



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:04 PM UTC

PDB ID : 3C0N / pdb_00003c0n
Title : Crystal structure of the proaerolysin mutant Y221G at 2.2 Å
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

<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

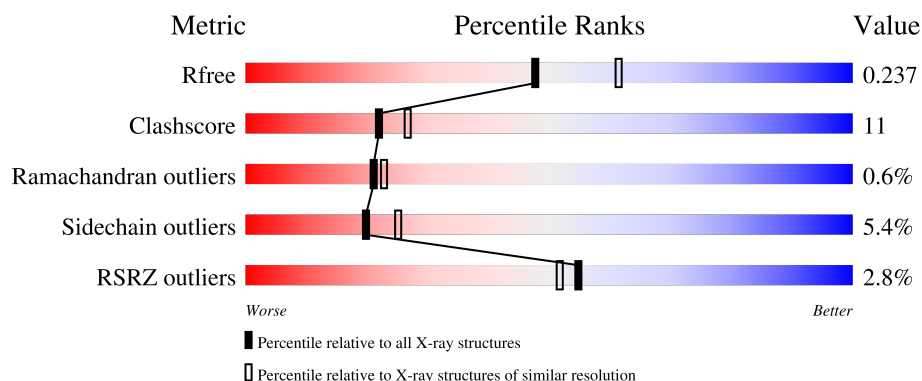
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

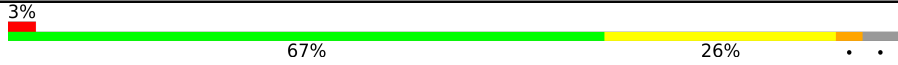
The reported resolution of this entry is 2.20 Å.

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	
1	B	470	

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			

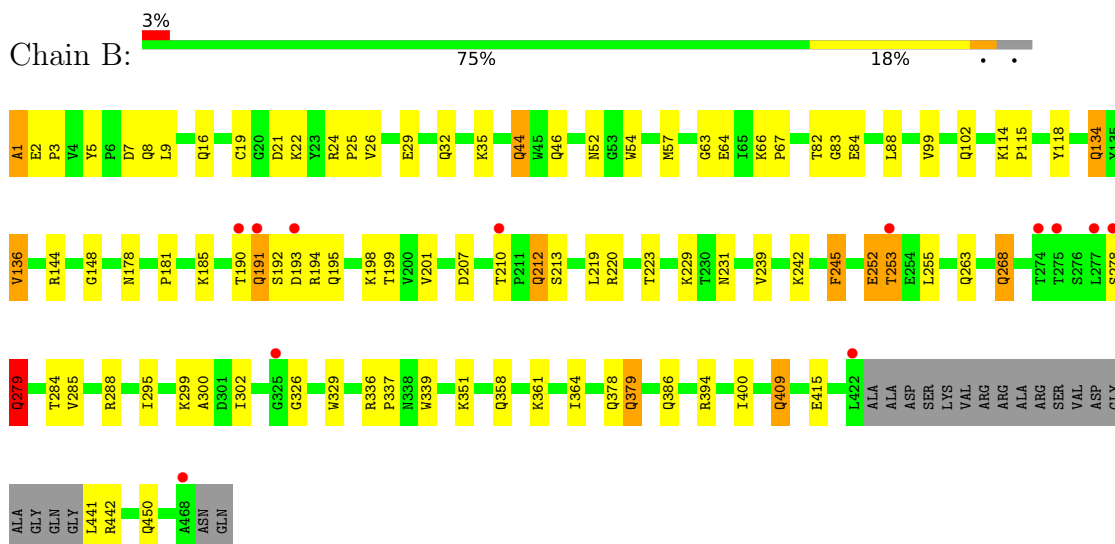
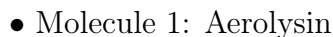
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 1: Aerolysin



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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	0.78	0/3616	1.29	43/4935 (0.9%)
1	B	0.80	1/3617 (0.0%)	1.29	43/4937 (0.9%)
All	All	0.79	1/7233 (0.0%)	1.29	86/9872 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	336	ARG	CA-C	-6.09	1.49	1.53

