Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 02:47 PM EDT

PDB ID	:	3G4O
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:

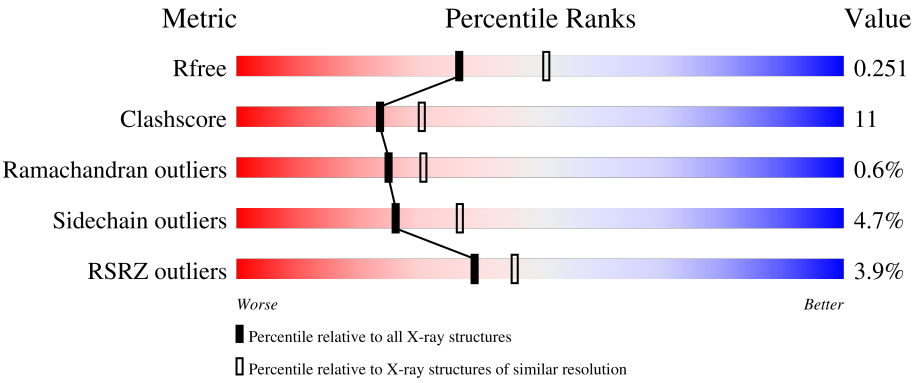
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	7% 68% 24% · 7%
1	B	470	% 73% 21% · ·

2 Entry composition (i)

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.

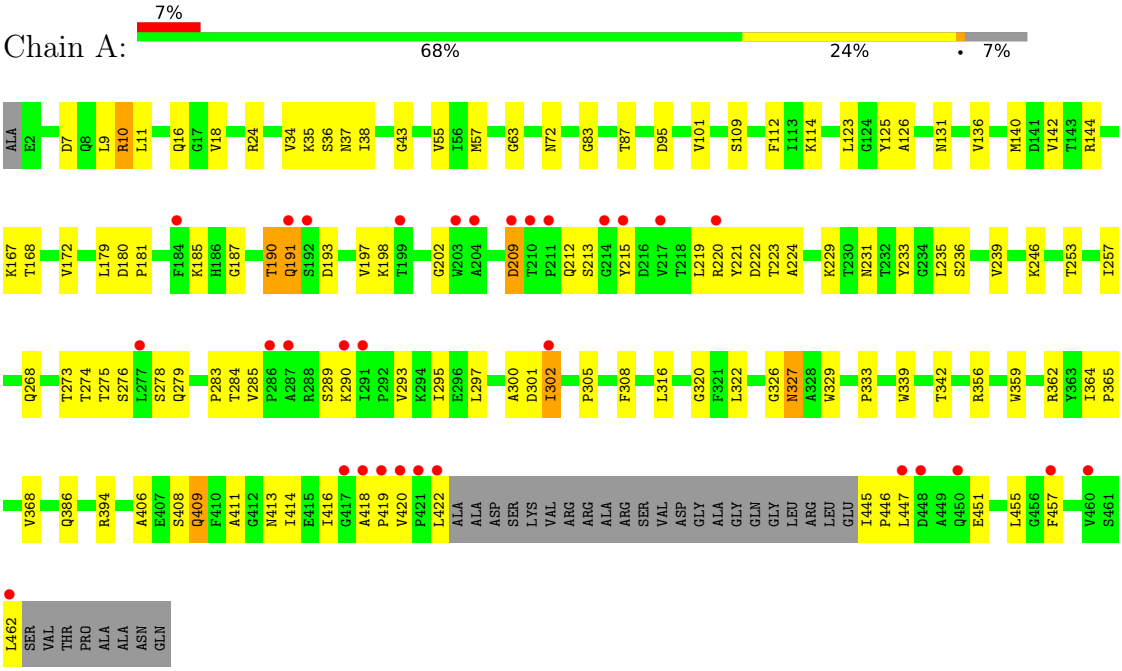
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	109	Total	O	0	0
			109	109		
2	B	78	Total	O	0	0
			78	78		

3 Residue-property plots (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.

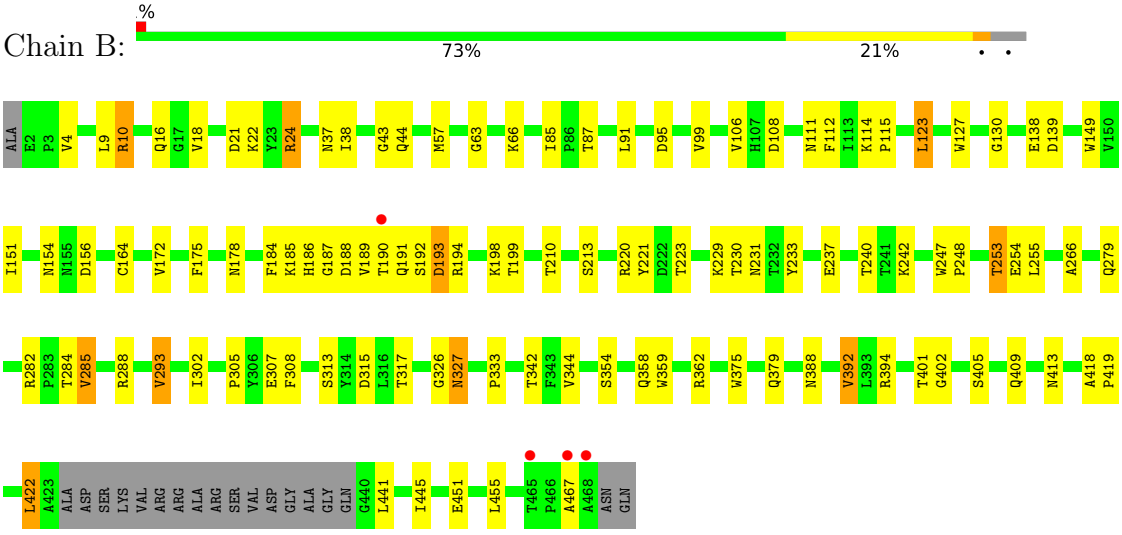
• Molecule 1: Aerolysin

Chain A:



• Molecule 1: Aerolysin

Chain B:



4 Data and refinement statistics (i)

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 55.50 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.2 (55.47-2.30) 95.2 (55.50-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.19 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.205 , 0.260 0.196 , 0.251	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)	0.30 , 45.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.31	0/3544	0.48	0/4837
1	B	0.30	0/3627	0.48	0/4951
All	All	0.31	0/7171	0.48	0/9788

There are no bond length outliers.

