Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 06:09 am BST

PDB ID	:	1YB4
Title	:	Crystal Structure of the Tartronic Semialdehyde Reductase from Salmonella typhimurium LT2
Authors	:	Kim, Y.; Wu, R.; Collart, F.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2004-12-20
Resolution	:	2.40 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 (i)

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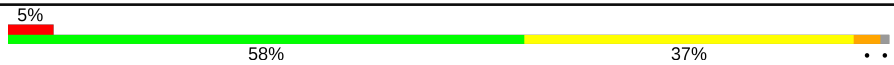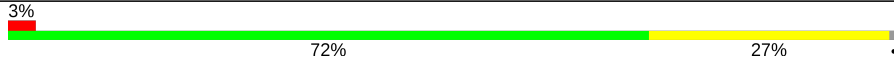*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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.
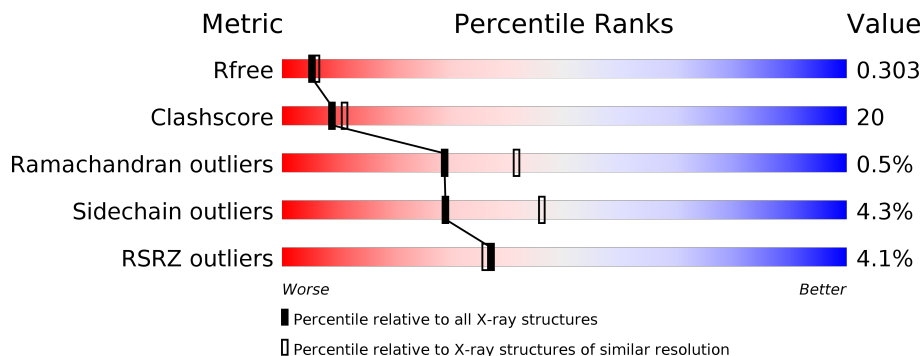
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	295	
1	B	295	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 4533 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 tartronic semialdehyde reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	291	Total 2161	C 1357	N 379	O 410	S 4	Se 11	0	0	0
1	B	291	Total 2161	C 1357	N 379	O 410	S 4	Se 11	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	CLONING ARTIFACT	UNP Q8ZR83
A	-1	ASN	-	CLONING ARTIFACT	UNP Q8ZR83
A	0	ALA	-	CLONING ARTIFACT	UNP Q8ZR83
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
A	11	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
A	15	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
A	62	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
A	92	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
A	110	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
A	134	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
A	205	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
A	221	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
A	279	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
A	286	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
B	-2	SER	-	CLONING ARTIFACT	UNP Q8ZR83
B	-1	ASN	-	CLONING ARTIFACT	UNP Q8ZR83
B	0	ALA	-	CLONING ARTIFACT	UNP Q8ZR83
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
B	11	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