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	GLN	OE1-CD-NE2	-10.72	111.88	122.60
1	A	279	GLN	OE1-CD-NE2	-10.62	111.98	122.60
1	B	195	GLN	OE1-CD-NE2	-10.35	112.25	122.60
1	B	263	GLN	OE1-CD-NE2	-10.33	112.27	122.60
1	B	102	GLN	OE1-CD-NE2	-10.32	112.28	122.60
1	B	134	GLN	OE1-CD-NE2	-10.26	112.34	122.60
1	A	44	GLN	OE1-CD-NE2	-10.17	112.43	122.60
1	B	212	GLN	OE1-CD-NE2	-10.14	112.46	122.60
1	B	268	GLN	OE1-CD-NE2	-10.13	112.47	122.60
1	A	32	GLN	OE1-CD-NE2	-10.07	112.53	122.60
1	A	450	GLN	OE1-CD-NE2	-10.06	112.54	122.60
1	A	379	GLN	OE1-CD-NE2	-10.02	112.58	122.60
1	A	268	GLN	OE1-CD-NE2	-10.01	112.59	122.60
1	A	386	GLN	OE1-CD-NE2	-9.86	112.74	122.60
1	A	191	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	B	16	GLN	OE1-CD-NE2	-9.84	112.76	122.60
1	B	386	GLN	OE1-CD-NE2	-9.82	112.78	122.60
1	B	32	GLN	OE1-CD-NE2	-9.80	112.80	122.60
1	A	134	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	A	46	GLN	OE1-CD-NE2	-9.74	112.86	122.60
1	A	409	GLN	OE1-CD-NE2	-9.67	112.93	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	GLN	OE1-CD-NE2	-9.59	113.01	122.60
1	A	8	GLN	OE1-CD-NE2	-9.57	113.03	122.60
1	B	450	GLN	OE1-CD-NE2	-9.52	113.08	122.60
1	A	102	GLN	OE1-CD-NE2	-9.41	113.19	122.60
1	B	409	GLN	OE1-CD-NE2	-9.40	113.20	122.60
1	B	44	GLN	OE1-CD-NE2	-9.39	113.21	122.60
1	B	279	GLN	OE1-CD-NE2	-9.36	113.24	122.60
1	A	378	GLN	OE1-CD-NE2	-9.27	113.33	122.60
1	B	46	GLN	OE1-CD-NE2	-9.21	113.39	122.60
1	A	263	GLN	OE1-CD-NE2	-9.11	113.49	122.60
1	B	8	GLN	OE1-CD-NE2	-9.10	113.50	122.60
1	B	379	GLN	OE1-CD-NE2	-9.06	113.54	122.60
1	A	16	GLN	OE1-CD-NE2	-8.98	113.62	122.60
1	B	378	GLN	OE1-CD-NE2	-8.91	113.69	122.60
1	A	195	GLN	OE1-CD-NE2	-8.88	113.72	122.60
1	B	191	GLN	OE1-CD-NE2	-8.71	113.89	122.60
1	B	358	GLN	OE1-CD-NE2	-8.54	114.06	122.60
1	A	379	GLN	CG-CD-NE2	7.47	127.61	116.40
1	A	212	GLN	CG-CD-NE2	7.45	127.58	116.40
1	B	263	GLN	CG-CD-NE2	7.37	127.45	116.40
1	B	212	GLN	CG-CD-NE2	7.20	127.20	116.40
1	B	386	GLN	CG-CD-NE2	7.10	127.05	116.40
1	A	279	GLN	CG-CD-NE2	7.03	126.95	116.40
1	A	358	GLN	CG-CD-NE2	7.02	126.94	116.40
1	B	409	GLN	CG-CD-NE2	6.96	126.84	116.40
1	A	386	GLN	CG-CD-NE2	6.94	126.81	116.40
1	B	268	GLN	CG-CD-NE2	6.76	126.54	116.40
1	A	16	GLN	CG-CD-NE2	6.75	126.53	116.40
1	A	263	GLN	CG-CD-NE2	6.75	126.52	116.40
1	A	44	GLN	CG-CD-NE2	6.71	126.47	116.40
1	B	195	GLN	CG-CD-NE2	6.71	126.47	116.40
1	B	378	GLN	CG-CD-NE2	6.67	126.40	116.40
1	A	378	GLN	CG-CD-NE2	6.66	126.39	116.40
1	A	32	GLN	CG-CD-NE2	6.65	126.38	116.40
1	A	8	GLN	CG-CD-NE2	6.62	126.34	116.40
1	A	102	GLN	CG-CD-NE2	6.59	126.28	116.40
1	A	191	GLN	CG-CD-NE2	6.58	126.27	116.40
1	A	409	GLN	CG-CD-NE2	6.57	126.26	116.40
1	B	32	GLN	CG-CD-NE2	6.51	126.16	116.40
1	B	379	GLN	CG-CD-NE2	6.51	126.16	116.40
1	B	279	GLN	CG-CD-NE2	6.50	126.15	116.40
1	A	450	GLN	CG-CD-NE2	6.49	126.14	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	GLN	CG-CD-NE2	6.47	126.11	116.40
1	B	16	GLN	CG-CD-NE2	6.46	126.09	116.40
1	B	8	GLN	CG-CD-NE2	6.44	126.07	116.40
1	A	195	GLN	CG-CD-NE2	6.43	126.05	116.40
1	B	134	GLN	CG-CD-NE2	6.43	126.04	116.40
1	B	450	GLN	CG-CD-NE2	6.39	125.99	116.40
1	A	46	GLN	CG-CD-NE2	6.39	125.98	116.40
1	A	268	GLN	CG-CD-NE2	6.34	125.91	116.40
1	B	358	GLN	CG-CD-NE2	6.30	125.86	116.40
1	B	44	GLN	CG-CD-NE2	6.26	125.80	116.40
1	B	191	GLN	CG-CD-NE2	6.25	125.78	116.40
1	A	134	GLN	CG-CD-NE2	6.19	125.69	116.40
1	B	46	GLN	CG-CD-NE2	6.17	125.65	116.40
1	B	52	ASN	N-CA-C	5.51	119.00	111.39
1	A	195	GLN	N-CA-C	5.39	117.75	109.07
1	B	1	ALA	CA-C-N	5.32	126.39	120.06
1	B	1	ALA	C-N-CA	5.32	126.39	120.06
1	A	184	PHE	N-CA-C	5.31	117.73	110.24
1	A	52	ASN	N-CA-C	5.24	118.47	111.24
1	B	337	PRO	CA-N-CD	-5.19	104.74	112.00
1	A	255	LEU	CA-C-N	-5.17	116.06	123.20
1	A	255	LEU	C-N-CA	-5.17	116.06	123.20
1	B	245	PHE	CA-CB-CG	5.16	118.96	113.80

