Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:48 PM GMT

PDB ID	:	1QO0
Title	:	AMIDE RECEPTOR OF THE AMIDASE OPERON OF PSEUDOMONAS AERUGINOSA (AMIC) COMPLEXED WITH THE POSITIVE 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

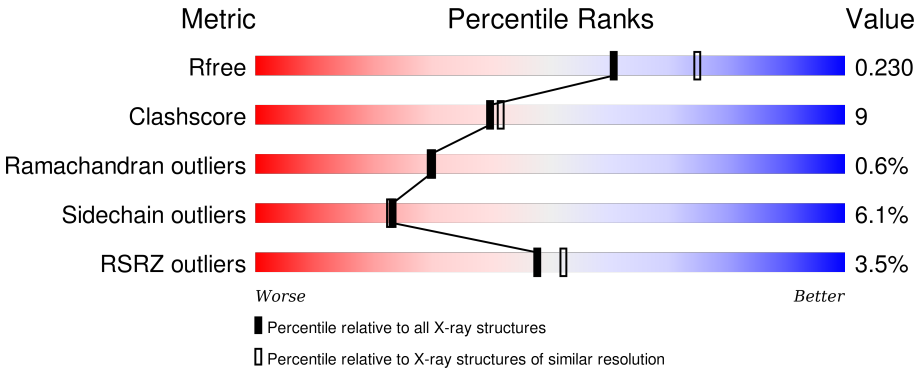
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	385	3% 73% 19%
1	B	385	2% 69% 23%
2	D	196	5% 74% 20%
2	E	196	6% 73% 20%

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
3	BMD	B	500	-	-	-	X

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

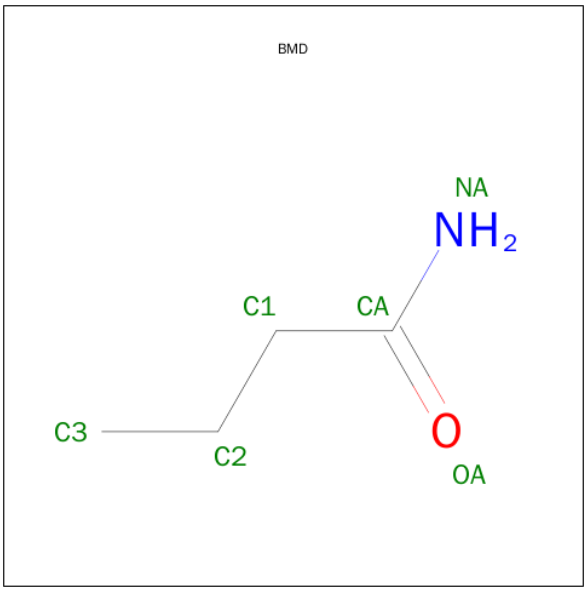
- Molecule 2 is a protein called AMIR.

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 (three-letter code: BMD) (formula: C_4H_9NO).



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

- Molecule 4 is water.

