



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 05:37 PM UTC

PDB ID : 2OAM / pdb_00002oam
Title : Apo RebH from Lechevalieria aerocolonigenes
Authors : Blasiak, L.C.; Drennan, C.L.
Deposited on : 2006-12-16
Resolution : 2.30 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
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

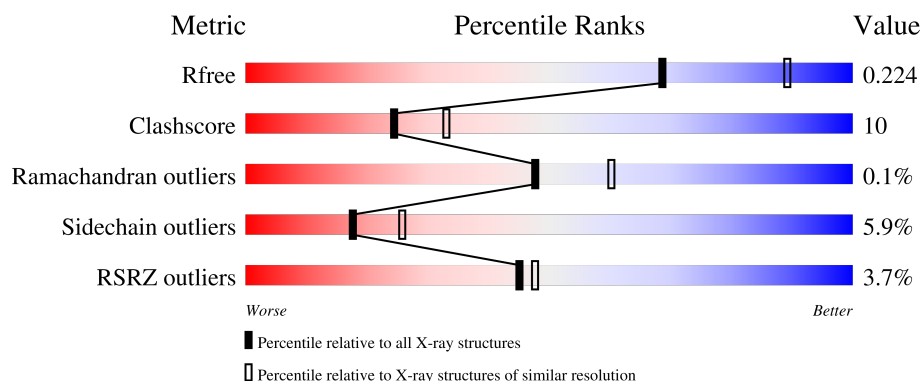
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	550	2% 72% 20% • 5%
1	B	550	5% 74% 19% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8973 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 Tryptophan halogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	523	Total	C	N	O	S	0	0	0
			4200	2668	732	781	19			
1	B	524	Total	C	N	O	S	0	0	0
			4199	2667	731	782	19			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8KHZ8
A	-18	GLY	-	cloning artifact	UNP Q8KHZ8
A	-17	SER	-	cloning artifact	UNP Q8KHZ8
A	-16	SER	-	cloning artifact	UNP Q8KHZ8
A	-15	HIS	-	expression tag	UNP Q8KHZ8
A	-14	HIS	-	expression tag	UNP Q8KHZ8
A	-13	HIS	-	expression tag	UNP Q8KHZ8
A	-12	HIS	-	expression tag	UNP Q8KHZ8
A	-11	HIS	-	expression tag	UNP Q8KHZ8
A	-10	HIS	-	expression tag	UNP Q8KHZ8
A	-9	SER	-	cloning artifact	UNP Q8KHZ8
A	-8	SER	-	cloning artifact	UNP Q8KHZ8
A	-7	GLY	-	cloning artifact	UNP Q8KHZ8
A	-6	LEU	-	cloning artifact	UNP Q8KHZ8
A	-5	VAL	-	cloning artifact	UNP Q8KHZ8
A	-4	PRO	-	cloning artifact	UNP Q8KHZ8
A	-3	ARG	-	cloning artifact	UNP Q8KHZ8
A	-2	GLY	-	cloning artifact	UNP Q8KHZ8
A	-1	SER	-	cloning artifact	UNP Q8KHZ8
A	0	HIS	-	cloning artifact	UNP Q8KHZ8
B	-19	MET	-	initiating methionine	UNP Q8KHZ8
B	-18	GLY	-	cloning artifact	UNP Q8KHZ8
B	-17	SER	-	cloning artifact	UNP Q8KHZ8
B	-16	SER	-	cloning artifact	UNP Q8KHZ8
B	-15	HIS	-	expression tag	UNP Q8KHZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q8KHZ8
B	-13	HIS	-	expression tag	UNP Q8KHZ8
B	-12	HIS	-	expression tag	UNP Q8KHZ8
B	-11	HIS	-	expression tag	UNP Q8KHZ8
B	-10	HIS	-	expression tag	UNP Q8KHZ8
B	-9	SER	-	cloning artifact	UNP Q8KHZ8
B	-8	SER	-	cloning artifact	UNP Q8KHZ8
B	-7	GLY	-	cloning artifact	UNP Q8KHZ8
B	-6	LEU	-	cloning artifact	UNP Q8KHZ8
B	-5	VAL	-	cloning artifact	UNP Q8KHZ8
B	-4	PRO	-	cloning artifact	UNP Q8KHZ8
B	-3	ARG	-	cloning artifact	UNP Q8KHZ8
B	-2	GLY	-	cloning artifact	UNP Q8KHZ8
B	-1	SER	-	cloning artifact	UNP Q8KHZ8
B	0	HIS	-	cloning artifact	UNP Q8KHZ8