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	73	0
2	A	177	0	0	6	0
2	B	240	0	0	7	0
All	All	7456	0	6711	146	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 (146) 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
1:A:41:MET:HE1	2:B:595:HOH:O	1.58	1.01
1:B:1:ALA:C	1:B:3:PRO:HD2	1.88	0.99
1:A:249:LEU:HD23	1:B:394:ARG:NH2	1.79	0.97
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:HG2	1:A:2:GLU:O	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:229:LYS:HZ2	1:B:231:ASN:HD21	1.33	0.71
1:B:1:ALA:CB	1:B:83:GLY:H	2.03	0.71
1:A:443:LEU:HG	1:A:464:VAL:HG22	1.73	0.69
1:B:178:ASN:HD21	1:B:242:LYS:H	1.41	0.69
1:B:229:LYS:HE3	1:B:268:GLN:O	1.91	0.69
1:A:202:GLY:HA3	1:A:445:ILE:HG12	1.76	0.68
1:A:368:VAL:HG13	1:A:368:VAL:O	1.92	0.67
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:A:132:HIS:HE1	1:A:154:ASN:OD1	1.78	0.66
1:B:118:TYR:CZ	1:B:136:VAL:HG13	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:191:GLN:O	1:B:302:ILE:HA	2.01	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: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: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:HH11	1:B:442:ARG:HG2	1.72	0.53
1:A:205:VAL:HG21	1:A:442:ARG:CZ	2.38	0.53
1:A:100:ASP:O	1:A:104:ARG:HG3	2.09	0.52
1:B:351:LYS:HG3	2:B:547:HOH:O	2.08	0.52
1:A:336:ARG:N	1:A:337:PRO:HD3	2.24	0.52
1:B:1:ALA:C	1:B:3:PRO:CD	2.73	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:B:57:MET:HE3	1:B:66:LYS:CD	2.40	0.51
1:A:151:ILE:HD12	1:A:151:ILE:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLN:NE2	1:A:35:LYS:HE3	2.27	0.50
1:A:296:GLU:OE1	1:A:298:TYR:OH	2.24	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
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:90:ALA:CB	1:A:397:ARG:HD2	2.43	0.49
1:A:139:ASP:OD2	1:A:154:ASN:HB3	2.13	0.49
1:A:144:ARG:NH2	2:A:544:HOH:O	2.46	0.49
1:A:281:VAL:HG11	1:A:416:ILE:CD1	2.42	0.49
1:A:24:ARG:O	1:A:24:ARG:HD3	2.13	0.48
1:A:163:ARG:HG3	1:A:166:ASP:OD2	2.13	0.48
1:A:365:PRO:O	1:A:368:VAL:HG12	2.14	0.47
1:B:54:TRP:CE3	1:B:67:PRO:HD3	2.48	0.47
1:B:57:MET:HE3	1:B:66:LYS:HD2	1.96	0.47
1:A:196:LEU:CD1	1:A:296:GLU:HB3	2.44	0.47
1:A:150:VAL:C	1:A:151:ILE:HD12	2.40	0.47
1:B:213:SER:HB2	1:B:284:THR:HG23	1.97	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:22:LYS:HB2	1:A:22:LYS:HE2	1.48	0.46
1:A:212:GLN:HE21	1:A:214:GLY:H	1.64	0.46
1:A:220:ARG:HG2	1:A:461:SER:OG	2.15	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:B:229:LYS:HZ3	1:B:231:ASN:HD21	1.62	0.44
1:A:117:SER:O	1:A:128:VAL:HG11	2.18	0.44
1:A:324:TRP:CD1	1:A:334:ASP:HB2	2.53	0.44
1:A:96:GLY:HA2	1:A:233:TYR:CD1	2.53	0.43
1:A:278:SER:O	1:A:279:GLN:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:188:ASP:O	1:A:190:THR:N	2.52	0.42
1:A:223:THR:HG23	1:A:277:LEU:CD1	2.41	0.42
1:A:114:LYS:NZ	1:B:415:GLU:OE1	2.41	0.42
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:279:GLN:HG3	2:B:553:HOH:O	2.20	0.41
1:B:442:ARG:NH1	1:B:442:ARG:HG2	2.34	0.41
1:B:229:LYS:HZ2	1:B:231:ASN:ND2	2.09	0.41
1:A:112:PHE:CZ	1:A:172:VAL:HG21	2.56	0.41
1:A:335:ASN:OD1	1:A:337:PRO:HG3	2.21	0.41
1:A:247:TRP:CG	1:A:248:PRO:HD2	2.56	0.41
1:A:246:LYS:O	1:A:247:TRP:C	2.63	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: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:99:VAL:CG2	1:B:144:ARG:HH21	2.33	0.41
1:B:379:GLN:NE2	2:B:580:HOH:O	2.54	0.41
1:B:24:ARG:HD2	1:B:24:ARG:C	2.46	0.40
1:B:253:THR:HB	1:B:300:ALA:HB3	2.04	0.40
1:A:57:MET:HG3	1:A:64:GLU:O	2.22	0.40
1:A:163:ARG:HD2	1:A:166:ASP:OD2	2.22	0.40
1:A:109:SER:HA	1:A:113:ILE:HB	2.03	0.40
1:B:118:TYR:CE1	1:B:136:VAL:HG13	2.56	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%)	18	19
1	B	446/470 (95%)	427 (96%)	17 (4%)	2 (0%)	30	34
All	All	892/940 (95%)	852 (96%)	35 (4%)	5 (1%)	21	23