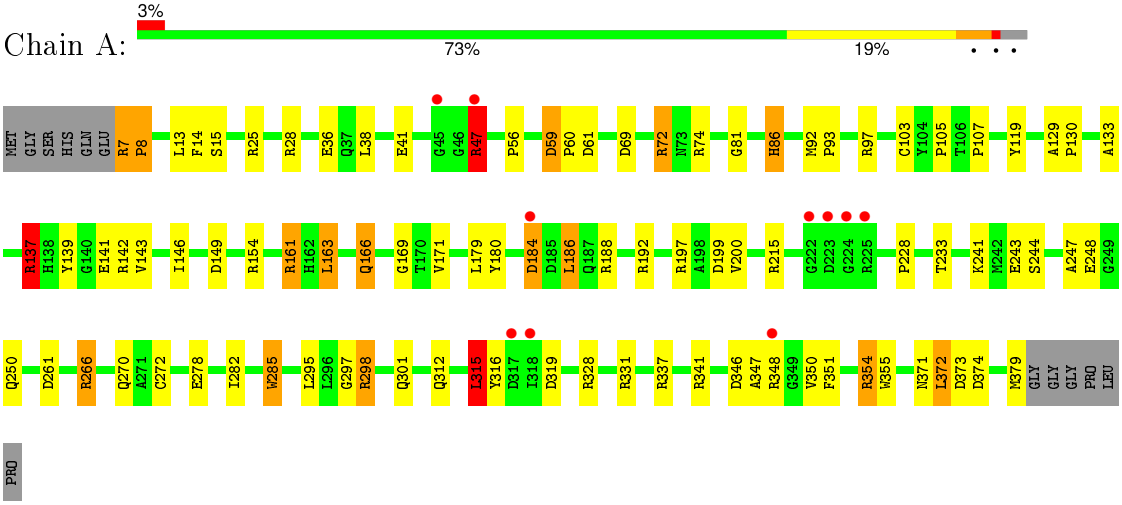
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	304	Total O 304 304	0	0
4	B	238	Total O 238 238	0	0
4	D	143	Total O 143 143	0	0
4	E	166	Total O 166 166	0	0

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.

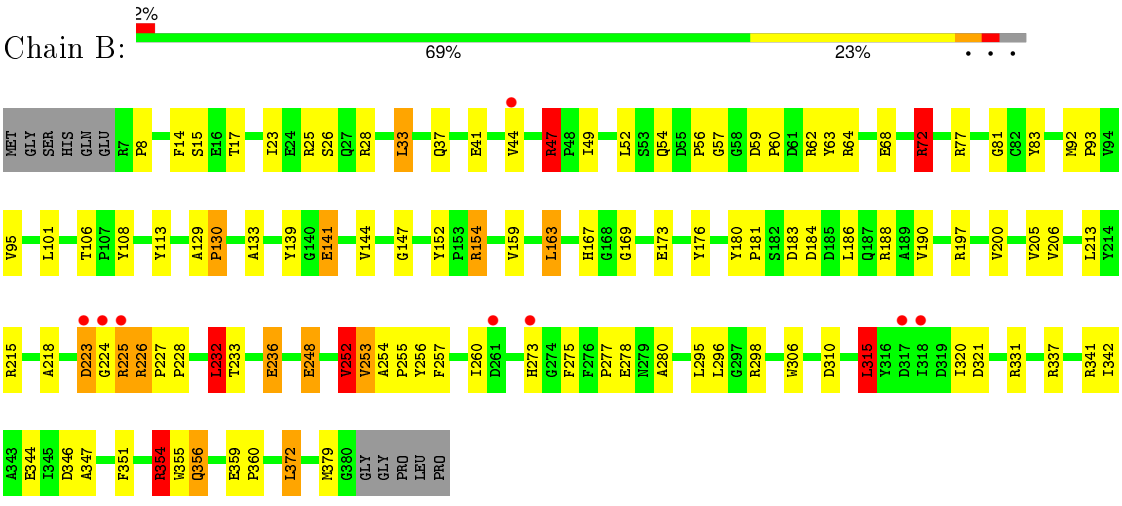
- Molecule 1: AMIC

Chain A:



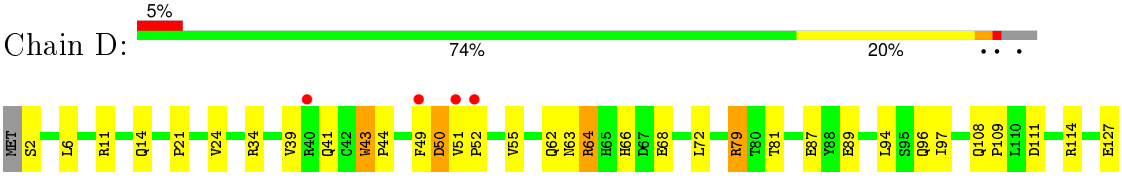
- Molecule 1: AMIC

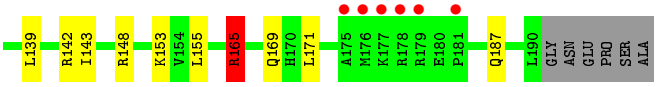
Chain B:



- Molecule 2: AMIR

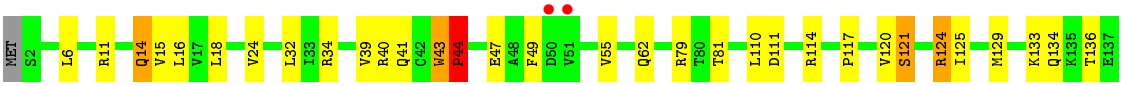
Chain D:

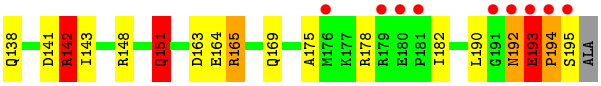




- Molecule 2: AMIR

Chain E:





4 Data and refinement statistics (i)

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 33.57 – 2.25	Depositor EDS
% Data completeness (in resolution range)	83.0 (20.00-2.25) 83.5 (33.57-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	4.74 (at 2.24Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.256 0.170 , 0.230	Depositor DCC
R_{free} test set	3055 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	19.5	Xtriage
Anisotropy	0.946	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 64.3	EDS
Estimated twinning fraction	0.021 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 60570 reflections	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.*

[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

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	0.61	0/3018	1.66	55/4114 (1.3%)
1	B	0.53	0/3019	1.43	36/4115 (0.9%)
2	D	0.55	0/1465	1.38	18/1999 (0.9%)
2	E	0.55	0/1497	1.51	25/2044 (1.2%)
All	All	0.57	0/8999	1.51	134/12272 (1.1%)

