



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:38 AM UTC

PDB ID : 1QO0 / pdb_00001qo0
Title : Amide receptor of the amidase operon of *Pseudomonas aeruginosa* (AmiC) complexed with the negative regulator AmiR.
Authors : Pearl, L.H.; O'Hara, B.P.; Roe, S.M.
Deposited on : 1999-10-26
Resolution : 2.25 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

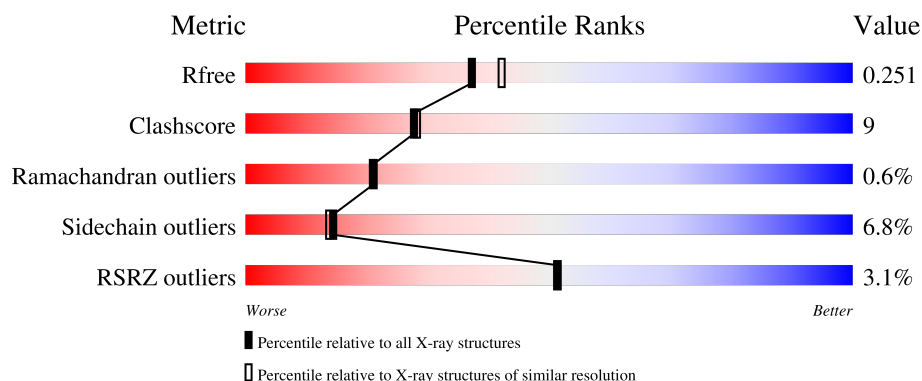
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	385	% 70% 22% • • •
1	B	385	3% 66% 26% 5% • •
2	D	196	4% 69% 21% 5% • •
2	E	196	6% 74% 16% 7% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9661 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 AMIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2943	1852	530	552	9			
1	B	374	Total	C	N	O	S	0	0	0
			2944	1853	531	551	9			

There are 4 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
B	27	GLN	HIS	conflict	UNP P27017
B	28	ARG	ALA	conflict	UNP P27017

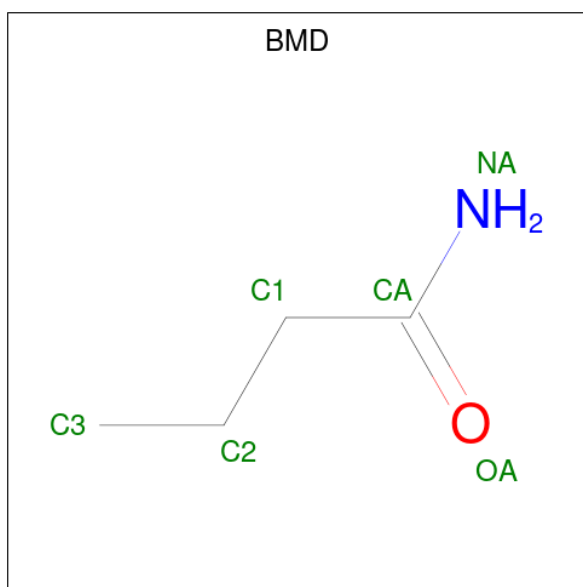
- Molecule 2 is a protein called AMIR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	189	Total	C	N	O	S	0	0	0
			1440	910	262	263	5			
2	E	194	Total	C	N	O	S	0	0	0
			1471	925	264	276	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	64	ARG	GLY	conflict	UNP P10932
E	64	ARG	GLY	conflict	UNP P10932

- Molecule 3 is BUTYRAMIDE (CCD ID: BMD) (formula: C₄H₉NO).



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

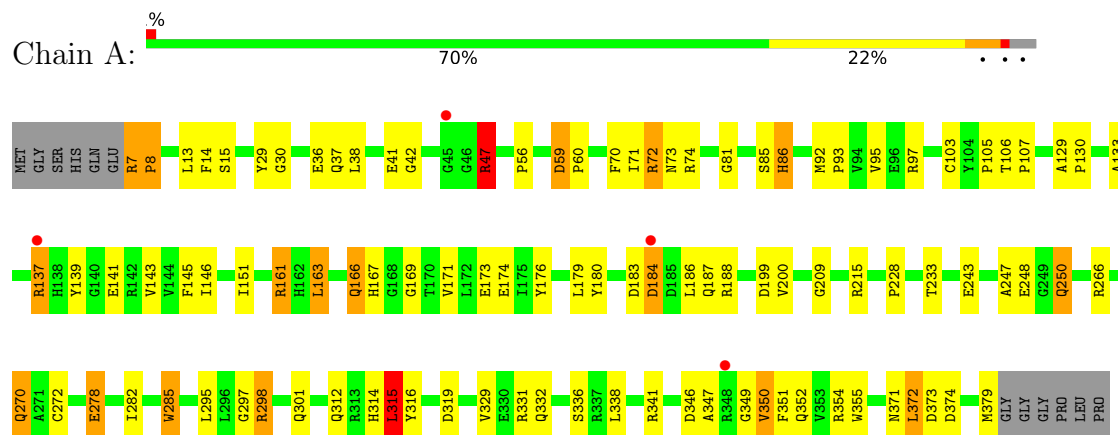
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	304	Total	O	0	0
			304	304		
4	B	238	Total	O	0	0
			238	238		
4	D	143	Total	O	0	0
			143	143		
4	E	166	Total	O	0	0
			166	166		