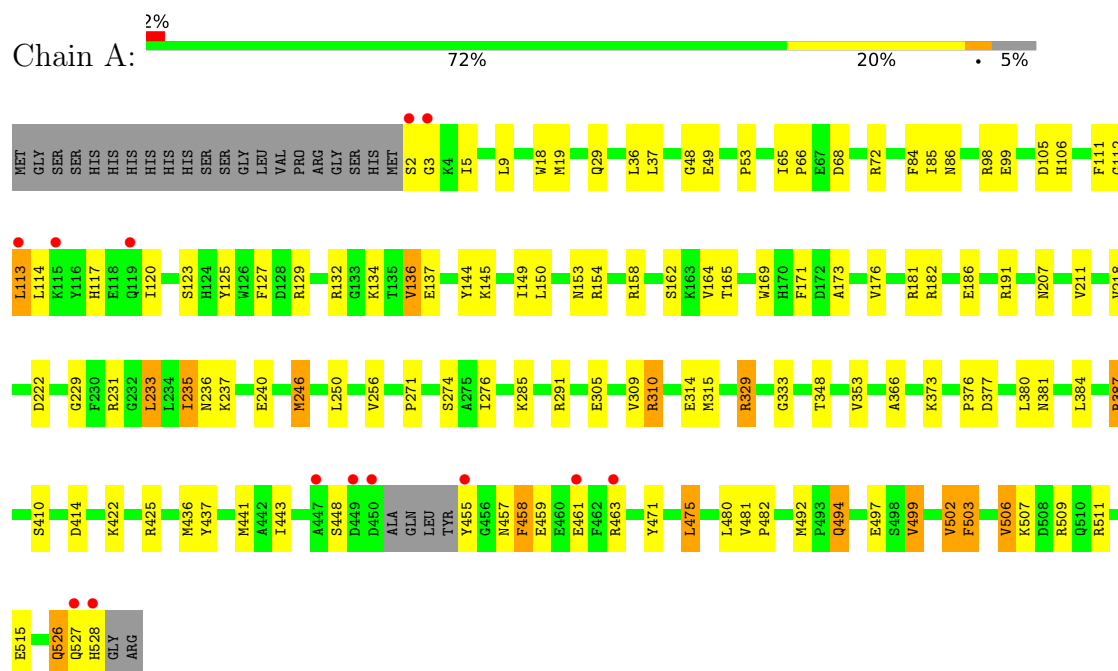
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	289	Total O 289 289	0	0
2	B	285	Total O 285 285	0	0

