



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 07:40 am BST

PDB ID : 1MO2
Title : Thioesterase Domain from 6-Deoxyerythronolide Synthase (DEBS TE), pH 8.5
Authors : Tsai, S.-C.; Lu, H.; Cane, D.E.; Khosla, C.; Stroud, R.M.
Deposited on : 2002-09-05
Resolution : 3.00 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

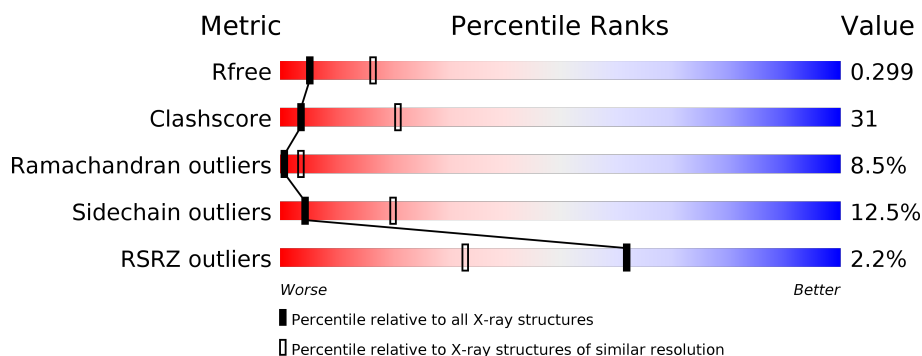
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 $\leq 5\%$. 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	294	<div> <div>2%</div> <div> <div></div> <div>40%</div> <div>37%</div> <div>7%</div> <div>15%</div> </div> </div>
1	B	294	<div> <div>2%</div> <div> <div></div> <div>43%</div> <div>33%</div> <div>8%</div> <div>15%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3830 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 Erythronolide synthase, modules 5 and 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1887	1192	329	357	9			
1	B	251	Total	C	N	O	S	0	0	0
			1887	1192	329	357	9			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INSERTION	UNP Q03133
A	2	ALA	-	INSERTION	UNP Q03133
A	3	SER	-	INSERTION	UNP Q03133
A	284	SER	-	INSERTION	UNP Q03133
A	285	SER	-	INSERTION	UNP Q03133
A	286	VAL	-	INSERTION	UNP Q03133
A	287	ASP	-	INSERTION	UNP Q03133
A	288	LYS	-	INSERTION	UNP Q03133
A	289	LEU	-	INSERTION	UNP Q03133
A	290	ALA	-	INSERTION	UNP Q03133
A	291	ALA	-	INSERTION	UNP Q03133
A	292	ALA	-	INSERTION	UNP Q03133
A	293	LEU	-	INSERTION	UNP Q03133
A	294	GLU	-	INSERTION	UNP Q03133
B	1	MET	-	INSERTION	UNP Q03133
B	2	ALA	-	INSERTION	UNP Q03133
B	3	SER	-	INSERTION	UNP Q03133
B	284	SER	-	INSERTION	UNP Q03133
B	285	SER	-	INSERTION	UNP Q03133
B	286	VAL	-	INSERTION	UNP Q03133
B	287	ASP	-	INSERTION	UNP Q03133
B	288	LYS	-	INSERTION	UNP Q03133
B	289	LEU	-	INSERTION	UNP Q03133
B	290	ALA	-	INSERTION	UNP Q03133
B	291	ALA	-	INSERTION	UNP Q03133

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	292	ALA	-	INSERTION	UNP Q03133
B	293	LEU	-	INSERTION	UNP Q03133
B	294	GLU	-	INSERTION	UNP Q03133

