Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:44 AM GMT

PDB ID	:	3C0N
Title	:	Crystal structure of the proaerolysin mutant Y221G at 2.2 A
Authors	:	Pernot, L.; Schiltz, M.; Thurnheer, S.; Burr, S.E.; van der Goot, G.
Deposited on	:	2008-01-21
Resolution	:	2.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

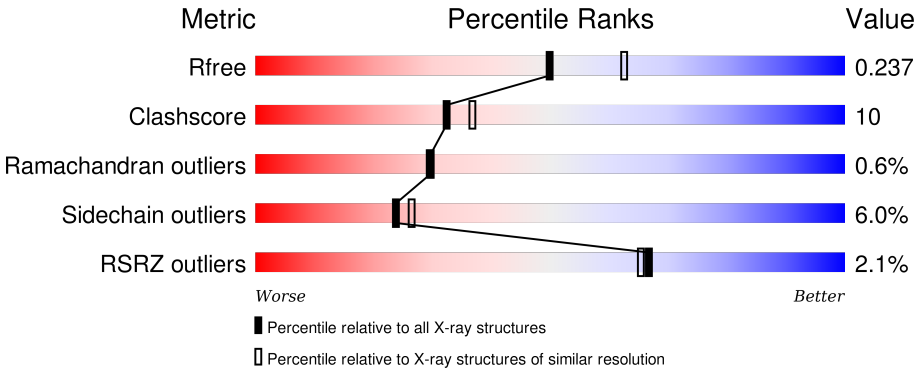
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	3% 71% 22%
1	B	470	% 79% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7456 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	450	Total	C	N	O	S	0	0	0
			3519	2223	606	681	9			
1	B	450	Total	C	N	O	S	0	0	0
			3520	2224	606	681	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	GLY	TYR	ENGINEERED	UNP P09167
B	221	GLY	TYR	ENGINEERED	UNP P09167

- Molecule 2 is water.

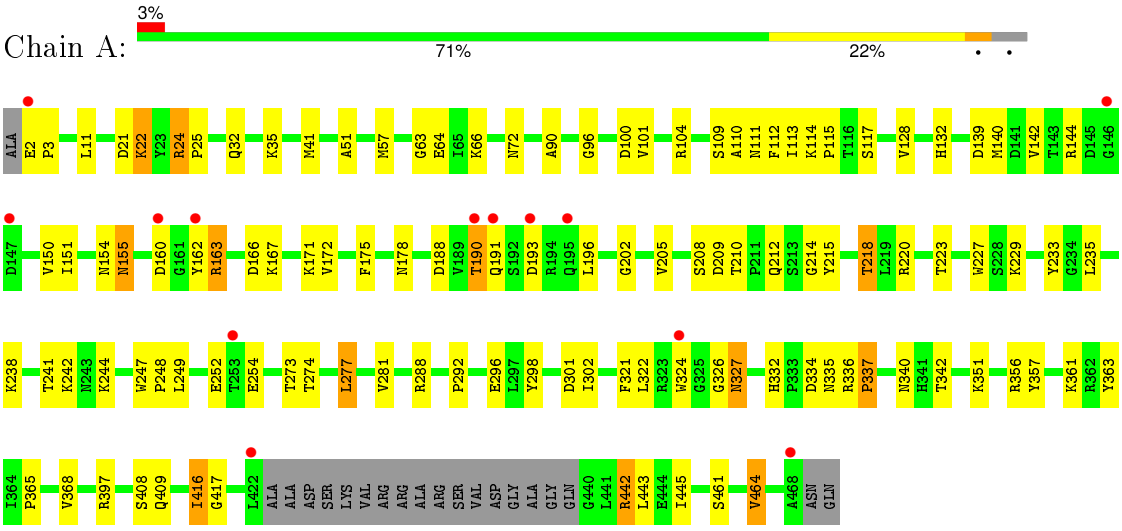
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	177	Total	O	0	0
			177	177		
2	B	240	Total	O	0	0
			240	240		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

