



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:47 PM EDT

PDB ID : 6XCS / pdb_00006xcs
Title : Erythromycin esterase mutant EreC H289N in its open conformation
Authors : Zielinski, M.; Berghuis, A.M.
Deposited on : 2020-06-09
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 ⓘ 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (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

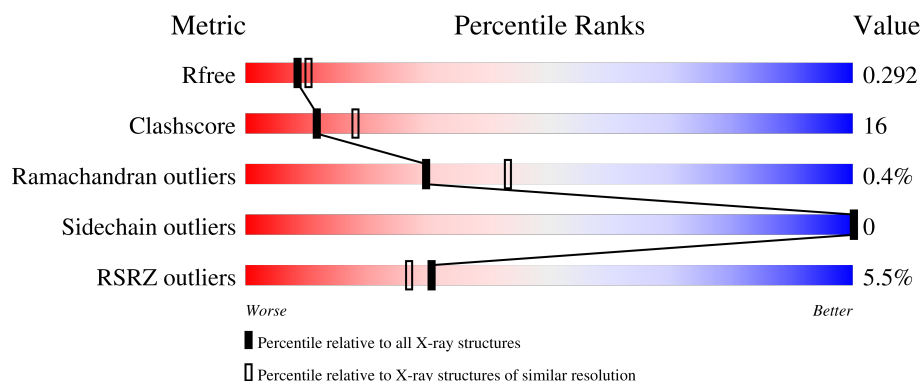
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	438	4% 68% 25% 7%
1	B	438	6% 64% 29% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6169 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 EreC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	Se	0	2	0
			3052	1928	514	596	4	10			
1	B	408	Total	C	N	O	S	Se	0	3	0
			3051	1912	532	593	4	10			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	initiating methionine	UNP C7C425
A	-18	GLY	-	expression tag	UNP C7C425
A	-17	SER	-	expression tag	UNP C7C425
A	-16	SER	-	expression tag	UNP C7C425
A	-15	HIS	-	expression tag	UNP C7C425
A	-14	HIS	-	expression tag	UNP C7C425
A	-13	HIS	-	expression tag	UNP C7C425
A	-12	HIS	-	expression tag	UNP C7C425
A	-11	HIS	-	expression tag	UNP C7C425
A	-10	HIS	-	expression tag	UNP C7C425
A	-9	SER	-	expression tag	UNP C7C425
A	-8	SER	-	expression tag	UNP C7C425
A	-7	GLY	-	expression tag	UNP C7C425
A	-6	LEU	-	expression tag	UNP C7C425
A	-5	VAL	-	expression tag	UNP C7C425
A	-4	PRO	-	expression tag	UNP C7C425
A	-3	ARG	-	expression tag	UNP C7C425
A	-2	GLY	-	expression tag	UNP C7C425
A	-1	SER	-	expression tag	UNP C7C425
A	0	HIS	-	expression tag	UNP C7C425
A	289	ASN	HIS	engineered mutation	UNP C7C425
B	-19	MSE	-	initiating methionine	UNP C7C425
B	-18	GLY	-	expression tag	UNP C7C425
B	-17	SER	-	expression tag	UNP C7C425
B	-16	SER	-	expression tag	UNP C7C425

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP C7C425
B	-14	HIS	-	expression tag	UNP C7C425
B	-13	HIS	-	expression tag	UNP C7C425
B	-12	HIS	-	expression tag	UNP C7C425
B	-11	HIS	-	expression tag	UNP C7C425
B	-10	HIS	-	expression tag	UNP C7C425
B	-9	SER	-	expression tag	UNP C7C425
B	-8	SER	-	expression tag	UNP C7C425
B	-7	GLY	-	expression tag	UNP C7C425
B	-6	LEU	-	expression tag	UNP C7C425
B	-5	VAL	-	expression tag	UNP C7C425
B	-4	PRO	-	expression tag	UNP C7C425
B	-3	ARG	-	expression tag	UNP C7C425
B	-2	GLY	-	expression tag	UNP C7C425
B	-1	SER	-	expression tag	UNP C7C425
B	0	HIS	-	expression tag	UNP C7C425
B	289	ASN	HIS	engineered mutation	UNP C7C425