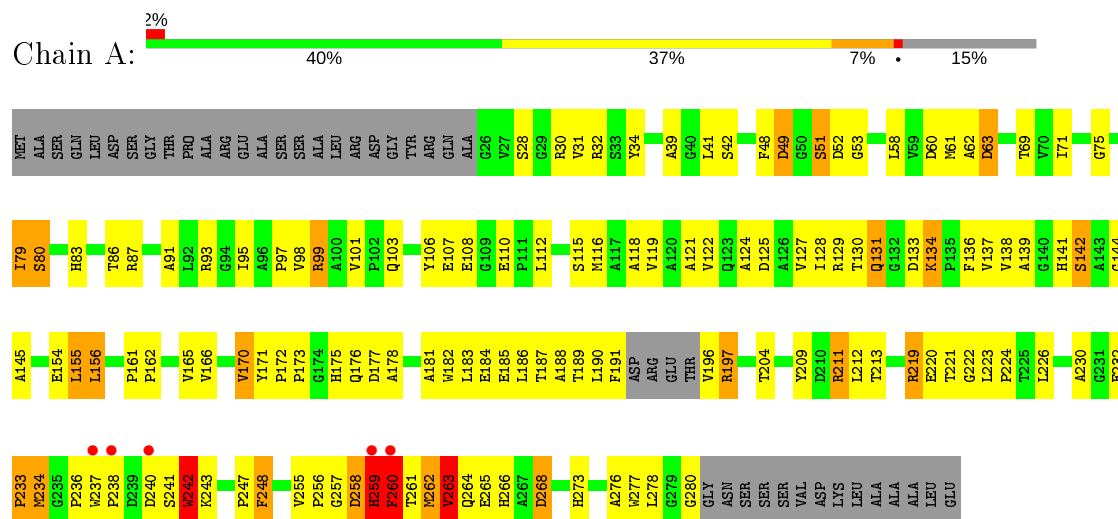
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	27	Total O 27 27	0	0

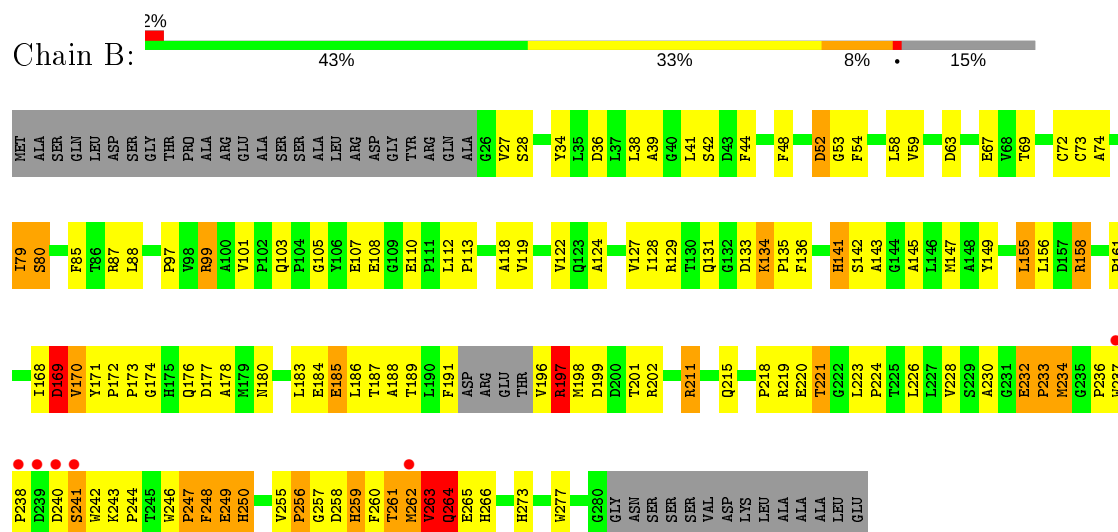
3 Residue-property plots

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: Erythronolide synthase, modules 5 and 6



- Molecule 1: Erythronolide synthase, modules 5 and 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.50Å 102.50Å 156.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 49.22 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.6 (30.00-3.00) 84.2 (49.22-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.1, CNS	Depositor
R, R_{free}	0.242 , 0.287 0.254 , 0.299	Depositor DCC
R_{free} test set	1082 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	67.2	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3830	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.48	0/1939	0.74	2/2651 (0.1%)
1	B	0.46	0/1939	0.73	1/2651 (0.0%)
All	All	0.47	0/3878	0.74	3/5302 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	PHE	N-CA-C	7.11	130.19	111.00
1	A	259	HIS	N-CA-C	5.28	125.24	111.00
1	B	266	HIS	N-CA-C	-5.06	97.35	111.00

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	1887	0	1810	124	1
1	B	1887	0	1810	111	1
2	A	29	0	0	3	0
2	B	27	0	0	4	0
All	All	3830	0	3620	231	1

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 31.