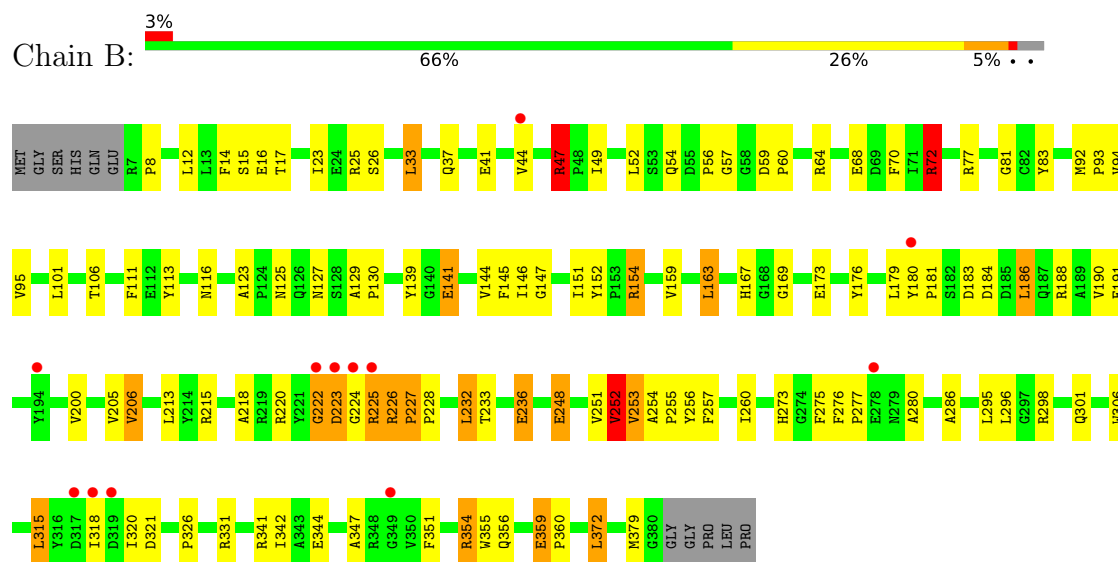
3 Residue-property plots [i](#)

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.

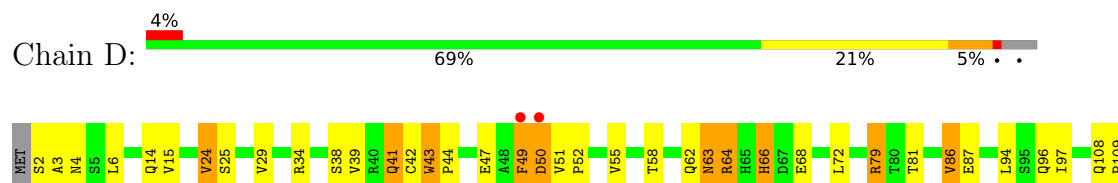
• Molecule 1: AMIC



• Molecule 1: AMIC

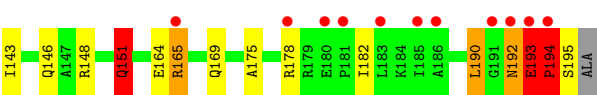


• Molecule 2: AMIR





● Molecule 2: AMIR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	308.44Å 67.15Å 76.41Å 90.00° 103.33° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 20.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	83.0 (20.00-2.25) 83.4 (20.00-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.74 (at 2.24Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.256 (Not available) , 0.251	Depositor DCC
R_{free} test set	3059 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.946	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9661	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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](#)

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	0.76	0/3018	1.89	58/4114 (1.4%)
1	B	0.68	0/3019	1.70	38/4115 (0.9%)
2	D	0.74	0/1465	1.84	35/1999 (1.8%)
2	E	0.73	0/1497	1.95	25/2044 (1.2%)
All	All	0.73	0/8999	1.83	156/12272 (1.3%)

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	2
2	D	0	2
2	E	0	3
All	All	0	7

There are no bond length outliers.

