



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:01 AM UTC

PDB ID : 3G4O / pdb_00003g4o
Title : Crystal structure of the activated aerolysin mutant H132N
Authors : Pernot, L.; Schiltz, M.; van der Goot, G.
Deposited on : 2009-02-04
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

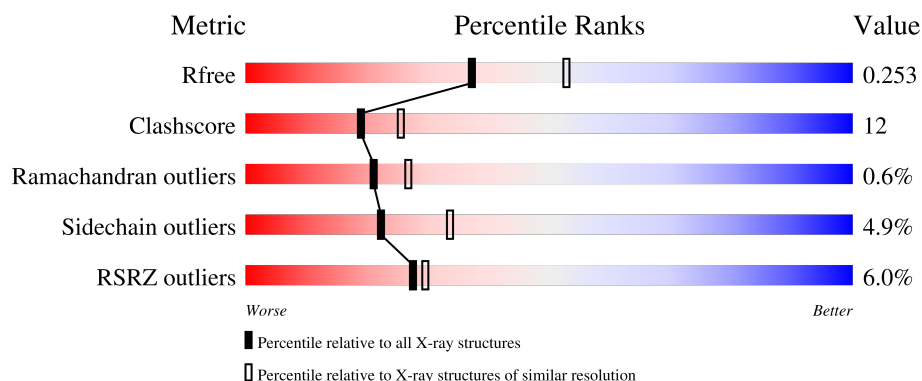
1 Overall quality at a glance

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	470	9% 67% 25% 7%
1	B	470	3% 71% 23% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7165 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 Aerolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3448	2180	591	668	9			
1	B	451	Total	C	N	O	S	0	0	0
			3530	2231	606	684	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	ASN	HIS	engineered mutation	UNP P09167
B	132	ASN	HIS	engineered mutation	UNP P09167

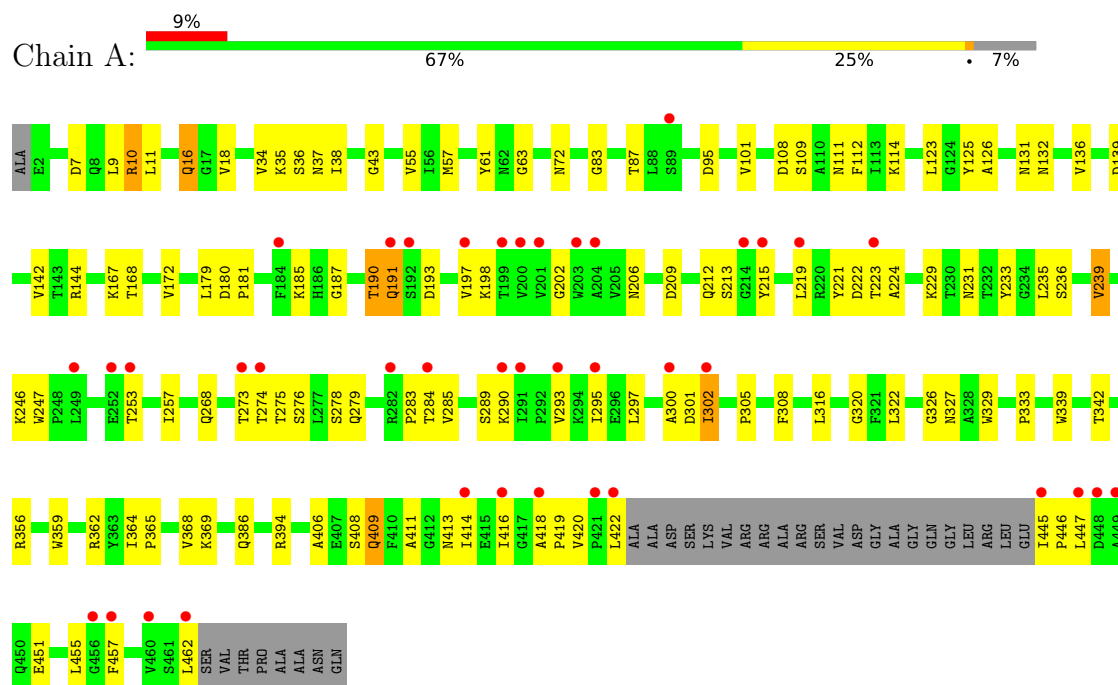
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	109	Total	O	0	0
			109	109		
2	B	78	Total	O	0	0
			78	78		

