Full wwPDB X-ray Structure Validation Report (i)

Dec 2, 2023 – 05:33 pm GMT

PDB ID	:	1QNL
Title	:	AMIDE RECEPTOR/NEGATIVE REGULATOR OF THE AMIDASE OPERON OF PSEUDOMONAS AERUGINOSA (AMIC) COMPLEXED WITH BUTYRAMIDE
Authors	:	Pearl, L.H.; O'Hara, B.P.; Roe, S.M.
Deposited on	:	1999-10-19
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

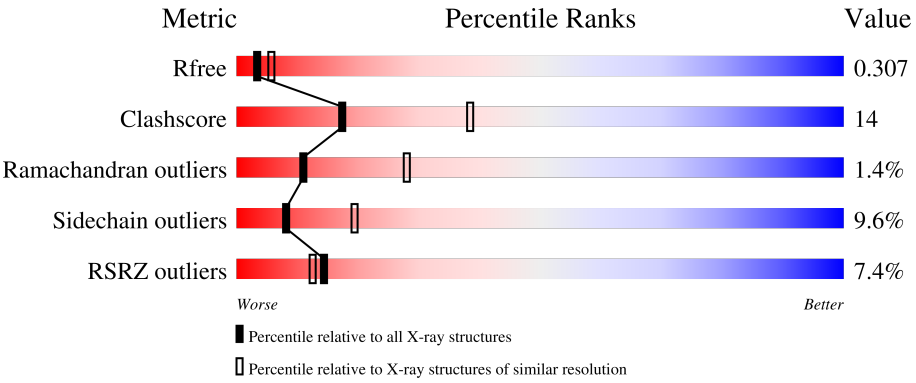
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	385	6% 59% 26% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BMD	A	1001	-	X	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2963 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.

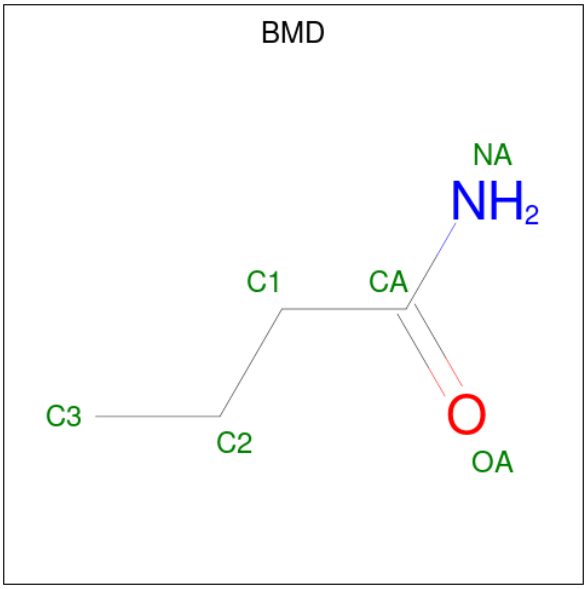
- Molecule 1 is a protein called ALIPHATIC AMIDASE EXPRESSION-REGULATING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	368	2914	1835	526	545	8	259	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLN	HIS	conflict	UNP P27017
A	28	ARG	ALA	conflict	UNP P27017

- Molecule 2 is BUTYRAMIDE (three-letter code: BMD) (formula: C_4H_9NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	6	4	1	1	0	0

- Molecule 3 is water.