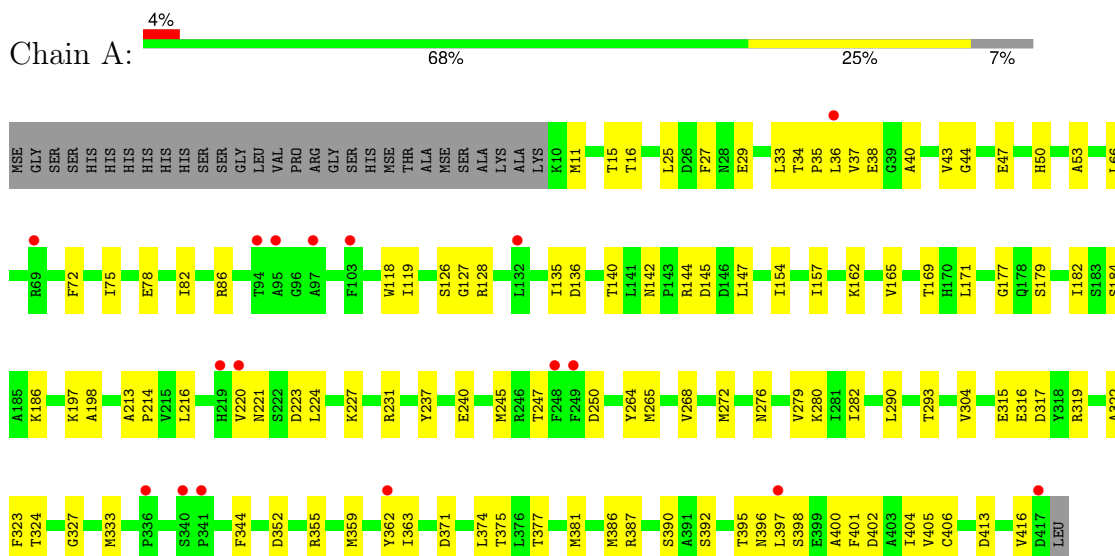
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	38	Total O 38 38	0	0
2	B	28	Total O 28 28	0	0

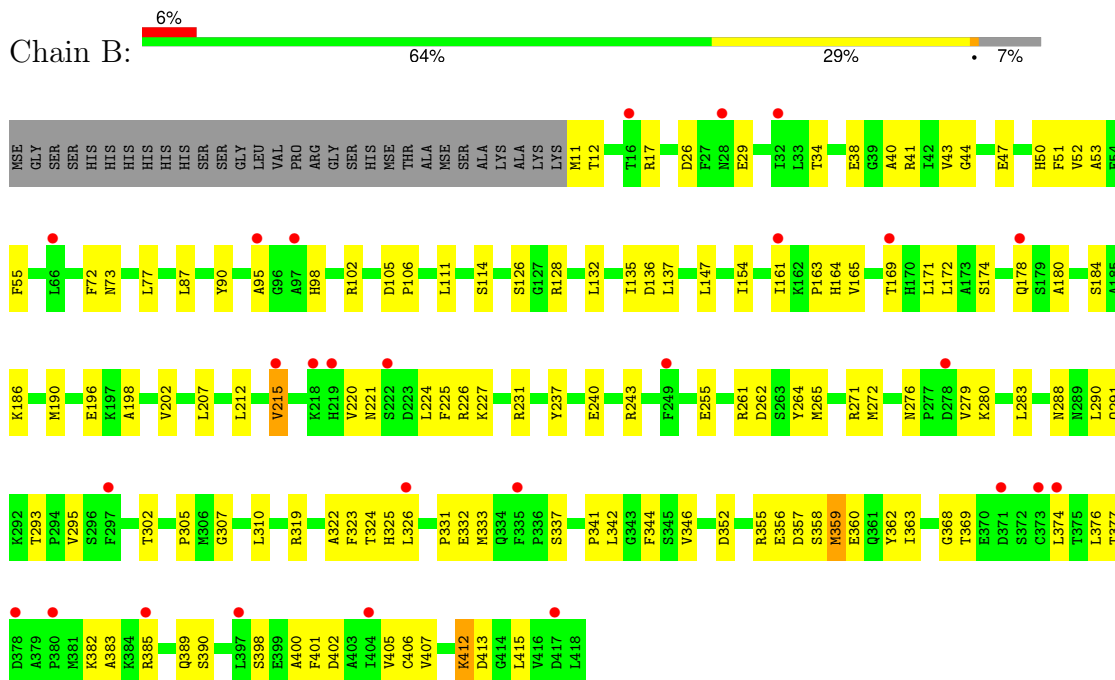
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: EreC