B	15	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
B	62	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
B	92	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
B	110	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
B	134	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
B	205	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	221	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
B	279	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83
B	286	MSE	MET	MODIFIED RESIDUE	UNP Q8ZR83

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	105	Total O 105 105	0	0
2	B	106	Total O 106 106	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: tartronic semialdehyde reductase
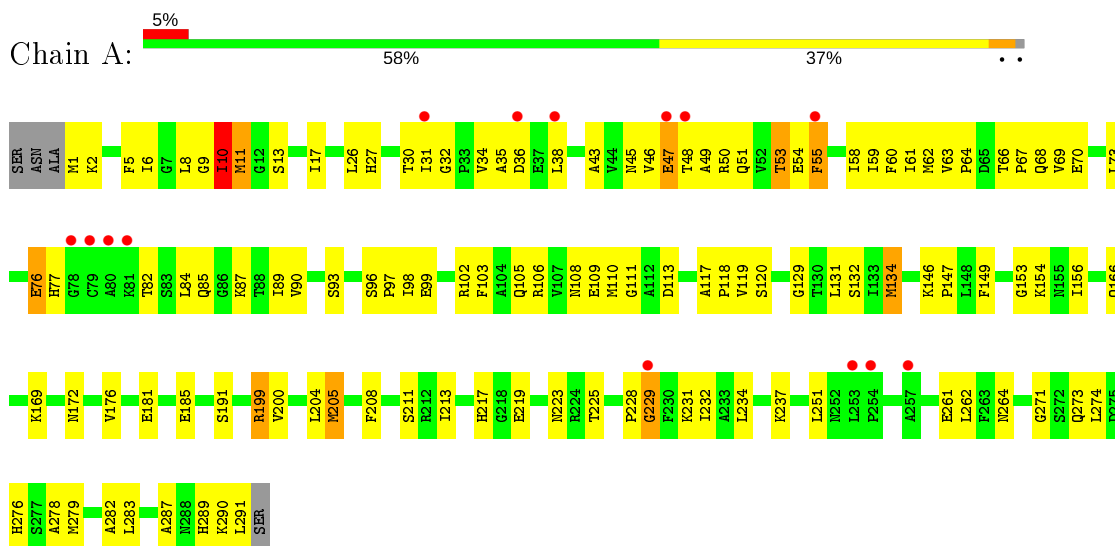
- Molecule 1: tartronic semialdehyde reductase
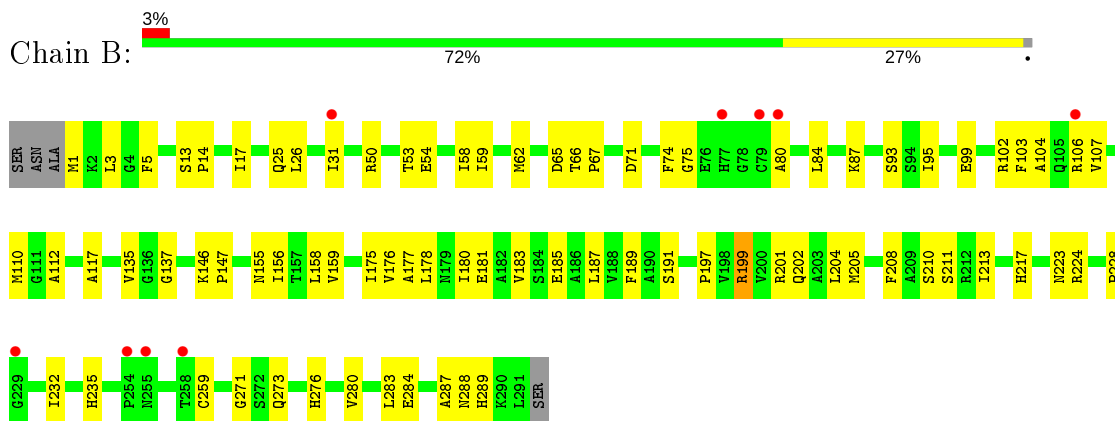
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	98.33Å 134.25Å 48.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.35 – 2.40 34.43 – 2.38	Depositor EDS
% Data completeness (in resolution range)	89.7 (33.35-2.40) 88.6 (34.43-2.38)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.78 (at 2.36Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.304 0.229 , 0.303	Depositor DCC
R_{free} test set	2305 reflections (8.93%)	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.3	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4533	wwPDB-VP
Average B, all atoms (Å^2)	40.0	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 78.46 % 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 6.8835e-07. 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, 0.333 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	0.40	0/2180	0.67	1/2929 (0.0%)
1	B	0.40	0/2180	0.67	0/2929
All	All	0.40	0/4360	0.67	1/5858 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	229	GLY	N-CA-C	-6.29	97.39	113.10

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	2161	0	2203	119	0
1	B	2161	0	2203	71	0
2	A	105	0	0	7	0
2	B	106	0	0	8	0
All	All	4533	0	4406	178	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 20.