All (231) 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:232:GLU:HB3	1:A:233:PRO:HD2	1.26	1.08
1:A:71:ILE:HD13	1:A:136:PHE:HB2	1.37	1.06
1:B:63:ASP:HA	1:B:97:PRO:HA	1.52	0.91
1:A:170:VAL:HG12	1:A:171:TYR:H	1.32	0.91
1:B:232:GLU:CB	1:B:233:PRO:HD2	2.00	0.91
1:B:232:GLU:HB3	1:B:233:PRO:HD2	1.55	0.88
1:A:232:GLU:CB	1:A:233:PRO:HD2	2.07	0.85
1:B:142:SER:HB3	1:B:169:ASP:HA	1.59	0.84
1:A:191:PHE:O	1:A:197:ARG:HD3	1.81	0.80
1:A:141:HIS:O	1:A:142:SER:HB3	1.84	0.78
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.49	0.78
1:B:142:SER:HA	1:B:145:ALA:HB2	1.67	0.77
1:B:196:VAL:HA	1:B:197:ARG:NH2	2.01	0.76
1:A:28:SER:HB2	1:A:183:LEU:HD23	1.67	0.74
1:A:263:VAL:HG22	1:A:263:VAL:O	1.84	0.74
1:B:127:VAL:HG11	1:B:155:LEU:HD21	1.70	0.73
1:B:211:ARG:HH11	1:B:211:ARG:HG3	1.52	0.73
1:B:107:GLU:HA	1:B:107:GLU:OE2	1.87	0.73
1:A:60:ASP:OD1	1:A:99:ARG:HD2	1.90	0.72
1:B:232:GLU:HB3	1:B:233:PRO:CD	2.19	0.72
1:A:93:ARG:HB2	1:A:93:ARG:HH11	1.54	0.71
1:A:71:ILE:CD1	1:A:136:PHE:HB2	2.17	0.71
1:B:172:PRO:HD2	1:B:178:ALA:HA	1.73	0.70
1:A:75:GLY:HA2	1:A:144:GLY:CA	2.22	0.69
1:A:48:PHE:CE1	1:A:122:VAL:HG21	2.27	0.68
1:B:174:GLY:HA3	1:B:241:SER:HB3	1.74	0.68
1:B:149:TYR:OH	1:B:221:THR:HG22	1.94	0.67
1:A:181:ALA:O	1:A:184:GLU:HB3	1.94	0.67
1:A:190:LEU:O	1:A:190:LEU:HD23	1.94	0.67
1:B:232:GLU:OE2	1:B:257:GLY:HA3	1.93	0.67
1:A:170:VAL:HG12	1:A:171:TYR:N	2.06	0.67
1:B:147:MET:HB3	2:B:297:HOH:O	1.95	0.66
1:B:198:MET:CE	1:B:198:MET:HA	2.25	0.66
1:A:136:PHE:CE1	1:A:162:PRO:HB3	2.31	0.66
1:A:128:ILE:HG13	1:A:129:ARG:N	2.10	0.66
1:A:247:PRO:O	1:A:248:PHE:HB2	1.96	0.65
1:A:232:GLU:HA	1:A:232:GLU:OE1	1.95	0.65
1:A:176:GLN:O	1:A:177:ASP:HB3	1.96	0.65
1:A:107:GLU:HA	1:A:107:GLU:OE2	1.96	0.64
1:B:99:ARG:HG3	1:B:99:ARG:HH11	1.63	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PHE:HE1	1:A:162:PRO:HB3	1.61	0.64
1:B:249:GLU:O	1:B:250:HIS:HB3	1.97	0.64
1:B:176:GLN:O	1:B:177:ASP:HB3	1.97	0.64
1:A:39:ALA:O	1:A:42:SER:HB3	1.98	0.63
1:B:230:ALA:HA	1:B:255:VAL:O	1.99	0.63
1:B:232:GLU:HB2	1:B:233:PRO:HD2	1.78	0.63
1:A:142:SER:HA	1:A:145:ALA:HB2	1.79	0.63
1:A:220:GLU:HG2	1:A:248:PHE:CE1	2.34	0.63
1:A:191:PHE:HD2	1:A:197:ARG:CZ	2.10	0.63
1:B:226:LEU:HD22	1:B:277:TRP:CG	2.34	0.63
1:B:105:GLY:HA2	1:B:110:GLU:HB2	1.80	0.62
1:A:139:ALA:HB2	1:A:166:VAL:HB	1.81	0.62
1:A:211:ARG:HG3	1:A:211:ARG:NH1	2.15	0.62
1:B:28:SER:HB2	1:B:183:LEU:HD21	1.81	0.62
1:A:141:HIS:O	1:A:142:SER:CB	2.48	0.61