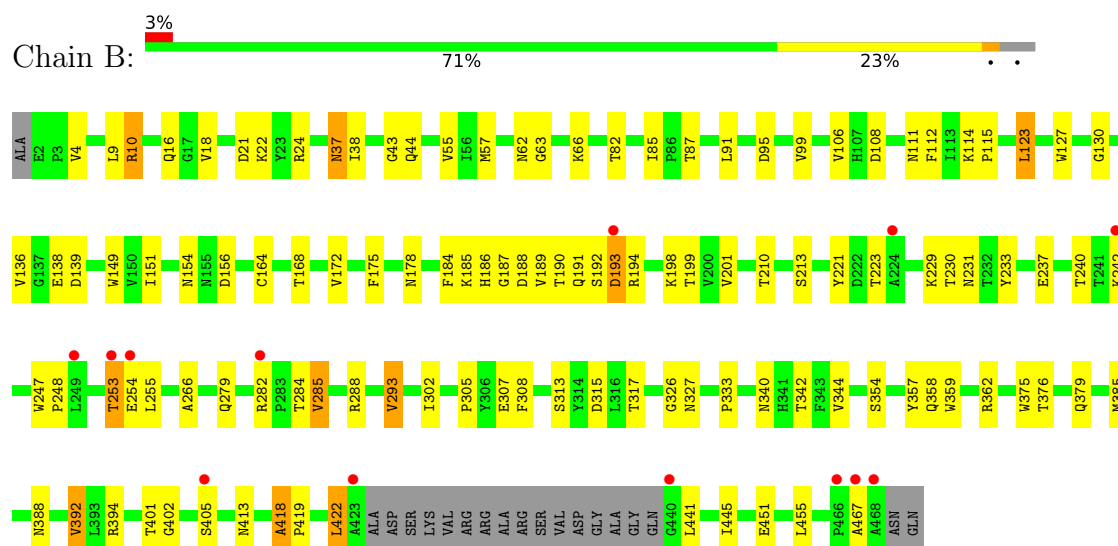
3 Residue-property plots

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: Aerolysin



• Molecule 1: Aerolysin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.98Å 69.31Å 165.23Å 90.00° 109.00° 90.00°	Depositor
Resolution (Å)	55.47 – 2.30 55.47 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.2 (55.47-2.30) 95.2 (55.47-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.205 , 0.260 0.200 , 0.253	Depositor DCC
R_{free} test set	2186 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.874	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7165	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.03% 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	0.38	0/3544	0.78	2/4837 (0.0%)
1	B	0.36	0/3627	0.76	2/4951 (0.0%)
All	All	0.37	0/7171	0.77	4/9788 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	418	ALA	CA-C-N	5.32	125.24	119.76
1	B	418	ALA	C-N-CA	5.32	125.24	119.76
1	A	247	TRP	CA-C-N	5.25	125.54	119.92
1	A	247	TRP	C-N-CA	5.25	125.54	119.92

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	3448	0	3276	92	0
1	B	3530	0	3363	73	0
2	A	109	0	0	1	0
2	B	78	0	0	1	0
All	All	7165	0	6639	160	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 12.