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 ⓘ

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%)	353 (93%)	25 (7%)	15	18
1	B	378/391 (97%)	362 (96%)	16 (4%)	26	36
All	All	756/782 (97%)	715 (95%)	41 (5%)	20	25

All (41) 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	218	THR
1	A	229	LYS
1	A	241	THR
1	A	244	LYS

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Mol	Chain	Res	Type
1	A	252	GLU
1	A	253	THR
1	A	254	GLU
1	A	274	THR
1	A	277	LEU
1	A	327	ASN
1	A	340	ASN
1	A	342	THR
1	A	408	SER
1	A	409	GLN
1	A	416	ILE
1	A	422	LEU
1	A	442	ARG
1	A	464	VAL
1	B	29	GLU
1	B	44	GLN
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	279	GLN
1	B	288	ARG
1	B	295	ILE
1	B	299	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	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	191	GLN

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Mol	Chain	Res	Type
1	A	195	GLN
1	A	212	GLN
1	A	263	GLN
1	A	327	ASN
1	A	386	GLN
1	A	387	ASN
1	A	409	GLN
1	A	413	ASN
1	B	32	GLN
1	B	79	ASN
1	B	107	HIS
1	B	111	ASN
1	B	178	ASN
1	B	191	GLN
1	B	212	GLN
1	B	226	ASN
1	B	231	ASN
1	B	379	GLN
1	B	387	ASN
1	B	409	GLN
1	B	413	ASN
1	B	450	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	450/470 (95%)	0.06	13 (2%) 53 50	15, 30, 61, 76	0
1	B	450/470 (95%)	-0.07	12 (2%) 56 53	13, 27, 61, 85	0
All	All	900/940 (95%)	-0.01	25 (2%) 55 52	13, 29, 61, 85	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	468	ALA	6.3
1	B	468	ALA	5.0
1	A	253	THR	4.4
1	A	190	THR	4.1
1	B	190	THR	3.9
1	A	146	GLY	3.5
1	B	191	GLN	3.3
1	A	195	GLN	3.2
1	A	193	ASP	3.1
1	A	191	GLN	3.1
1	A	252	GLU	3.0
1	A	324	TRP	3.0
1	A	192	SER	2.9
1	B	277	LEU	2.9
1	B	325	GLY	2.8
1	A	147	ASP	2.8
1	B	422	LEU	2.8
1	A	2	GLU	2.6
1	B	193	ASP	2.5
1	B	274	THR	2.5
1	A	422	LEU	2.4
1	B	210	THR	2.3
1	B	253	THR	2.3
1	B	275	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	278	SER	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.