Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 10:04 am BST

PDB ID	:	4GGP
Title	:	Crystal Structure of Selenomethionine containing Trans-2-Enoyl-CoA Reductase from Treponema denticola
Authors	:	Bond-Watts, B.B.; Weeks, A.M.; Chang, M.C.Y.
Deposited on	:	2012-08-06
Resolution	:	2.05 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
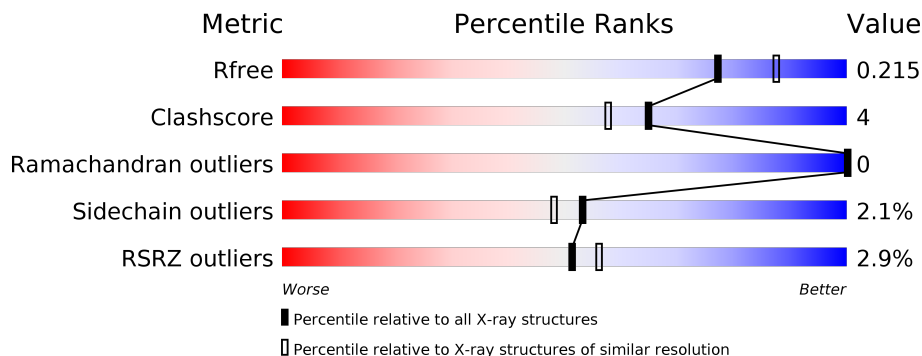with specific help available everywhere you see the (i) symbol.

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
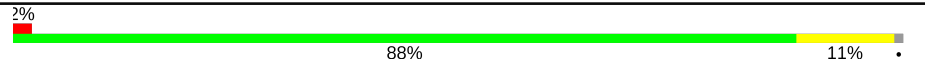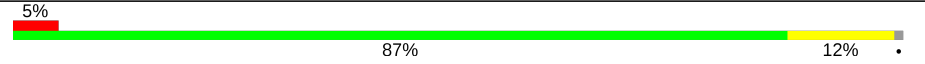*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	Percentile Ranks	Value
Rfree		0.215
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		2.1%
RSRZ outliers		2.9%

Worse   Better

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 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	401	2% 88% 11% •
1	B	401	5% 87% 12% •
1	C	401	% 89% 9% •
1	D	401	3% 89% 9% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12861 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 Trans-2-enoyl-CoA reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	Se	0	0	0
			3079	1946	525	597	5	6			
1	B	397	Total	C	N	O	S	Se	0	0	0
			3079	1946	525	597	5	6			
1	C	397	Total	C	N	O	S	Se	0	0	0
			3079	1946	525	597	5	6			
1	D	397	Total	C	N	O	S	Se	0	0	0
			3079	1946	525	597	5	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q73Q47
A	-2	THR	-	EXPRESSION TAG	UNP Q73Q47
A	-1	GLY	-	EXPRESSION TAG	UNP Q73Q47
A	0	ALA	-	EXPRESSION TAG	UNP Q73Q47
B	-3	GLY	-	EXPRESSION TAG	UNP Q73Q47
B	-2	THR	-	EXPRESSION TAG	UNP Q73Q47
B	-1	GLY	-	EXPRESSION TAG	UNP Q73Q47
B	0	ALA	-	EXPRESSION TAG	UNP Q73Q47
C	-3	GLY	-	EXPRESSION TAG	UNP Q73Q47
C	-2	THR	-	EXPRESSION TAG	UNP Q73Q47
C	-1	GLY	-	EXPRESSION TAG	UNP Q73Q47
C	0	ALA	-	EXPRESSION TAG	UNP Q73Q47
D	-3	GLY	-	EXPRESSION TAG	UNP Q73Q47
D	-2	THR	-	EXPRESSION TAG	UNP Q73Q47
D	-1	GLY	-	EXPRESSION TAG	UNP Q73Q47
D	0	ALA	-	EXPRESSION TAG	UNP Q73Q47