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 (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	ARG	CD-NE-CZ	25.22	158.91	123.60
1	A	97	ARG	CD-NE-CZ	20.50	152.30	123.60
2	E	192	ASN	CA-CB-CG	15.31	147.09	113.40
1	A	215	ARG	CD-NE-CZ	14.86	144.40	123.60
2	E	114	ARG	NE-CZ-NH2	-13.60	113.50	120.30
1	A	97	ARG	NE-CZ-NH2	-12.47	114.07	120.30
1	A	331	ARG	NE-CZ-NH2	12.33	126.46	120.30
1	A	7	ARG	CA-C-O	-11.75	95.43	120.10
1	A	72	ARG	NE-CZ-NH1	11.32	125.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	331	ARG	CD-NE-CZ	11.06	139.09	123.60
1	B	154	ARG	CD-NE-CZ	10.97	138.96	123.60
1	A	315	LEU	CA-CB-CG	10.89	140.35	115.30
1	B	28	ARG	NE-CZ-NH2	-10.88	114.86	120.30
2	D	43	TRP	CA-C-O	-10.21	98.67	120.10
2	E	40	ARG	NE-CZ-NH2	-10.11	115.25	120.30
1	B	64	ARG	NE-CZ-NH2	-9.96	115.32	120.30
1	B	225	ARG	NE-CZ-NH1	9.94	125.27	120.30
2	E	43	TRP	CA-C-O	-9.84	99.44	120.10
2	E	124	ARG	N-CA-CB	9.74	128.14	110.60
1	A	161	ARG	NE-CZ-NH2	-9.63	115.48	120.30
2	E	124	ARG	CA-CB-CG	9.62	134.56	113.40
2	D	79	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	B	64	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	A	47	ARG	CD-NE-CZ	9.45	136.82	123.60
1	A	298	ARG	NE-CZ-NH1	-9.06	115.77	120.30
1	B	47	ARG	CD-NE-CZ	8.80	135.92	123.60
1	A	8	PRO	CA-N-CD	-8.65	99.39	111.50
1	A	192	ARG	NE-CZ-NH2	-8.63	115.98	120.30
2	D	44	PRO	N-CA-CB	8.63	113.66	103.30
1	B	331	ARG	NE-CZ-NH1	8.32	124.46	120.30
2	D	34	ARG	CD-NE-CZ	8.22	135.11	123.60
1	A	161	ARG	NE-CZ-NH1	-8.05	116.27	120.30
1	A	161	ARG	NH1-CZ-NH2	8.04	128.24	119.40
1	A	341	ARG	CD-NE-CZ	8.00	134.79	123.60
1	B	331	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	B	47	ARG	NE-CZ-NH1	7.82	124.21	120.30
2	D	11	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	B	25	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	A	188	ARG	CD-NE-CZ	7.60	134.24	123.60
2	D	44	PRO	CA-N-CD	-7.55	100.93	111.50
2	D	34	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	A	266	ARG	NE-CZ-NH2	-7.43	116.59	120.30
2	D	79	ARG	CD-NE-CZ	7.39	133.94	123.60
2	E	39	VAL	CB-CA-C	-7.35	97.43	111.40
1	B	64	ARG	CD-NE-CZ	7.23	133.72	123.60
1	A	97	ARG	NE-CZ-NH1	7.22	123.91	120.30
2	E	114	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	328	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	B	225	ARG	CD-NE-CZ	6.98	133.38	123.60
1	A	337	ARG	NE-CZ-NH1	-6.98	116.81	120.30
2	E	165	ARG	CD-NE-CZ	6.91	133.28	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	44	PRO	CA-N-CD	-6.86	101.89	111.50
2	E	165	ARG	NE-CZ-NH1	-6.75	116.92	120.30
1	A	74	ARG	CD-NE-CZ	6.73	133.02	123.60
1	A	25	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	B	62	ARG	NE-CZ-NH1	6.64	123.62	120.30
2	D	89	GLU	OE1-CD-OE2	-6.50	115.50	123.30
1	B	77	ARG	CD-NE-CZ	6.47	132.66	123.60
2	E	11	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	184	ASP	CB-CG-OD1	6.41	124.07	118.30
2	D	44	PRO	N-CD-CG	6.39	112.79	103.20
2	E	34	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	149	ASP	CB-CG-OD1	6.35	124.01	118.30
1	B	77	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	A	69	ASP	CB-CG-OD2	6.32	123.99	118.30
1	A	74	ARG	NE-CZ-NH1	-6.31	117.14	120.30
1	A	72	ARG	CG-CD-NE	6.31	125.05	111.80