All (178) 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:48:THR:HG22	1:A:49:ALA:H	1.23	1.02
1:A:205:MSE:HE2	2:A:314:HOH:O	1.71	0.90
1:A:205:MSE:HA	1:A:205:MSE:HE3	1.56	0.87
1:A:48:THR:HG22	1:A:49:ALA:N	1.95	0.81
1:A:262:LEU:HB3	1:A:279:MSE:HE1	1.64	0.80
1:A:48:THR:CG2	1:A:49:ALA:H	1.98	0.76
1:A:66:THR:HG21	1:A:99:GLU:HG3	1.67	0.76
1:A:50:ARG:HG3	1:A:82:THR:OG1	1.85	0.76
1:A:66:THR:HB	1:A:67:PRO:HD3	1.68	0.76
1:A:172:ASN:HD22	1:B:204:LEU:HD22	1.52	0.75
1:B:185:GLU:HG2	1:B:283:LEU:CD2	2.17	0.75
1:A:76:GLU:HG2	1:A:77:HIS:H	1.55	0.70
1:A:63:VAL:CG1	1:A:69:VAL:HG23	2.22	0.70
1:A:279:MSE:HE3	1:A:282:ALA:HB3	1.74	0.69
1:A:63:VAL:HG22	1:A:64:PRO:HD2	1.75	0.69
1:B:205:MSE:HE3	1:B:205:MSE:HA	1.74	0.69
1:B:185:GLU:HG2	1:B:283:LEU:HD21	1.72	0.69
1:A:46:VAL:HG11	1:A:55:PHE:CZ	2.27	0.69
1:A:98:ILE:HD13	2:A:303:HOH:O	1.93	0.67
1:A:98:ILE:HD12	1:A:98:ILE:H	1.59	0.67
1:B:183:VAL:HG12	1:B:187:LEU:HD12	1.75	0.67
1:A:271:GLY:HA2	1:A:274:LEU:HD12	1.76	0.67
1:A:119:VAL:HG21	1:A:131:LEU:HD13	1.78	0.66
1:A:279:MSE:CE	1:A:282:ALA:HB3	2.26	0.66
1:A:154:LYS:O	1:A:156:ILE:HD12	1.96	0.65
1:A:217:HIS:HE1	1:B:208:PHE:HD1	1.44	0.65
1:B:66:THR:HG21	1:B:99:GLU:HG3	1.78	0.65
1:A:279:MSE:HE2	1:A:283:LEU:CD1	2.26	0.65
1:A:31:ILE:HD12	1:A:32:GLY:N	2.12	0.65
1:A:35:ALA:O	1:A:38:LEU:HD23	1.97	0.64
1:A:279:MSE:HE3	1:A:279:MSE:O	1.98	0.64
1:A:99:GLU:OE1	1:A:102:ARG:NH2	2.31	0.63
1:A:6:ILE:HG22	1:A:6:ILE:O	1.98	0.63
1:B:201:ARG:HH11	1:B:201:ARG:HG2	1.63	0.62
1:B:228:PRO:HG3	1:B:273:GLN:O	1.99	0.61
1:A:279:MSE:HE2	1:A:283:LEU:HD11	1.81	0.61
1:A:217:HIS:HE1	1:B:208:PHE:CD1	2.18	0.60
1:A:199:ARG:HB3	1:B:159:VAL:HG13	1.83	0.60
1:A:98:ILE:N	1:A:98:ILE:HD12	2.16	0.60
1:B:224:ARG:NH2	1:B:284:GLU:OE2	2.35	0.60
1:A:231:LYS:HD3	1:A:273:GLN:OE1	2.01	0.60
1:B:62:MSE:HE1	1:B:93:SER:HA	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:MSE:HE1	1:A:93:SER:HA	1.83	0.59
1:A:205:MSE:HA	1:A:205:MSE:CE	2.31	0.58
1:A:63:VAL:HG12	1:A:69:VAL:HG23	1.86	0.57
1:A:290:LYS:O	1:A:291:LEU:HB2	2.03	0.57
1:B:59:ILE:N	1:B:59:ILE:HD12	2.20	0.57
1:A:8:LEU:HB2	1:A:30:THR:HG21	1.87	0.57
1:B:53:THR:O	1:B:87:LYS:HE3	2.04	0.57
1:B:62:MSE:CE	1:B:93:SER:HA	2.36	0.56
1:A:119:VAL:CG2	1:A:131:LEU:HB3	2.36	0.56
1:B:50:ARG:O	1:B:54:GLU:HG3	2.06	0.56
1:B:65:ASP:OD1	1:B:67:PRO:HD2	2.05	0.56
1:A:185:GLU:HG2	1:A:283:LEU:CD2	2.36	0.56