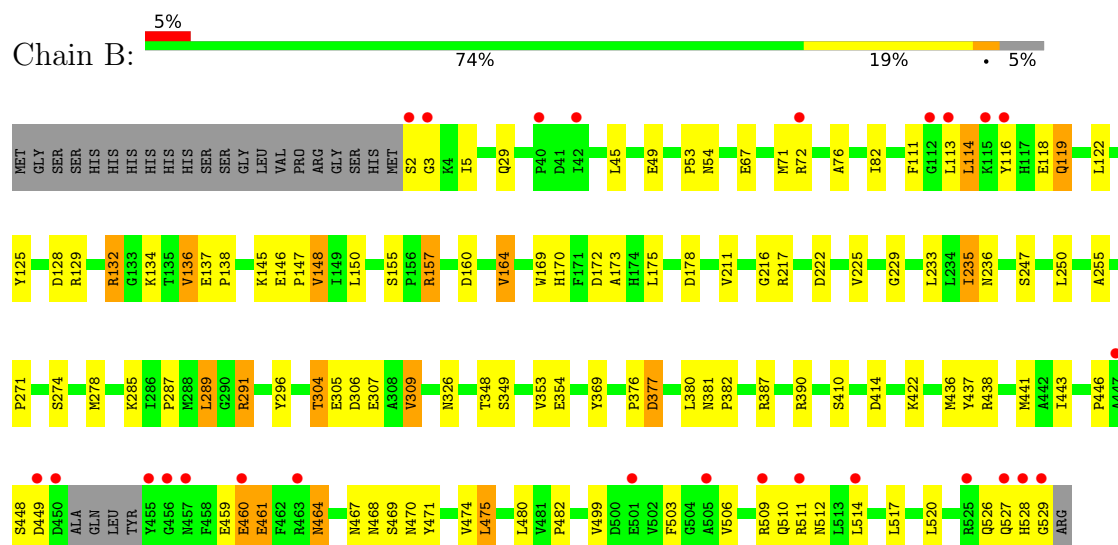
3 Residue-property plots

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: Tryptophan halogenase



• Molecule 1: Tryptophan halogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	114.82Å 114.82Å 230.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.70 – 2.30 41.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (41.70-2.30) 99.7 (41.70-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.224 0.198 , 0.224	Depositor DCC
R_{free} test set	3797 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8973	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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	0.47	0/4315	0.93	13/5854 (0.2%)
1	B	0.40	0/4313	0.93	9/5851 (0.2%)
All	All	0.44	0/8628	0.93	22/11705 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	GLY	N-CA-C	-10.82	95.13	112.66
1	A	48	GLY	N-CA-C	7.25	121.25	112.48
1	A	377	ASP	N-CA-C	-6.99	98.74	109.65
1	A	414	ASP	N-CA-C	6.51	120.48	112.54
1	A	136	VAL	N-CA-C	-6.51	106.95	113.20
1	A	503	PHE	N-CA-C	-6.48	104.86	112.89
1	A	235	ILE	N-CA-C	6.39	117.07	110.36
1	B	414	ASP	N-CA-C	6.20	120.11	112.54
1	A	19	MET	N-CA-C	-6.18	104.62	111.36
1	B	377	ASP	N-CA-C	-6.02	101.02	109.69
1	B	354	GLU	CA-C-N	5.93	127.25	119.84
1	B	354	GLU	C-N-CA	5.93	127.25	119.84
1	A	85	ILE	N-CA-C	5.88	116.39	108.17
1	A	169	TRP	N-CA-C	5.83	118.56	109.52
1	A	3	GLY	N-CA-C	-5.68	99.71	113.18
1	B	169	TRP	N-CA-C	5.51	118.55	109.85
1	B	349	SER	N-CA-C	-5.42	105.93	112.54
1	B	235	ILE	N-CA-C	5.36	115.57	110.42
1	A	381	ASN	CA-C-N	5.29	125.60	119.47
1	A	381	ASN	C-N-CA	5.29	125.60	119.47
1	B	82	ILE	N-CA-C	-5.22	100.80	108.11
1	A	458	PHE	N-CA-C	5.20	116.64	111.07

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	4200	0	4004	86	0
1	B	4199	0	4002	81	0
2	A	289	0	0	6	0
2	B	285	0	0	4	0
All	All	8973	0	8006	163	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 10.