1:A:93:ARG:NH1	1:A:93:ARG:HB2	2.15	0.61
1:A:232:GLU:HB3	1:A:233:PRO:CD	2.17	0.61
1:B:174:GLY:CA	1:B:241:SER:HB3	2.29	0.61
1:B:156:LEU:O	1:B:156:LEU:HD12	2.00	0.61
1:B:218:PRO:O	1:B:248:PHE:HZ	1.83	0.61
1:A:48:PHE:HE1	1:A:122:VAL:HG21	1.65	0.61
1:B:107:GLU:HB2	1:B:110:GLU:OE2	2.00	0.60
1:A:258:ASP:O	1:A:259:HIS:HB3	2.01	0.60
1:B:72:CYS:HB3	1:B:85:PHE:CZ	2.37	0.60
1:B:141:HIS:O	1:B:143:ALA:N	2.34	0.60
1:A:107:GLU:O	1:A:110:GLU:HB2	2.02	0.59
1:B:118:ALA:O	1:B:122:VAL:HG23	2.03	0.59
1:B:232:GLU:CB	1:B:233:PRO:CD	2.74	0.59
1:B:67:GLU:O	1:B:135:PRO:HD2	2.02	0.59
1:A:71:ILE:N	1:A:71:ILE:HD12	2.17	0.59
1:A:79:ILE:HG22	1:A:80:SER:N	2.16	0.58
1:A:86:THR:HG23	1:A:87:ARG:H	1.68	0.58
1:A:58:LEU:CD2	1:A:101:VAL:HG22	2.32	0.58
1:A:69:THR:HG22	1:A:71:ILE:HD12	1.83	0.58
1:A:139:ALA:CB	1:A:166:VAL:HB	2.34	0.58
1:A:176:GLN:C	1:A:178:ALA:H	2.08	0.57
1:B:191:PHE:HD2	1:B:197:ARG:HH22	1.52	0.57
1:B:232:GLU:O	1:B:233:PRO:C	2.41	0.57
1:B:170:VAL:HG12	1:B:171:TYR:H	1.71	0.56
1:B:211:ARG:HG3	1:B:211:ARG:NH1	2.20	0.56
1:B:79:ILE:O	1:B:202:ARG:NH1	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLU:HB2	1:A:110:GLU:OE2	2.06	0.56
1:A:247:PRO:O	1:A:248:PHE:CB	2.53	0.56
1:A:265:GLU:OE2	1:A:265:GLU:HA	2.06	0.56
1:B:215:GLN:HB2	2:B:303:HOH:O	2.04	0.56
1:A:236:PRO:HD2	1:A:242:TRP:CZ3	2.40	0.55
1:A:226:LEU:HD22	1:A:277:TRP:CG	2.41	0.55
1:B:168:ILE:O	1:B:169:ASP:HB3	2.07	0.55
1:A:83:HIS:O	1:A:86:THR:HG22	2.07	0.55
1:B:133:ASP:O	1:B:134:LYS:O	2.25	0.55
1:B:263:VAL:O	1:B:264:GLN:NE2	2.40	0.55
1:A:58:LEU:HD22	1:A:101:VAL:HG22	1.89	0.55
1:B:180:ASN:O	1:B:184:GLU:HB2	2.06	0.55
1:A:175:HIS:HA	1:A:243:LYS:HB3	1.88	0.55
1:A:263:VAL:CG2	1:A:263:VAL:O	2.55	0.55
1:A:75:GLY:HA2	1:A:144:GLY:HA3	1.87	0.55
1:A:30:ARG:HH21	1:B:44:PHE:HD1	1.54	0.54
1:B:198:MET:HE2	1:B:198:MET:HA	1.90	0.54
1:A:99:ARG:HG3	1:A:99:ARG:HH11	1.73	0.54
1:B:263:VAL:O	1:B:263:VAL:HG22	2.08	0.54
1:A:127:VAL:O	1:A:131:GLN:HB3	2.07	0.54
1:A:93:ARG:CB	1:A:93:ARG:HH11	2.19	0.54
1:A:41:LEU:HD11	1:B:41:LEU:HD11	1.90	0.54
1:A:196:VAL:HG12	1:A:196:VAL:O	2.08	0.53
1:B:88:LEU:O	1:B:88:LEU:HG	2.08	0.53
1:A:28:SER:HB2	1:A:183:LEU:CD2	2.37	0.53
1:A:86:THR:HG23	1:A:87:ARG:N	2.24	0.53
1:B:173:PRO:O	1:B:243:LYS:HG2	2.09	0.53
1:A:131:GLN:O	1:A:133:ASP:O	2.26	0.53
1:A:142:SER:C	1:A:144:GLY:N	2.63	0.52
1:A:137:VAL:HG11	1:A:278:LEU:HD21	1.91	0.52
1:B:156:LEU:HD13	1:B:161:PRO:HB3	1.92	0.52
1:B:247:PRO:O	1:B:248:PHE:O	2.27	0.52
1:B:124:ALA:HB3	1:B:158:ARG:HH21	1.73	0.51