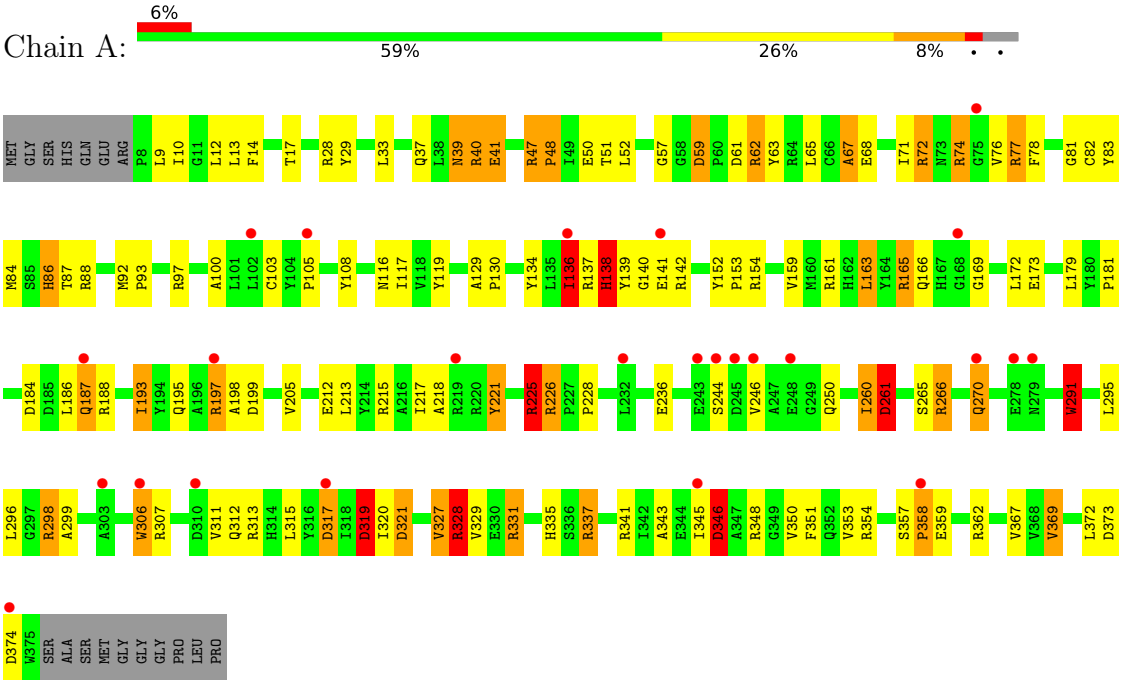
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	43	Total O 43 43	5	0

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: ALIPHATIC AMIDASE EXPRESSION-REGULATING PROTEIN

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	104.15Å 104.15Å 65.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 26.84 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (15.00-2.70) 97.1 (26.84-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.08 (at 2.72Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.269 , 0.314 0.244 , 0.307	Depositor DCC
R_{free} test set	480 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	41.1	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 57.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	2963	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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

Bond lengths and bond angles in the following residue types are not validated in this section: BMD

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	0.86	14/2989 (0.5%)	1.99	77/4074 (1.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	13

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	261	ASP	C-N	-15.77	0.97	1.34
1	A	221	TYR	C-N	-13.55	1.08	1.33
1	A	307	ARG	C-N	11.81	1.61	1.34
1	A	67	ALA	C-N	10.73	1.58	1.34
1	A	317	ASP	C-N	-9.62	1.11	1.34
1	A	72	ARG	C-N	9.46	1.55	1.34
1	A	50	GLU	C-N	-9.30	1.12	1.34
1	A	328	ARG	C-N	-8.29	1.15	1.34
1	A	327	VAL	C-N	-7.37	1.17	1.34
1	A	68	GLU	C-N	-7.29	1.17	1.34
1	A	37	GLN	CB-CG	-7.29	1.32	1.52
1	A	358	PRO	C-N	-5.88	1.20	1.34
1	A	136	ILE	C-N	-5.77	1.20	1.34
1	A	71	ILE	C-N	5.37	1.46	1.34