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	192	ASN	CA-CB-CG	34.49	147.09	112.60
1	A	72	ARG	CD-NE-CZ	24.65	158.91	124.40
1	A	97	ARG	CD-NE-CZ	19.93	152.30	124.40
2	D	43	TRP	CA-C-O	-15.69	98.67	120.16
2	E	43	TRP	CA-C-O	-15.12	99.44	120.16
1	A	7	ARG	CA-C-O	-14.92	95.43	120.80
1	A	215	ARG	CD-NE-CZ	14.28	144.40	124.40
2	E	124	ARG	N-CA-CB	12.15	128.14	110.16
1	A	145	PHE	CA-CB-CG	11.85	125.64	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	44	PRO	N-CA-CB	10.90	113.66	103.08
1	B	331	ARG	CD-NE-CZ	10.49	139.09	124.40
1	B	154	ARG	CD-NE-CZ	10.40	138.96	124.40
1	B	70	PHE	CA-CB-CG	10.25	124.05	113.80
2	E	124	ARG	CA-CB-CG	10.23	134.56	114.10
2	D	115	VAL	N-CA-C	9.56	119.52	110.53
1	A	270	GLN	OE1-CD-NE2	9.51	132.11	122.60
1	A	8	PRO	CA-N-CD	-9.01	99.39	112.00
1	A	47	ARG	CD-NE-CZ	8.88	136.82	124.40
2	D	49	PHE	CA-C-O	-8.52	111.93	120.70
2	E	39	VAL	CB-CA-C	-8.29	97.43	110.69
1	B	47	ARG	CD-NE-CZ	8.23	135.92	124.40
1	A	331	ARG	NE-CZ-NH2	8.07	126.46	119.20
1	A	151	ILE	N-CA-C	8.06	118.84	110.62
2	D	44	PRO	CA-N-CD	-7.91	100.93	112.00
1	B	151	ILE	N-CA-C	7.79	117.90	110.42
1	A	319	ASP	CA-CB-CG	-7.79	104.81	112.60
2	D	34	ARG	CD-NE-CZ	7.65	135.11	124.40
1	A	319	ASP	O-C-N	7.61	131.58	123.06
2	D	43	TRP	CA-C-N	7.56	128.17	120.38
2	D	43	TRP	C-N-CA	7.56	128.17	120.38
1	B	179	LEU	CA-C-O	-7.54	112.56	120.55
2	E	44	PRO	N-CA-CB	7.44	110.30	103.08
1	A	341	ARG	CD-NE-CZ	7.42	134.79	124.40
2	D	49	PHE	N-CA-C	7.39	119.12	111.14
1	B	25	ARG	N-CA-C	-7.37	103.33	111.36
2	E	44	PRO	CA-N-CD	-7.22	101.89	112.00
1	B	252	VAL	N-CA-CB	-7.20	97.95	111.62
2	D	49	PHE	CA-CB-CG	-7.18	106.62	113.80
2	D	39	VAL	CB-CA-C	-7.14	99.90	110.33
1	B	276	PHE	CA-CB-CG	7.06	120.86	113.80
1	A	314	HIS	CA-CB-CG	-7.04	106.76	113.80
1	A	188	ARG	CD-NE-CZ	7.03	134.24	124.40
1	A	250	GLN	CB-CG-CD	6.96	124.43	112.60
1	A	7	ARG	CA-C-N	6.93	128.51	119.84
1	A	7	ARG	C-N-CA	6.93	128.51	119.84
2	D	63	ASN	CA-CB-CG	6.91	119.51	112.60
1	A	161	ARG	NH1-CZ-NH2	6.88	128.24	119.30
1	A	315	LEU	CA-CB-CG	6.87	140.35	116.30
1	A	315	LEU	N-CA-CB	-6.86	99.74	110.44
2	D	4	ASN	CA-CB-CG	-6.86	105.74	112.60
2	D	79	ARG	CD-NE-CZ	6.82	133.94	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	GLY	CA-C-O	-6.80	112.40	119.27
1	B	64	ARG	CD-NE-CZ	6.65	133.72	124.40
1	A	184	ASP	CA-CB-CG	6.64	119.24	112.60
1	B	113	TYR	N-CA-CB	6.64	121.59	110.77
1	A	42	GLY	N-CA-C	6.62	124.76	115.43
1	B	145	PHE	CA-CB-CG	6.61	120.41	113.80
1	B	116	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	A	319	ASP	N-CA-CB	6.57	121.12	110.41
1	B	224	GLY	CA-C-O	6.50	131.89	120.57
2	E	146	GLN	OE1-CD-NE2	-6.48	116.12	122.60
1	B	72	ARG	CB-CA-C	-6.45	99.95	110.79
1	B	225	ARG	CD-NE-CZ	6.41	133.38	124.40
1	B	123	ALA	N-CA-C	-6.40	102.78	110.13
2	D	44	PRO	N-CD-CG	6.39	112.79	103.20
2	E	165	ARG	CD-NE-CZ	6.34	133.28	124.40
2	E	114	ARG	NE-CZ-NH2	-6.33	113.50	119.20
1	A	332	GLN	OE1-CD-NE2	-6.29	116.31	122.60
2	D	3	ALA	CA-C-O	6.25	127.04	120.42
1	B	94	VAL	O-C-N	6.24	128.39	121.90
1	A	8	PRO	N-CA-CB	6.24	109.80	103.25
1	B	127	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	A	209	GLY	N-CA-C	-6.17	106.60	114.37
2	E	193	GLU	N-CA-C	-6.17	96.18	109.81
1	A	346	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	74	ARG	CD-NE-CZ	6.16	133.02	124.40
1	A	73	ASN	CA-CB-CG	-6.15	106.45	112.60
1	A	85	SER	N-CA-C	6.14	117.97	111.28
1	B	222	GLY	CA-C-N	6.12	133.22	121.54
