Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:42 PM GMT

PDB ID	:	1GUB
Title	:	HINGE-BENDING MOTION OF D-ALLOSE BINDING PROTEIN FROM ESCHERICHIA COLI: THREE OPEN CONFORMATIONS
Authors	:	Magnusson, U.; Chaudhuri, B.N.; Ko, J.; Park, C.; Jones, T.A.; Mowbray, S.L.
Deposited on	:	2002-01-24
Resolution	:	3.10 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:

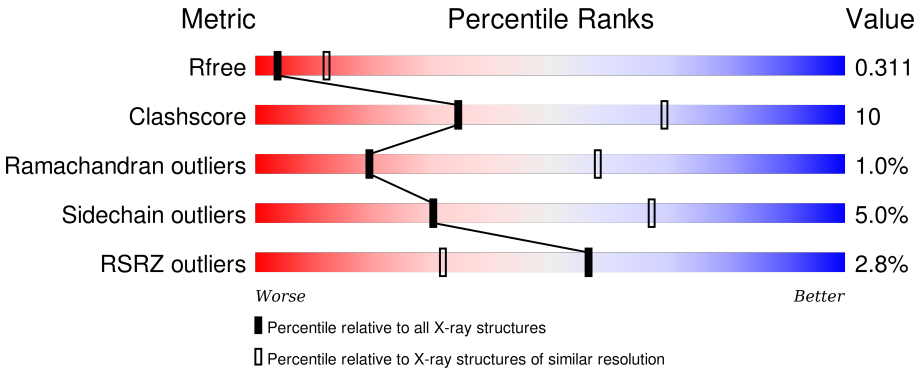
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	288	3%, 37%, 52%, 9%

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	NI	A	1289	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2144 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 D-ALLOSE-BINDING PERIPLASMIC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2133	1346	362	416	9			

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		

- Molecule 3 is water.

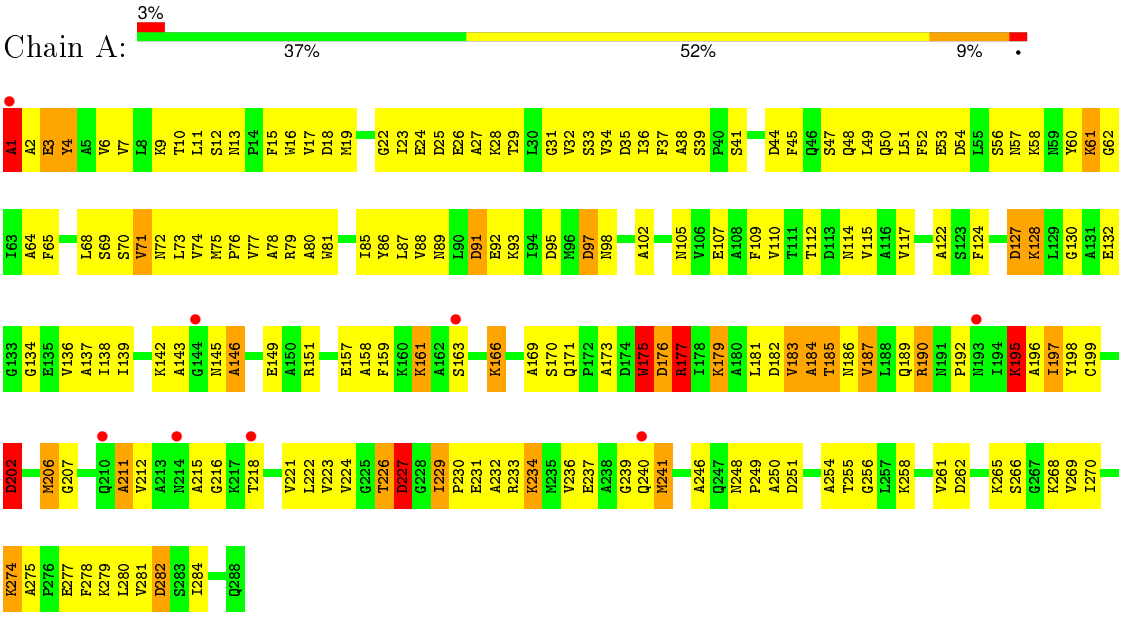
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		