• Molecule 1: EreC



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.37Å 74.21Å 129.29Å 90.00° 96.50° 90.00°	Depositor
Resolution (Å)	44.80 – 2.40 44.80 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.80-2.40) 99.5 (44.80-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.15.1_3469	Depositor
R, R_{free}	0.240 , 0.290 0.243 , 0.292	Depositor DCC
R_{free} test set	1912 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6169	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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

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	0/3091	0.68	0/4187
1	B	0.44	0/3092	0.85	14/4190 (0.3%)
All	All	0.42	0/6183	0.77	14/8377 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	ARG	CB-CG-CD	-13.75	79.69	111.30
1	B	226	ARG	CA-CB-CG	10.83	135.76	114.10
1	B	226	ARG	CB-CA-C	-8.47	96.73	110.79
1	B	226	ARG	CG-CD-NE	7.73	129.00	112.00
1	B	412	LYS	CB-CG-CD	-6.83	95.59	111.30
1	B	226	ARG	N-CA-CB	6.77	120.08	110.12
1	B	359	MSE	CA-CB-CG	-5.67	102.77	114.10
1	B	226	ARG	NE-CZ-NH1	-5.66	115.84	121.50
1	B	355	ARG	CA-CB-CG	-5.60	102.91	114.10
1	B	412	LYS	CA-CB-CG	5.42	124.95	114.10
1	B	215	VAL	CG1-CB-CG2	5.28	122.42	110.80
1	B	226	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	B	225	PHE	CA-C-N	-5.06	113.50	120.28
1	B	225	PHE	C-N-CA	-5.06	113.50	120.28

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	3052	0	2982	93	0
1	B	3051	0	2934	104	0
2	A	38	0	0	3	0
2	B	28	0	0	7	0
All	All	6169	0	5916	191	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 16.