1:A:90:VAL:O	1:A:90:VAL:HG23	2.05	0.56
1:A:119:VAL:HG22	1:A:120:SER:N	2.22	0.54
1:B:191:SER:OG	1:B:289:HIS:HE1	1.90	0.54
1:A:208:PHE:CD1	1:B:217:HIS:HE1	2.24	0.54
1:B:224:ARG:HH22	1:B:284:GLU:CD	2.11	0.54
1:B:280:VAL:O	1:B:284:GLU:HG3	2.07	0.54
1:A:76:GLU:HG2	1:A:77:HIS:N	2.20	0.54
1:A:61:ILE:HD11	1:A:89:ILE:HD11	1.90	0.54
1:A:1:MSE:HE3	1:A:58:ILE:HD11	1.89	0.54
1:A:172:ASN:HD22	1:B:204:LEU:CD2	2.20	0.54
1:A:106:ARG:O	1:A:109:GLU:HG2	2.07	0.53
1:B:1:MSE:HG3	1:B:3:LEU:HD21	1.89	0.53
1:A:200:VAL:O	1:A:204:LEU:HD13	2.09	0.53
1:B:273:GLN:HG2	2:B:353:HOH:O	2.07	0.53
1:A:62:MSE:CE	1:A:93:SER:HA	2.38	0.53
1:B:66:THR:HB	1:B:67:PRO:HD3	1.89	0.53
1:A:47:GLU:HB2	2:A:361:HOH:O	2.08	0.53
1:A:53:THR:O	1:A:87:LYS:HE3	2.08	0.52
1:A:204:LEU:HD23	1:B:175:ILE:HD12	1.92	0.52
1:A:85:GLN:HA	1:A:111:GLY:O	2.10	0.52
1:B:74:PHE:CZ	1:B:106:ARG:HG3	2.44	0.52
1:B:223:ASN:O	1:B:224:ARG:HB2	2.10	0.52
1:A:231:LYS:HG3	2:A:294:HOH:O	2.10	0.51
1:A:17:ILE:HG12	1:A:38:LEU:HB3	1.93	0.51
1:A:172:ASN:O	1:A:176:VAL:HG23	2.10	0.51
1:B:159:VAL:HG12	1:B:159:VAL:O	2.10	0.51
1:A:60:PHE:CE1	1:A:90:VAL:HG21	2.46	0.50
1:B:13:SER:O	1:B:17:ILE:HG13	2.11	0.50
1:B:65:ASP:HB2	1:B:67:PRO:HD2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:HIS:HA	2:A:328:HOH:O	2.11	0.50
1:A:98:ILE:CD1	1:A:98:ILE:H	2.25	0.50
1:A:146:LYS:HB3	1:A:147:PRO:HD3	1.93	0.49
1:A:271:GLY:HA2	1:A:274:LEU:CD1	2.42	0.49
1:B:199:ARG:NH1	2:B:315:HOH:O	2.43	0.49
1:A:219:GLU:HB3	2:A:324:HOH:O	2.12	0.49
1:B:201:ARG:HG2	1:B:201:ARG:NH1	2.24	0.49
1:B:104:ALA:O	1:B:107:VAL:HG22	2.13	0.49
1:B:103:PHE:O	1:B:107:VAL:HG13	2.13	0.49
1:A:63:VAL:HG22	1:A:64:PRO:CD	2.43	0.49
1:B:155:ASN:HB2	2:B:338:HOH:O	2.13	0.49
1:A:63:VAL:HG21	1:A:68:GLN:HB3	1.94	0.48
1:A:63:VAL:HG12	1:A:69:VAL:CG2	2.43	0.48
1:A:27:HIS:CG	1:A:55:PHE:CD1	3.02	0.48
1:A:59:ILE:HB	1:A:89:ILE:HD12	1.94	0.48
1:B:183:VAL:CG1	1:B:187:LEU:HD12	2.42	0.48
1:A:6:ILE:CG2	1:A:6:ILE:O	2.60	0.48
1:A:89:ILE:HG22	1:A:113:ASP:O	2.13	0.48
1:A:46:VAL:HG11	1:A:55:PHE:CE1	2.48	0.48
1:B:66:THR:OG1	1:B:95:ILE:HB	2.14	0.48
1:B:177:ALA:HB2	1:B:235:HIS:NE2	2.29	0.48
1:B:80:ALA:HB1	1:B:110:MSE:HE1	1.96	0.47
1:B:31:ILE:HG13	2:B:359:HOH:O	2.14	0.47
1:A:59:ILE:N	1:A:59:ILE:HD12	2.30	0.47
1:A:120:SER:HB3	1:A:169:LYS:HE3	1.96	0.47
1:A:261:GLU:O	1:A:264:ASN:HB2	2.15	0.47