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: D-ALLOSE-BINDING PERIPLASMIC PROTEIN

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 3 2	Depositor
Cell constants a, b, c, α, β, γ	133.10Å 133.10Å 133.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.10 29.76 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.75-3.10) 99.5 (29.76-3.00)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.62 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.280 , 0.339 0.251 , 0.311	Depositor DCC
R_{free} test set	550 reflections (7.65%)	DCC
Wilson B-factor (Å^2)	49.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 31.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 8517 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	2144	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: NI

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	3.45	242/2161 (11.2%)	1.80	44/2920 (1.5%)

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	1	2

All (242) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	ALA	CA-CB	43.46	2.43	1.52
1	A	1	ALA	C-O	26.52	1.73	1.23
1	A	37	PHE	CD1-CE1	-17.07	1.05	1.39
1	A	1	ALA	CA-C	-16.80	1.09	1.52
1	A	9	LYS	C-O	14.01	1.50	1.23
1	A	266	SER	CB-OG	-13.36	1.24	1.42
1	A	132	GLU	CD-OE2	13.26	1.40	1.25
1	A	221	VAL	CB-CG2	-12.92	1.25	1.52
1	A	52	PHE	CE2-CZ	-12.52	1.13	1.37
1	A	74	VAL	CB-CG2	-12.22	1.27	1.52
1	A	37	PHE	CD2-CE2	-12.09	1.15	1.39
1	A	234	LYS	CD-CE	11.62	1.80	1.51
1	A	146	ALA	CA-CB	11.34	1.76	1.52
1	A	277	GLU	CD-OE1	11.24	1.38	1.25
1	A	1	ALA	N-CA	11.23	1.68	1.46
1	A	277	GLU	CD-OE2	11.21	1.38	1.25
1	A	149	GLU	CD-OE2	11.13	1.37	1.25
1	A	61	LYS	CE-NZ	11.04	1.76	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	PHE	CE1-CZ	11.01	1.58	1.37
1	A	53	GLU	CD-OE1	-10.82	1.13	1.25
1	A	72	ASN	CA-C	-10.77	1.25	1.52
1	A	16	TRP	CE3-CZ3	-10.53	1.20	1.38
1	A	24	GLU	CD-OE1	-10.48	1.14	1.25
1	A	69	SER	CB-OG	-10.43	1.28	1.42
1	A	38	ALA	CA-CB	-10.13	1.31	1.52
1	A	175	TRP	CG-CD1	10.05	1.50	1.36
1	A	281	VAL	CB-CG1	-9.93	1.31	1.52
1	A	17	VAL	CB-CG1	-9.74	1.32	1.52
1	A	166	LYS	CD-CE	9.74	1.75	1.51
1	A	161	LYS	CD-CE	9.70	1.75	1.51
1	A	109	PHE	CE1-CZ	-9.50	1.19	1.37