All (160) 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:126:ALA:O	1:A:168:THR:HG23	1.71	0.90
1:A:229:LYS:HZ2	1:A:231:ASN:HD21	1.20	0.87
1:A:253:THR:HG22	1:A:300:ALA:HB1	1.63	0.81
1:A:198:LYS:HB3	1:A:297:LEU:HD12	1.61	0.81
1:B:317:THR:OG1	1:B:342:THR:HG22	1.82	0.80
1:A:112:PHE:HZ	1:A:172:VAL:HG11	1.46	0.79
1:A:125:TYR:HB3	1:A:168:THR:HG21	1.65	0.78
1:A:202:GLY:HA3	1:A:445:ILE:HG22	1.66	0.78
1:A:198:LYS:HB2	1:A:455:LEU:HD23	1.66	0.78
1:A:229:LYS:NZ	1:A:231:ASN:HD21	1.83	0.77
1:A:191:GLN:O	1:A:302:ILE:HA	1.85	0.75
1:B:282:ARG:NH2	1:B:467:ALA:H	1.84	0.75
1:B:344:VAL:HG23	2:B:542:HOH:O	1.87	0.74
1:B:112:PHE:HE2	1:B:151:ILE:HD11	1.54	0.73
1:A:289:SER:HA	1:A:422:LEU:H	1.54	0.71
1:A:215:TYR:O	1:A:283:PRO:HD2	1.91	0.71
1:A:447:LEU:HD11	1:A:462:LEU:HB3	1.73	0.69
1:A:43:GLY:HA3	1:B:10:ARG:NH2	2.10	0.67
1:A:213:SER:HB2	1:A:284:THR:HG23	1.77	0.67
1:B:327:ASN:HD21	1:B:333:PRO:HD2	1.60	0.67
1:B:189:VAL:HG11	1:B:192:SER:HB2	1.77	0.67
1:A:253:THR:OG1	1:A:302:ILE:HD12	1.96	0.66
1:B:359:TRP:NE1	1:B:362:ARG:HH21	1.94	0.65
1:B:178:ASN:ND2	1:B:242:LYS:HD2	2.11	0.65
1:A:198:LYS:HE2	1:A:451:GLU:OE2	1.97	0.65
1:A:290:LYS:HZ2	1:A:420:VAL:HB	1.61	0.64
1:B:91:LEU:HB2	1:B:394:ARG:HE	1.61	0.64
1:A:112:PHE:CZ	1:A:172:VAL:HG11	2.32	0.64
1:A:302:ILE:N	1:A:302:ILE:HD13	2.15	0.62
1:A:219:LEU:HB3	1:A:414:ILE:HD11	1.83	0.60
1:B:114:LYS:HE2	1:B:138:GLU:HG2	1.83	0.59
1:A:187:GLY:HA3	1:A:305:PRO:HG2	1.82	0.59
1:A:223:THR:O	1:A:274:THR:HA	2.02	0.58
1:B:282:ARG:HH22	1:B:467:ALA:H	1.49	0.58
1:A:11:LEU:HD21	1:A:72:ASN:HD22	1.68	0.58
1:A:329:TRP:CE2	1:A:339:TRP:HZ2	2.21	0.58
1:B:178:ASN:HD21	1:B:242:LYS:H	1.52	0.58
1:A:302:ILE:HD13	1:A:302:ILE:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LYS:HE3	1:A:268:GLN:O	2.05	0.57
1:B:229:LYS:NZ	1:B:231:ASN:HD21	2.02	0.57
1:A:293:VAL:HG12	1:A:416:ILE:HG22	1.86	0.56
1:A:219:LEU:O	1:A:278:SER:HA	2.06	0.56
1:B:87:THR:HG23	1:B:87:THR:O	2.05	0.56
1:A:368:VAL:O	1:A:368:VAL:HG23	2.05	0.56
1:A:35:LYS:HE3	1:A:63:GLY:O	2.04	0.56
1:A:197:VAL:HG23	1:A:198:LYS:N	2.20	0.55
1:B:24:ARG:O	1:B:24:ARG:HD3	2.07	0.55
1:A:219:LEU:CB	1:A:414:ILE:HD11	2.38	0.54
1:B:178:ASN:HD21	1:B:242:LYS:N	2.06	0.54
1:B:288:ARG:C	1:B:422:LEU:HD22	2.33	0.54
1:A:109:SER:O	1:A:114:LYS:HB2	2.08	0.54
1:B:108:ASP:CG	1:B:111:ASN:HB2	2.33	0.53
1:A:329:TRP:CE2	1:A:339:TRP:CZ2	2.96	0.53
1:A:445:ILE:HD11	1:A:462:LEU:HD22	1.89	0.53
1:A:224:ALA:HB3	1:A:409:GLN:NE2	2.24	0.53
1:B:285:VAL:HG11	1:B:441:LEU:HD11	1.90	0.53