There are no bond angle outliers.

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	3448	0	3276	88	0
1	B	3530	0	3363	69	0
2	A	109	0	0	1	0
2	B	78	0	0	1	0
All	All	7165	0	6639	152	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 11.

All (152) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:290:LYS:HZ2	1:A:420:VAL:HB	1.55	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: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: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
1:A:197:VAL:HG23	1:A:198:LYS:N	2.20	0.57
1:A:229:LYS:HZ3	1:A:231:ASN:HD21	1.48	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:109:SER:O	1:A:114:LYS:HB2	2.08	0.54
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: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:131:ASN:HD21	1:A:167:LYS:HZ2	1.60	0.49
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:288:ARG:C	1:B:422:LEU:HD22	2.33	0.49
1:B:359:TRP:NE1	1:B:362:ARG:NH2	2.60	0.49
1:A:221:TYR:O	1:A:276:SER:HA	2.13	0.49
1:B:108:ASP:CG	1:B:111:ASN:HB2	2.33	0.48
1:A:451:GLU:O	1:A:455:LEU:HD13	2.13	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:237:GLU:HA	1:B:266:ALA:HB3	1.96	0.47
1:A:229:LYS:HZ2	1:A:231:ASN:HD21	1.58	0.47
1:A:197:VAL:CG2	1:A:198:LYS:N	2.78	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: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:B:229:LYS:HZ2	1:B:231:ASN:HD21	1.63	0.44
1:A:83:GLY:HA2	1:A:386:GLN:NE2	2.32	0.44
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:HIS:HD2	1:B:187:GLY:O	2.01	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:95:ASP:CG	1:B:233:TYR:HD2	2.23	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:198:LYS:HE2	1:A:451:GLU:CD	2.39	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: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%)	29	35
1	B	447/470 (95%)	425 (95%)	19 (4%)	3 (1%)	22	26
All	All	882/940 (94%)	832 (94%)	45 (5%)	5 (1%)	25	31

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%)	352 (95%)	19 (5%)	24	33
1	B	379/392 (97%)	363 (96%)	16 (4%)	30	42
All	All	750/784 (96%)	715 (95%)	35 (5%)	26	37

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	24	ARG
1	A	36	SER
1	A	55	VAL
1	A	123	LEU
1	A	136	VAL
1	A	140	MET
1	A	142	VAL
1	A	190	THR
1	A	191	GLN
1	A	193	ASP

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Mol	Chain	Res	Type
1	A	209	ASP
1	A	220	ARG
1	A	285	VAL
1	A	302	ILE
1	A	322	LEU
1	A	327	ASN
1	A	342	THR
1	A	409	GLN
1	B	4	VAL
1	B	10	ARG
1	B	24	ARG
1	B	99	VAL
1	B	123	LEU
1	B	199	THR
1	B	210	THR
1	B	220	ARG
1	B	254	GLU
1	B	285	VAL
1	B	293	VAL
1	B	327	ASN
1	B	392	VAL
1	B	409	GLN
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
1	A	72	ASN
1	A	131	ASN
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	388	ASN
1	A	409	GLN
1	B	37	ASN
1	B	62	ASN

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Mol	Chain	Res	Type
1	B	72	ASN
1	B	178	ASN
1	B	186	HIS
1	B	212	GLN
1	B	231	ASN
1	B	269	ASN
1	B	327	ASN
1	B	374	ASN
1	B	387	ASN
1	B	388	ASN
1	B	409	GLN
1	B	459	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.30	31 (7%) 16 21	21, 51, 132, 167	0
1	B	451/470 (95%)	-0.05	4 (0%) 84 88	31, 50, 85, 124	0
All	All	890/940 (94%)	0.13	35 (3%) 39 46	21, 50, 112, 167	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	468	ALA	10.2
1	A	460	VAL	4.2
1	A	420	VAL	4.2
1	A	291	ILE	4.1
1	A	418	ALA	3.7
1	A	462	LEU	3.6
1	A	422	LEU	3.4
1	A	421	PRO	3.4
1	A	448	ASP	3.3
1	A	220	ARG	3.3
1	A	184	PHE	3.3
1	A	277	LEU	3.2
1	A	450	GLN	3.1
1	A	191	GLN	3.1
1	A	457	PHE	3.1
1	A	286	PRO	2.8
1	A	215	TYR	2.8
1	A	217	VAL	2.8
1	A	203	TRP	2.7
1	A	287	ALA	2.6
1	A	192	SER	2.5
1	A	204	ALA	2.5
1	B	190	THR	2.4
1	A	302	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	419	PRO	2.4
1	A	417	GLY	2.3
1	A	209	ASP	2.3
1	A	447	LEU	2.3
1	A	199	THR	2.2
1	A	214	GLY	2.2
1	B	467	ALA	2.2
1	A	290	LYS	2.2
1	B	465	THR	2.2
1	A	210	THR	2.1
1	A	211	PRO	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 monosaccharides 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.