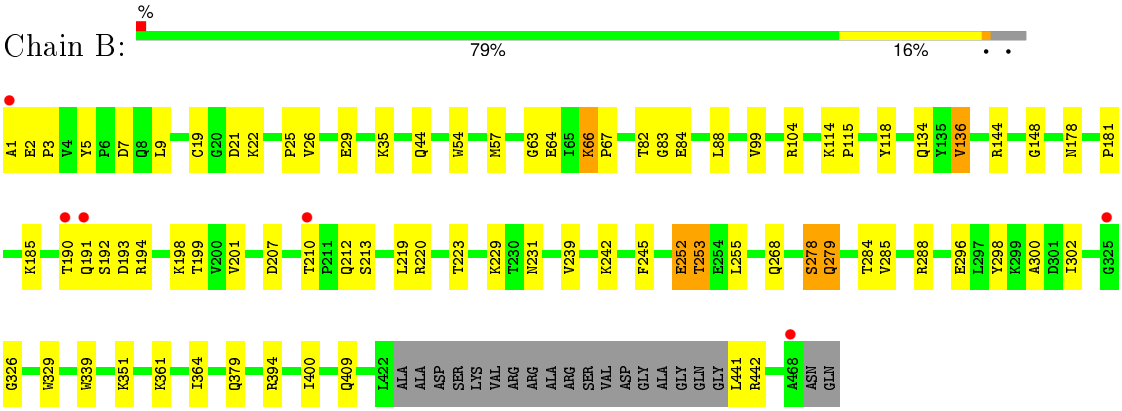
- Molecule 1: Aerolysin

Chain A:



- Molecule 1: Aerolysin

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.36Å 89.77Å 166.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.82 – 2.20 64.82 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.82-2.20) 100.0 (64.82-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	6.23 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.3.0008	Depositor
R, R_{free}	0.189 , 0.238 0.196 , 0.237	Depositor DCC
R_{free} test set	2755 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 54335 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7456	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.57	0/3616	0.86	0/4935
1	B	0.58	0/3617	0.86	0/4937
All	All	0.57	0/7233	0.86	0/9872