1:A:236:SER:HA	1:A:239:VAL:HG13	1.91	0.52
1:A:219:LEU:HD22	1:A:295:ILE:HG21	1.92	0.52
1:A:219:LEU:HD22	1:A:295:ILE:HD13	1.92	0.52
1:A:16:GLN:O	1:A:18:VAL:HG23	2.09	0.52
1:A:221:TYR:CZ	1:A:411:ALA:HB3	2.45	0.52
1:B:112:PHE:CE2	1:B:151:ILE:HD11	2.39	0.51
1:B:190:THR:HG22	1:B:191:GLN:OE1	2.11	0.51
1:A:212:GLN:O	1:A:284:THR:HA	2.10	0.51
1:A:101:VAL:HG21	1:A:235:LEU:HD22	1.93	0.51
1:A:57:MET:HE2	1:A:61:TYR:CG	2.46	0.51
1:B:187:GLY:HA3	1:B:305:PRO:HG2	1.93	0.50
1:A:297:LEU:HB3	1:A:457:PHE:CZ	2.46	0.50
1:B:37:ASN:HD22	1:B:37:ASN:H	1.60	0.50
1:A:359:TRP:CD1	1:A:362:ARG:HH21	2.30	0.50
1:A:289:SER:HA	1:A:422:LEU:N	2.26	0.49
1:A:327:ASN:HD22	1:A:329:TRP:H	1.60	0.49
1:B:114:LYS:HB3	1:B:115:PRO:HD3	1.94	0.49
1:B:21:ASP:O	1:B:22:LYS:HB2	2.12	0.49
1:B:376:THR:HB	1:B:385:MET:HE2	1.94	0.49
1:B:359:TRP:NE1	1:B:362:ARG:NH2	2.60	0.49
1:A:359:TRP:NE1	1:A:362:ARG:HH21	2.11	0.49
1:A:221:TYR:O	1:A:276:SER:HA	2.13	0.49
1:A:451:GLU:O	1:A:455:LEU:HD13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:PHE:HB2	1:B:308:PHE:CE2	2.48	0.48
1:A:131:ASN:HD21	1:A:167:LYS:NZ	2.10	0.48
1:A:9:LEU:HD13	1:A:38:ILE:HG12	1.95	0.48
1:A:43:GLY:HA3	1:B:10:ARG:HH21	1.78	0.48
1:B:112:PHE:HE2	1:B:151:ILE:CD1	2.23	0.48
1:B:189:VAL:CG1	1:B:192:SER:HB2	2.42	0.48
1:A:297:LEU:HB3	1:A:457:PHE:CE2	2.48	0.48
1:B:247:TRP:CD1	1:B:248:PRO:HD2	2.49	0.48
1:B:315:ASP:OD1	1:B:344:VAL:HG12	2.13	0.48
1:B:221:TYR:CD2	1:B:223:THR:HG23	2.49	0.47
1:B:354:SER:O	1:B:358:GLN:HG3	2.15	0.47
1:B:95:ASP:CG	1:B:233:TYR:HD2	2.23	0.47
1:B:237:GLU:HA	1:B:266:ALA:HB3	1.96	0.47
1:B:359:TRP:CD1	1:B:362:ARG:HH21	2.32	0.47
1:A:197:VAL:CG2	1:A:198:LYS:N	2.78	0.47
1:A:198:LYS:HE2	1:A:451:GLU:CD	2.39	0.47
1:A:327:ASN:HD21	1:A:333:PRO:HD2	1.80	0.47
1:A:95:ASP:OD2	1:A:233:TYR:HD2	1.97	0.47
1:B:230:THR:O	1:B:402:GLY:HA3	2.16	0.46
1:B:302:ILE:O	1:B:405:SER:HA	2.15	0.46
1:A:179:LEU:HD11	1:A:308:PHE:HB2	1.98	0.46
1:A:394:ARG:HD2	2:A:530:HOH:O	2.15	0.46
1:B:253:THR:HG22	1:B:255:LEU:HG	1.97	0.46
1:A:246:LYS:HA	1:A:257:ILE:O	2.16	0.45
1:B:198:LYS:HE2	1:B:451:GLU:OE1	2.17	0.45
1:B:279:GLN:OE1	1:B:413:ASN:HA	2.16	0.45
1:B:85:ILE:HG13	1:B:359:TRP:CD1	2.51	0.45
1:B:229:LYS:HZ2	1:B:231:ASN:HD21	1.62	0.45
1:A:418:ALA:HA	1:A:419:PRO:HD2	1.83	0.45
1:A:34:VAL:HB	1:A:37:ASN:HD22	1.82	0.45
1:A:301:ASP:HB2	1:A:406:ALA:O	2.16	0.45
1:B:57:MET:SD	1:B:66:LYS:HD3	2.57	0.45
1:A:87:THR:HG22	1:A:356:ARG:NH2	2.32	0.45
1:B:188:ASP:OD1	1:B:188:ASP:N	2.49	0.45
1:A:222:ASP:HA	1:A:275:THR:O	2.16	0.44