All (163) 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:113:LEU:HD22	1:A:113:LEU:H	1.08	1.13
1:B:45:LEU:H	1:B:326:ASN:HD21	1.11	0.97
1:A:113:LEU:H	1:A:113:LEU:CD2	1.81	0.93
1:A:113:LEU:HD22	1:A:113:LEU:N	1.89	0.86
1:A:49:GLU:HG3	1:A:173:ALA:HB2	1.62	0.79
1:A:145:LYS:NZ	1:A:165:THR:HG22	2.01	0.76
1:A:441:MET:HE1	1:B:387:ARG:HG3	1.70	0.74
1:B:172:ASP:HB3	1:B:175:LEU:HD13	1.67	0.74
1:B:506:VAL:O	1:B:510:GLN:HG3	1.90	0.72
1:A:329:ARG:HH11	1:A:329:ARG:HB2	1.56	0.71
1:B:467:ASN:H	1:B:470:ASN:HD22	1.38	0.70
1:B:471:TYR:O	1:B:475:LEU:HB2	1.94	0.68
1:B:528:HIS:O	1:B:529:GLY:C	2.38	0.67
1:B:503:PHE:O	1:B:506:VAL:HG22	1.94	0.66
1:B:467:ASN:HD22	1:B:469:SER:H	1.43	0.66
1:B:369:TYR:OH	1:B:459:GLU:HG2	1.96	0.66
1:A:231:ARG:HG3	2:A:776:HOH:O	1.95	0.66
1:B:509:ARG:HH11	1:B:509:ARG:HG3	1.60	0.65
1:A:526:GLN:HG3	1:A:527:GLN:N	2.11	0.64
1:B:148:VAL:HG21	1:B:510:GLN:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ARG:O	1:A:314:GLU:HG3	2.00	0.61
1:A:499:VAL:O	1:A:502:VAL:HG13	2.00	0.61
1:B:304:THR:HB	1:B:307:GLU:HG3	1.81	0.61
1:A:117:HIS:CD2	1:A:499:VAL:HG13	2.35	0.61
1:A:129:ARG:HD3	2:A:780:HOH:O	2.01	0.60
1:A:471:TYR:O	1:A:475:LEU:HB2	2.01	0.60
1:B:437:TYR:HB2	1:B:443:ILE:HD11	1.83	0.59
1:A:164:VAL:HG23	1:A:165:THR:HG23	1.84	0.58
1:B:45:LEU:N	1:B:326:ASN:HD21	1.91	0.58
1:A:117:HIS:HB3	1:A:125:TYR:CE2	2.39	0.57
1:B:526:GLN:C	1:B:528:HIS:H	2.12	0.57
1:A:499:VAL:HA	1:A:502:VAL:CG1	2.34	0.57
1:A:233:LEU:O	1:A:237:LYS:HB3	2.05	0.56
1:A:511:ARG:O	1:A:515:GLU:HG2	2.05	0.56
1:A:182:ARG:O	1:A:186:GLU:HB2	2.05	0.56
1:B:116:TYR:HD2	1:B:449:ASP:HB3	1.71	0.56
1:A:455:TYR:HA	1:A:461:GLU:CD	2.31	0.55
1:A:246:MET:HG3	1:A:333:GLY:HA2	1.88	0.55
1:A:459:GLU:HG3	1:A:463:ARG:HH11	1.72	0.55
1:A:145:LYS:HZ1	1:A:165:THR:HG22	1.69	0.54
1:B:125:TYR:CG	1:B:499:VAL:HG21	2.43	0.54
1:B:49:GLU:HG3	1:B:173:ALA:HB2	1.90	0.54
1:B:72:ARG:HH11	1:B:72:ARG:HG3	1.72	0.53
1:A:154:ARG:HD2	1:A:154:ARG:N	2.21	0.53
1:A:410:SER:O	1:A:422:LYS:NZ	2.42	0.53
1:B:436:MET:HA	1:B:441:MET:HE3	1.90	0.53
1:B:306:ASP:HA	1:B:309:VAL:HG13	1.91	0.53
1:A:475:LEU:HG	1:A:480:LEU:HD23	1.90	0.53
1:B:129:ARG:HB3	1:B:134:LYS:HB3	1.90	0.53
1:A:459:GLU:O	1:A:463:ARG:HD3	2.08	0.53
1:B:305:GLU:O	1:B:309:VAL:HG12	2.10	0.52
1:B:304:THR:HG22	1:B:306:ASP:N	2.23	0.52
1:A:236:ASN:O	1:A:240:GLU:HA	2.09	0.52
1:B:72:ARG:HG3	1:B:72:ARG:NH1	2.24	0.52
1:B:128:ASP:OD2	1:B:132:ARG:NH2	2.42	0.52
1:A:114:LEU:HD21	1:A:123:SER:HB3	1.92	0.52
