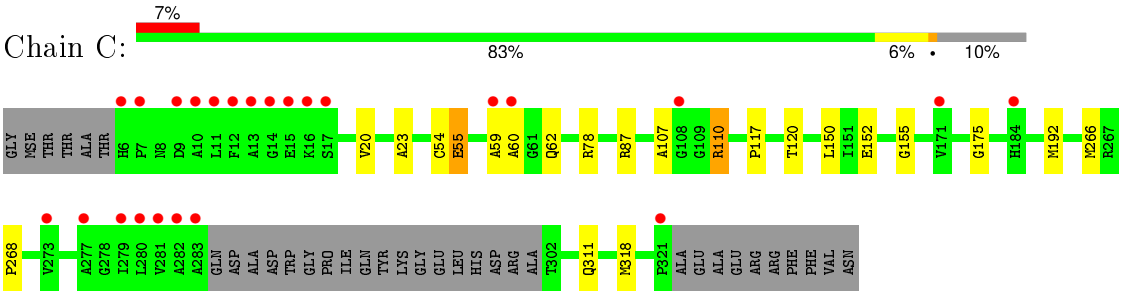
- Molecule 1: Putative citrate lyase

Chain B:



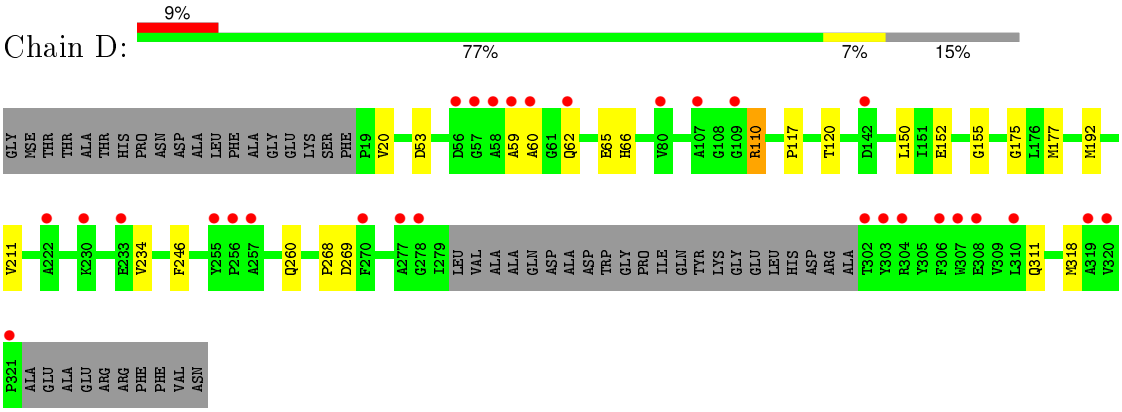
- Molecule 1: Putative citrate lyase

Chain C:



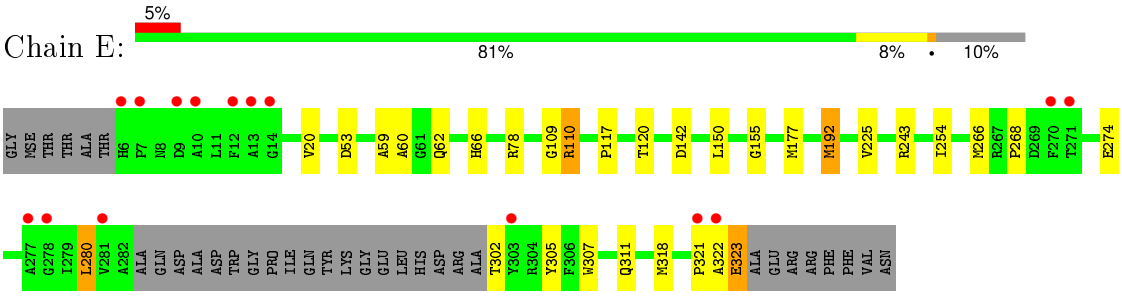
- Molecule 1: Putative citrate lyase

Chain D:



