



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:50 AM UTC

PDB ID : 1MO2 / pdb_00001mo2
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

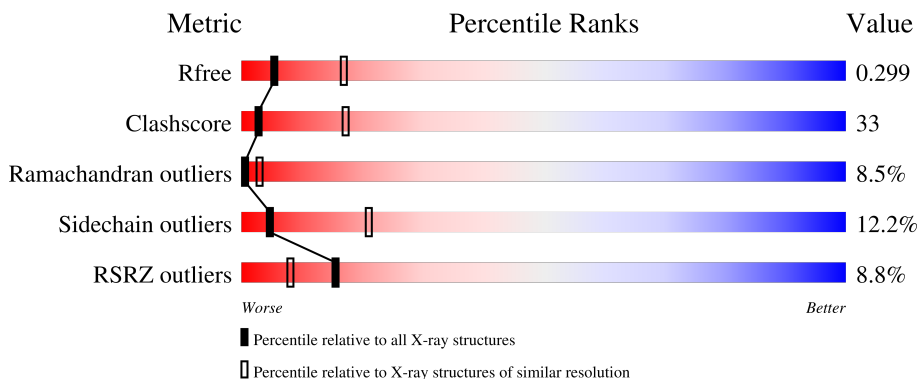
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 of 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	
1	B	294	

2 Entry composition i

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
			Total	C	N	O	S			
1	A	251	1887	1192	329	357	9	0	0	0
1	B	251	1887	1192	329	357	9	0	0	0

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

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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

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 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.6 (30.00-3.00) 84.1 (30.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.01Å)	Xtrriage
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	Xtrriage
Anisotropy	0.063	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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	0.61	1/1939 (0.1%)	1.18	21/2651 (0.8%)
1	B	0.60	1/1939 (0.1%)	1.14	16/2651 (0.6%)
All	All	0.61	2/3878 (0.1%)	1.16	37/5302 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	PHE	CA-C	5.45	1.61	1.53
1	B	261	THR	CA-CB	5.38	1.62	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	266	HIS	N-CA-C	-12.54	97.35	112.89
1	A	260	PHE	N-CA-C	10.47	130.19	108.53
1	A	176	GLN	N-CA-C	-8.69	98.36	110.35
1	A	266	HIS	N-CA-C	-8.04	103.92	112.93
1	A	143	ALA	N-CA-C	-7.80	103.51	112.87
1	B	259	HIS	N-CA-C	7.52	121.38	109.65
1	A	29	GLY	N-CA-C	-7.44	102.85	115.80
1	A	116	MET	N-CA-C	-7.19	103.45	111.28
1	B	64	GLY	CA-C-N	7.17	127.33	119.87
1	B	64	GLY	C-N-CA	7.17	127.33	119.87
1	A	30	ARG	N-CA-C	-6.94	104.81	113.28
1	A	267	ALA	N-CA-C	-6.87	103.72	111.14
1	A	259	HIS	N-CA-C	6.78	125.24	110.80
1	A	178	ALA	N-CA-C	-6.70	104.74	113.12
1	A	255	VAL	CA-C-N	6.68	128.19	119.84
1	A	255	VAL	C-N-CA	6.68	128.19	119.84
1	B	243	LYS	N-CA-C	6.37	118.69	109.84
1	A	64	GLY	CA-C-N	6.04	126.15	119.87
1	A	64	GLY	C-N-CA	6.04	126.15	119.87
1	A	265	GLU	N-CA-C	5.88	117.99	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	ARG	N-CA-C	-5.59	105.33	111.82
1	A	247	PRO	N-CA-C	-5.53	101.50	110.40
1	B	30	ARG	N-CA-C	-5.42	105.53	111.82
1	B	143	ALA	N-CA-C	-5.39	104.86	111.75
1	A	179	MET	N-CA-C	-5.34	105.53	111.36
1	B	265	GLU	CA-C-N	5.33	130.47	121.14
1	B	265	GLU	C-N-CA	5.33	130.47	121.14
1	B	138	VAL	N-CA-C	-5.32	100.82	108.53
1	B	171	TYR	CA-C-N	5.20	125.74	120.38
1	B	171	TYR	C-N-CA	5.20	125.74	120.38
1	A	237	TRP	CA-C-N	5.17	126.30	119.84
1	A	237	TRP	C-N-CA	5.17	126.30	119.84
1	B	101	VAL	CA-C-N	5.16	125.61	120.14
1	B	101	VAL	C-N-CA	5.16	125.61	120.14
1	B	252	THR	N-CA-C	5.10	116.95	109.24
1	A	150	ALA	N-CA-C	-5.06	105.68	111.14
1	B	176	GLN	N-CA-C	-5.03	103.41	110.35