1	B	197	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	B	224	GLY	CA-C-O	6.27	131.89	120.60
1	A	331	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	A	261	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	B	252	VAL	N-CA-CB	-6.16	97.95	111.50
1	A	137	ARG	NE-CZ-NH2	6.11	123.36	120.30
1	B	113	TYR	N-CA-CB	6.11	121.59	110.60
1	A	374	ASP	CB-CG-OD1	6.08	123.78	118.30
2	E	44	PRO	N-CD-CG	6.08	112.32	103.20
2	D	39	VAL	CB-CA-C	-6.05	99.90	111.40
1	B	225	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	61	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	142	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	241	LYS	CD-CE-NZ	5.97	125.44	111.70
1	A	346	ASP	CB-CG-OD1	5.96	123.66	118.30
2	E	79	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	D	142	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	47	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	337	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	197	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	319	ASP	N-CA-CB	5.84	121.12	110.60
2	E	44	PRO	N-CA-CB	5.83	110.30	103.30
1	B	63	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	B	346	ASP	CB-CG-OD1	5.82	123.54	118.30
2	E	169	GLN	CA-CB-CG	5.81	126.19	113.40
1	A	348	ARG	NE-CZ-NH2	-5.81	117.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	ARG	NE-CZ-NH1	5.78	123.19	120.30
2	E	11	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	E	141	ASP	CB-CG-OD1	5.71	123.44	118.30
2	E	151	GLN	CA-CB-CG	5.64	125.82	113.40
2	D	165	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	B	180	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	B	25	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	215	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	186	LEU	CA-CB-CG	5.56	128.10	115.30
1	A	319	ASP	O-C-N	5.55	131.58	122.70
1	B	310	ASP	CB-CG-OD2	5.55	123.30	118.30
2	E	163	ASP	CB-CG-OD1	5.54	123.29	118.30
2	E	114	ARG	CG-CD-NE	-5.52	100.20	111.80
1	A	154	ARG	CD-NE-CZ	5.52	131.32	123.60
2	E	193	GLU	N-CA-C	-5.49	96.18	111.00
1	B	180	TYR	N-CA-CB	5.45	120.41	110.60
1	B	47	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	180	TYR	CB-CG-CD2	5.43	124.26	121.00
1	A	8	PRO	N-CA-CB	5.42	109.80	103.30
1	A	285	TRP	CB-CA-C	5.41	121.22	110.40
1	A	354	ARG	NE-CZ-NH2	5.39	123.00	120.30
2	E	142	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	192	ARG	CD-NE-CZ	5.35	131.09	123.60
1	A	59	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	315	LEU	N-CA-CB	-5.33	99.74	110.40
1	B	62	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	224	GLY	N-CA-C	5.29	126.32	113.10
2	D	165	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	A	28	ARG	NE-CZ-NH2	5.26	122.93	120.30
2	D	114	ARG	CD-NE-CZ	5.23	130.92	123.60
1	B	72	ARG	CB-CA-C	-5.22	99.95	110.40
1	A	215	ARG	CG-CD-NE	5.22	122.77	111.80
2	E	111	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	315	LEU	CA-CB-CG	5.17	127.18	115.30
1	A	166	GLN	CA-CB-CG	5.09	124.60	113.40
2	D	11	ARG	CD-NE-CZ	5.07	130.70	123.60
1	B	232	LEU	CA-CB-CG	5.05	126.91	115.30
2	D	2	SER	N-CA-CB	5.03	118.04	110.50
1	A	119	TYR	CB-CG-CD1	5.01	124.00	121.00
2	D	111	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	354	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