1	A	86	TYR	CG-CD1	-9.41	1.26	1.39
1	A	274	LYS	CE-NZ	9.39	1.72	1.49
1	A	54	ASP	CB-CG	9.35	1.71	1.51
1	A	196	ALA	CA-CB	-9.33	1.32	1.52
1	A	78	ALA	CA-CB	-9.23	1.33	1.52
1	A	136	VAL	CA-CB	9.20	1.74	1.54
1	A	189	GLN	CG-CD	8.97	1.71	1.51
1	A	237	GLU	CD-OE2	8.97	1.35	1.25
1	A	50	GLN	CG-CD	-8.87	1.30	1.51
1	A	60	TYR	CG-CD2	-8.86	1.27	1.39
1	A	169	ALA	CA-CB	8.84	1.71	1.52
1	A	198	TYR	CD1-CE1	-8.84	1.26	1.39
1	A	110	VAL	CA-CB	-8.81	1.36	1.54
1	A	223	VAL	CB-CG2	8.80	1.71	1.52
1	A	269	VAL	CB-CG2	-8.80	1.34	1.52
1	A	109	PHE	CE2-CZ	-8.75	1.20	1.37
1	A	157	GLU	CD-OE2	8.65	1.35	1.25
1	A	107	GLU	CD-OE2	8.65	1.35	1.25
1	A	4	TYR	CD2-CE2	8.47	1.52	1.39
1	A	95	ASP	C-O	-8.47	1.07	1.23
1	A	81	TRP	CE3-CZ3	-8.39	1.24	1.38
1	A	102	ALA	CA-CB	-8.39	1.34	1.52
1	A	15	PHE	CE2-CZ	-8.38	1.21	1.37
1	A	71	VAL	CB-CG1	8.28	1.70	1.52
1	A	27	ALA	CA-CB	8.22	1.69	1.52
1	A	157	GLU	CD-OE1	8.13	1.34	1.25
1	A	231	GLU	CD-OE2	8.12	1.34	1.25
1	A	110	VAL	CB-CG1	8.11	1.69	1.52
1	A	115	VAL	N-CA	-8.10	1.30	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	ARG	NE-CZ	8.08	1.43	1.33
1	A	56	SER	CA-CB	-8.08	1.40	1.52
1	A	184	ALA	CA-CB	8.08	1.69	1.52
1	A	240	GLN	CG-CD	8.07	1.69	1.51
1	A	173	ALA	CA-CB	8.04	1.69	1.52
1	A	177	ARG	CZ-NH2	7.90	1.43	1.33
1	A	254	ALA	CA-CB	-7.86	1.35	1.52
1	A	179	LYS	CE-NZ	7.82	1.68	1.49
1	A	215	ALA	C-O	7.75	1.38	1.23
1	A	35	ASP	C-O	-7.73	1.08	1.23
1	A	13	ASN	CG-ND2	7.70	1.52	1.32
1	A	62	GLY	C-O	-7.66	1.11	1.23
1	A	124	PHE	CD1-CE1	-7.64	1.24	1.39
1	A	41	SER	CB-OG	7.63	1.52	1.42
1	A	32	VAL	CB-CG1	-7.61	1.36	1.52
1	A	255	THR	C-O	-7.60	1.08	1.23
1	A	71	VAL	CB-CG2	7.59	1.68	1.52
1	A	109	PHE	CG-CD1	-7.57	1.27	1.38
1	A	265	LYS	CB-CG	7.54	1.73	1.52
1	A	212	VAL	CB-CG2	7.53	1.68	1.52
1	A	163	SER	CB-OG	7.52	1.52	1.42
1	A	110	VAL	N-CA	-7.51	1.31	1.46
1	A	130	GLY	C-O	7.50	1.35	1.23
1	A	17	VAL	CB-CG2	-7.45	1.37	1.52
1	A	68	LEU	CG-CD1	-7.37	1.24	1.51
1	A	246	ALA	CA-CB	-7.37	1.36	1.52
1	A	81	TRP	CG-CD1	7.29	1.47	1.36
1	A	37	PHE	CE1-CZ	-7.27	1.23	1.37
1	A	268	LYS	CB-CG	7.26	1.72	1.52
1	A	70	SER	C-O	-7.26	1.09	1.23
1	A	240	GLN	CB-CG	7.24	1.72	1.52
1	A	37	PHE	CE2-CZ	-7.24	1.23	1.37
1	A	58	LYS	C-O	7.24	1.37	1.23