1:B:127:TRP:CE2	1:B:164:CYS:HA	2.52	0.44
1:A:172:VAL:HG12	1:A:316:LEU:HD12	1.98	0.44
1:A:409:GLN:HE21	1:A:409:GLN:HB2	1.64	0.44
1:B:149:TRP:HB2	1:B:172:VAL:CG1	2.48	0.44
1:B:194:ARG:O	1:B:194:ARG:HG3	2.17	0.44
1:A:83:GLY:HA2	1:A:386:GLN:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:HH11	1:A:144:ARG:HG3	1.83	0.44
1:A:445:ILE:HA	1:A:446:PRO:HD2	1.89	0.44
1:B:357:TYR:C	1:B:357:TYR:CD1	2.96	0.44
1:A:445:ILE:O	1:A:445:ILE:HD12	2.18	0.44
1:B:192:SER:O	1:B:193:ASP:HB3	2.18	0.43
1:A:185:LYS:HE3	1:A:185:LYS:HB3	1.86	0.43
1:B:293:VAL:HG21	1:B:445:ILE:CD1	2.48	0.43
1:A:359:TRP:NE1	1:A:362:ARG:NH2	2.66	0.43
1:A:185:LYS:CD	1:B:185:LYS:HD3	2.49	0.43
1:A:7:ASP:HB2	1:B:44:GLN:HB2	1.99	0.43
1:B:130:GLY:HA3	1:B:139:ASP:O	2.19	0.43
1:B:186:HIS:HD2	1:B:187:GLY:O	2.01	0.43
1:A:108:ASP:CG	1:A:111:ASN:HB2	2.44	0.43
1:A:190:THR:HB	1:A:191:GLN:OE1	2.19	0.43
1:B:175:PHE:HA	1:B:313:SER:O	2.18	0.43
1:B:9:LEU:HD13	1:B:38:ILE:HG12	2.01	0.42
1:B:123:LEU:HD12	1:B:123:LEU:HA	1.77	0.42
1:B:307:GLU:HG3	1:B:401:THR:HG22	2.01	0.42
1:A:212:GLN:NE2	1:A:215:TYR:CE1	2.87	0.42
1:B:114:LYS:CB	1:B:115:PRO:HD3	2.50	0.42
1:A:206:ASN:CG	1:A:212:GLN:HB2	2.45	0.42
1:B:57:MET:O	1:B:63:GLY:HA2	2.20	0.42
1:B:106:VAL:HG11	1:B:172:VAL:HG11	2.02	0.42
1:A:57:MET:O	1:A:63:GLY:HA2	2.20	0.42
1:B:418:ALA:HA	1:B:419:PRO:HD3	1.87	0.41
1:B:178:ASN:HA	1:B:240:THR:O	2.20	0.41
1:A:224:ALA:O	1:A:408:SER:HA	2.19	0.41
1:B:154:ASN:OD1	1:B:156:ASP:HB2	2.20	0.41
1:A:168:THR:HG22	1:A:320:GLY:HA3	2.02	0.41
1:A:224:ALA:HA	1:A:273:THR:O	2.20	0.41
1:A:180:ASP:HA	1:A:181:PRO:HD2	1.85	0.41
1:A:10:ARG:NH2	1:B:43:GLY:HA3	2.35	0.41
1:A:132:ASN:HB3	1:A:139:ASP:CG	2.45	0.41
1:A:253:THR:HG21	1:A:302:ILE:HG23	2.02	0.41
1:A:279:GLN:HG2	1:A:413:ASN:HA	2.02	0.41
1:B:375:TRP:CZ2	1:B:379:GLN:HG3	2.55	0.41
1:B:213:SER:HB3	1:B:284:THR:HG23	2.03	0.41
1:B:388:ASN:O	1:B:392:VAL:HG13	2.21	0.40
1:B:16:GLN:O	1:B:18:VAL:HG23	2.21	0.40
1:A:364:ILE:HA	1:A:365:PRO:HD2	1.83	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	435/470 (93%)	407 (94%)	26 (6%)	2 (0%)	24	31
1	B	447/470 (95%)	425 (95%)	19 (4%)	3 (1%)	18	23
All	All	882/940 (94%)	832 (94%)	45 (5%)	5 (1%)	21	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	253	THR
1	B	193	ASP
1	A	209	ASP
1	A	326	GLY
1	B	326	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/392 (95%)	354 (95%)	17 (5%)	24	36
1	B	379/392 (97%)	359 (95%)	20 (5%)	20	30
All	All	750/784 (96%)	713 (95%)	37 (5%)	22	34