1:B:113:LEU:HD13	1:B:449:ASP:O	2.10	0.52
1:B:509:ARG:HG3	1:B:509:ARG:NH1	2.25	0.51
1:A:84:PHE:O	1:A:106:HIS:HA	2.10	0.51
1:B:250:LEU:HD13	1:B:353:VAL:HG23	1.93	0.51
1:B:255:ALA:HA	1:B:296:TYR:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:LEU:HG	1:B:480:LEU:HD23	1.93	0.50
1:B:438:ARG:HA	1:B:482:PRO:HA	1.93	0.50
1:A:171:PHE:CE1	1:A:176:VAL:HG21	2.47	0.50
1:B:271:PRO:HB3	1:B:520:LEU:HD22	1.93	0.50
1:A:387:ARG:HG3	1:B:441:MET:HE1	1.94	0.49
1:A:527:GLN:O	1:A:528:HIS:O	2.29	0.49
1:A:18:TRP:CE2	1:A:181:ARG:HG3	2.47	0.49
1:B:29:GLN:NE2	2:B:709:HOH:O	2.44	0.49
1:A:125:TYR:CG	1:A:499:VAL:HG11	2.47	0.49
1:B:467:ASN:H	1:B:470:ASN:ND2	2.08	0.49
1:B:377:ASP:OD1	1:B:377:ASP:C	2.56	0.49
1:B:216:GLY:HA2	2:B:698:HOH:O	2.12	0.49
1:A:18:TRP:CZ2	1:A:181:ARG:HG3	2.48	0.49
1:B:526:GLN:C	1:B:528:HIS:N	2.71	0.49
1:A:310:ARG:HD2	1:A:314:GLU:OE2	2.13	0.48
1:A:120:ILE:HD12	1:A:492:MET:HE1	1.96	0.48
1:B:53:PRO:HD3	1:B:111:PHE:CE1	2.48	0.47
1:A:276:ILE:HG21	1:A:315:MET:CE	2.45	0.47
1:B:304:THR:HG22	1:B:307:GLU:H	1.78	0.47
1:B:467:ASN:ND2	1:B:469:SER:H	2.09	0.47
1:A:145:LYS:HZ2	1:A:165:THR:HG22	1.79	0.47
1:B:128:ASP:O	1:B:132:ARG:HG3	2.13	0.47
1:B:136:VAL:HG13	1:B:136:VAL:O	2.15	0.47
1:B:150:LEU:HD22	1:B:271:PRO:HG2	1.97	0.47
1:B:274:SER:HB2	1:B:285:LYS:HB3	1.96	0.47
1:A:387:ARG:HA	1:A:387:ARG:HE	1.79	0.47
1:A:113:LEU:CD2	1:A:113:LEU:N	2.55	0.46
1:A:207:ASN:ND2	2:A:669:HOH:O	2.47	0.46
1:A:384:LEU:HD23	1:B:441:MET:HE2	1.97	0.46
1:A:9:LEU:HD11	1:A:37:LEU:HD13	1.98	0.45
1:A:36:LEU:C	1:A:36:LEU:HD23	2.41	0.45
1:A:112:GLY:O	1:A:144:TYR:HE2	1.99	0.45
1:B:526:GLN:O	1:B:528:HIS:N	2.48	0.45
1:B:145:LYS:HA	1:B:510:GLN:HG2	1.99	0.45
1:A:229:GLY:HA2	1:A:348:THR:OG1	2.16	0.45
1:B:164:VAL:O	1:B:164:VAL:HG23	2.16	0.45
1:B:71:MET:HB2	1:B:76:ALA:HB3	1.99	0.45
1:A:503:PHE:O	1:A:506:VAL:CG1	2.64	0.45
1:A:503:PHE:O	1:A:506:VAL:HG13	2.17	0.45
1:B:305:GLU:O	1:B:309:VAL:CG1	2.65	0.45
1:A:158:ARG:HD2	1:A:162:SER:OG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:VAL:HG11	1:B:517:LEU:HD21	1.99	0.45
1:B:304:THR:HG22	1:B:306:ASP:H	1.83	0.45
1:A:218:VAL:O	1:A:218:VAL:HG23	2.17	0.44
1:A:125:TYR:O	1:A:129:ARG:HG3	2.17	0.44
1:A:68:ASP:O	1:A:72:ARG:HG2	2.18	0.44
1:A:237:LYS:HD3	2:A:677:HOH:O	2.18	0.44
1:A:329:ARG:HH11	1:A:329:ARG:CB	2.28	0.44
1:A:437:TYR:HB2	1:A:443:ILE:HD11	2.00	0.44
1:B:235:ILE:HG23	1:B:236:ASN:N	2.32	0.44
1:A:153:ASN:ND2	2:A:591:HOH:O	2.51	0.44