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

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	2943	0	2836	34	0
1	B	2944	0	2837	62	0
2	D	1440	0	1448	27	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	153	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 (153) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:86:HIS:CD2	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
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
2:E:193:GLU:N	2:E:194:PRO:CD	2.67	0.57
1:B:344:GLU:HB2	1:B:354:ARG:HD2	1.86	0.57
2:D:165:ARG:H	2:D:165:ARG:CD	2.03	0.57
2:D:143:ILE:HG12	2:E:143:ILE:CG1	2.35	0.57
1:B:47:ARG:HH11	1:B:47:ARG:HG2	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:87:GLU:O	2:D:87:GLU:HG2	2.08	0.53
1:A:47:ARG:HH11	1:A:47:ARG:HB3	1.74	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
2:E:175:ALA:HB2	2:E:182:ILE:HA	1.92	0.51
1:B:188:ARG:HD2	4:B:2123:HOH:O	2.10	0.51
2:D:94:LEU:HA	2:D:97:ILE:HD12	1.91	0.51
2:D:49:PHE:O	2:D:50:ASP:CB	2.59	0.50
1:A:41:GLU:OE2	1:A:298:ARG:NH2	2.29	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
1:A:297:GLY:O	1:A:301:GLN:HG3	2.11	0.49
1:A:247:ALA:O	1:A:250:GLN:HG2	2.12	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:E:142:ARG:HG2	2:E:142:ARG:HH11	1.77	0.48
2:D:153:LYS:HG3	2:D:171:LEU:HD11	1.95	0.48
1:B:206:VAL:HG12	1:B:233:THR:HG21	1.96	0.48
1:A:266:ARG:O	1:A:270:GLN:HG3	2.14	0.48
1:B:354:ARG:HB3	1:B:354:ARG:HH11	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
2:E:125:ILE:O	2:E:129:MET:HG3	2.15	0.47
1:B:41:GLU:OE1	1:B:298:ARG:NH1	2.47	0.47
2:E:165:ARG:HD2	4:E:2159:HOH:O	2.14	0.47
2:D:148:ARG:HG3	2:D:187:GLN:HE21	1.78	0.47
2:D:24:VAL:HG23	4:D:2028:HOH:O	2.13	0.47
1:A:163:LEU:HG	1:A:372:LEU:HD21	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:179:LEU:O	1:A:180:TYR:HB2	2.15	0.46
1:A:14:PHE:CZ	1:A:81:GLY:HA2	2.51	0.46
1:B:181:PRO:HB2	1:B:186:LEU:CD1	2.45	0.46
1:A:272:CYS:HB2	1:A:282:ILE:HD11	1.97	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
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
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:354:ARG:HH11	1:B:354:ARG:CB	2.31	0.44
1:B:215:ARG:O	1:B:218:ALA:HB3	2.18	0.44
2:E:15:VAL:HG11	2:E:32:LEU:HD13	2.00	0.44
1:A:351:PHE:N	1:A:351:PHE:CD1	2.86	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:B:133:ALA:HB1	1:B:379:MET:HE1	1.99	0.43
1:A:92:MET:HB3	1:A:93:PRO:HD3	2.00	0.43
1:B:59:ASP:HA	1:B:60:PRO:HD2	1.85	0.43
2:E:194:PRO:HB2	2:E:195:SER:H	1.39	0.43
1:A:233:THR:HG22	3:A:400:BMD:H31	2.01	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: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:B:355:TRP:NE1	1:B:379:MET:HG2	2.34	0.42
1:A:248:GLU:OE2	1:A:347:ALA:HB2	2.20	0.42
2:E:192:ASN:ND2	2:E:194:PRO:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ARG:NH1	4:B:2023:HOH:O	2.52	0.42
1:B:320:ILE:HG22	1:B:321:ASP:N	2.35	0.42
1:A:38:LEU:HD13	1:A:297:GLY:HA3	2.01	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:256:TYR:CD1	1:B:260:ILE:HD12	2.55	0.41
1:B:17:THR:O	1:B:57:GLY:HA2	2.20	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:HG2	2:E:165:ARG:H	1.72	0.41
1:B:129:ALA:N	1:B:130:PRO:HD2	2.35	0.41
1:B:372:LEU:HA	1:B:372:LEU:HD12	1.92	0.41
1:A:355:TRP:CD1	1:A:379:MET:HG2	2.56	0.41
2:D:165:ARG:N	2:D:165:ARG:HD2	2.14	0.41
1:B:226:ARG:HD3	1:B:226:ARG:HH11	1.73	0.41
2:E:142:ARG:NH1	2:E:142:ARG:HG2	2.36	0.41
2:D:108:GLN:HB3	2:D:109:PRO:HA	2.02	0.40
2:E:16:LEU:HD22	2:E:49:PHE:CE1	2.56	0.40
2:D:64:ARG:HB3	4:D:2066:HOH:O	2.20	0.40
1:B:154:ARG:HD3	2:E:62:GLN:HB3	2.04	0.40
1:A:15:SER:HA	1:A:56:PRO:HD2	2.03	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%)	46	52
1	B	372/385 (97%)	356 (96%)	14 (4%)	2 (0%)	34	34
2	D	187/196 (95%)	179 (96%)	7 (4%)	1 (0%)	34	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	E	192/196 (98%)	179 (93%)	10 (5%)	3 (2%)	12 7
All	All	1122/1162 (97%)	1075 (96%)	40 (4%)	7 (1%)	30 30

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 (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	306/315 (97%)	289 (94%)	17 (6%)	26 27
1	B	305/315 (97%)	279 (92%)	26 (8%)	13 11
2	D	153/169 (90%)	148 (97%)	5 (3%)	45 56
2	E	157/169 (93%)	149 (95%)	8 (5%)	29 32
All	All	921/968 (95%)	865 (94%)	56 (6%)	23 23

All (56) 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	137	ARG
1	A	146	ILE