1	B	222	GLY	C-N-CA	6.12	133.22	121.54
1	A	167	HIS	CA-CB-CG	-6.10	107.70	113.80
2	E	44	PRO	N-CD-CG	6.08	112.32	103.20
1	A	59	ASP	CA-C-N	6.06	125.78	119.05
1	A	59	ASP	C-N-CA	6.06	125.78	119.05
2	D	15	VAL	CA-C-O	6.06	127.62	120.72
2	E	41	GLN	OE1-CD-NE2	6.05	128.65	122.60
2	E	169	GLN	CA-CB-CG	6.05	126.19	114.10
2	D	2	SER	CA-C-O	-6.02	110.56	120.80
1	B	180	TYR	N-CA-CB	6.00	120.41	110.38
2	E	123	ARG	CA-C-O	-6.00	114.06	120.42
1	B	301	GLN	OE1-CD-NE2	-5.98	116.62	122.60
1	A	278	GLU	CB-CG-CD	5.97	122.75	112.60
1	A	72	ARG	CG-CD-NE	5.93	125.05	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	66	HIS	CA-CB-CG	-5.91	107.89	113.80
1	B	77	ARG	CD-NE-CZ	5.90	132.66	124.40
1	B	16	GLU	CA-C-O	5.87	125.88	119.24
2	E	151	GLN	CA-CB-CG	5.86	125.82	114.10
2	D	86	VAL	CB-CA-C	-5.75	102.06	110.62
1	A	270	GLN	CA-CB-CG	-5.74	102.62	114.10
1	A	298	ARG	NE-CZ-NH1	-5.73	115.77	121.50
2	D	41	GLN	CA-C-O	-5.72	114.08	120.66
1	A	97	ARG	NE-CZ-NH2	-5.71	114.07	119.20
1	A	37	GLN	OE1-CD-NE2	5.69	128.29	122.60
2	D	38	SER	N-CA-C	-5.67	100.75	109.76
2	D	143	ILE	CB-CA-C	-5.65	104.52	112.14
2	D	121	SER	CA-C-O	-5.59	114.62	120.55
1	B	224	GLY	N-CA-C	5.54	126.32	113.18
2	D	42	CYS	CA-C-O	-5.54	114.64	121.06
1	A	374	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	106	THR	N-CA-CB	-5.49	101.84	111.17
2	E	76	GLY	N-CA-C	5.49	119.61	112.25
1	A	30	GLY	N-CA-C	-5.47	105.77	112.77
1	B	125	ASN	N-CA-CB	5.45	119.44	110.39
1	B	318	ILE	N-CA-C	5.44	115.07	106.32
1	A	338	LEU	N-CA-C	5.42	118.07	109.50
1	B	286	ALA	N-CA-C	-5.42	105.45	111.36
1	A	336	SER	N-CA-C	5.42	118.39	109.72
1	B	72	ARG	CD-NE-CZ	-5.39	116.85	124.40
1	B	12	LEU	CA-C-O	-5.39	114.94	120.54
1	A	285	TRP	CB-CA-C	5.38	121.22	109.99
1	A	329	VAL	CA-C-O	-5.37	114.78	120.48
2	D	157	MET	CA-C-N	5.37	127.91	120.29
2	D	157	MET	C-N-CA	5.37	127.91	120.29
2	E	114	ARG	CG-CD-NE	-5.36	100.20	112.00
1	B	25	ARG	CA-C-O	5.34	126.08	120.42
1	B	227	PRO	N-CA-C	-5.31	104.22	110.70
2	D	44	PRO	N-CA-C	-5.27	104.27	110.70
1	B	94	VAL	CB-CA-C	-5.27	105.12	112.02
1	B	251	VAL	CA-C-O	5.27	126.72	120.72
2	D	164	GLU	CA-C-N	5.25	127.27	120.44
2	D	164	GLU	C-N-CA	5.25	127.27	120.44
1	A	166	GLN	CA-CB-CG	5.25	124.60	114.10
1	B	326	PRO	CA-C-O	-5.23	114.85	120.97
1	A	161	ARG	NE-CZ-NH1	-5.23	116.27	121.50
2	D	24	VAL	CA-C-O	-5.21	115.71	121.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	29	VAL	CA-C-O	-5.21	115.65	121.17
1	A	183	ASP	CA-CB-CG	-5.20	107.40	112.60
1	B	111	PHE	CA-CB-CG	-5.20	108.60	113.80
2	E	194	PRO	CB-CA-C	-5.18	103.01	111.56
2	D	58	THR	CA-C-O	-5.18	115.71	121.51
2	E	190	LEU	CA-C-O	5.17	127.44	122.01
1	B	127	ASN	CA-CB-CG	5.16	117.75	112.60
1	A	298	ARG	CA-CB-CG	-5.15	103.80	114.10
1	A	350	VAL	N-CA-CB	5.13	119.06	110.86
1	A	71	ILE	N-CA-C	5.11	115.33	110.53
2	E	120	VAL	CA-C-N	5.10	127.07	120.44
2	E	120	VAL	C-N-CA	5.10	127.07	120.44
2	E	115	VAL	CA-C-O	-5.09	114.42	120.78
1	A	29	TYR	CA-CB-CG	-5.07	104.78	113.90
2	E	133	LYS	CA-C-N	5.05	127.36	120.54
2	E	133	LYS	C-N-CA	5.05	127.36	120.54
2	D	25	SER	CA-C-N	5.02	126.97	120.44
2	D	25	SER	C-N-CA	5.02	126.97	120.44
1	A	349	GLY	CA-C-N	-5.01	115.74	122.91
1	A	349	GLY	C-N-CA	-5.01	115.74	122.91
1	A	70	PHE	CA-CB-CG	5.01	118.81	113.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	7	ARG	Peptide,Mainchain
2	D	43	TRP	Peptide,Mainchain
2	E	193	GLU	Mainchain
2	E	43	TRP	Peptide,Mainchain