1:A:49:GLU:CG	1:A:173:ALA:HB2	2.41	0.43
1:A:436:MET:HA	1:A:441:MET:HE3	2.00	0.43
1:A:191:ARG:HD3	2:A:657:HOH:O	2.17	0.43
1:B:460:GLU:O	1:B:460:GLU:CD	2.61	0.43
1:B:512:ASN:OD1	1:B:512:ASN:C	2.61	0.43
1:A:274:SER:HB2	1:A:285:LYS:HB3	1.99	0.43
1:B:53:PRO:HD3	1:B:111:PHE:CZ	2.53	0.43
1:A:5:ILE:HG23	1:A:222:ASP:HB2	2.01	0.43
1:B:157:ARG:NH1	2:B:741:HOH:O	2.52	0.43
1:B:446:PRO:HB2	1:B:448:SER:O	2.18	0.43
1:B:155:SER:HB2	1:B:520:LEU:HA	2.01	0.43
1:A:305:GLU:O	1:A:309:VAL:HG23	2.19	0.43
1:A:366:ALA:HA	1:A:458:PHE:CZ	2.54	0.43
1:B:5:ILE:HG23	1:B:222:ASP:HB2	2.00	0.42
1:A:53:PRO:HD3	1:A:111:PHE:CE1	2.54	0.42
1:B:114:LEU:HD22	1:B:122:LEU:HB3	2.02	0.42
1:A:276:ILE:HG21	1:A:315:MET:HE1	2.01	0.42
1:B:118:GLU:O	1:B:119:GLN:HB2	2.18	0.42
1:B:122:LEU:HD11	1:B:503:PHE:CE1	2.55	0.42
1:B:467:ASN:N	1:B:470:ASN:HD22	2.12	0.42
1:A:145:LYS:CD	1:A:509:ARG:HG2	2.50	0.42
1:A:494:GLN:H	1:A:494:GLN:HG2	1.45	0.42
1:A:150:LEU:HD22	1:A:271:PRO:HG2	2.00	0.42
1:A:235:ILE:HG23	1:A:236:ASN:N	2.35	0.42
1:B:229:GLY:HA2	1:B:348:THR:OG1	2.19	0.42
1:A:132:ARG:HH12	1:A:134:LYS:HG3	1.85	0.42
1:A:457:ASN:OD1	1:A:457:ASN:C	2.63	0.42
1:B:170:HIS:CE1	1:B:287:PRO:HD2	2.54	0.42
1:A:250:LEU:HD13	1:A:353:VAL:HG23	2.02	0.42
1:A:86:ASN:HB3	1:A:98:ARG:NH2	2.35	0.42
1:A:436:MET:HG2	1:A:441:MET:CE	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:GLU:O	1:B:71:MET:HG2	2.20	0.41
1:A:86:ASN:HA	1:A:105:ASP:OD2	2.21	0.41
1:B:247:SER:HA	1:B:250:LEU:O	2.19	0.41
1:B:468:ASN:HB3	2:B:633:HOH:O	2.19	0.41
1:A:463:ARG:NH2	1:B:464:ASN:OD1	2.53	0.41
1:B:54:ASN:HD22	1:B:461:GLU:CD	2.28	0.41
1:B:146:GLU:HB2	1:B:147:PRO:HD3	2.03	0.41
1:A:65:ILE:HA	1:A:66:PRO:HD3	1.91	0.41
1:A:127:PHE:CE1	1:A:481:VAL:HB	2.55	0.41
1:A:149:ILE:O	1:A:154:ARG:HG2	2.21	0.41
1:A:106:HIS:CD2	1:A:106:HIS:C	2.99	0.41
1:A:127:PHE:CE2	1:A:482:PRO:HB2	2.56	0.41
1:A:329:ARG:HB2	1:A:329:ARG:NH1	2.32	0.41
1:B:137:GLU:HA	1:B:138:PRO:HD3	1.92	0.41
1:B:278:MET:HG3	1:B:296:TYR:CE1	2.56	0.41
1:B:160:ASP:OD1	1:B:160:ASP:C	2.64	0.41
1:A:137:GLU:OE2	1:A:507:LYS:NZ	2.54	0.40
1:B:289:LEU:O	1:B:291:ARG:HD2	2.21	0.40
1:B:410:SER:O	1:B:422:LYS:NZ	2.50	0.40
1:B:381:ASN:HA	1:B:382:PRO:HD3	1.97	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	519/550 (94%)	506 (98%)	13 (2%)	0	100	100
1	B	520/550 (94%)	500 (96%)	19 (4%)	1 (0%)	43	55
All	All	1039/1100 (94%)	1006 (97%)	32 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	527	GLN