All (191) 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:359:MSE:HE2	1:A:404:ILE:HG13	1.52	0.89
1:A:184[B]:SER:HB2	1:A:245:MSE:HE3	1.63	0.81
1:A:16:THR:HG22	1:A:29:GLU:HB3	1.66	0.76
1:A:184[A]:SER:HB2	1:A:245:MSE:HE3	1.66	0.76
1:B:44:GLY:HA3	1:B:290:LEU:HD22	1.68	0.76
1:A:359:MSE:HG2	1:A:397:LEU:HD13	1.69	0.73
1:B:40:ALA:HB2	1:B:319:ARG:HE	1.55	0.72
1:A:47:GLU:OE2	1:A:50:HIS:ND1	2.22	0.71
1:B:161:ILE:CG1	1:B:164:HIS:HB2	2.21	0.71
1:B:231:ARG:NH1	2:B:501:HOH:O	2.23	0.71
1:B:332:GLU:HG3	1:B:389:GLN:HE21	1.58	0.68
1:B:106:PRO:HB2	1:B:342:LEU:HD21	1.76	0.68
1:A:374:LEU:HD13	1:A:405:VAL:HG22	1.74	0.67
1:B:147:LEU:HB3	1:B:169:THR:HG22	1.76	0.66
1:A:272:MSE:HE3	1:A:279:VAL:HG11	1.76	0.66
1:B:12:THR:HG23	1:B:376:LEU:HB2	1.78	0.65
1:A:11:MSE:HE2	1:A:362:TYR:CE2	2.33	0.65
1:B:161:ILE:HG13	1:B:164:HIS:CB	2.27	0.64
1:A:386:MSE:HE1	1:A:404:ILE:HD12	1.77	0.64
1:A:53:ALA:HB2	1:A:413:ASP:HA	1.79	0.64
1:A:140:THR:HG21	2:A:537:HOH:O	1.99	0.63
1:A:34:THR:O	1:A:38:GLU:HG2	2.00	0.62
1:A:327:GLY:O	1:A:387:ARG:NH1	2.29	0.62
1:B:332:GLU:HG2	1:B:333:MSE:H	1.65	0.62
1:B:261:ARG:HG2	1:B:265:MSE:HE2	1.81	0.62
1:B:154:ILE:HA	2:B:509:HOH:O	1.99	0.61
1:B:47:GLU:OE2	1:B:50:HIS:ND1	2.34	0.61
1:A:386:MSE:O	1:A:392:SER:OG	2.18	0.60
1:B:272:MSE:HE2	1:B:279:VAL:HG11	1.82	0.60
1:A:157:ILE:O	1:A:216:LEU:HD22	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ILE:HG12	1:A:186:LYS:HE2	1.85	0.58
1:B:50:HIS:HD2	1:B:333:MSE:CE	2.15	0.58
1:A:78:GLU:HG2	1:A:265:MSE:HE1	1.86	0.58
1:A:140:THR:HG23	1:A:142:ASN:H	1.68	0.58
1:A:324:THR:HG21	1:A:386:MSE:HE2	1.86	0.58
1:B:276:ASN:O	1:B:279:VAL:HG12	2.03	0.58
1:B:34:THR:O	1:B:38:GLU:HG2	2.04	0.58
1:A:304:VAL:HG21	1:B:215:VAL:CG2	2.34	0.57
1:B:43:VAL:HG23	1:B:319:ARG:HB2	1.85	0.57
1:B:95:ALA:O	1:B:98:HIS:ND1	2.36	0.57
1:B:106:PRO:HD2	1:B:178:GLN:OE1	2.04	0.57
1:B:332:GLU:HG2	1:B:333:MSE:N	2.20	0.57
1:A:221:ASN:HB3	1:A:224:LEU:HD12	1.87	0.57
1:B:72:PHE:HA	1:B:280:LYS:HB2	1.87	0.57
1:A:247:THR:HA	1:A:250:ASP:HB2	1.86	0.56
1:A:154:ILE:HD11	1:A:162:LYS:HA	1.88	0.56
1:B:377:THR:HB	1:B:398:SER:HA	1.88	0.56
1:A:197:LYS:NZ	1:B:196:GLU:OE2	2.39	0.56
1:A:184[B]:SER:HB2	1:A:245:MSE:CE	2.35	0.56
1:A:182:ILE:O	1:A:186:LYS:HG3	2.06	0.55
1:A:319:ARG:HA	1:A:402:ASP:OD2	2.05	0.55
1:A:304:VAL:CG2	1:B:215:VAL:HG22	2.36	0.55
1:A:304:VAL:CG2	1:B:215:VAL:CG2	2.84	0.55
1:B:135:ILE:HD13	1:B:283:LEU:HD22	1.89	0.55
1:A:184[A]:SER:HB2	1:A:245:MSE:CE	2.37	0.54
1:A:237:TYR:CD2	1:A:264:TYR:HB2	2.43	0.54
1:A:66:LEU:HD13	1:A:282:ILE:HG12	1.88	0.54
1:B:161:ILE:CG1	1:B:164:HIS:CB	2.85	0.54
1:A:182:ILE:CG1	1:A:186:LYS:HE2	2.38	0.54
1:B:174:SER:O	1:B:186:LYS:HE2	2.08	0.54
1:B:374:LEU:HD13	1:B:405:VAL:HG22	1.90	0.53
1:B:11:MSE:HE3	1:B:376:LEU:O	2.08	0.53