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Mol	Chain	Res	Type
1	A	163	LEU
1	A	166	GLN
1	A	184	ASP
1	A	186	LEU
1	A	244	SER
1	A	278	GLU
1	A	315	LEU
1	A	350	VAL
1	A	354	ARG
1	A	372	LEU
1	B	33	LEU
1	B	47	ARG
1	B	52	LEU
1	B	54	GLN
1	B	72	ARG
1	B	95	VAL
1	B	101	LEU
1	B	108	TYR
1	B	130	PRO
1	B	141	GLU
1	B	163	LEU
1	B	183	ASP
1	B	223	ASP
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	278	GLU
1	B	296	LEU
1	B	315	LEU
1	B	354	ARG
1	B	356	GLN
1	B	372	LEU
2	D	6	LEU
2	D	14	GLN
2	D	21	PRO
2	D	64	ARG
2	D	165	ARG
2	E	6	LEU

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Mol	Chain	Res	Type
2	E	14	GLN
2	E	47	GLU
2	E	121	SER
2	E	124	ARG
2	E	142	ARG
2	E	151	GLN
2	E	164	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	86	HIS
1	A	312	GLN
1	B	138	HIS
1	B	195	GLN
1	B	270	GLN
1	B	312	GLN
1	B	356	GLN
2	D	14	GLN
2	D	96	GLN
2	D	158	GLN
2	D	187	GLN
2	E	14	GLN
2	E	150	ASN
2	E	187	GLN
2	E	192	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 (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	0.63	0	5,5,5	1.14	1 (20%)
3	BMD	B	500	-	5,5,5	0.51	0	5,5,5	1.73	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	0/0/0/0
3	BMD	B	500	-	-	0/3/3/3	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	400	BMD	C1-CA-NA	-2.13	109.85	116.53
3	B	500	BMD	C2-C1-CA	3.34	121.23	112.80

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

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	373/385 (96%)	-0.14	10 (2%) 58 62	8, 20, 43, 67	0
1	B	374/385 (97%)	-0.10	8 (2%) 67 71	13, 31, 53, 77	0
2	D	189/196 (96%)	0.13	10 (5%) 30 33	13, 28, 69, 98	0
2	E	194/196 (98%)	0.02	11 (5%) 27 30	11, 26, 72, 95	0
All	All	1130/1162 (97%)	-0.06	39 (3%) 48 52	8, 26, 60, 98	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	192	ASN	8.6
2	E	193	GLU	7.1
1	B	317	ASP	5.0
2	E	194	PRO	4.7
2	E	191	GLY	4.1
2	D	181	PRO	4.1
1	A	222	GLY	3.9
2	D	179	ARG	3.8
2	D	175	ALA	3.8
2	E	180	GLU	3.7
1	A	224	GLY	3.5
1	B	225	ARG	3.4
2	E	179	ARG	3.3
2	D	178	ARG	3.3
1	B	44	VAL	3.3
1	A	223	ASP	3.3
2	E	50	ASP	3.0
2	E	181	PRO	2.9
1	A	317	ASP	2.9
1	B	223	ASP	2.9
1	A	45	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	261	ASP	2.7
1	A	225	ARG	2.6
1	B	224	GLY	2.6
2	E	176	MET	2.6
2	D	49	PHE	2.5
1	B	318	ILE	2.4
2	D	51	VAL	2.4
2	E	51	VAL	2.3
1	A	348	ARG	2.3
2	D	52	PRO	2.3
2	D	40	ARG	2.2
1	A	318	ILE	2.2
1	B	273	HIS	2.1
2	E	195	SER	2.1
2	D	177	LYS	2.1
1	A	47	ARG	2.0
1	A	184	ASP	2.0
2	D	176	MET	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	BMD	B	500	6/6	0.98	0.23	3.00	16,19,20,22	0
3	BMD	A	400	6/6	0.99	0.20	1.55	6,9,13,16	0

6.5 Other polymers (i)

There are no such residues in this entry.