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	130	1
1	B	1887	0	1810	116	1
2	A	29	0	0	3	0
2	B	27	0	0	4	0
All	All	3830	0	3620	242	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 33.

All (242) 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:198:MET:HE2	1:B:198:MET:HA	1.45	0.96
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:O	1:A:263:VAL:HG22	1.84	0.74
1:B:127:VAL:HG11	1:B:155:LEU:HD21	1.70	0.73
1:B:211:ARG:HG3	1:B:211:ARG:HH11	1.52	0.73
1:B:107:GLU:OE2	1:B:107:GLU:HA	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:HH11	1:A:93:ARG:HB2	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:116:MET:HE1	1:B:213:THR:HG22	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:HD23	1:A:190:LEU:O	1.94	0.67
1:B:232:GLU:OE2	1:B:257:GLY:HA3	1.93	0.67
1:B:147:MET:HB3	2:B:297:HOH:O	1.95	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:170:VAL:HG12	1:A:171:TYR:N	2.06	0.65
1:A:107:GLU:OE2	1:A:107:GLU:HA	1.96	0.64
1:B:99:ARG:HG3	1:B:99:ARG:HH11	1.63	0.64
1:A:136:PHE:HE1	1:A:162:PRO:HB3	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLU:O	1:B:250:HIS: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:B:176:GLN:O	1:B:177:ASP:HB3	1.97	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:A:176:GLN:C	1:A:178:ALA:H	2.08	0.62
1:B:28:SER:HB2	1:B:183:LEU:HD21	1.81	0.62
1:A:93:ARG:HB2	1:A:93:ARG:NH1	2.15	0.61
1:A:141:HIS:O	1:A:142:SER:CB	2.48	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:HD12	1:B:156:LEU:O	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:198:MET:HA	1:B:198:MET:CE	2.25	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:B:232:GLU:O	1:B:233:PRO:C	2.41	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:B:191:PHE:HD2	1:B:197:ARG:HH22	1.52	0.57
1:A:142:SER:C	1:A:144:GLY:N	2.63	0.56
1:B:79:ILE:O	1:B:202:ARG:NH1	2.38	0.56
1:B:170:VAL:HG12	1:B:171:TYR:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ARG:HG3	1:B:211:ARG:NH1	2.20	0.56
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:75:GLY:HA2	1:A:144:GLY:HA3	1.87	0.55
1:A:263:VAL:O	1:A:263:VAL:CG2	2.55	0.55
1:A:30:ARG:HH21	1:B:44:PHE:HD1	1.54	0.54
1:A:99:ARG:HH11	1:A:99:ARG:HG3	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:41:LEU:HD11	1:B:41:LEU:HD11	1.90	0.54
1:A:93:ARG:HH11	1:A:93:ARG:CB	2.19	0.54
1:A:187:THR:C	1:A:189:THR:H	2.15	0.53
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:A:116:MET:HE1	1:A:213:THR:HG22	1.91	0.53
1:A:233:PRO:O	1:A:234:MET:C	2.52	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: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:79:ILE:O	1:A:80:SER:O	2.28	0.51
1:A:230:ALA:HA	1:A:255:VAL:O	2.09	0.51
1:A:172:PRO:HD2	1:A:178:ALA:HA	1.93	0.51
1:A:142:SER:C	1:A:144:GLY:H	2.17	0.51
1:A:93:ARG:HG3	2:A:300:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ALA:HB2	2:B:313:HOH:O	2.10	0.50
1:B:260:PHE:O	1:B:261:THR:OG1	2.24	0.50
1:B:170:VAL:O	1:B:171:TYR:HB2	2.10	0.50
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:A:181:ALA:C	1:A:184:GLU:HB3	2.36	0.49
1:B:105:GLY:HA3	1:B:112:LEU:HD23	1.93	0.49
1:B:142:SER:HB3	1:B:169:ASP:CA	2.39	0.49