1:B:174:GLY:HA2	1:B:242:TRP:N	2.25	0.51
1:A:230:ALA:HA	1:A:255:VAL:O	2.09	0.51
1:A:79:ILE:O	1:A:80:SER:O	2.28	0.51
1:A:172:PRO:HD2	1:A:178:ALA:HA	1.93	0.51
1:B:260:PHE:O	1:B:261:THR:OG1	2.24	0.51
1:A:93:ARG:HG3	2:A:300:HOH:O	2.12	0.50
1:B:143:ALA:HB2	2:B:313:HOH:O	2.10	0.50
1:B:170:VAL:O	1:B:171:TYR:HB2	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:PRO:CD	1:B:242:TRP:CE3	2.95	0.49
1:A:221:THR:O	1:A:223:LEU:N	2.46	0.49
1:B:191:PHE:HD2	1:B:197:ARG:NH2	2.10	0.49
1:B:105:GLY:HA3	1:B:112:LEU:HD23	1.93	0.49
1:A:187:THR:C	1:A:189:THR:H	2.15	0.49
1:B:142:SER:HB3	1:B:169:ASP:CA	2.39	0.49
1:A:103:GLN:O	1:A:106:TYR:HD2	1.96	0.49
1:A:49:ASP:OD1	1:A:51:SER:HB3	2.13	0.49
1:B:36:ASP:O	1:B:39:ALA:HB3	2.13	0.49
1:B:185:GLU:O	1:B:188:ALA:HB3	2.12	0.48
1:A:133:ASP:O	1:A:134:LYS:HB3	2.14	0.48
1:A:116:MET:HE3	1:A:213:THR:HA	1.95	0.48
1:A:233:PRO:O	1:A:234:MET:C	2.52	0.48
1:A:71:ILE:N	1:A:71:ILE:CD1	2.76	0.48
1:B:48:PHE:CE1	1:B:122:VAL:HG21	2.49	0.48
1:B:124:ALA:O	1:B:128:ILE:HG23	2.14	0.48
1:A:87:ARG:HG2	1:A:87:ARG:HH11	1.78	0.48
1:A:170:VAL:O	1:A:171:TYR:HB2	2.14	0.48
1:B:34:TYR:CE2	1:B:38:LEU:HD11	2.48	0.48
1:A:124:ALA:HB2	1:A:154:GLU:CG	2.45	0.47
1:B:177:ASP:HA	1:B:180:ASN:ND2	2.29	0.47
1:A:28:SER:HB3	1:A:31:VAL:HG23	1.97	0.47
1:B:220:GLU:HG2	1:B:248:PHE:CE1	2.49	0.47
1:B:262:MET:CE	1:B:262:MET:HA	2.42	0.47
1:A:30:ARG:NH2	1:B:44:PHE:HD1	2.12	0.47
1:A:124:ALA:HB2	1:A:154:GLU:HG2	1.96	0.47
1:A:142:SER:C	1:A:144:GLY:H	2.17	0.47
1:B:177:ASP:H	1:B:180:ASN:ND2	2.13	0.47
1:B:133:ASP:HB2	2:B:321:HOH:O	2.14	0.47
1:B:168:ILE:HG22	1:B:169:ASP:N	2.28	0.47
1:B:52:ASP:O	1:B:54:PHE:N	2.36	0.46
1:B:174:GLY:HA2	1:B:242:TRP:H	1.79	0.46
1:B:236:PRO:HG3	1:B:242:TRP:HE3	1.80	0.46
1:A:176:GLN:O	1:A:177:ASP:CB	2.61	0.46
1:B:176:GLN:O	1:B:177:ASP:CB	2.58	0.46
1:A:182:TRP:CE3	1:A:183:LEU:HD12	2.51	0.46
1:A:115:SER:O	1:A:119:VAL:HG12	2.16	0.46
1:A:63:ASP:HA	1:A:97:PRO:HA	1.98	0.45
1:A:276:ALA:O	1:A:280:GLY:O	2.34	0.45
1:B:223:LEU:HA	1:B:224:PRO:HD3	1.85	0.45
1:B:243:LYS:HB2	1:B:244:PRO:HD2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLU:HG2	1:A:248:PHE:HE1	1.80	0.45
1:A:61:MET:O	1:A:62:ALA:HB2	2.16	0.45
1:B:69:THR:O	1:B:136:PHE:HA	2.16	0.45
1:B:173:PRO:HG3	1:B:233:PRO:O	2.16	0.45
1:B:73:CYS:O	1:B:85:PHE:HE2	2.00	0.45
1:A:122:VAL:O	1:A:125:ASP:HB2	2.17	0.45
1:A:87:ARG:HG2	1:A:87:ARG:NH1	2.31	0.45
1:A:172:PRO:HA	1:A:173:PRO:HD3	1.77	0.44
1:A:87:ARG:NH1	1:A:265:GLU:HG3	2.32	0.44