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	2943	0	2836	35	0
1	B	2944	0	2837	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1440	0	1448	28	0
2	E	1471	0	1457	33	0
3	A	6	0	9	1	0
3	B	6	0	9	0	0
4	A	304	0	0	1	0
4	B	238	0	0	5	0
4	D	143	0	0	5	0
4	E	166	0	0	6	0
All	All	9661	0	8596	156	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 9.

All (156) 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:D:165:ARG:HD2	2:D:165:ARG:H	1.31	0.95
2:E:192:ASN:HB2	2:E:194:PRO:HB3	1.46	0.94
2:E:192:ASN:CB	2:E:194:PRO:HB3	2.07	0.83
1:B:253:VAL:HG23	1:B:342:ILE:HG12	1.62	0.80
2:E:151:GLN:HG2	2:E:190:LEU:HD11	1.64	0.79
2:D:62:GLN:HE21	2:D:96:GLN:HE22	1.30	0.78
1:A:143:VAL:HG23	1:A:200:VAL:HG23	1.66	0.78
1:B:253:VAL:HG22	4:B:2202:HOH:O	1.86	0.75
2:E:165:ARG:NE	4:E:2158:HOH:O	2.22	0.73
2:E:193:GLU:N	2:E:194:PRO:HD3	2.06	0.71
1:A:243:GLU:HG2	4:A:2192:HOH:O	1.91	0.70
2:D:139:LEU:O	2:D:143:ILE:HG13	1.93	0.68
2:D:41:GLN:HG2	4:D:2045:HOH:O	1.94	0.68
2:E:117:PRO:O	2:E:121:SER:HB2	1.94	0.67
1:B:141:GLU:HB2	1:B:169:GLY:HA2	1.74	0.67
1:A:86:HIS:CD2	1:A:86:HIS:H	2.12	0.66
2:E:14:GLN:HG2	4:E:2054:HOH:O	1.96	0.65
2:D:148:ARG:HG3	2:D:187:GLN:NE2	2.12	0.65
2:E:193:GLU:H	2:E:194:PRO:HD3	1.63	0.64
1:B:92:MET:HB3	1:B:93:PRO:HD3	1.78	0.64
2:E:165:ARG:CZ	4:E:2158:HOH:O	2.44	0.64
2:D:165:ARG:O	2:D:169:GLN:HG3	1.99	0.63
1:B:248:GLU:HG3	1:B:347:ALA:HA	1.81	0.62
1:B:68:GLU:O	1:B:72:ARG:HB2	2.00	0.61
1:A:133:ALA:O	1:A:137:ARG:HD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ASN:OD1	1:A:373:ASP:HB2	2.01	0.60
1:B:144:VAL:HG23	1:B:173:GLU:HB2	1.83	0.59
1:B:253:VAL:HG23	1:B:342:ILE:CG1	2.33	0.59
1:A:86:HIS:H	1:A:86:HIS:HD2	1.51	0.59
1:B:257:PHE:O	1:B:260:ILE:HG13	2.04	0.58
1:A:295:LEU:HG	1:A:315:LEU:HD22	1.85	0.58
2:E:148:ARG:HA	2:E:151:GLN:HE21	1.69	0.58
1:B:344:GLU:HB2	1:B:354:ARG:HD2	1.86	0.57
2:E:193:GLU:N	2:E:194:PRO:CD	2.67	0.57
1:B:47:ARG:HH11	1:B:47:ARG:HG2	1.69	0.57
2:D:143:ILE:HG12	2:E:143:ILE:CG1	2.35	0.57
2:D:165:ARG:H	2:D:165:ARG:CD	2.03	0.57
2:D:94:LEU:HD13	2:E:120:VAL:HG21	1.86	0.56
1:B:252:VAL:HG11	1:B:351:PHE:CE1	2.40	0.56
1:B:181:PRO:HB2	1:B:186:LEU:HD13	1.88	0.55
2:E:192:ASN:HB2	2:E:194:PRO:CB	2.27	0.55
1:B:355:TRP:CD1	1:B:379:MET:HG2	2.41	0.55
2:E:16:LEU:HD23	2:E:18:LEU:HB2	1.89	0.55
1:B:226:ARG:HB3	1:B:227:PRO:HD2	1.88	0.55
1:B:139:TYR:HB3	1:B:200:VAL:HG22	1.90	0.54
1:B:295:LEU:HA	1:B:320:ILE:HD11	1.89	0.54
1:B:23:ILE:O	1:B:26:SER:HB3	2.07	0.54
2:D:79:ARG:HD2	2:D:127:GLU:OE2	2.07	0.54
1:B:341:ARG:HG2	1:B:356:GLN:HG3	1.90	0.53