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	132	Total 132	O 132	0	0
2	B	110	Total 110	O 110	0	0
2	C	161	Total 161	O 161	0	0
2	D	142	Total 142	O 142	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 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.
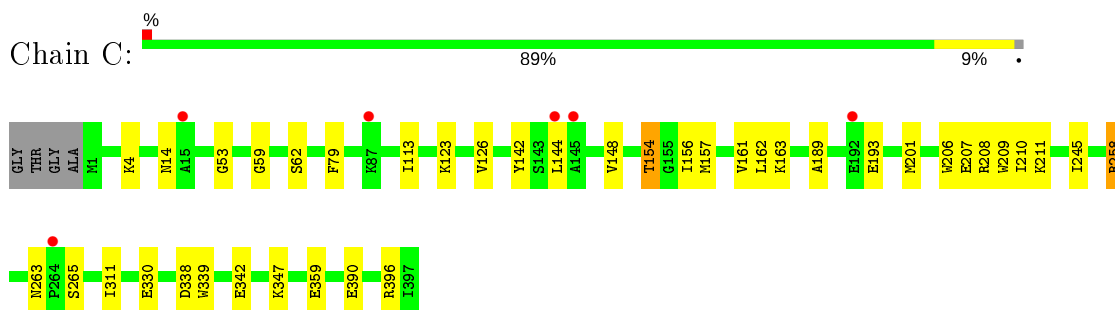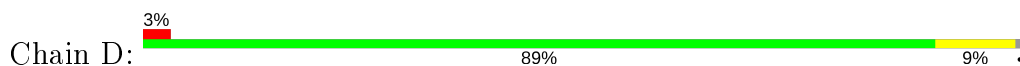
- Molecule 1: Trans-2-enoyl-CoA reductase
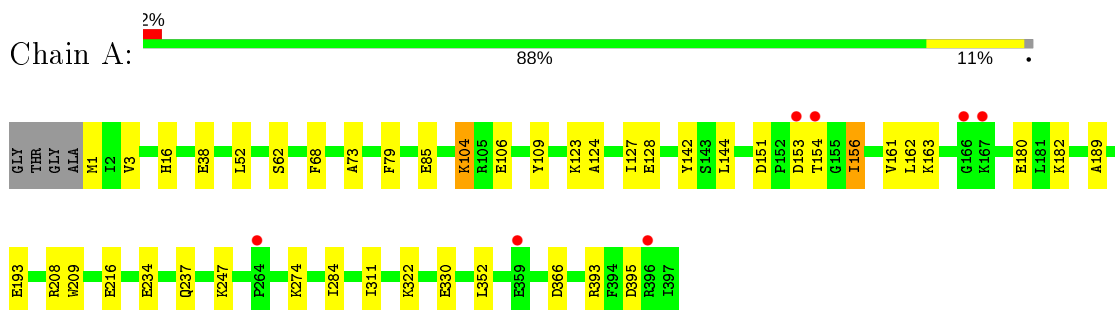
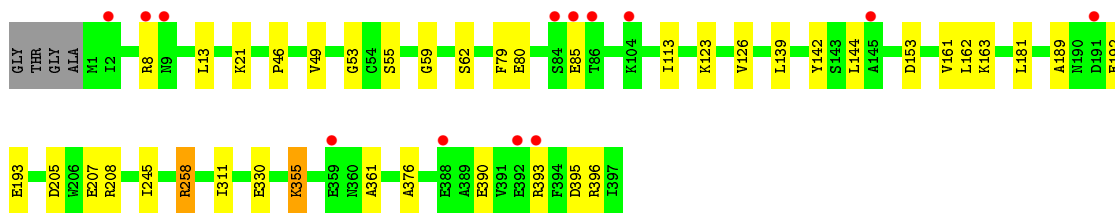- Molecule 1: Trans-2-enoyl-CoA reductase
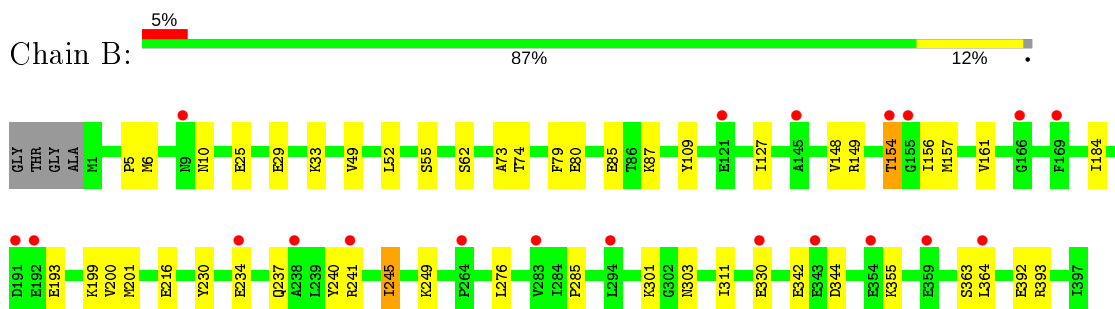
- Molecule 1: Trans-2-enoyl-CoA reductase