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	221	TYR	O-C-N	-28.43	74.87	123.20
1	A	328	ARG	O-C-N	-26.59	80.16	122.70
1	A	317	ASP	O-C-N	-22.25	87.10	122.70
1	A	39	ASN	O-C-N	-20.12	90.51	122.70
1	A	328	ARG	C-N-CA	19.57	170.62	121.70
1	A	266	ARG	NE-CZ-NH2	-18.16	111.22	120.30
1	A	346	ASP	O-C-N	-17.74	94.31	122.70
1	A	74	ARG	NE-CZ-NH1	-17.52	111.54	120.30
1	A	47	ARG	NE-CZ-NH1	17.39	129.00	120.30
1	A	328	ARG	CA-C-N	15.74	151.82	117.20
1	A	348	ARG	NE-CZ-NH2	15.73	128.16	120.30
1	A	260	ILE	O-C-N	-14.27	99.87	122.70
1	A	261	ASP	C-N-CA	13.96	156.60	121.70
1	A	261	ASP	CB-CG-OD1	13.44	130.40	118.30
1	A	193	ILE	O-C-N	-12.55	102.62	122.70
1	A	50	GLU	O-C-N	-12.17	103.23	122.70
1	A	50	GLU	C-N-CA	11.77	151.13	121.70
1	A	68	GLU	O-C-N	-10.65	105.65	122.70
1	A	337	ARG	NE-CZ-NH2	-9.79	115.40	120.30
1	A	50	GLU	OE1-CD-OE2	-9.79	111.55	123.30
1	A	165	ARG	CD-NE-CZ	9.75	137.25	123.60
1	A	328	ARG	CD-NE-CZ	9.62	137.07	123.60
1	A	266	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	A	328	ARG	NE-CZ-NH2	9.54	125.07	120.30
1	A	47	ARG	N-CA-CB	9.01	126.81	110.60
1	A	68	GLU	C-N-CA	8.85	143.83	121.70
1	A	47	ARG	CD-NE-CZ	8.71	135.79	123.60
1	A	61	ASP	CB-CG-OD1	8.69	126.12	118.30
1	A	261	ASP	O-C-N	-8.61	108.93	122.70
1	A	348	ARG	NE-CZ-NH1	-8.42	116.09	120.30
1	A	215	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	137	ARG	CD-NE-CZ	8.31	135.24	123.60
1	A	41	GLU	CG-CD-OE2	8.29	134.88	118.30
1	A	327	VAL	O-C-N	-8.23	109.53	122.70
1	A	319	ASP	O-C-N	7.89	135.32	122.70
1	A	62	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	A	307	ARG	C-N-CA	-7.54	102.84	121.70
1	A	266	ARG	CD-NE-CZ	7.43	134.00	123.60
1	A	328	ARG	NH1-CZ-NH2	-7.35	111.31	119.40
1	A	331	ARG	CD-NE-CZ	7.31	133.83	123.60
1	A	221	TYR	CA-C-N	7.22	130.65	116.20
1	A	154	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	50	GLU	CA-C-N	7.06	132.73	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	161	ARG	NE-CZ-NH1	-7.05	116.78	120.30
1	A	74	ARG	NH1-CZ-NH2	7.02	127.12	119.40
1	A	41	GLU	OE1-CD-OE2	-7.01	114.89	123.30
1	A	68	GLU	OE1-CD-OE2	6.99	131.69	123.30
1	A	72	ARG	CB-CG-CD	6.91	129.57	111.60
1	A	261	ASP	CA-C-N	6.86	132.30	117.20
1	A	29	TYR	CA-CB-CG	-6.68	100.71	113.40
1	A	225	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	A	328	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	72	ARG	NE-CZ-NH2	6.55	123.58	120.30
1	A	197	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	319	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	A	40	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	A	47	ARG	NH1-CZ-NH2	-6.03	112.76	119.40
1	A	319	ASP	C-N-CA	-5.93	106.86	121.70
1	A	341	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	261	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	137	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	A	193	ILE	CA-C-N	5.73	129.80	117.20
1	A	307	ARG	CD-NE-CZ	5.71	131.59	123.60
1	A	307	ARG	CB-CA-C	5.68	121.76	110.40
1	A	88	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	A	226	ARG	O-C-N	5.62	131.77	121.10
1	A	306	TRP	CA-CB-CG	-5.53	103.19	113.70
1	A	319	ASP	CB-CG-OD1	5.48	123.24	118.30
1	A	359	GLU	OE1-CD-OE2	-5.44	116.78	123.30
1	A	97	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	291	TRP	CA-CB-CG	5.28	123.73	113.70
1	A	77	ARG	NE-CZ-NH2	5.15	122.87	120.30
1	A	195	GLN	CG-CD-OE1	5.14	131.87	121.60
1	A	48	PRO	O-C-N	5.13	130.90	122.70
1	A	319	ASP	CA-C-O	-5.12	109.36	120.10
1	A	165	ARG	CB-CG-CD	5.02	124.66	111.60
1	A	59	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	ILE	Mainchain
1	A	193	ILE	Mainchain
1	A	221	TYR	Mainchain

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Mol	Chain	Res	Type	Group
1	A	260	ILE	Mainchain
1	A	261	ASP	Peptide
1	A	306	TRP	Mainchain
1	A	317	ASP	Mainchain
1	A	319	ASP	Mainchain
1	A	327	VAL	Mainchain
1	A	328	ARG	Mainchain,Peptide
1	A	346	ASP	Mainchain
1	A	39	ASN	Mainchain

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	2914	0	2801	63	0
2	A	6	0	4	12	0
3	A	43	0	0	0	0
All	All	2963	0	2805	72	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 14.