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	3519	0	3353	80	0
1	B	3520	0	3358	69	0
2	A	177	0	0	6	0
2	B	240	0	0	9	0
All	All	7456	0	6711	143	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 (143) 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:249:LEU:HD23	1:B:394:ARG:HH22	1.07	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LEU:HD23	1:B:394:ARG:NH2	1.79	0.97
1:B:1:ALA:C	1:B:3:PRO:HD2	1.88	0.94
1:A:249:LEU:CD2	1:B:394:ARG:HH22	1.80	0.94
1:B:1:ALA:HB2	1:B:83:GLY:H	1.36	0.91
1:B:54:TRP:CZ3	1:B:67:PRO:HD3	2.07	0.90
1:B:2:GLU:N	1:B:3:PRO:HD2	1.86	0.90
1:A:218:THR:HG23	2:A:560:HOH:O	1.72	0.88
1:B:229:LYS:NZ	1:B:231:ASN:HD21	1.73	0.86
1:A:292:PRO:HG2	1:A:417:GLY:HA3	1.60	0.83
1:B:2:GLU:N	1:B:3:PRO:CD	2.41	0.83
1:A:2:GLU:O	1:A:2:GLU:HG2	1.80	0.82
1:A:322:LEU:HD13	1:A:327:ASN:OD1	1.80	0.81
1:A:223:THR:HG23	1:A:277:LEU:HD11	1.61	0.80
1:B:99:VAL:HG22	1:B:144:ARG:NH2	1.98	0.79
1:B:35:LYS:HE3	1:B:63:GLY:O	1.88	0.73
1:A:208:SER:O	1:A:288:ARG:HD2	1.88	0.73
1:A:327:ASN:HD21	1:A:332:HIS:HA	1.52	0.72
1:A:351:LYS:HG2	1:A:357:TYR:CE1	2.25	0.72
1:B:1:ALA:CB	1:B:83:GLY:H	2.03	0.71
1:B:178:ASN:HD21	1:B:242:LYS:H	1.41	0.69
1:A:443:LEU:HG	1:A:464:VAL:HG22	1.73	0.69
1:B:229:LYS:HE3	1:B:268:GLN:O	1.91	0.69
1:A:368:VAL:HG13	1:A:368:VAL:O	1.92	0.69
1:A:202:GLY:HA3	1:A:445:ILE:HG12	1.76	0.68
1:B:223:THR:HG21	1:B:409:GLN:O	1.94	0.67
1:A:163:ARG:HG2	1:A:321:PHE:CE2	2.30	0.67
1:B:118:TYR:CZ	1:B:136:VAL:HG13	2.30	0.66
1:A:132:HIS:HE1	1:A:154:ASN:OD1	1.78	0.66
1:A:11:LEU:HD11	1:A:72:ASN:HD22	1.60	0.66
1:A:111:ASN:HD21	1:B:252:GLU:HG2	1.61	0.65
1:B:1:ALA:HB3	1:B:82:THR:HB	1.79	0.65
1:A:220:ARG:HD2	2:A:480:HOH:O	1.96	0.65
1:B:1:ALA:CA	1:B:3:PRO:HD2	2.27	0.64
1:A:57:MET:O	1:A:63:GLY:HA2	1.97	0.64
1:B:229:LYS:HZ3	1:B:231:ASN:HD21	1.44	0.64
1:A:227:TRP:HE1	1:A:273:THR:HG23	1.64	0.63
1:A:90:ALA:HB1	1:A:397:ARG:HG3	1.81	0.62
1:A:41:MET:CE	2:B:595:HOH:O	2.48	0.61
1:A:114:LYS:HB2	1:A:115:PRO:HD3	1.81	0.61
1:B:88:LEU:HB2	1:B:394:ARG:HG3	1.83	0.61
1:B:21:ASP:O	1:B:22:LYS:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:GLN:O	1:B:302:ILE:HA	2.01	0.60
1:B:229:LYS:HZ2	1:B:231:ASN:HD21	1.49	0.60
1:A:215:TYR:HB3	1:A:464:VAL:HG12	1.82	0.60
2:A:549:HOH:O	1:B:136:VAL:HG12	2.01	0.60
1:B:253:THR:HG21	1:B:302:ILE:HB	1.83	0.59
1:A:2:GLU:N	1:A:3:PRO:HD3	2.17	0.59
1:B:64:GLU:OE2	1:B:66:LYS:HE3	2.02	0.59
1:A:443:LEU:HG	1:A:464:VAL:CG2	2.33	0.58
1:B:207:ASP:OD2	1:B:442:ARG:NH1	2.37	0.57
1:A:210:THR:HG22	2:A:534:HOH:O	2.04	0.56
1:A:2:GLU:N	1:A:3:PRO:CD	2.69	0.56
1:A:101:VAL:HG21	1:A:235:LEU:HD22	1.88	0.56
1:A:292:PRO:HG3	1:B:134:GLN:OE1	2.06	0.56
1:B:1:ALA:HA	1:B:3:PRO:HD2	1.88	0.55
1:B:134:GLN:HG2	2:B:532:HOH:O	2.05	0.55
1:A:41:MET:HE1	2:B:595:HOH:O	2.06	0.55
1:B:19:CYS:SG	1:B:25:PRO:HD3	2.47	0.55
1:B:114:LYS:HB2	1:B:115:PRO:HD3	1.90	0.54
1:A:191:GLN:O	1:A:302:ILE:HA	2.08	0.54
1:A:155:ASN:ND2	1:A:167:LYS:HZ3	2.06	0.54
1:B:57:MET:O	1:B:63:GLY:HA2	2.07	0.53
1:B:9:LEU:CD2	1:B:26:VAL:HG21	2.38	0.53
1:B:442:ARG:HG2	1:B:442:ARG:HH11	1.72	0.53
1:A:205:VAL:HG21	1:A:442:ARG:CZ	2.38	0.53
1:B:351:LYS:HG3	2:B:547:HOH:O	2.08	0.52
1:A:100:ASP:O	1:A:104:ARG:HG3	2.09	0.52
1:A:336:ARG:N	1:A:337:PRO:HD3	2.24	0.52
1:B:181:PRO:HG3	1:B:245:PHE:CD1	2.44	0.52
1:B:219:LEU:O	1:B:278:SER:HA	2.09	0.52
1:A:227:TRP:HE1	1:A:273:THR:CG2	2.22	0.52
1:B:178:ASN:HD21	1:B:242:LYS:N	2.07	0.51
1:B:9:LEU:HD22	1:B:26:VAL:HG21	1.92	0.51