- Molecule 1: Trans-2-enoyl-CoA reductase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	62.58Å　87.68Å　91.99Å 106.25°　109.85°　98.33°	Depositor
Resolution (Å)	19.47　–　2.05 19.85　–　2.05	Depositor EDS
% Data completeness (in resolution range)	97.1 (19.47-2.05) 97.1 (19.85-2.05)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.83 (at 2.06Å)	Xtriage
Refinement program	PHENIX AutoRefine	Depositor
R, R_{free}	0.182　,　0.214 0.183　,　0.215	Depositor DCC
R_{free} test set	5183 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 53.7	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	12861	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

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	0.26	0/3129	0.43	0/4214
1	B	0.26	0/3129	0.43	0/4214
1	C	0.27	0/3129	0.44	0/4214
1	D	0.25	0/3129	0.42	0/4214
All	All	0.26	0/12516	0.43	0/16856

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	3079	0	3080	26	0
1	B	3079	0	3080	29	0
1	C	3079	0	3080	23	0
1	D	3079	0	3080	24	0
2	A	132	0	0	2	0
2	B	110	0	0	5	0
2	C	161	0	0	2	0
2	D	142	0	0	5	0
All	All	12861	0	12320	101	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 (101) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:GLU:OE1	2:B:463:HOH:O	1.91	0.86
1:A:38:GLU:O	1:A:322:LYS:NZ	2.15	0.80
1:D:361:ALA:N	2:D:522:HOH:O	2.17	0.74
1:B:230:TYR:O	1:B:249:LYS:NZ	2.21	0.72
1:C:342:GLU:OE2	2:C:482:HOH:O	2.08	0.72
1:B:303:ASN:ND2	2:B:497:HOH:O	2.17	0.71
1:C:123:LYS:HE2	1:C:208:ARG:HG2	1.73	0.70
1:D:207:GLU:OE1	1:D:258:ARG:NH2	2.28	0.66
1:D:85:GLU:HG2	1:D:393:ARG:HH22	1.62	0.64
1:A:1:MSE:N	2:A:468:HOH:O	2.13	0.59
1:B:301:LYS:NZ	1:B:342:GLU:OE1	2.36	0.59
1:B:149:ARG:HB3	1:B:200:VAL:HG22	1.85	0.58
1:D:153:ASP:OD2	1:D:208:ARG:NH2	2.36	0.58
1:A:127:ILE:HD13	1:A:216:GLU:HG3	1.83	0.58
1:C:154:THR:HG22	1:C:156:ILE:H	1.70	0.57
1:B:73:ALA:HB1	1:B:109:TYR:HD2	1.69	0.57
1:D:46:PRO:O	2:D:535:HOH:O	2.17	0.57
1:C:62:SER:HA	1:C:311:ILE:HG21	1.87	0.56
1:D:62:SER:HA	1:D:311:ILE:HG21	1.87	0.56
1:A:142:TYR:CZ	1:A:144:LEU:HD12	2.40	0.55
1:B:29:GLU:OE2	1:B:33:LYS:NZ	2.38	0.55
1:D:123:LYS:HE2	1:D:208:ARG:HG2	1.88	0.55
1:A:153:ASP:OD2	1:A:208:ARG:NH2	2.40	0.55
1:D:162:LEU:HD22	1:D:245:ILE:HD11	1.89	0.55
1:B:127:ILE:HD13	1:B:216:GLU:HG3	1.90	0.54
1:B:201:MSE:SE	1:B:245:ILE:HG22	2.57	0.54
1:C:4:LYS:O	1:C:14:ASN:ND2	2.32	0.54
1:B:161:VAL:HG21	1:B:193:GLU:HB3	1.90	0.53
1:B:355:LYS:HG2	1:B:364:LEU:HD21	1.91	0.52
1:A:62:SER:HA	1:A:311:ILE:HG21	1.91	0.52
1:C:162:LEU:HD21	1:C:201:MSE:HE1	1.91	0.52
1:A:330:GLU:CD	1:A:330:GLU:H	2.13	0.51
1:A:366:ASP:OD1	2:A:464:HOH:O	2.19	0.51
1:B:240:TYR:HA	1:B:245:ILE:HG13	1.91	0.51
1:B:330:GLU:H	1:B:330:GLU:CD	2.14	0.51
1:A:163:LYS:HB2	1:A:189:ALA:HB2	1.93	0.50
1:D:8:ARG:HG2	1:D:13:LEU:HD11	1.93	0.50
1:A:151:ASP:HB3	1:A:154:THR:HG22	1.93	0.50
1:D:161:VAL:HG21	1:D:193:GLU:HB3	1.92	0.50
1:D:163:LYS:HB2	1:D:189:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:LYS:NZ	2:D:525:HOH:O	2.29	0.50
1:B:237:GLN:OE1	1:B:241:ARG:NE	2.44	0.50
1:B:49:VAL:HB	1:B:74:THR:HG22	1.95	0.49