1:A:304:VAL:HG21	1:B:215:VAL:HG22	1.89	0.53
1:A:11:MSE:SE	1:A:381:MSE:HE3	2.59	0.53
1:A:43:VAL:HG12	1:A:72:PHE:CE2	2.43	0.53
1:B:227:LYS:O	1:B:231:ARG:HG2	2.09	0.53
1:A:171:LEU:HD23	1:A:198:ALA:HB2	1.91	0.53
1:B:172:LEU:HD23	1:B:190:MSE:HE1	1.92	0.52
1:A:413:ASP:O	1:A:416:VAL:HG12	2.10	0.52
1:B:291:GLN:HG3	1:B:401:PHE:CE2	2.45	0.52
1:A:227:LYS:O	1:A:231:ARG:HG2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ILE:HG12	1:B:164:HIS:HB2	1.92	0.51
1:B:105:ASP:HB2	2:B:517:HOH:O	2.10	0.51
1:B:358:SER:HB2	2:B:510:HOH:O	2.10	0.51
1:A:359:MSE:HE2	1:A:404:ILE:CG1	2.34	0.51
1:B:17:ARG:N	1:B:29:GLU:OE2	2.44	0.51
1:B:319:ARG:HA	1:B:402:ASP:OD2	2.11	0.50
1:A:395:THR:HG22	1:A:396:ASN:N	2.25	0.50
1:A:36:LEU:O	1:A:319:ARG:NE	2.44	0.50
1:A:144:ARG:HG3	1:A:145:ASP:N	2.26	0.50
1:B:73[A]:ASN:OD1	1:B:280:LYS:N	2.40	0.50
1:B:272:MSE:HE1	1:B:279:VAL:HG21	1.94	0.50
1:A:136:ASP:CB	1:A:265:MSE:HE3	2.41	0.49
1:B:50:HIS:HD2	1:B:333:MSE:HE1	1.77	0.49
1:A:221:ASN:ND2	1:A:223:ASP:HB2	2.27	0.49
1:B:161:ILE:HG13	1:B:164:HIS:H	1.76	0.49
1:A:147:LEU:HB3	1:A:169:THR:HG22	1.93	0.49
1:A:34:THR:N	1:A:35:PRO:HD2	2.28	0.49
1:B:337:SER:HB3	1:B:344:PHE:HA	1.95	0.48
1:A:11:MSE:HE3	1:A:375:THR:OG1	2.13	0.48
1:A:36:LEU:HD23	1:A:36:LEU:H	1.78	0.48
1:B:52:VAL:HG12	1:B:55:PHE:H	1.79	0.48
1:A:333:MSE:HE3	1:A:344:PHE:CZ	2.48	0.48
1:B:161:ILE:HG13	1:B:164:HIS:HB3	1.95	0.48
1:B:307:GLY:HA2	1:B:310:LEU:HB2	1.95	0.48
1:A:165:VAL:O	1:A:169:THR:HG23	2.13	0.48
1:A:386:MSE:HE1	1:A:404:ILE:CG2	2.44	0.48
1:B:262:ASP:HA	1:B:265:MSE:HE3	1.95	0.48
1:B:51:PHE:CE1	1:B:111:LEU:HD23	2.49	0.47
1:A:240:GLU:HG2	1:B:207:LEU:HD13	1.96	0.47
1:B:198:ALA:O	1:B:202:VAL:HG23	2.15	0.47
1:A:118:TRP:CE3	1:A:119:ILE:HG13	2.50	0.47
1:A:315:GLU:N	1:A:315:GLU:OE2	2.48	0.47
1:B:161:ILE:HG13	1:B:161:ILE:O	2.15	0.47
1:A:213:ALA:HB3	1:A:214:PRO:HD3	1.97	0.47
1:A:316:GLU:HA	2:A:501:HOH:O	2.14	0.47
1:A:363:ILE:HG21	1:A:406:CYS:SG	2.55	0.47
1:B:26:ASP:HB3	1:B:29:GLU:OE1	2.14	0.47
1:B:114:SER:N	1:B:415:LEU:HD21	2.30	0.47
1:B:41:ARG:HG2	1:B:279:VAL:O	2.15	0.47
1:B:237:TYR:CD2	1:B:264:TYR:HB2	2.50	0.47
1:B:288:ASN:O	1:B:305:PRO:HB3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:PRO:HG3	1:B:412:LYS:HB2	1.98	0.47
1:B:352:ASP:HB2	1:B:390:SER:O	2.15	0.47
1:B:356:GLU:OE1	1:B:382:LYS:NZ	2.35	0.46
1:A:25:LEU:HD23	1:A:27:PHE:CE2	2.50	0.46
1:B:53:ALA:HB2	1:B:413:ASP:HA	1.95	0.46
1:B:106:PRO:CB	1:B:342:LEU:HD21	2.45	0.46
1:B:165:VAL:O	1:B:169:THR:HG23	2.15	0.46
1:A:377:THR:HB	1:A:398:SER:HA	1.97	0.46
1:B:212:LEU:O	1:B:215:VAL:HG23	2.16	0.46
1:B:341:PRO:C	1:B:342:LEU:HD23	2.39	0.46
1:A:293:THR:OG1	1:A:395:THR:HG21	2.15	0.46
1:B:240:GLU:OE2	1:B:243:ARG:NH2	2.32	0.46
1:B:221:ASN:O	1:B:224:LEU:HD12	2.15	0.46
1:B:77:LEU:HD21	1:B:132:LEU:HD22	1.97	0.46