1:A:49:ASP:OD1	1:A:51:SER:HB3	2.13	0.49
1:A:103:GLN:O	1:A:106:TYR:HD2	1.96	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:71:ILE:CD1	1:A:71:ILE:N	2.76	0.48
1:B:48:PHE:CE1	1:B:122:VAL:HG21	2.49	0.48
1:B:262:MET:HE3	1:B:262:MET:HA	1.95	0.48
1:B:124:ALA:O	1:B:128:ILE:HG23	2.14	0.48
1:A:87:ARG:HH11	1:A:87:ARG:HG2	1.78	0.48
1:A:98:VAL:C	1:A:99:ARG:HG2	2.39	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:A:30:ARG:NH2	1:B:44:PHE:HD1	2.12	0.47
1:B:220:GLU:HG2	1:B:248:PHE:CE1	2.49	0.47
1:B:262:MET:HA	1:B:262:MET:CE	2.42	0.47
1:A:124:ALA:HB2	1:A:154:GLU:HG2	1.96	0.47
1:B:187:THR:C	1:B:189:THR:N	2.73	0.47
1:A:257:GLY:C	1:A:258:ASP:CG	2.83	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:A:187:THR:C	1:A:189:THR:N	2.74	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:A:176:GLN:C	1:A:178:ALA:N	2.73	0.46
1:B:176:GLN:O	1:B:177:ASP:CB	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:87:ARG:HG2	1:A:87:ARG:NH1	2.31	0.45
1:A:122:VAL:O	1:A:125:ASP:HB2	2.17	0.45
1:A:87:ARG:NH1	1:A:265:GLU:HG3	2.32	0.44
1:A:172:PRO:HA	1:A:173:PRO:HD3	1.77	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:87:ARG:HD3	1:B:265:GLU:OE2	2.17	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: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:B:187:THR:C	1:B:189:THR:H	2.24	0.44
1:A:61:MET:HB2	1:A:98:VAL:HG12	1.99	0.44
1:A:226:LEU:HD22	1:A:277:TRP:CD2	2.53	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:A:116:MET:HE1	1:A:213:THR:CG2	2.48	0.43
1:B:48:PHE:HE1	1:B:122:VAL:HG21	1.83	0.43
1:B:236:PRO:HD2	1:B:242:TRP:CZ3	2.54	0.43
1:B:267:ALA:O	1:B:268:ASP:C	2.61	0.43
1:B:79:ILE:O	1:B:80:SER:O	2.37	0.43
1:A:48:PHE:CD1	1:A:48:PHE:C	2.97	0.43
1:A:219:ARG:HE	1:A:219:ARG:HB3	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:GLN:HE21	1:B:264:GLN:HB3	1.56	0.42
1:B:56:LEU:C	1:B:56:LEU:HD12	2.44	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: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
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:N	1:A:95:ILE:HD12	2.33	0.42
1:B:196:VAL:HA	1:B:197:ARG:CZ	2.49	0.42
1:A:99:ARG:NH2	1:A:130:THR:O	2.51	0.42
1:A:191:PHE:CD2	1:A:197:ARG:CZ	2.98	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: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:221:THR:O	1:A:222:GLY:C	2.63	0.41
1:A:245:THR:O	1:A:246:TRP:C	2.63	0.41
1:B:168:ILE:O	1:B:228:VAL:O	2.38	0.41
1:A:34:TYR:CE1	1:B:41:LEU:HD22	2.56	0.41
1:A:260:PHE:O	1:A:260:PHE:CG	2.72	0.41
1:B:246:TRP:CD1	1:B:247:PRO:O	2.73	0.41
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.90	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:B:142:SER:C	1:B:144:GLY:N	2.74	0.40
1:A:180:ASN:O	1:A:181:ALA:C	2.64	0.40
1:A:91:ALA:HB1	1:A:268:ASP:HA	2.04	0.40
1:B:74:ALA:HB3	1:B:103:GLN:HG2	2.03	0.40
1:B:113:PRO:HB3	1:B:119:VAL:HB	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 [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	247/294 (84%)	194 (78%)	32 (13%)	21 (8%)	0	3
1	B	247/294 (84%)	201 (81%)	25 (10%)	21 (8%)	0	3
All	All	494/588 (84%)	395 (80%)	57 (12%)	42 (8%)	0	3