1:A:73:ALA:HB1	1:A:109:TYR:HD2	1.77	0.49
1:B:73:ALA:HB1	1:B:109:TYR:CD2	2.48	0.49
1:A:3:VAL:HG13	1:A:16:HIS:CD2	2.48	0.48
1:A:85:GLU:HG3	1:A:393:ARG:HG2	1.94	0.48
1:C:161:VAL:HG21	1:C:193:GLU:HB3	1.94	0.48
1:C:162:LEU:HD22	1:C:245:ILE:HD11	1.94	0.47
1:B:62:SER:HA	1:B:311:ILE:HG21	1.95	0.47
1:D:376:ALA:O	2:D:476:HOH:O	2.20	0.47
1:C:113:ILE:HD12	1:C:126:VAL:HG22	1.96	0.47
1:D:113:ILE:HD12	1:D:126:VAL:HG22	1.96	0.47
1:D:355:LYS:NZ	2:D:524:HOH:O	2.42	0.46
1:B:154:THR:HG22	1:B:156:ILE:H	1.80	0.46
1:A:124:ALA:O	1:A:128:GLU:HG2	2.16	0.46
1:B:392:GLU:H	1:B:392:GLU:CD	2.18	0.46
1:A:234:GLU:HA	1:A:237:GLN:HG2	1.98	0.45
1:D:142:TYR:CZ	1:D:144:LEU:HD12	2.51	0.45
1:A:161:VAL:HG21	1:A:193:GLU:HB3	1.98	0.45
1:C:142:TYR:CZ	1:C:144:LEU:HD12	2.51	0.45
1:B:10:ASN:O	2:B:470:HOH:O	2.21	0.45
1:B:184:ILE:HG13	1:B:285:PRO:HB3	1.99	0.45
1:C:123:LYS:HE3	1:C:209:TRP:CD1	2.53	0.44
1:A:154:THR:HG23	1:A:156:ILE:H	1.82	0.44
1:D:393:ARG:HE	1:D:396:ARG:HH12	1.65	0.44
1:D:330:GLU:H	1:D:330:GLU:CD	2.20	0.44
1:D:85:GLU:HG2	1:D:393:ARG:NH2	2.31	0.43
1:B:149:ARG:HD3	1:B:199:LYS:O	2.18	0.43
1:B:276:LEU:HB2	2:B:443:HOH:O	2.19	0.43
1:A:104:LYS:N	1:A:104:LYS:HD3	2.33	0.43
1:C:148:VAL:HG21	1:C:157:MSE:HE3	1.99	0.43
1:C:263:ASN:OD1	1:C:265:SER:OG	2.26	0.43
1:A:123:LYS:HE3	1:A:209:TRP:CD1	2.54	0.42
1:C:207:GLU:OE1	1:C:258:ARG:NH2	2.51	0.42
1:C:330:GLU:CD	1:C:330:GLU:H	2.22	0.42
1:D:49:VAL:HG22	1:D:139:LEU:HB3	2.02	0.42
1:A:322:LYS:HD3	1:C:339:TRP:CZ2	2.55	0.42
1:D:393:ARG:NH2	1:D:395:ASP:OD2	2.53	0.42
1:B:148:VAL:HG11	1:B:157:MSE:HE3	2.02	0.42
1:C:211:LYS:HD3	1:C:211:LYS:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLU:HG2	1:A:182:LYS:HG3	2.01	0.41
1:D:55:SER:OG	1:D:80:GLU:OE2	2.31	0.41
1:C:123:LYS:HE3	1:C:209:TRP:CG	2.55	0.41
1:B:55:SER:OG	1:B:80:GLU:OE2	2.29	0.41
1:C:163:LYS:HB2	1:C:189:ALA:HB2	2.01	0.41
1:C:338:ASP:OD1	1:C:338:ASP:N	2.52	0.41
1:A:162:LEU:HD13	1:A:284:ILE:HD11	2.02	0.41
1:B:6:MSE:HE3	1:B:6:MSE:HB3	1.84	0.41
1:C:263:ASN:HB2	2:C:498:HOH:O	2.20	0.41
1:C:53:GLY:O	1:C:59:GLY:HA3	2.21	0.41
1:A:247:LYS:HD3	1:A:247:LYS:HA	1.92	0.41
1:A:274:LYS:HE2	1:A:274:LYS:HB2	1.95	0.41
1:D:53:GLY:O	1:D:59:GLY:HA3	2.21	0.41
1:B:85:GLU:HG3	1:B:393:ARG:HD2	2.02	0.41
1:B:5:PRO:O	2:B:467:HOH:O	2.21	0.41
1:C:206:TRP:O	1:C:210:ILE:HG12	2.21	0.40
1:A:123:LYS:HE2	1:A:208:ARG:HG2	2.04	0.40
1:A:68:PHE:HE1	1:A:106:GLU:HG3	1.87	0.40
1:B:249:LYS:HE2	1:B:249:LYS:HB2	1.95	0.40
1:D:142:TYR:OH	1:D:205:ASP:HB3	2.21	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	395/401 (98%)	385 (98%)	10 (2%)	0	100	100
1	B	395/401 (98%)	384 (97%)	11 (3%)	0	100	100
1	C	395/401 (98%)	384 (97%)	11 (3%)	0	100	100
1	D	395/401 (98%)	389 (98%)	6 (2%)	0	100	100
All	All	1580/1604 (98%)	1542 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	323/318 (102%)	317 (98%)	6 (2%)	57	53
1	B	323/318 (102%)	315 (98%)	8 (2%)	47	40
1	C	323/318 (102%)	316 (98%)	7 (2%)	52	46
1	D	323/318 (102%)	317 (98%)	6 (2%)	57	53
All	All	1292/1272 (102%)	1265 (98%)	27 (2%)	53	48