1:B:43:VAL:HG12	1:B:72:PHE:CE2	2.51	0.46
1:A:179:SER:HB3	1:A:182:ILE:HG22	1.98	0.45
1:B:368:GLY:HA3	2:B:503:HOH:O	2.15	0.45
1:A:324:THR:O	1:A:406:CYS:HA	2.16	0.45
1:B:180:ALA:O	1:B:184:SER:HB3	2.16	0.45
1:B:161:ILE:HD12	1:B:163:PRO:HB2	1.99	0.45
1:B:369:THR:N	2:B:503:HOH:O	2.49	0.45
1:A:140:THR:OG1	1:A:177:GLY:O	2.35	0.45
1:A:276:ASN:O	1:A:279:VAL:HG12	2.17	0.45
1:B:271:ARG:NH1	2:B:502:HOH:O	2.47	0.45
1:B:332:GLU:CG	1:B:333:MSE:H	2.27	0.45
1:A:75:ILE:CD1	1:A:282:ILE:HB	2.47	0.45
1:A:126:SER:C	1:A:128:ARG:H	2.25	0.45
1:B:322:ALA:C	1:B:323:PHE:HD1	2.24	0.45
1:A:82:ILE:O	1:A:86:ARG:HG3	2.17	0.44
1:A:352:ASP:HB2	1:A:390:SER:O	2.16	0.44
1:A:147:LEU:HD13	1:A:169:THR:HA	1.99	0.44
1:B:326:LEU:HD23	1:B:360:GLU:HB3	2.00	0.44
1:B:147:LEU:HD13	1:B:169:THR:HA	1.99	0.44
1:B:324:THR:O	1:B:406:CYS:HA	2.18	0.44
1:B:11:MSE:HE2	1:B:362:TYR:CE2	2.53	0.44
1:B:325:HIS:HA	1:B:407:VAL:O	2.18	0.43
1:A:44:GLY:HA3	1:A:290:LEU:HD22	2.00	0.43
1:B:77:LEU:CD2	1:B:132:LEU:HD22	2.49	0.43
1:B:126:SER:C	1:B:128:ARG:H	2.26	0.43
1:B:135:ILE:O	1:B:265:MSE:HG2	2.18	0.43
1:A:359:MSE:CB	1:A:386:MSE:HE3	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:THR:CG2	1:A:396:ASN:N	2.81	0.43
1:B:363:ILE:HG21	1:B:406:CYS:SG	2.59	0.43
1:B:293:THR:HG23	1:B:400:ALA:HA	1.99	0.43
1:A:38:GLU:HA	1:A:38:GLU:OE1	2.18	0.43
1:A:395:THR:HG21	1:A:400:ALA:HB2	2.01	0.43
1:A:136:ASP:CG	1:A:265:MSE:HE3	2.43	0.42
1:B:102:ARG:HA	1:B:102:ARG:HD3	1.87	0.42
1:A:75:ILE:HD13	1:A:282:ILE:HB	2.01	0.42
1:B:359:MSE:O	1:B:363:ILE:HG12	2.20	0.42
1:A:47:GLU:HA	1:A:323:PHE:HB2	2.00	0.42
1:A:322:ALA:C	1:A:323:PHE:HD1	2.27	0.42
1:A:355:ARG:NH1	2:A:506:HOH:O	2.52	0.42
1:B:47:GLU:HA	1:B:323:PHE:HB2	2.02	0.42
1:B:358:SER:HA	1:B:385:ARG:HB3	2.02	0.42
1:A:15:THR:HG23	1:A:371:ASP:HB3	2.02	0.42
1:A:135:ILE:HA	1:A:268:VAL:HG11	2.01	0.42
1:A:72:PHE:HA	1:A:280:LYS:HB2	2.01	0.42
1:B:255[B]:GLU:OE1	1:B:255[B]:GLU:N	2.46	0.42
1:B:295:VAL:O	1:B:302:THR:HB	2.20	0.41
1:A:33:LEU:HD23	1:A:36:LEU:HD21	2.02	0.41
1:A:33:LEU:O	1:A:37:VAL:HG23	2.20	0.41
1:A:324:THR:CG2	1:A:386:MSE:HE2	2.48	0.41
1:A:136:ASP:HB2	1:A:265:MSE:HE3	2.01	0.41
1:B:272:MSE:CE	1:B:279:VAL:HG11	2.49	0.41
1:B:359:MSE:HE3	1:B:362:TYR:HD2	1.86	0.41
1:B:136:ASP:OD1	1:B:137:LEU:N	2.54	0.41
1:B:161:ILE:HG13	1:B:164:HIS:HB2	1.93	0.41
1:B:171:LEU:O	1:B:190:MSE:HE2	2.21	0.41
1:A:40:ALA:HA	1:A:317:ASP:HB2	2.02	0.41
1:A:221:ASN:HB3	1:A:224:LEU:CD1	2.50	0.41
1:B:357:ASP:O	1:B:383:ALA:HA	2.20	0.41
1:A:322:ALA:HB2	1:A:401:PHE:CD1	2.56	0.40
1:B:87:LEU:O	1:B:90:TYR:HB3	2.21	0.40
1:B:357:ASP:OD1	1:B:357:ASP:N	2.51	0.40
1:A:43:VAL:HA	1:A:319:ARG:O	2.22	0.40
1:A:142:ASN:ND2	1:A:144:ARG:HG2	2.37	0.40
1:B:51:PHE:CD2	1:B:346:VAL:HG11	2.56	0.40
1:B:332:GLU:CG	1:B:333:MSE:N	2.84	0.40