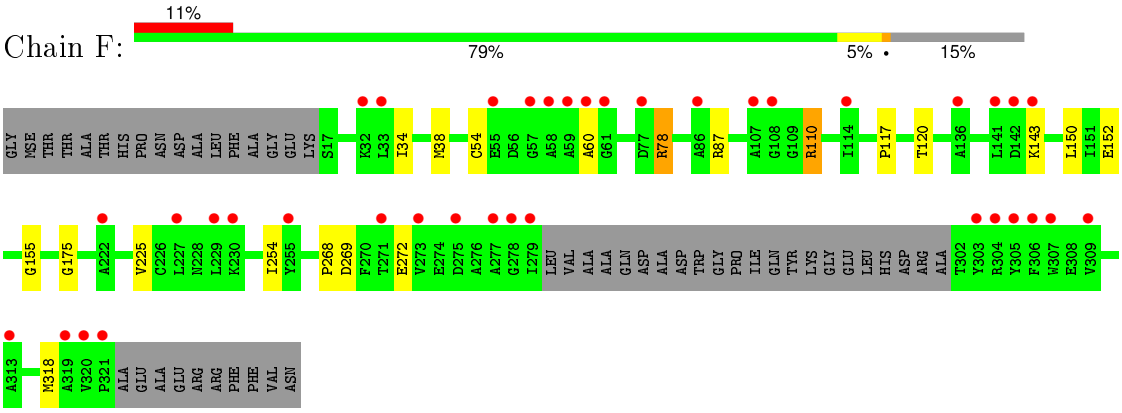
- Molecule 1: Putative citrate lyase

Chain E:



- Molecule 1: Putative citrate lyase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	226.40Å 73.83Å 149.25Å 90.00° 125.31° 90.00°	Depositor
Resolution (Å)	29.79 – 2.44 29.79 – 2.44	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.79-2.44) 99.5 (29.79-2.44)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.202 , 0.231 0.212 , 0.241	Depositor DCC
R_{free} test set	3766 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 51.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 74753 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13240	wwPDB-VP
Average B, all atoms (Å^2)	57.0	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 33.21 % 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 8.2994e-04.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: 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	0.49	0/2167	0.62	0/2933
1	B	0.47	0/2228	0.62	0/3018
1	C	0.52	0/2255	0.64	0/3056
1	D	0.50	0/2109	0.63	0/2858
1	E	0.55	0/2311	0.66	0/3126
1	F	0.48	0/2133	0.62	0/2888
All	All	0.50	0/13203	0.63	0/17879

There are no bond length outliers.

There are no bond angle outliers.