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	79	PHE
1	A	104	LYS
1	A	156	ILE
1	A	352	LEU
1	A	395	ASP
1	B	52	LEU
1	B	79	PHE
1	B	87	LYS
1	B	154	THR
1	B	234	GLU
1	B	245	ILE
1	B	344	ASP
1	B	363	SER
1	C	79	PHE
1	C	154	THR
1	C	258	ARG
1	C	347	LYS
1	C	359	GLU
1	C	390	GLU
1	C	396	ARG
1	D	79	PHE

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Mol	Chain	Res	Type
1	D	181	LEU
1	D	192	GLU
1	D	258	ARG
1	D	355	LYS
1	D	390	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	9	ASN

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 (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	391/401 (97%)	-0.04	7 (1%)	68	71	20, 38, 60, 72	0
1	B	391/401 (97%)	0.20	20 (5%)	28	30	20, 41, 65, 79	0
1	C	391/401 (97%)	-0.05	6 (1%)	73	76	18, 35, 57, 75	0
1	D	391/401 (97%)	-0.01	13 (3%)	46	50	21, 36, 62, 80	0
All	All	1564/1604 (97%)	0.03	46 (2%)	51	56	18, 37, 62, 80	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	145	ALA	4.4
1	C	145	ALA	4.3
1	B	166	GLY	4.2
1	B	264	PRO	4.0
1	B	354	GLU	4.0
1	D	86	THR	3.7
1	D	9	ASN	3.6
1	B	192	GLU	3.5
1	B	238	ALA	3.3
1	A	359	GLU	3.3
1	C	144	LEU	3.2
1	B	169	PHE	3.2
1	A	166	GLY	3.1
1	B	9	ASN	3.0
1	B	364	LEU	3.0
1	B	359	GLU	2.9
1	A	396	ARG	2.8
1	D	388	GLU	2.8
1	C	264	PRO	2.8
1	A	264	PRO	2.7
1	D	85	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	155	GLY	2.6
1	D	2	ILE	2.6
1	D	393	ARG	2.6
1	D	392	GLU	2.6
1	B	154	THR	2.5
1	D	359	GLU	2.5
1	B	343	GLU	2.4
1	C	192	GLU	2.4
1	A	154	THR	2.4
1	B	241	ARG	2.3
1	A	167	LYS	2.3
1	B	283	VAL	2.3
1	B	330	GLU	2.2
1	D	145	ALA	2.2
1	B	121	GLU	2.2
1	B	191	ASP	2.2
1	B	294	LEU	2.2
1	D	8	ARG	2.2
1	D	84	SER	2.2
1	D	191	ASP	2.1
1	C	87	LYS	2.1
1	C	15	ALA	2.1
1	D	104	LYS	2.0
1	A	153	ASP	2.0
1	B	234	GLU	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.