All (72) 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)
2:A:1001:BMD:NA	2:A:1001:BMD:CA	1.69	1.51
2:A:1001:BMD:CA	2:A:1001:BMD:C1	1.89	1.50
2:A:1001:BMD:C1	2:A:1001:BMD:C3	2.15	1.24
2:A:1001:BMD:C3	2:A:1001:BMD:C2	0.90	0.90
1:A:9:LEU:HD11	1:A:52:LEU:HD13	1.54	0.87
1:A:141:GLU:HB2	1:A:169:GLY:HA2	1.60	0.82
2:A:1001:BMD:CA	2:A:1001:BMD:C3	2.62	0.77
2:A:1001:BMD:C1	2:A:1001:BMD:C2	2.66	0.74
1:A:346:ASP:HB2	1:A:350:VAL:H	1.54	0.72
1:A:92:MET:HG3	1:A:117:ILE:HD11	1.71	0.71
1:A:337:ARG:HH21	1:A:362:ARG:HH11	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:HD11	1:A:67:ALA:HB2	1.79	0.64
1:A:134:TYR:O	1:A:138:HIS:HB2	2.00	0.62
1:A:136:ILE:HA	1:A:140:GLY:O	2.00	0.61
2:A:1001:BMD:NA	2:A:1001:BMD:OA	2.32	0.59
1:A:81:GLY:O	1:A:82:CYS:HB2	2.03	0.58
1:A:236:GLU:HG3	1:A:351:PHE:CE1	2.39	0.58
1:A:337:ARG:HG2	1:A:362:ARG:HA	1.87	0.57
1:A:139:TYR:CE1	1:A:228:PRO:HG3	2.40	0.57
1:A:213:LEU:O	1:A:217:ILE:HG13	2.05	0.56
1:A:92:MET:HG3	1:A:117:ILE:CD1	2.34	0.56
1:A:346:ASP:HB2	1:A:350:VAL:N	2.21	0.56
1:A:84:MET:HA	2:A:1001:BMD:OA	2.06	0.55
1:A:172:LEU:HD12	1:A:198:ALA:HB2	1.90	0.53
1:A:103:CYS:O	1:A:105:PRO:HD3	2.08	0.53
1:A:298:ARG:HD2	1:A:298:ARG:H	1.74	0.52
1:A:134:TYR:OH	1:A:354:ARG:HG3	2.10	0.51
1:A:320:ILE:HG22	1:A:321:ASP:N	2.26	0.51
1:A:298:ARG:HD2	1:A:298:ARG:N	2.25	0.51
1:A:59:ASP:HB3	1:A:62:ARG:HD3	1.93	0.50
1:A:312:GLN:O	1:A:313:ARG:C	2.49	0.49
1:A:184:ASP:HB3	1:A:188:ARG:NH1	2.28	0.49
1:A:218:ALA:CB	1:A:246:VAL:HG22	2.41	0.49
1:A:369:VAL:O	1:A:372:LEU:HB2	2.13	0.49
1:A:78:PHE:HD2	1:A:296:LEU:HD11	1.78	0.48
1:A:83:TYR:CE2	2:A:1001:BMD:C3	2.97	0.48
1:A:343:ALA:HA	1:A:353:VAL:HA	1.95	0.48
1:A:100:ALA:O	1:A:116:ASN:HB3	2.14	0.47
1:A:159:VAL:HG11	1:A:367:VAL:HG11	1.96	0.47
1:A:291:TRP:HZ3	1:A:295:LEU:HD22	1.80	0.47
1:A:14:PHE:CE1	1:A:81:GLY:HA2	2.50	0.47
1:A:10:ILE:O	1:A:51:THR:HA	2.14	0.47
1:A:86:HIS:CD2	1:A:86:HIS:H	2.32	0.46
1:A:236:GLU:HG3	1:A:351:PHE:HE1	1.79	0.46
1:A:152:TYR:HB3	1:A:153:PRO:HD3	1.98	0.46
1:A:187:GLN:NE2	1:A:187:GLN:HA	2.31	0.46
1:A:205:VAL:HG21	1:A:213:LEU:HD22	1.98	0.45
1:A:17:THR:O	1:A:57:GLY:HA2	2.17	0.45
1:A:299:ALA:HB3	1:A:311:VAL:HG13	1.99	0.45
1:A:129:ALA:HB3	1:A:130:PRO:CD	2.46	0.45
1:A:63:TYR:CD1	1:A:87:THR:HB	2.52	0.45
1:A:142:ARG:NH1	1:A:197:ARG:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LEU:O	1:A:181:PRO:HD3	2.17	0.44
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.83	0.43
1:A:129:ALA:HB3	1:A:130:PRO:HD3	2.00	0.43
1:A:357:SER:HA	1:A:358:PRO:HD3	1.86	0.43
1:A:152:TYR:CG	2:A:1001:BMD:CA	3.02	0.43
1:A:184:ASP:HB3	1:A:188:ARG:HH12	1.84	0.43
1:A:10:ILE:HD13	1:A:10:ILE:HG21	1.87	0.42
1:A:266:ARG:O	1:A:270:GLN:HG2	2.19	0.42
1:A:163:LEU:HD13	1:A:369:VAL:HG22	2.00	0.42
2:A:1001:BMD:NA	2:A:1001:BMD:C1	2.80	0.42
1:A:9:LEU:HG	1:A:76:VAL:HG22	2.02	0.42
1:A:331:ARG:HE	1:A:331:ARG:HB3	1.68	0.41
1:A:119:TYR:HB2	1:A:335:HIS:HA	2.02	0.41
1:A:12:LEU:HD13	1:A:28:ARG:HG3	2.01	0.41
1:A:92:MET:HB3	1:A:93:PRO:HD3	2.03	0.41
1:A:186:LEU:HD11	1:A:212:GLU:HB3	2.02	0.41
1:A:250:GLN:O	1:A:345:ILE:HG13	2.20	0.41
1:A:199:ASP:O	1:A:228:PRO:HD2	2.21	0.41
2:A:1001:BMD:CA	2:A:1001:BMD:C2	2.99	0.41
1:A:166:GLN:HA	1:A:166:GLN:OE1	2.21	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	366/385 (95%)	335 (92%)	26 (7%)	5 (1%)	11 28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	HIS