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	441/463 (95%)	416 (94%)	25 (6%)	18	27
1	B	440/463 (95%)	413 (94%)	27 (6%)	17	24
All	All	881/926 (95%)	829 (94%)	52 (6%)	18	26

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	29	GLN
1	A	99	GLU
1	A	113	LEU
1	A	136	VAL
1	A	211	VAL
1	A	233	LEU
1	A	246	MET
1	A	256	VAL
1	A	291	ARG
1	A	310	ARG
1	A	329	ARG
1	A	373	LYS
1	A	376	PRO
1	A	380	LEU
1	A	387	ARG
1	A	425	ARG
1	A	448	SER
1	A	475	LEU
1	A	494	GLN
1	A	497	GLU
1	A	499	VAL
1	A	502	VAL

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Mol	Chain	Res	Type
1	A	506	VAL
1	A	526	GLN
1	B	2	SER
1	B	114	LEU
1	B	119	GLN
1	B	132	ARG
1	B	136	VAL
1	B	148	VAL
1	B	157	ARG
1	B	164	VAL
1	B	178	ASP
1	B	211	VAL
1	B	217	ARG
1	B	225	VAL
1	B	233	LEU
1	B	289	LEU
1	B	291	ARG
1	B	304	THR
1	B	309	VAL
1	B	376	PRO
1	B	380	LEU
1	B	390	ARG
1	B	460	GLU
1	B	461	GLU
1	B	464	ASN
1	B	474	VAL
1	B	475	LEU
1	B	511	ARG
1	B	514	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	153	ASN
1	A	166	ASN
1	A	199	HIS
1	A	205	ASN
1	A	207	ASN
1	A	494	GLN
1	A	510	GLN
1	A	526	GLN

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Mol	Chain	Res	Type
1	B	29	GLN
1	B	38	GLN
1	B	119	GLN
1	B	124	HIS
1	B	166	ASN
1	B	199	HIS
1	B	205	ASN
1	B	207	ASN
1	B	323	GLN
1	B	326	ASN
1	B	457	ASN
1	B	467	ASN
1	B	470	ASN
1	B	494	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	523/550 (95%)	0.03	13 (2%) 58 60	19, 34, 58, 96	0
1	B	524/550 (95%)	0.16	26 (4%) 34 35	21, 37, 66, 96	0
All	All	1047/1100 (95%)	0.09	39 (3%) 45 48	19, 35, 64, 96	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	ALA	5.2
1	A	528	HIS	4.8
1	B	447	ALA	4.3
1	A	455	TYR	4.0
1	A	2	SER	3.8
1	B	455	TYR	3.7
1	B	2	SER	3.6
1	A	113	LEU	3.6
1	B	42	ILE	3.5
1	B	456	GLY	3.4
1	B	113	LEU	3.4
1	B	112	GLY	3.3
1	B	525	ARG	3.2
1	A	463	ARG	3.1
1	B	529	GLY	3.1
1	A	449	ASP	3.1
1	B	3	GLY	3.0
1	B	450	ASP	3.0
1	B	463	ARG	2.8
1	B	501	GLU	2.8
1	B	115	LYS	2.7
1	B	528	HIS	2.6
1	A	119	GLN	2.5
1	A	450	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	527	GLN	2.4
1	A	115	LYS	2.4
1	B	449	ASP	2.4
1	B	40	PRO	2.4
1	B	457	ASN	2.3
1	B	509	ARG	2.3
1	A	3	GLY	2.3
1	B	116	TYR	2.3
1	B	460	GLU	2.2
1	B	72	ARG	2.2
1	B	511	ARG	2.1
1	B	514	LEU	2.1
1	A	461	GLU	2.1
1	B	505	ALA	2.1
1	B	527	GLN	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.