1	A	33	SER	N-CA	-7.16	1.32	1.46
1	A	91	ASP	CB-CG	-7.11	1.36	1.51
1	A	132	GLU	CD-OE1	7.06	1.33	1.25
1	A	199	CYS	CB-SG	-7.03	1.70	1.82
1	A	92	GLU	CB-CG	6.98	1.65	1.52
1	A	50	GLN	CD-OE1	-6.96	1.08	1.24
1	A	198	TYR	CD2-CE2	-6.95	1.28	1.39
1	A	212	VAL	CB-CG1	6.94	1.67	1.52
1	A	158	ALA	CA-CB	-6.87	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	TRP	C-O	-6.86	1.10	1.23
1	A	12	SER	CB-OG	6.79	1.51	1.42
1	A	107	GLU	CD-OE1	-6.76	1.18	1.25
1	A	171	GLN	CG-CD	6.70	1.66	1.51
1	A	279	LYS	CB-CG	-6.68	1.34	1.52
1	A	32	VAL	CB-CG2	-6.65	1.38	1.52
1	A	93	LYS	CB-CG	-6.65	1.34	1.52
1	A	19	MET	CG-SD	-6.64	1.63	1.81
1	A	92	GLU	CD-OE1	6.57	1.32	1.25
1	A	57	ASN	CA-CB	6.52	1.70	1.53
1	A	105	ASN	CB-CG	6.52	1.66	1.51
1	A	248	ASN	C-O	-6.51	1.10	1.23
1	A	23	ILE	CB-CG2	-6.46	1.32	1.52
1	A	229	ILE	CB-CG2	6.46	1.72	1.52
1	A	181	LEU	CA-C	6.45	1.69	1.52
1	A	51	LEU	C-O	-6.44	1.11	1.23
1	A	249	PRO	C-O	-6.44	1.10	1.23
1	A	279	LYS	C-O	-6.43	1.11	1.23
1	A	6	VAL	CA-CB	-6.39	1.41	1.54
1	A	261	VAL	CA-CB	-6.39	1.41	1.54
1	A	279	LYS	CD-CE	6.38	1.67	1.51
1	A	233	ARG	CZ-NH1	6.36	1.41	1.33
1	A	185	THR	CA-CB	6.32	1.69	1.53
1	A	95	ASP	CA-C	-6.30	1.36	1.52
1	A	24	GLU	C-O	-6.29	1.11	1.23
1	A	142	LYS	CD-CE	6.28	1.67	1.51
1	A	262	ASP	CA-CB	-6.23	1.40	1.53
1	A	4	TYR	CA-CB	-6.23	1.40	1.53
1	A	7	VAL	CB-CG1	-6.17	1.39	1.52
1	A	36	ILE	C-O	-6.16	1.11	1.23
1	A	109	PHE	CD2-CE2	-6.15	1.26	1.39
1	A	85	ILE	CA-CB	-6.14	1.40	1.54
1	A	251	ASP	CA-C	-6.14	1.36	1.52
1	A	175	TRP	CB-CG	6.14	1.61	1.50
1	A	61	LYS	C-O	-6.12	1.11	1.23
1	A	218	THR	CA-CB	6.09	1.69	1.53
1	A	44	ASP	CA-C	-6.05	1.37	1.52
1	A	37	PHE	CB-CG	6.05	1.61	1.51
1	A	270	ILE	CB-CG1	-6.04	1.37	1.54
1	A	80	ALA	CA-CB	-6.04	1.39	1.52
1	A	185	THR	N-CA	6.04	1.58	1.46
1	A	278	PHE	CE1-CZ	-6.03	1.25	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	ASP	CG-OD1	6.02	1.39	1.25
1	A	112	THR	C-O	-6.01	1.11	1.23
1	A	65	PHE	CE1-CZ	-6.00	1.25	1.37
1	A	91	ASP	C-O	-6.00	1.11	1.23
1	A	163	SER	CA-CB	5.94	1.61	1.52
1	A	44	ASP	CB-CG	5.94	1.64	1.51
1	A	206	MET	SD-CE	5.92	2.10	1.77
1	A	159	PHE	CD2-CE2	-5.91	1.27	1.39
1	A	157	GLU	CG-CD	5.86	1.60	1.51
1	A	11	LEU	CG-CD2	-5.85	1.30	1.51
1	A	282	ASP	CB-CG	-5.84	1.39	1.51