There are no symmetry-related clashes.

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	408/438 (93%)	392 (96%)	14 (3%)	2 (0%)	24	37
1	B	409/438 (93%)	393 (96%)	15 (4%)	1 (0%)	43	58
All	All	817/876 (93%)	785 (96%)	29 (4%)	3 (0%)	30	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	220	VAL
1	A	220	VAL
1	A	127	GLY

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	318/359 (89%)	318 (100%)	0	100	100
1	B	312/359 (87%)	312 (100%)	0	100	100
All	All	630/718 (88%)	630 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	149	GLN
1	A	289	ASN
1	A	361	GLN
1	B	131	GLN
1	B	194	GLN
1	B	334	GLN

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	398/438 (90%)	0.66	17 (4%) 40 36	32, 70, 98, 109	2 (0%)
1	B	398/438 (90%)	0.81	27 (6%) 23 20	30, 72, 100, 120	3 (0%)
All	All	796/876 (90%)	0.74	44 (5%) 30 27	30, 71, 99, 120	5 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	95	ALA	3.5
1	B	215	VAL	3.5
1	A	97	ALA	3.2
1	B	97	ALA	3.2
1	A	132	LEU	3.1
1	B	219	HIS	3.0
1	A	219	HIS	2.9
1	A	95	ALA	2.9
1	B	169	THR	2.8
1	B	335	PHE	2.8
1	B	385	ARG	2.8
1	B	161	ILE	2.7
1	A	362	TYR	2.7
1	A	397	LEU	2.7
1	B	380	PRO	2.7
1	A	69	ARG	2.6
1	B	417	ASP	2.5
1	B	28	ASN	2.5
1	B	222	SER	2.5
1	B	297	PHE	2.5
1	A	103	PHE	2.4
1	B	371	ASP	2.4
1	B	378	ASP	2.4
1	A	220	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	336	PRO	2.4
1	A	248	PHE	2.4
1	B	66	LEU	2.3
1	B	374	LEU	2.3
1	B	373	CYS	2.3
1	B	16	THR	2.3
1	B	326	LEU	2.3
1	B	278	ASP	2.3
1	A	36	LEU	2.2
1	B	218	LYS	2.1
1	B	404	ILE	2.1
1	A	341	PRO	2.1
1	A	249	PHE	2.1
1	A	94	THR	2.1
1	A	340	SER	2.1
1	B	178	GLN	2.0
1	B	397	LEU	2.0
1	B	32	ILE	2.0
1	A	417	ASP	2.0
1	B	249	PHE	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.