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	2119	0	2040	23	0
1	B	2181	0	2080	17	0
1	C	2209	0	2101	15	0
1	D	2071	0	1972	15	0
1	E	2259	0	2189	17	0
1	F	2097	0	2014	12	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
3	A	41	0	0	1	0
3	B	34	0	0	0	0
3	C	60	0	0	1	0
3	D	41	0	0	0	0
3	E	82	0	0	2	0
3	F	37	0	0	0	0
All	All	13240	0	12396	95	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 (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ALA:HB1	1:D:234:VAL:HG22	1.45	0.99
1:E:110:ARG:HH11	1:E:110:ARG:HG2	1.38	0.88
1:C:110:ARG:HH11	1:C:110:ARG:HG2	1.38	0.86
1:D:110:ARG:HH11	1:D:110:ARG:HG2	1.41	0.85
1:B:110:ARG:HH11	1:B:110:ARG:HG2	1.43	0.83
1:F:110:ARG:HG2	1:F:110:ARG:HH11	1.43	0.83
1:A:110:ARG:HH11	1:A:110:ARG:HG2	1.42	0.82
1:B:243[B]:ARG:HD3	1:B:266:MSE:SE	2.40	0.72
1:F:268:PRO:HD2	1:F:318:MSE:SE	2.42	0.69
1:A:177:MSE:HG3	1:A:192[B]:MSE:SE	2.43	0.68
1:A:60:ALA:CB	1:D:234:VAL:HG22	2.23	0.68
1:A:177:MSE:HE3	1:A:192[B]:MSE:SE	2.44	0.67
1:F:38:MSE:HE3	1:F:78:ARG:HG2	1.75	0.67
1:B:177[B]:MSE:H	1:B:177[B]:MSE:SE	2.29	0.66
1:E:268:PRO:HD2	1:E:318:MSE:SE	2.45	0.66
1:A:268:PRO:HD2	1:A:318:MSE:SE	2.50	0.62
1:B:268:PRO:HD2	1:B:318:MSE:SE	2.50	0.62
1:B:177[B]:MSE:HE1	1:B:224:ASN:HB2	1.82	0.61
1:E:243[A]:ARG:HD3	1:E:266:MSE:SE	2.52	0.60
1:A:177:MSE:CE	1:A:192[B]:MSE:SE	2.99	0.59
1:E:20:VAL:HG11	1:E:311:GLN:HB3	1.85	0.59
1:D:177:MSE:HB2	1:D:192[B]:MSE:HE1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:CG1	1:A:192[A]:MSE:HE2	2.33	0.58
1:B:117:PRO:HA	1:B:150:LEU:HB2	1.85	0.58
1:D:268:PRO:HD2	1:D:318:MSE:SE	2.54	0.58
1:C:268:PRO:HD2	1:C:318:MSE:SE	2.54	0.57
1:D:117:PRO:HA	1:D:150:LEU:HB2	1.87	0.56
1:A:120:THR:O	1:A:155:GLY:HA3	2.06	0.56
1:C:55:GLU:HB2	1:C:87:ARG:HG2	1.90	0.53
1:D:177:MSE:HA	1:D:192[B]:MSE:SE	2.59	0.53
1:D:120:THR:O	1:D:155:GLY:HA3	2.09	0.53
1:F:120:THR:O	1:F:155:GLY:HA3	2.10	0.52
1:A:192[B]:MSE:HE1	3:A:652:HOH:O	2.09	0.52
1:C:120:THR:O	1:C:155:GLY:HA3	2.10	0.52
1:A:177:MSE:HA	1:A:192[B]:MSE:SE	2.59	0.51
1:E:110:ARG:CG	1:E:110:ARG:HH11	2.17	0.51
1:A:269:ASP:HB3	1:A:272:GLU:HB2	1.93	0.51
1:A:117:PRO:HA	1:A:150:LEU:HB2	1.91	0.51
1:C:110:ARG:CG	1:C:110:ARG:HH11	2.16	0.51
1:A:186:ALA:HA	1:B:243[B]:ARG:HH12	1.76	0.51
1:B:120:THR:O	1:B:155:GLY:HA3	2.11	0.51
1:E:109:GLY:HA2	3:E:686:HOH:O	2.11	0.50
1:E:120:THR:O	1:E:155:GLY:HA3	2.11	0.50
1:D:110:ARG:HH11	1:D:110:ARG:CG	2.19	0.49
1:F:117:PRO:HA	1:F:150:LEU:HB2	1.94	0.49
1:C:20:VAL:HG11	1:C:311:GLN:HB3	1.95	0.48
1:E:110:ARG:NH1	1:E:110:ARG:HG2	2.17	0.48