1:A:47:ARG:HH11	1:A:47:ARG:HB3	1.74	0.53
2:D:87:GLU:O	2:D:87:GLU:HG2	2.08	0.53
2:D:55:VAL:HG22	2:D:81:THR:HB	1.90	0.52
1:B:273:HIS:HB3	4:B:2164:HOH:O	2.08	0.52
1:B:252:VAL:HG11	1:B:351:PHE:HE1	1.74	0.52
1:A:141:GLU:HB2	1:A:169:GLY:HA2	1.93	0.51
1:B:295:LEU:HG	1:B:315:LEU:HD22	1.91	0.51
2:D:62:GLN:HE21	2:D:96:GLN:NE2	2.05	0.51
2:D:155:LEU:HD12	4:D:2133:HOH:O	2.10	0.51
2:E:41:GLN:HB2	4:E:2042:HOH:O	2.11	0.51
1:B:188:ARG:HD2	4:B:2123:HOH:O	2.10	0.51
2:E:175:ALA:HB2	2:E:182:ILE:HA	1.92	0.51
2:D:94:LEU:HA	2:D:97:ILE:HD12	1.91	0.51
1:A:41:GLU:OE2	1:A:298:ARG:NH2	2.29	0.50
2:D:49:PHE:O	2:D:50:ASP:CB	2.59	0.50
1:B:15:SER:HA	1:B:56:PRO:HD2	1.94	0.50
2:E:44:PRO:HB2	4:E:2045:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ALA:O	1:A:250:GLN:HG2	2.12	0.49
1:A:297:GLY:O	1:A:301:GLN:HG3	2.11	0.49
2:E:24:VAL:HG13	2:E:110:LEU:HD21	1.94	0.49
2:D:62:GLN:O	2:D:63:ASN:HB3	2.12	0.49
1:B:139:TYR:HB3	1:B:200:VAL:CG2	2.42	0.49
2:D:64:ARG:HG3	2:D:68:GLU:OE2	2.13	0.49
1:B:236:GLU:HG3	1:B:351:PHE:CE2	2.48	0.48
1:B:226:ARG:CB	1:B:227:PRO:HD2	2.42	0.48
2:D:153:LYS:HG3	2:D:171:LEU:HD11	1.95	0.48
2:E:142:ARG:HH11	2:E:142:ARG:HG2	1.77	0.48
1:A:266:ARG:O	1:A:270:GLN:HG3	2.14	0.48
1:B:206:VAL:HG12	1:B:233:THR:HG21	1.96	0.48
1:B:354:ARG:HH11	1:B:354:ARG:HB3	1.79	0.48
1:B:129:ALA:HB3	1:B:130:PRO:HD3	1.95	0.47
1:B:8:PRO:HA	1:B:306:TRP:CE2	2.48	0.47
1:B:205:VAL:HG21	1:B:213:LEU:CD2	2.44	0.47
1:B:14:PHE:CZ	1:B:81:GLY:HA2	2.50	0.47
1:B:33:LEU:HD22	4:B:2012:HOH:O	2.13	0.47
1:B:41:GLU:OE1	1:B:298:ARG:NH1	2.47	0.47
2:E:125:ILE:O	2:E:129:MET:HG3	2.15	0.47
1:A:163:LEU:HG	1:A:372:LEU:HD21	1.94	0.47
2:D:24:VAL:HG23	4:D:2028:HOH:O	2.13	0.47
2:D:148:ARG:HG3	2:D:187:GLN:HE21	1.78	0.47
2:E:165:ARG:HD2	4:E:2159:HOH:O	2.14	0.47
1:A:161:ARG:HB2	1:A:171:VAL:HG21	1.97	0.47
1:A:103:CYS:O	1:A:105:PRO:HD3	2.15	0.47
2:E:134:GLN:O	2:E:138:GLN:HG3	2.15	0.46
1:B:83:TYR:O	1:B:106:THR:HG21	2.16	0.46
1:A:14:PHE:CZ	1:A:81:GLY:HA2	2.51	0.46
1:A:179:LEU:O	1:A:180:TYR:HB2	2.15	0.46
1:A:272:CYS:HB2	1:A:282:ILE:HD11	1.97	0.46
1:B:181:PRO:HB2	1:B:186:LEU:CD1	2.45	0.46
1:B:152:TYR:OH	1:B:232:LEU:HD13	2.16	0.45
1:B:277:PRO:HD2	1:B:280:ALA:HB3	1.98	0.45
1:B:147:GLY:O	1:B:176:TYR:HA	2.16	0.45
1:A:129:ALA:HB3	1:A:130:PRO:HD3	1.99	0.45
2:E:55:VAL:HG22	2:E:81:THR:HB	1.98	0.45
1:A:199:ASP:O	1:A:228:PRO:HD2	2.15	0.45
1:A:174:GLU:OE2	1:A:176:TYR:OH	2.28	0.45
2:E:192:ASN:HD22	2:E:194:PRO:HB3	1.82	0.45
2:D:49:PHE:CZ	2:D:72:LEU:HD21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLN:O	1:B:41:GLU:HG3	2.18	0.44