1:A:251:LEU:CD1	1:B:189:PHE:HA	2.45	0.47
1:A:185:GLU:CG	1:A:283:LEU:CD2	2.93	0.46
1:A:118:PRO:HG3	1:A:166:GLN:HA	1.98	0.46
1:A:211:SER:HA	1:B:211:SER:HA	1.96	0.46
1:B:84:LEU:HB3	1:B:112:ALA:HB2	1.97	0.46
1:A:283:LEU:N	1:A:283:LEU:HD12	2.30	0.46
1:B:146:LYS:HB3	1:B:147:PRO:HD3	1.97	0.46
1:B:213:ILE:HD13	1:B:217:HIS:CE1	2.50	0.46
1:B:102:ARG:HG2	1:B:102:ARG:HH11	1.81	0.46
1:B:205:MSE:HA	1:B:205:MSE:CE	2.42	0.46
1:A:10:ILE:N	1:A:10:ILE:HD12	2.31	0.46
1:A:96:SER:HA	1:A:97:PRO:HD3	1.86	0.45
1:B:117:ALA:CB	1:B:135:VAL:HG22	2.46	0.45
1:A:105:GLN:HA	1:A:108:ASN:HB2	1.99	0.45
1:B:185:GLU:HG2	1:B:283:LEU:HD22	1.95	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LEU:HD23	1:B:287:ALA:HB1	1.98	0.45
1:A:129:GLY:O	1:A:153:GLY:HA2	2.16	0.45
1:B:156:ILE:HD12	1:B:156:ILE:N	2.31	0.45
1:B:178:LEU:HD12	1:B:259:CYS:SG	2.57	0.45
1:B:205:MSE:HE2	1:B:210:SER:OG	2.16	0.45
1:A:223:ASN:HB2	1:A:225:THR:HG23	1.98	0.45
1:A:51:GLN:O	1:A:55:PHE:CE1	2.70	0.45
1:A:27:HIS:HD2	2:A:376:HOH:O	1.99	0.45
1:A:34:VAL:HG13	1:A:38:LEU:HD21	1.99	0.45
1:B:137:GLY:O	1:B:158:LEU:HD11	2.16	0.45
1:A:191:SER:OG	1:A:289:HIS:HE1	1.99	0.44
1:A:34:VAL:CG1	1:A:38:LEU:HD21	2.47	0.44
1:A:48:THR:CG2	1:A:49:ALA:N	2.65	0.44
1:A:181:GLU:OE2	1:A:185:GLU:OE2	2.36	0.44
1:A:60:PHE:CD1	1:A:90:VAL:CG2	3.00	0.44
1:B:232:ILE:HD12	1:B:271:GLY:O	2.17	0.44
1:B:181:GLU:OE2	1:B:185:GLU:OE2	2.36	0.44
1:B:25:GLN:HG3	2:B:363:HOH:O	2.17	0.44
1:B:65:ASP:CB	1:B:67:PRO:HD2	2.47	0.44
1:A:2:LYS:HG3	1:A:2:LYS:O	2.18	0.44
1:B:66:THR:N	1:B:67:PRO:CD	2.80	0.44
1:A:251:LEU:HD11	1:B:189:PHE:HA	2.00	0.43
1:A:283:LEU:HD12	1:A:283:LEU:H	1.83	0.43
1:A:50:ARG:O	1:A:54:GLU:HG3	2.18	0.43
1:A:232:ILE:HD11	1:A:278:ALA:HB3	1.99	0.43
1:A:90:VAL:CG2	1:A:90:VAL:O	2.66	0.43
1:B:187:LEU:HD22	1:B:197:PRO:HB3	2.01	0.43
1:A:149:PHE:HB3	1:A:156:ILE:HG12	2.01	0.42
1:B:25:GLN:O	1:B:26:LEU:HD12	2.19	0.42
1:B:284:GLU:O	1:B:288:ASN:N	2.52	0.42
1:A:96:SER:HB3	1:A:99:GLU:CG	2.50	0.42
1:A:287:ALA:HB2	2:B:294:HOH:O	2.18	0.42
1:A:106:ARG:O	1:A:110:MSE:HG3	2.19	0.42
1:A:26:LEU:O	1:A:43:ALA:HA	2.20	0.41
1:A:96:SER:OG	1:A:99:GLU:HG2	2.19	0.41
1:B:1:MSE:HE2	1:B:58:ILE:HD12	2.02	0.41
1:A:49:ALA:HB3	1:A:77:HIS:O	2.20	0.41
1:B:1:MSE:HB2	2:B:369:HOH:O	2.20	0.41
1:A:85:GLN:NE2	1:A:111:GLY:HA3	2.35	0.41
1:A:31:ILE:CD1	1:A:32:GLY:N	2.81	0.41