1:A:41:MET:HE3	2:B:595:HOH:O	2.10	0.51
1:A:151:ILE:N	1:A:151:ILE:HD12	2.24	0.51
1:A:142:VAL:HG22	1:A:151:ILE:HG13	1.92	0.50
1:B:1:ALA:HB1	1:B:5:TYR:OH	2.10	0.50
1:B:99:VAL:CG2	1:B:144:ARG:NH2	2.71	0.50
1:B:361:LYS:HD2	1:B:364:ILE:HD12	1.93	0.50
1:A:32:GLN:NE2	1:A:35:LYS:HE3	2.27	0.50
1:B:1:ALA:HB3	1:B:82:THR:CB	2.41	0.50
1:B:7:ASP:OD1	1:B:84:GLU:OE2	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLU:OE1	1:A:298:TYR:OH	2.24	0.50
1:A:273:THR:HG21	2:A:635:HOH:O	2.12	0.50
1:A:110:ALA:HB2	1:B:194:ARG:NH2	2.27	0.49
1:B:99:VAL:HB	2:B:694:HOH:O	2.13	0.49
1:A:209:ASP:OD1	1:A:288:ARG:NH1	2.45	0.49
1:B:212:GLN:OE1	1:B:441:LEU:N	2.45	0.49
1:A:139:ASP:OD2	1:A:154:ASN:HB3	2.13	0.49
1:A:90:ALA:CB	1:A:397:ARG:HD2	2.43	0.49
1:A:281:VAL:HG11	1:A:416:ILE:CD1	2.42	0.49
1:A:144:ARG:NH2	2:A:544:HOH:O	2.46	0.49
1:A:24:ARG:HD3	1:A:24:ARG:O	2.13	0.48
1:A:163:ARG:HG3	1:A:166:ASP:OD2	2.13	0.48
1:B:54:TRP:CE3	1:B:67:PRO:HD3	2.48	0.47
1:A:365:PRO:O	1:A:368:VAL:HG12	2.14	0.47
1:A:196:LEU:CD1	1:A:296:GLU:HB3	2.44	0.47
1:B:213:SER:HB2	1:B:284:THR:HG23	1.97	0.47
1:B:296:GLU:OE1	1:B:298:TYR:OH	2.28	0.47
1:B:54:TRP:CH2	1:B:67:PRO:HD3	2.50	0.46
1:A:25:PRO:HB2	1:A:51:ALA:HB2	1.97	0.46
1:B:19:CYS:SG	1:B:25:PRO:CD	3.04	0.46
1:A:220:ARG:HG2	1:A:461:SER:OG	2.15	0.46
1:A:212:GLN:HE21	1:A:214:GLY:H	1.64	0.46
1:A:22:LYS:HB2	1:A:22:LYS:HE2	1.48	0.46
1:B:144:ARG:HD2	1:B:148:GLY:O	2.15	0.46
1:A:292:PRO:HG2	1:A:417:GLY:CA	2.41	0.45
1:A:162:TYR:O	1:A:163:ARG:HB3	2.17	0.45
1:B:329:TRP:CE2	1:B:339:TRP:HZ2	2.34	0.45
1:B:285:VAL:HG21	1:B:441:LEU:HD11	1.98	0.45
1:A:357:TYR:CZ	1:A:361:LYS:HG3	2.52	0.45
1:B:178:ASN:ND2	2:B:632:HOH:O	2.48	0.44
1:A:363:TYR:O	1:A:365:PRO:HD3	2.17	0.44
1:A:196:LEU:HD13	1:A:296:GLU:HB3	1.98	0.44
1:A:324:TRP:CD1	1:A:334:ASP:HB2	2.53	0.44
1:A:117:SER:O	1:A:128:VAL:HG11	2.18	0.44
1:A:96:GLY:HA2	1:A:233:TYR:CD1	2.53	0.43
1:B:239:VAL:HG21	1:B:400:ILE:CD1	2.48	0.43
1:B:198:LYS:HG3	1:B:199:THR:N	2.33	0.43
1:A:209:ASP:OD1	1:A:288:ARG:HD3	2.20	0.42
1:A:223:THR:HG23	1:A:277:LEU:CD1	2.41	0.42
1:A:188:ASP:O	1:A:190:THR:N	2.52	0.42
1:B:57:MET:HE3	1:B:66:LYS:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ASN:HD21	1:A:242:LYS:H	1.68	0.42
1:A:368:VAL:O	1:A:368:VAL:CG1	2.63	0.42
1:B:442:ARG:NH1	1:B:442:ARG:HG2	2.34	0.41
1:A:150:VAL:C	1:A:151:ILE:HD12	2.40	0.41
1:B:279:GLN:HG3	2:B:553:HOH:O	2.20	0.41
1:A:335:ASN:OD1	1:A:337:PRO:HG3	2.21	0.41
1:A:112:PHE:CZ	1:A:172:VAL:HG21	2.56	0.41
1:A:247:TRP:CG	1:A:248:PRO:HD2	2.56	0.41
1:B:1:ALA:CB	1:B:82:THR:HB	2.48	0.41
1:B:118:TYR:CE1	1:B:136:VAL:CG1	3.03	0.41
1:B:99:VAL:CG2	1:B:144:ARG:HH21	2.33	0.41
1:A:150:VAL:HG22	1:A:171:LYS:HG2	2.02	0.41
1:A:172:VAL:HG12	1:A:175:PHE:CZ	2.56	0.41
1:B:379:GLN:NE2	2:B:580:HOH:O	2.54	0.41
1:B:253:THR:HB	1:B:300:ALA:HB3	2.04	0.40
1:A:163:ARG:HD2	1:A:166:ASP:OD2	2.22	0.40
1:A:57:MET:HG3	1:A:64:GLU:O	2.22	0.40
1:B:118:TYR:CE1	1:B:136:VAL:HG13	2.56	0.40
1:A:109:SER:HA	1:A:113:ILE:HB	2.03	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	446/470 (95%)	425 (95%)	18 (4%)	3 (1%)	26	25
1	B	446/470 (95%)	427 (96%)	17 (4%)	2 (0%)	39	42
All	All	892/940 (95%)	852 (96%)	35 (4%)	5 (1%)	30	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	THR
1	B	193	ASP
1	B	326	GLY
1	A	193	ASP
1	A	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	378/391 (97%)	350 (93%)	28 (7%)	17	17
1	B	378/391 (97%)	361 (96%)	17 (4%)	34	41
All	All	756/782 (97%)	711 (94%)	45 (6%)	24	26