1:A:181:ALA:C	1:A:184:GLU:HB3	2.36	0.44
1:B:79:ILE:HG22	1:B:80:SER:N	2.31	0.44
1:A:196:VAL:HA	1:A:197:ARG:NH1	2.32	0.44
1:A:258:ASP:O	1:A:259:HIS:CB	2.63	0.44
1:B:107:GLU:O	1:B:110:GLU:HG3	2.17	0.44
1:B:172:PRO:HB3	1:B:177:ASP:OD1	2.16	0.44
1:B:58:LEU:HG	1:B:101:VAL:HG22	1.97	0.44
1:B:170:VAL:HG12	1:B:171:TYR:N	2.33	0.44
1:B:236:PRO:CG	1:B:242:TRP:HE3	2.31	0.44
1:B:87:ARG:HD3	1:B:265:GLU:OE2	2.17	0.44
1:B:73:CYS:O	1:B:85:PHE:CE2	2.70	0.44
1:B:99:ARG:HG3	1:B:99:ARG:NH1	2.30	0.44
1:A:226:LEU:HD22	1:A:277:TRP:CD2	2.53	0.44
1:A:61:MET:HB2	1:A:98:VAL:HG12	1.99	0.44
1:A:118:ALA:O	1:A:122:VAL:HG23	2.18	0.43
1:A:138:VAL:O	1:A:165:VAL:HA	2.18	0.43
1:A:155:LEU:HD13	1:A:155:LEU:HA	1.86	0.43
1:A:223:LEU:HA	1:A:224:PRO:HD2	1.97	0.43
1:B:59:VAL:O	1:B:99:ARG:HA	2.18	0.43
1:B:48:PHE:HE1	1:B:122:VAL:HG21	1.83	0.43
1:A:98:VAL:C	1:A:99:ARG:HG2	2.39	0.43
1:B:236:PRO:HD2	1:B:242:TRP:CZ3	2.54	0.43
1:B:79:ILE:O	1:B:80:SER:O	2.37	0.43
1:A:219:ARG:HB3	1:A:219:ARG:HE	1.60	0.43
1:B:264:GLN:HE21	1:B:264:GLN:HB3	1.56	0.42
1:B:191:PHE:CD2	1:B:197:ARG:NH1	2.87	0.42
1:A:209:TYR:HA	1:A:212:LEU:HD12	2.00	0.42
1:A:116:MET:N	2:A:302:HOH:O	2.49	0.42
1:B:187:THR:C	1:B:189:THR:N	2.73	0.42
1:B:174:GLY:HA3	1:B:241:SER:CB	2.47	0.42
1:B:199:ASP:OD1	1:B:201:THR:HB	2.19	0.42
1:B:234:MET:HG2	1:B:256:PRO:HG2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:HG	1:A:161:PRO:HB3	2.01	0.42
1:B:128:ILE:HG13	1:B:129:ARG:N	2.35	0.42
1:B:168:ILE:O	1:B:169:ASP:CB	2.68	0.42
1:A:71:ILE:HA	1:A:99:ARG:O	2.20	0.42
1:A:95:ILE:HD12	1:A:95:ILE:N	2.33	0.42
1:B:196:VAL:HA	1:B:197:ARG:CZ	2.49	0.42
1:A:191:PHE:CD2	1:A:197:ARG:CZ	2.98	0.42
1:A:99:ARG:NH2	1:A:130:THR:O	2.51	0.42
1:A:220:GLU:HG2	1:A:248:PHE:CD1	2.53	0.42
1:B:72:CYS:HB3	1:B:85:PHE:CE1	2.54	0.42
1:B:263:VAL:O	1:B:264:GLN:CB	2.68	0.41
1:A:176:GLN:C	1:A:178:ALA:N	2.73	0.41
1:A:175:HIS:H	1:A:241:SER:CB	2.33	0.41
1:A:116:MET:HB3	2:A:302:HOH:O	2.20	0.41
1:A:127:VAL:O	1:A:131:GLN:CB	2.68	0.41
1:A:187:THR:C	1:A:189:THR:N	2.74	0.41
1:B:168:ILE:O	1:B:228:VAL:O	2.38	0.41
1:A:260:PHE:O	1:A:260:PHE:CG	2.72	0.41
1:A:34:TYR:CE1	1:B:41:LEU:HD22	2.56	0.41
1:B:246:TRP:CD1	1:B:247:PRO:O	2.73	0.41
1:A:112:LEU:HA	1:A:112:LEU:HD23	1.90	0.41
1:B:103:GLN:HA	1:B:103:GLN:OE1	2.21	0.41
1:A:58:LEU:HD21	1:A:101:VAL:HG22	2.01	0.40
1:A:118:ALA:O	1:A:121:ALA:HB3	2.21	0.40
1:A:91:ALA:HB1	1:A:268:ASP:HA	2.04	0.40
1:B:113:PRO:HB3	1:B:119:VAL:HB	2.03	0.40
1:B:74:ALA:HB3	1:B:103:GLN:HG2	2.03	0.40