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

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Mol	Chain	Res	Type
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
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 [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	192/224 (86%)	170 (88%)	22 (12%)	5	24
1	B	192/224 (86%)	167 (87%)	25 (13%)	4	19
All	All	384/448 (86%)	337 (88%)	47 (12%)	5	21

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG

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Mol	Chain	Res	Type
1	A	49	ASP
1	A	63	ASP
1	A	71	ILE
1	A	93	ARG
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
1	A	219	ARG
1	A	234	MET
1	A	242	TRP
1	A	252	THR
1	A	258	ASP
1	A	260	PHE
1	A	263	VAL
1	A	264	GLN
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	128	ILE
1	B	141	HIS
1	B	155	LEU
1	B	158	ARG
1	B	168	ILE
1	B	169	ASP
1	B	185	GLU
1	B	186	LEU
1	B	197	ARG
1	B	211	ARG
1	B	215	GLN
1	B	219	ARG
1	B	234	MET
1	B	249	GLU
1	B	258	ASP
1	B	259	HIS

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Mol	Chain	Res	Type
1	B	262	MET
1	B	263	VAL
1	B	264	GLN
1	B	273	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	141	HIS
1	A	259	HIS
1	A	264	GLN
1	A	266	HIS
1	B	123	GLN
1	B	180	ASN
1	B	250	HIS
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 oligosaccharides 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

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, 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%)	0.27	21 (8%) 17 9	34, 52, 94, 120	0
1	B	251/294 (85%)	0.32	23 (9%) 14 8	35, 51, 91, 123	0
All	All	502/588 (85%)	0.30	44 (8%) 15 8	34, 52, 94, 123	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	HIS	6.1
1	A	260	PHE	5.9
1	A	196	VAL	4.9
1	B	233	PRO	4.9
1	B	234	MET	4.4
1	B	262	MET	4.2
1	A	280	GLY	4.0
1	B	237	TRP	3.9
1	A	237	TRP	3.6
1	B	190	LEU	3.5
1	B	260	PHE	3.5
1	B	240	ASP	3.5
1	A	262	MET	3.4
1	A	27	VAL	3.4
1	B	261	THR	3.3
1	A	234	MET	3.3
1	B	259	HIS	3.2
1	A	240	ASP	3.1
1	A	265	GLU	3.1
1	B	264	GLN	3.0
1	A	261	THR	2.9
1	B	27	VAL	2.9
1	B	238	PRO	2.8
1	A	242	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	196	VAL	2.7
1	B	241	SER	2.7
1	A	263	VAL	2.6
1	B	242	TRP	2.5
1	B	28	SER	2.5
1	A	189	THR	2.5
1	A	28	SER	2.4
1	B	263	VAL	2.4
1	B	133	ASP	2.3
1	A	258	ASP	2.3
1	B	265	GLU	2.2
1	B	239	ASP	2.2
1	B	235	GLY	2.2
1	B	191	PHE	2.2
1	A	238	PRO	2.2
1	B	236	PRO	2.2
1	A	190	LEU	2.2
1	A	233	PRO	2.1
1	A	191	PHE	2.1
1	A	241	SER	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 oligosaccharides 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.