1:B:186:LEU:O	1:B:190:VAL:HG23	2.18	0.44
1:B:184:ASP:O	1:B:188:ARG:HG3	2.17	0.44
1:B:215:ARG:O	1:B:218:ALA:HB3	2.18	0.44
1:B:354:ARG:HH11	1:B:354:ARG:CB	2.31	0.44
1:A:351:PHE:N	1:A:351:PHE:CD1	2.86	0.44
2:D:108:GLN:HA	2:D:109:PRO:C	2.42	0.44
2:E:15:VAL:HG11	2:E:32:LEU:HD13	2.00	0.44
1:A:59:ASP:HA	1:A:60:PRO:HD2	1.74	0.44
1:B:44:VAL:HG23	1:B:49:ILE:HD11	1.99	0.43
1:A:92:MET:HB3	1:A:93:PRO:HD3	2.00	0.43
1:B:222:GLY:O	1:B:223:ASP:C	2.61	0.43
1:B:59:ASP:HA	1:B:60:PRO:HD2	1.85	0.43
1:A:233:THR:HG22	3:A:400:BMD:H31	2.01	0.43
2:E:194:PRO:HB2	2:E:195:SER:H	1.39	0.43
1:B:227:PRO:HA	1:B:228:PRO:HD3	1.92	0.43
2:E:133:LYS:O	2:E:136:THR:HB	2.19	0.43
1:B:359:GLU:HB2	1:B:360:PRO:HD2	1.99	0.43
1:A:312:GLN:HG2	1:A:316:TYR:CE2	2.54	0.43
1:B:191:GLU:CD	1:B:220:ARG:HH21	2.25	0.43
1:A:14:PHE:CE1	1:A:81:GLY:HA2	2.54	0.43
1:A:107:PRO:HG3	1:A:285:TRP:CZ2	2.54	0.42
2:D:66:HIS:HB3	4:D:2069:HOH:O	2.17	0.42
1:A:133:ALA:HA	1:A:137:ARG:NH1	2.34	0.42
1:A:248:GLU:OE2	1:A:347:ALA:HB2	2.20	0.42
1:B:355:TRP:NE1	1:B:379:MET:HG2	2.34	0.42
1:B:47:ARG:NH1	4:B:2023:HOH:O	2.52	0.42
2:E:192:ASN:ND2	2:E:194:PRO:HB3	2.34	0.42
1:A:38:LEU:HD13	1:A:297:GLY:HA3	2.01	0.42
1:B:320:ILE:HG22	1:B:321:ASP:N	2.35	0.42
1:A:139:TYR:HB3	1:A:200:VAL:CG1	2.49	0.42
1:B:159:VAL:HG12	1:B:163:LEU:HD22	2.02	0.42
1:B:17:THR:O	1:B:57:GLY:HA2	2.20	0.41
1:B:256:TYR:CD1	1:B:260:ILE:HD12	2.55	0.41
2:D:51:VAL:HG13	2:D:52:PRO:HD2	2.01	0.41
1:B:254:ALA:HB1	1:B:255:PRO:CD	2.49	0.41
2:E:165:ARG:H	2:E:165:ARG:HG2	1.72	0.41
1:A:355:TRP:CD1	1:A:379:MET:HG2	2.56	0.41
1:B:129:ALA:N	1:B:130:PRO:HD2	2.35	0.41
1:B:372:LEU:HD12	1:B:372:LEU:HA	1.92	0.41
2:D:165:ARG:HD2	2:D:165:ARG:N	2.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ARG:HH11	1:B:226:ARG:HD3	1.73	0.41
2:E:142:ARG:HG2	2:E:142:ARG:NH1	2.36	0.41
2:D:108:GLN:HB3	2:D:109:PRO:HA	2.02	0.40
1:A:15:SER:HA	1:A:56:PRO:HD2	2.03	0.40
1:B:154:ARG:HD3	2:E:62:GLN:HB3	2.04	0.40
2:D:64:ARG:HB3	4:D:2066:HOH:O	2.20	0.40
2:E:16:LEU:HD22	2:E:49:PHE:CE1	2.56	0.40
1:B:163:LEU:O	1:B:167:HIS:HD2	2.05	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	371/385 (96%)	361 (97%)	9 (2%)	1 (0%)	36	40
1	B	372/385 (97%)	356 (96%)	14 (4%)	2 (0%)	24	24
2	D	187/196 (95%)	179 (96%)	7 (4%)	1 (0%)	24	24
2	E	192/196 (98%)	179 (93%)	10 (5%)	3 (2%)	7	4
All	All	1122/1162 (97%)	1075 (96%)	40 (4%)	7 (1%)	21	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	50	ASP
2	E	178	ARG
2	E	194	PRO
1	B	275	PHE
2	E	44	PRO
1	B	223	ASP
1	A	8	PRO