1:C:54:CYS:HB2	1:C:87:ARG:O	2.13	0.48
1:A:180:VAL:HG11	1:A:192[A]:MSE:HE2	1.96	0.48
1:A:180:VAL:HG12	1:A:192[A]:MSE:HE2	1.96	0.47
1:B:20:VAL:HG11	1:B:311:GLN:HB3	1.96	0.47
1:E:142:ASP:HA	3:E:688:HOH:O	2.14	0.46
1:C:107:ALA:HB3	3:C:556:HOH:O	2.14	0.46
1:A:243:ARG:HD3	1:A:266:MSE:SE	2.65	0.46
1:C:59:ALA:HB3	1:C:62:GLN:HB2	1.98	0.46
1:E:117:PRO:HA	1:E:150:LEU:HB2	1.97	0.45
1:F:54:CYS:HB2	1:F:87:ARG:O	2.16	0.45
1:B:53:ASP:O	1:B:66:HIS:HE1	2.00	0.45
1:E:59:ALA:HB3	1:E:62:GLN:HB2	1.98	0.44
1:D:20:VAL:HG11	1:D:311:GLN:HB3	1.99	0.44
1:E:53:ASP:O	1:E:66:HIS:HE1	2.00	0.44
1:B:269:ASP:HB3	1:B:272:GLU:HB2	1.98	0.44
1:D:211:VAL:HG11	1:D:246:PHE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ARG:HH11	1:B:110:ARG:CG	2.20	0.44
1:D:53:ASP:O	1:D:66:HIS:HE1	2.01	0.44
1:D:59:ALA:HB3	1:D:62:GLN:HB2	2.00	0.43
1:F:34:ILE:HG22	1:F:38:MSE:HE2	2.00	0.43
1:E:302:THR:O	1:E:305:TYR:HB3	2.19	0.43
1:E:280:LEU:HD21	1:E:307:TRP:HA	2.01	0.43
1:F:269:ASP:HB3	1:F:272:GLU:HB2	2.01	0.43
1:C:117:PRO:HA	1:C:150:LEU:HB2	2.00	0.42
1:C:192:MSE:HB3	1:C:192:MSE:HE2	1.96	0.42
1:A:225:VAL:HG11	1:A:254:ILE:HG23	2.02	0.42
1:C:152:GLU:HB3	1:C:175:GLY:HA3	2.02	0.42
1:E:177:MSE:HG3	1:E:192[A]:MSE:HE1	2.02	0.42
1:B:23:ALA:HB1	1:B:266:MSE:HG3	2.02	0.41
1:B:152:GLU:HB3	1:B:175:GLY:HA3	2.02	0.41
1:B:280:LEU:HD21	1:B:307:TRP:HA	2.02	0.41
1:F:225:VAL:HG11	1:F:254:ILE:HG23	2.03	0.41
1:A:110:ARG:CG	1:A:110:ARG:HH11	2.20	0.41
1:C:55:GLU:HG3	1:C:117:PRO:HG3	2.02	0.41
1:E:225:VAL:HG11	1:E:254:ILE:HG23	2.02	0.41
1:B:225:VAL:HG11	1:B:254:ILE:HG23	2.02	0.41
1:C:23:ALA:HB1	1:C:266:MSE:HG2	2.02	0.41
1:F:110:ARG:HH11	1:F:110:ARG:CG	2.20	0.41
1:A:152:GLU:HB3	1:A:175:GLY:HA3	2.02	0.41
1:D:152:GLU:HB3	1:D:175:GLY:HA3	2.02	0.41
1:F:110:ARG:NH1	1:F:110:ARG:HG2	2.22	0.41
1:A:154:HIS:CG	1:B:216:ALA:HA	2.56	0.41
1:A:23:ALA:HB1	1:A:266:MSE:HG3	2.03	0.41
1:C:110:ARG:NH1	1:C:110:ARG:HG2	2.18	0.40
1:F:152:GLU:HB3	1:F:175:GLY:HA3	2.03	0.40
1:E:321:PRO:O	1:E:323:GLU:N	2.55	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	284/332 (86%)	275 (97%)	8 (3%)	1 (0%)	39	49
1	B	293/332 (88%)	278 (95%)	15 (5%)	0	100	100
1	C	297/332 (90%)	285 (96%)	11 (4%)	1 (0%)	46	56
1	D	278/332 (84%)	268 (96%)	9 (3%)	1 (0%)	39	49
1	E	299/332 (90%)	285 (95%)	12 (4%)	2 (1%)	26	32
1	F	279/332 (84%)	268 (96%)	10 (4%)	1 (0%)	39	49
All	All	1730/1992 (87%)	1659 (96%)	65 (4%)	6 (0%)	46	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	322	ALA
1	E	60	ALA
1	A	60	ALA
1	C	60	ALA
1	D	60	ALA
1	F	60	ALA