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	A	22	LYS
1	A	24	ARG
1	A	66	LYS
1	A	140	MET
1	A	155	ASN
1	A	160	ASP
1	A	163	ARG
1	A	218	THR
1	A	229	LYS
1	A	238	LYS
1	A	241	THR
1	A	244	LYS
1	A	252	GLU
1	A	254	GLU
1	A	274	THR
1	A	277	LEU
1	A	301	ASP
1	A	327	ASN

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Mol	Chain	Res	Type
1	A	337	PRO
1	A	340	ASN
1	A	342	THR
1	A	356	ARG
1	A	408	SER
1	A	409	GLN
1	A	416	ILE
1	A	442	ARG
1	A	464	VAL
1	B	29	GLU
1	B	44	GLN
1	B	66	LYS
1	B	104	ARG
1	B	136	VAL
1	B	185	LYS
1	B	190	THR
1	B	192	SER
1	B	201	VAL
1	B	210	THR
1	B	220	ARG
1	B	252	GLU
1	B	253	THR
1	B	255	LEU
1	B	278	SER
1	B	279	GLN
1	B	288	ARG

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

Mol	Chain	Res	Type
1	A	16	GLN
1	A	32	GLN
1	A	62	ASN
1	A	72	ASN
1	A	111	ASN
1	A	132	HIS
1	A	155	ASN
1	A	178	ASN
1	A	212	GLN
1	A	231	ASN
1	A	327	ASN
1	A	387	ASN

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Mol	Chain	Res	Type
1	A	409	GLN
1	A	413	ASN
1	B	62	ASN
1	B	79	ASN
1	B	107	HIS
1	B	178	ASN
1	B	212	GLN
1	B	231	ASN
1	B	379	GLN
1	B	387	ASN
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 carbohydrates 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	450/470 (95%)	-0.21	13 (2%) 55 54	15, 30, 61, 76	0
1	B	450/470 (95%)	-0.22	6 (1%) 79 78	13, 27, 61, 85	0
All	All	900/940 (95%)	-0.22	19 (2%) 67 65	13, 29, 61, 85	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	ASP	5.3
1	A	190	THR	4.5
1	A	324	TRP	3.8
1	A	191	GLN	3.8
1	B	468	ALA	3.8
1	B	191	GLN	3.3
1	A	422	LEU	3.3
1	A	146	GLY	3.2
1	B	190	THR	3.0
1	A	162	TYR	2.9
1	A	253	THR	2.9
1	A	2	GLU	2.8
1	B	325	GLY	2.8
1	B	1	ALA	2.6
1	A	160	ASP	2.6
1	A	195	GLN	2.4
1	B	210	THR	2.3
1	A	193	ASP	2.0
1	A	468	ALA	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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.