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Mol	Chain	Res	Type
1	A	261	ASP
1	A	329	VAL
1	A	225	ARG
1	A	41	GLU

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	303/315 (96%)	274 (90%)	29 (10%)	8 19

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	40	ARG
1	A	47	ARG
1	A	48	PRO
1	A	65	LEU
1	A	72	ARG
1	A	74	ARG
1	A	86	HIS
1	A	108	TYR
1	A	138	HIS
1	A	163	LEU
1	A	165	ARG
1	A	173	GLU
1	A	187	GLN
1	A	225	ARG
1	A	226	ARG
1	A	244	SER
1	A	261	ASP
1	A	265	SER
1	A	270	GLN
1	A	291	TRP
1	A	298	ARG

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Mol	Chain	Res	Type
1	A	315	LEU
1	A	319	ASP
1	A	321	ASP
1	A	328	ARG
1	A	369	VAL
1	A	373	ASP
1	A	374	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	HIS
1	A	187	GLN
1	A	270	GLN
1	A	312	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BMD	A	1001	-	5,5,5	12.67	5 (100%)	4,5,5	11.26	4 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMD	A	1001	-	-	1/3/3/3	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	BMD	C2-C1	21.97	2.66	1.51
2	A	1001	BMD	CA-NA	11.35	1.69	1.32
2	A	1001	BMD	C1-CA	9.73	1.89	1.51
2	A	1001	BMD	C3-C2	-7.21	0.90	1.49
2	A	1001	BMD	OA-CA	6.71	1.44	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	BMD	C3-C2-C1	-15.43	46.71	112.67
2	A	1001	BMD	OA-CA-C1	12.25	157.03	121.07
2	A	1001	BMD	OA-CA-NA	-9.98	95.27	122.50
2	A	1001	BMD	C1-CA-NA	-4.42	102.76	116.51

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	BMD	CA-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	BMD	12	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	8

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	307:ARG	C	308:VAL	N	1.61
1	A	68:GLU	C	69:ASP	N	1.17
1	A	327:VAL	C	328:ARG	N	1.17
1	A	328:ARG	C	329:VAL	N	1.15
1	A	50:GLU	C	51:THR	N	1.12
1	A	317:ASP	C	318:ILE	N	1.11
1	A	221:TYR	C	222:GLY	N	1.08
1	A	261:ASP	C	262:THR	N	0.97

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	338/385 (87%)	0.50	25 (7%)	14	12	10, 29, 51, 64	3 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	SER	5.2
1	A	303	ALA	4.1
1	A	374	ASP	4.0
1	A	246	VAL	3.6
1	A	136	ILE	3.4
1	A	245	ASP	3.4
1	A	270	GLN	3.3
1	A	248	GLU	3.1
1	A	243	GLU	2.7
1	A	317	ASP	2.7
1	A	306	TRP	2.6
1	A	279	ASN	2.6
1	A	168	GLY	2.5
1	A	232	LEU	2.5
1	A	141	GLU	2.4
1	A	102	LEU	2.4
1	A	278	GLU	2.3
1	A	219	ARG	2.3
1	A	345	ILE	2.2
1	A	310	ASP	2.2
1	A	105	PRO	2.2
1	A	358	PRO	2.2
1	A	75	GLY	2.1
1	A	197	ARG	2.1
1	A	187	GLN	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMD	A	1001	6/6	0.95	0.27	3,4,12,16	0

6.5 Other polymers (i)

There are no such residues in this entry.