All (1) 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)
1:A:261:THR:N	1:B:259:HIS:N[2_564]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	247/294 (84%)	194 (78%)	32 (13%)	21 (8%)	1	4
1	B	247/294 (84%)	201 (81%)	25 (10%)	21 (8%)	1	4
All	All	494/588 (84%)	395 (80%)	57 (12%)	42 (8%)	1	4

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	233	PRO
1	A	240	ASP
1	A	256	PRO
1	A	259	HIS
1	A	263	VAL
1	B	80	SER
1	B	131	GLN
1	B	232	GLU
1	B	233	PRO
1	B	240	ASP
1	B	248	PHE
1	B	261	THR
1	A	79	ILE
1	A	108	GLU
1	A	131	GLN
1	A	142	SER
1	A	222	GLY
1	A	257	GLY
1	B	53	GLY
1	B	79	ILE
1	B	264	GLN
1	A	51	SER
1	B	197	ARG
1	B	241	SER
1	B	250	HIS
1	B	256	PRO
1	A	134	LYS
1	A	262	MET
1	B	134	LYS
1	B	170	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	170	VAL
1	A	188	ALA
1	A	242	TRP
1	B	169	ASP
1	B	221	THR
1	B	247	PRO
1	A	53	GLY
1	A	238	PRO
1	A	248	PHE
1	B	263	VAL
1	B	238	PRO