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	306/315 (97%)	286 (94%)	20 (6%)	15	14
1	B	305/315 (97%)	280 (92%)	25 (8%)	10	9
2	D	153/169 (90%)	146 (95%)	7 (5%)	24	28
2	E	157/169 (93%)	146 (93%)	11 (7%)	14	13
All	All	921/968 (95%)	858 (93%)	63 (7%)	14	14

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	36	GLU
1	A	47	ARG
1	A	72	ARG
1	A	86	HIS
1	A	95	VAL
1	A	137	ARG
1	A	146	ILE
1	A	163	LEU
1	A	166	GLN
1	A	173	GLU
1	A	184	ASP
1	A	186	LEU
1	A	187	GLN
1	A	278	GLU
1	A	315	LEU
1	A	350	VAL
1	A	352	GLN
1	A	354	ARG
1	A	372	LEU
1	B	33	LEU
1	B	47	ARG
1	B	52	LEU
1	B	54	GLN

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Mol	Chain	Res	Type
1	B	72	ARG
1	B	95	VAL
1	B	101	LEU
1	B	141	GLU
1	B	146	ILE
1	B	163	LEU
1	B	183	ASP
1	B	186	LEU
1	B	206	VAL
1	B	225	ARG
1	B	226	ARG
1	B	232	LEU
1	B	236	GLU
1	B	248	GLU
1	B	252	VAL
1	B	253	VAL
1	B	296	LEU
1	B	315	LEU
1	B	354	ARG
1	B	359	GLU
1	B	372	LEU
2	D	6	LEU
2	D	14	GLN
2	D	47	GLU
2	D	64	ARG
2	D	86	VAL
2	D	110	LEU
2	D	143	ILE
2	E	6	LEU
2	E	14	GLN
2	E	39	VAL
2	E	47	GLU
2	E	51	VAL
2	E	121	SER
2	E	124	ARG
2	E	129	MET
2	E	136	THR
2	E	151	GLN
2	E	164	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	A	162	HIS
1	A	187	GLN
1	A	312	GLN
1	B	54	GLN
1	B	73	ASN
1	B	187	GLN
1	B	195	GLN
1	B	270	GLN
1	B	301	GLN
1	B	332	GLN
1	B	356	GLN
2	D	14	GLN
2	D	41	GLN
2	D	96	GLN
2	D	158	GLN
2	E	14	GLN
2	E	187	GLN
2	E	192	ASN

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](#)

2 ligands are 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	$\# Z > 2$
3	BMD	A	400	-	5,5,5	0.66	0	5,5,5	1.27	1 (20%)
3	BMD	B	500	-	5,5,5	0.53	0	5,5,5	2.55	1 (20%)

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
3	BMD	A	400	-	-	0/3/3/3	-
3	BMD	B	500	-	-	0/3/3/3	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	500	BMD	C2-C1-CA	5.33	121.23	113.19
3	A	400	BMD	C1-CA-NA	-2.07	109.85	116.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	BMD	1	0

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	373/385 (96%)	-0.49	4 (1%) 78 79	8, 20, 43, 67	0
1	B	374/385 (97%)	-0.14	12 (3%) 50 50	13, 31, 53, 77	0
2	D	189/196 (96%)	-0.03	7 (3%) 45 45	13, 28, 69, 98	0
2	E	194/196 (98%)	-0.16	12 (6%) 26 24	11, 26, 72, 95	0
All	All	1130/1162 (97%)	-0.24	35 (3%) 51 51	8, 26, 60, 98	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	192	ASN	4.8
2	E	193	GLU	4.5
1	B	224	GLY	4.4
2	E	180	GLU	3.7
1	B	225	ARG	3.6
1	B	222	GLY	3.3
2	E	181	PRO	3.2
2	D	178	ARG	3.1
2	E	185	ILE	3.0
1	B	317	ASP	2.9
1	B	318	ILE	2.9
2	D	176	MET	2.9
2	D	50	ASP	2.9
1	B	319	ASP	2.9
1	B	44	VAL	2.8
2	D	174	GLU	2.7
1	B	223	ASP	2.7
2	E	186	ALA	2.6
1	B	180	TYR	2.6
1	A	348	ARG	2.6
2	E	191	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	178	ARG	2.5
2	E	194	PRO	2.5
2	E	165	ARG	2.4
2	D	49	PHE	2.4
1	B	349	GLY	2.4
2	E	183	LEU	2.4
2	E	50	ASP	2.3
1	A	45	GLY	2.3
1	A	184	ASP	2.3
1	A	137	ARG	2.3
1	B	278	GLU	2.2
2	D	183	LEU	2.1
2	D	190	LEU	2.1
1	B	194	TYR	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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
3	BMD	A	400	6/6	0.97	0.06	6,9,13,16	0
3	BMD	B	500	6/6	0.98	0.05	16,19,20,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.