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	206/244 (84%)	204 (99%)	2 (1%)	82	88
1	B	209/244 (86%)	204 (98%)	5 (2%)	57	72
1	C	212/244 (87%)	209 (99%)	3 (1%)	74	84
1	D	199/244 (82%)	195 (98%)	4 (2%)	63	77
1	E	222/244 (91%)	215 (97%)	7 (3%)	46	62
1	F	203/244 (83%)	200 (98%)	3 (2%)	72	83
All	All	1251/1464 (86%)	1227 (98%)	24 (2%)	65	78

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	A	110	ARG
1	B	78	ARG
1	B	101	ASP
1	B	110	ARG
1	B	280	LEU
1	B	303	TYR
1	C	55	GLU
1	C	78	ARG
1	C	110	ARG
1	D	65	GLU
1	D	110	ARG
1	D	260	GLN
1	D	269	ASP
1	E	78	ARG
1	E	110	ARG
1	E	192[A]	MSE
1	E	192[B]	MSE
1	E	274	GLU
1	E	280	LEU
1	E	323	GLU
1	F	78	ARG
1	F	110	ARG
1	F	143	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	B	264	ASN
1	D	264	ASN
1	E	244	ASN
1	E	260	GLN
1	E	264	ASN

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 9 ligands modelled in this entry, 9 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	275/332 (82%)	0.36	27 (9%) 10 8	36, 59, 97, 115	0
1	B	285/332 (85%)	0.27	27 (9%) 10 9	32, 59, 100, 115	0
1	C	289/332 (87%)	0.11	24 (8%) 14 13	30, 48, 97, 117	0
1	D	272/332 (81%)	0.34	29 (10%) 8 6	33, 56, 107, 130	0
1	E	290/332 (87%)	-0.01	15 (5%) 31 30	26, 41, 81, 96	0
1	F	274/332 (82%)	0.47	38 (13%) 4 3	32, 59, 109, 124	0
All	All	1685/1992 (84%)	0.25	160 (9%) 10 9	26, 54, 100, 130	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	56	ASP	8.7
1	B	12	PHE	8.4
1	D	303	TYR	8.2
1	D	59	ALA	7.8
1	D	58	ALA	7.6
1	F	271	THR	7.3
1	C	281	VAL	6.2
1	D	321	PRO	5.9
1	F	321	PRO	5.8
1	D	60	ALA	5.7
1	A	304	ARG	5.7
1	A	303	TYR	5.4
1	C	7	PRO	5.3
1	F	305	TYR	5.3
1	C	273	VAL	5.2
1	D	320	VAL	5.1
1	E	14	GLY	5.1
1	F	60	ALA	5.0
1	F	309	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	308	GLU	4.8
1	D	307	TRP	4.8
1	A	270	PHE	4.7
1	F	142	ASP	4.7
1	E	13	ALA	4.6
1	F	136	ALA	4.6
1	D	270	PHE	4.5
1	B	9	ASP	4.3
1	F	306	PHE	4.3
1	D	304	ARG	4.3
1	F	320	VAL	4.3
1	C	6	HIS	4.2
1	A	277	ALA	4.2
1	B	11	LEU	4.1
1	A	60	ALA	4.1
1	B	60	ALA	4.1
1	F	143	LYS	4.1
1	C	14	GLY	4.1
1	F	303	TYR	4.0
1	B	319	ALA	4.0
1	D	302	THR	4.0
1	B	304	ARG	4.0
1	C	10	ALA	4.0
1	C	282	ALA	4.0
1	A	58	ALA	3.9
1	A	107	ALA	3.8
1	F	279	ILE	3.8
1	E	270	PHE	3.8
1	F	58	ALA	3.7
1	F	307	TRP	3.7
1	E	7	PRO	3.7
1	B	140	GLY	3.7
1	D	142	ASP	3.6
1	B	14	GLY	3.6
1	B	271	THR	3.6
1	F	278	GLY	3.6
1	F	230	LYS	3.6