5.3.2 Protein sidechains ⓘ

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	192/224 (86%)	167 (87%)	25 (13%)	4	19
1	B	192/224 (86%)	169 (88%)	23 (12%)	5	22
All	All	384/448 (86%)	336 (88%)	48 (12%)	4	20

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	49	ASP
1	A	52	ASP
1	A	63	ASP
1	A	99	ARG
1	A	155	LEU
1	A	156	LEU
1	A	185	GLU
1	A	186	LEU
1	A	197	ARG
1	A	204	THR
1	A	211	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	219	ARG
1	A	234	MET
1	A	237	TRP
1	A	242	TRP
1	A	258	ASP
1	A	259	HIS
1	A	260	PHE
1	A	262	MET
1	A	263	VAL
1	A	264	GLN
1	A	266	HIS
1	A	268	ASP
1	A	273	HIS
1	B	27	VAL
1	B	42	SER
1	B	52	ASP
1	B	99	ARG
1	B	108	GLU
1	B	141	HIS
1	B	155	LEU
1	B	158	ARG
1	B	169	ASP
1	B	185	GLU
1	B	186	LEU
1	B	197	ARG
1	B	211	ARG
1	B	219	ARG
1	B	234	MET
1	B	237	TRP
1	B	249	GLU
1	B	258	ASP
1	B	259	HIS
1	B	262	MET
1	B	263	VAL
1	B	264	GLN
1	B	273	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	141	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	259	HIS
1	A	264	GLN
1	A	266	HIS
1	B	123	GLN
1	B	180	ASN
1	B	259	HIS
1	B	264	GLN
1	B	273	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 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	251/294 (85%)	-0.28	5 (1%) 65 36	34, 52, 94, 120	0
1	B	251/294 (85%)	-0.28	6 (2%) 59 30	35, 51, 91, 123	0
All	All	502/588 (85%)	-0.28	11 (2%) 62 33	34, 52, 94, 123	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	ASP	3.7
1	A	237	TRP	3.5
1	A	240	ASP	3.5
1	B	238	PRO	3.4
1	A	259	HIS	3.2
1	B	239	ASP	3.0
1	B	237	TRP	2.6
1	A	260	PHE	2.3
1	B	262	MET	2.3
1	A	238	PRO	2.1
1	B	241	SER	2.1

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.