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG

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Mol	Chain	Res	Type
1	A	16	GLN
1	A	36	SER
1	A	55	VAL
1	A	123	LEU
1	A	136	VAL
1	A	142	VAL
1	A	190	THR
1	A	191	GLN
1	A	193	ASP
1	A	239	VAL
1	A	285	VAL
1	A	302	ILE
1	A	322	LEU
1	A	342	THR
1	A	369	LYS
1	A	409	GLN
1	B	4	VAL
1	B	10	ARG
1	B	37	ASN
1	B	55	VAL
1	B	62	ASN
1	B	82	THR
1	B	99	VAL
1	B	123	LEU
1	B	136	VAL
1	B	168	THR
1	B	199	THR
1	B	201	VAL
1	B	210	THR
1	B	254	GLU
1	B	285	VAL
1	B	293	VAL
1	B	340	ASN
1	B	392	VAL
1	B	422	LEU
1	B	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	62	ASN

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Mol	Chain	Res	Type
1	A	72	ASN
1	A	131	ASN
1	A	134	GLN
1	A	212	GLN
1	A	226	ASN
1	A	231	ASN
1	A	279	GLN
1	A	327	ASN
1	A	340	ASN
1	A	387	ASN
1	A	409	GLN
1	B	37	ASN
1	B	62	ASN
1	B	178	ASN
1	B	186	HIS
1	B	226	ASN
1	B	231	ASN
1	B	269	ASN
1	B	327	ASN
1	B	374	ASN
1	B	378	GLN
1	B	379	GLN
1	B	387	ASN
1	B	409	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	439/470 (93%)	0.43	40 (9%) 15 16	21, 51, 132, 167	0
1	B	451/470 (95%)	0.21	13 (2%) 53 56	31, 50, 85, 124	0
All	All	890/940 (94%)	0.32	53 (5%) 27 29	21, 50, 112, 167	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	468	ALA	7.2
1	A	291	ILE	4.6
1	B	440	GLY	4.2
1	A	462	LEU	4.1
1	A	249	LEU	4.0
1	A	253	THR	3.9
1	B	253	THR	3.9
1	A	199	THR	3.7
1	A	89	SER	3.4
1	A	302	ILE	3.3
1	A	422	LEU	3.2
1	A	457	PHE	3.1
1	A	418	ALA	3.1
1	A	184	PHE	2.9
1	A	456	GLY	2.8
1	A	204	ALA	2.8
1	A	200	VAL	2.8
1	A	191	GLN	2.7
1	A	290	LYS	2.7
1	B	249	LEU	2.7
1	A	421	PRO	2.7
1	B	254	GLU	2.6
1	A	192	SER	2.6
1	A	300	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	467	ALA	2.6
1	A	460	VAL	2.6
1	A	223	THR	2.6
1	A	214	GLY	2.5
1	A	293	VAL	2.5
1	A	416	ILE	2.5
1	A	215	TYR	2.5
1	A	448	ASP	2.5
1	A	295	ILE	2.4
1	B	466	PRO	2.3
1	A	273	THR	2.3
1	A	197	VAL	2.3
1	A	447	LEU	2.3
1	B	242	LYS	2.3
1	A	284	THR	2.3
1	A	201	VAL	2.3
1	A	282	ARG	2.2
1	B	423	ALA	2.2
1	A	274	THR	2.2
1	B	405	SER	2.2
1	B	224	ALA	2.2
1	A	414	ILE	2.1
1	A	203	TRP	2.1
1	A	449	ALA	2.1
1	B	193	ASP	2.1
1	A	445	ILE	2.1
1	B	282	ARG	2.1
1	A	252	GLU	2.0
1	A	219	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.