1	F	141	LEU	3.4
1	C	283	ALA	3.3
1	C	277	ALA	3.3
1	F	319	ALA	3.3
1	A	305	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	280	LEU	3.3
1	B	108	GLY	3.3
1	A	17	SER	3.3
1	D	277	ALA	3.3
1	B	142	ASP	3.2
1	B	280	LEU	3.2
1	E	6	HIS	3.2
1	C	17	SER	3.1
1	C	16	LYS	3.1
1	D	230	LYS	3.0
1	F	273	VAL	3.0
1	E	277	ALA	3.0
1	C	11	LEU	3.0
1	E	303	TYR	3.0
1	A	108	GLY	2.9
1	D	310	LEU	2.9
1	F	313	ALA	2.9
1	E	281	VAL	2.9
1	E	321	PRO	2.8
1	A	276	ALA	2.8
1	B	229	LEU	2.8
1	D	308	GLU	2.8
1	A	56	ASP	2.8
1	A	269	ASP	2.8
1	B	235	ILE	2.8
1	F	86	ALA	2.8
1	B	273	VAL	2.7
1	C	12	PHE	2.7
1	F	107	ALA	2.7
1	C	108	GLY	2.7
1	E	278	GLY	2.7
1	D	233	GLU	2.7
1	F	255	TYR	2.7
1	F	275	ASP	2.7
1	D	319	ALA	2.7
1	F	114	ILE	2.7
1	A	307	TRP	2.7
1	D	278	GLY	2.7
1	F	77	ASP	2.6
1	D	109	GLY	2.6
1	A	320	VAL	2.6
1	F	32	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	59	ALA	2.6
1	E	10	ALA	2.6
1	C	321	PRO	2.6
1	B	307	TRP	2.6
1	A	130	ARG	2.6
1	B	57	GLY	2.6
1	D	62	GLN	2.6
1	A	57	GLY	2.5
1	B	58	ALA	2.5
1	F	55	GLU	2.5
1	B	274	GLU	2.5
1	C	60	ALA	2.5
1	F	227	LEU	2.5
1	A	321	PRO	2.5
1	F	108	GLY	2.5
1	D	107	ALA	2.5
1	C	171	VAL	2.5
1	B	139	ALA	2.5
1	D	80	VAL	2.4
1	D	256	PRO	2.4
1	C	184	HIS	2.4
1	D	222	ALA	2.4
1	F	229	LEU	2.4
1	C	9	ASP	2.4
1	A	221	PRO	2.4
1	F	304	ARG	2.4
1	B	308	GLU	2.4
1	B	13	ALA	2.4
1	D	57	GLY	2.3
1	E	271	THR	2.3
1	C	13	ALA	2.3
1	E	322	ALA	2.3
1	F	33	LEU	2.3
1	A	142	ASP	2.3
1	B	303	TYR	2.3
1	A	59	ALA	2.3
1	F	222	ALA	2.3
1	F	277	ALA	2.2
1	A	255	TYR	2.2
1	F	59	ALA	2.2
1	F	57	GLY	2.2
1	B	236	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	275	ASP	2.2
1	A	309	VAL	2.2
1	E	12	PHE	2.2
1	B	171	VAL	2.2
1	F	61	GLY	2.1
1	C	15	GLU	2.1
1	B	305	TYR	2.1
1	A	271	THR	2.1
1	B	51	THR	2.1
1	A	222	ALA	2.0
1	D	255	TYR	2.0
1	D	306	PHE	2.0
1	D	257	ALA	2.0
1	C	279	ILE	2.0
1	E	9	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	C	401	1/1	0.95	0.06	-2.13	47,47,47,47	0
2	CL	D	402	1/1	0.95	0.08	-	62,62,62,62	0
2	CL	A	405	1/1	0.98	0.06	-	60,60,60,60	0
2	CL	F	408	1/1	0.97	0.13	-	58,58,58,58	0
2	CL	B	400	1/1	0.88	0.16	-	88,88,88,88	0
2	CL	C	406	1/1	0.98	0.10	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CL	B	404	1/1	0.49	0.40	-	98,98,98,98	0
2	CL	E	407	1/1	0.98	0.13	-	46,46,46,46	0
2	CL	E	403	1/1	0.88	0.15	-	81,81,81,81	0

6.5 Other polymers (i)

There are no such residues in this entry.