1:A:50:ARG:HH11	1:A:50:ARG:HG2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:O	1:A:46:VAL:CG2	2.68	0.41
1:B:71:ASP:O	1:B:75:GLY:N	2.51	0.41
1:A:228:PRO:HG3	1:A:273:GLN:O	2.21	0.41
1:A:119:VAL:CG2	1:A:120:SER:N	2.83	0.41
1:A:13:SER:O	1:A:17:ILE:HG13	2.21	0.41
1:A:119:VAL:HG23	1:A:132:SER:O	2.22	0.40
1:A:213:ILE:HG12	2:B:312:HOH:O	2.22	0.40
1:A:117:ALA:HA	1:A:134:MSE:O	2.22	0.40
1:A:251:LEU:HD23	1:B:287:ALA:CB	2.51	0.40
1:A:9:GLY:O	1:A:11:MSE:N	2.55	0.40
1:B:13:SER:HB3	1:B:14:PRO:CD	2.52	0.40
1:A:70:GLU:HB2	1:A:103:PHE:CZ	2.56	0.40
1:B:176:VAL:O	1:B:180:ILE:HG13	2.20	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	289/295 (98%)	261 (90%)	25 (9%)	3 (1%)	15	23
1	B	289/295 (98%)	270 (93%)	19 (7%)	0	100	100
All	All	578/590 (98%)	531 (92%)	44 (8%)	3 (0%)	29	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	47	GLU
1	A	229	GLY

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	230/222 (104%)	214 (93%)	16 (7%)	15	24
1	B	230/222 (104%)	226 (98%)	4 (2%)	60	78
All	All	460/444 (104%)	440 (96%)	20 (4%)	29	46

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	10	ILE
1	A	11	MSE
1	A	36	ASP
1	A	45	ASN
1	A	53	THR
1	A	55	PHE
1	A	73	LEU
1	A	76	GLU
1	A	84	LEU
1	A	134	MSE
1	A	199	ARG
1	A	205	MSE
1	A	234	LEU
1	A	237	LYS
1	A	276	HIS
1	B	5	PHE
1	B	199	ARG
1	B	202	GLN
1	B	276	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	85	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	108	ASN
1	A	172	ASN
1	A	236	GLN
1	A	289	HIS
1	B	51	GLN
1	B	162	ASN
1	B	172	ASN
1	B	217	HIS
1	B	223	ASN
1	B	236	GLN
1	B	289	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 ⓘ

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 (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	280/295 (94%)	0.02	14 (5%)	28	27	19, 37, 70, 97	0
1	B	280/295 (94%)	-0.09	9 (3%)	47	46	21, 36, 58, 89	0
All	All	560/590 (94%)	-0.04	23 (4%)	37	36	19, 37, 64, 97	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	ALA	4.9
1	A	47	GLU	4.5
1	A	79	CYS	4.1
1	A	81	LYS	3.5
1	B	80	ALA	3.2
1	A	48	THR	3.1
1	B	31	ILE	3.1
1	A	78	GLY	3.1
1	A	55	PHE	3.1
1	B	79	CYS	3.0
1	A	31	ILE	2.6
1	B	255	ASN	2.4
1	A	229	GLY	2.4
1	A	254	PRO	2.4
1	B	106	ARG	2.2
1	A	257	ALA	2.1
1	A	36	ASP	2.1
1	A	38	LEU	2.1
1	B	77	HIS	2.1
1	B	258	THR	2.0
1	B	229	GLY	2.0
1	A	253	LEU	2.0
1	B	254	PRO	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.