1	A	60	TYR	CZ-OH	5.83	1.47	1.37
1	A	86	TYR	CE1-CZ	-5.81	1.30	1.38
1	A	86	TYR	N-CA	-5.81	1.34	1.46
1	A	122	ALA	C-O	-5.81	1.12	1.23
1	A	241	MET	SD-CE	-5.78	1.45	1.77
1	A	216	GLY	N-CA	5.77	1.54	1.46
1	A	215	ALA	C-N	5.75	1.43	1.33
1	A	237	GLU	CG-CD	5.75	1.60	1.51
1	A	187	VAL	CA-CB	5.75	1.66	1.54
1	A	45	PHE	CD1-CE1	-5.73	1.27	1.39
1	A	256	GLY	C-O	-5.72	1.14	1.23
1	A	78	ALA	N-CA	-5.71	1.34	1.46
1	A	202	ASP	C-O	5.71	1.34	1.23
1	A	284	ILE	C-O	-5.69	1.12	1.23
1	A	179	LYS	CD-CE	5.66	1.65	1.51
1	A	149	GLU	CD-OE1	5.66	1.31	1.25
1	A	37	PHE	CG-CD1	-5.61	1.30	1.38
1	A	89	ASN	CG-OD1	-5.60	1.11	1.24
1	A	223	VAL	CA-CB	5.58	1.66	1.54
1	A	199	CYS	CA-CB	-5.58	1.41	1.53
1	A	79	ARG	CZ-NH2	5.57	1.40	1.33
1	A	281	VAL	CA-CB	-5.57	1.43	1.54
1	A	211	ALA	CA-CB	5.57	1.64	1.52
1	A	17	VAL	CA-CB	5.54	1.66	1.54
1	A	47	SER	C-O	5.54	1.33	1.23
1	A	88	VAL	CB-CG2	-5.52	1.41	1.52
1	A	157	GLU	N-CA	-5.52	1.35	1.46
1	A	136	VAL	C-O	5.51	1.33	1.23
1	A	64	ALA	CA-CB	-5.50	1.41	1.52
1	A	91	ASP	N-CA	5.47	1.57	1.46
1	A	15	PHE	CA-CB	-5.46	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	GLY	C-O	-5.46	1.15	1.23
1	A	195	LYS	CE-NZ	5.46	1.62	1.49
1	A	3	GLU	CA-C	-5.45	1.38	1.52
1	A	31	GLY	CA-C	-5.45	1.43	1.51
1	A	258	LYS	CE-NZ	-5.44	1.35	1.49
1	A	26	GLU	CA-C	-5.44	1.38	1.52
1	A	277	GLU	C-O	-5.41	1.13	1.23
1	A	117	VAL	CB-CG2	5.41	1.64	1.52
1	A	38	ALA	CA-C	-5.38	1.39	1.52
1	A	65	PHE	CA-CB	-5.37	1.42	1.53
1	A	132	GLU	CG-CD	5.36	1.59	1.51
1	A	216	GLY	CA-C	5.34	1.60	1.51
1	A	249	PRO	N-CA	-5.32	1.38	1.47
1	A	18	ASP	N-CA	-5.32	1.35	1.46
1	A	105	ASN	N-CA	-5.32	1.35	1.46
1	A	77	VAL	C-O	-5.31	1.13	1.23
1	A	256	GLY	CA-C	-5.29	1.43	1.51
1	A	239	GLY	CA-C	-5.28	1.43	1.51
1	A	114	ASN	CB-CG	-5.27	1.39	1.51
1	A	226	THR	N-CA	-5.26	1.35	1.46
1	A	81	TRP	CE2-CZ2	-5.26	1.30	1.39
1	A	74	VAL	CA-CB	-5.25	1.43	1.54
1	A	48	GLN	CD-OE1	-5.25	1.12	1.24
1	A	33	SER	CA-C	-5.24	1.39	1.52
1	A	177	ARG	CZ-NH1	5.24	1.39	1.33
1	A	236	VAL	CA-CB	-5.24	1.43	1.54
1	A	50	GLN	C-O	-5.24	1.13	1.23
1	A	184	ALA	CA-C	-5.23	1.39	1.52
1	A	143	ALA	CA-CB	5.22	1.63	1.52
1	A	87	LEU	C-O	-5.22	1.13	1.23
1	A	58	LYS	CA-CB	-5.21	1.42	1.53
1	A	182	ASP	CB-CG	5.21	1.62	1.51
1	A	189	GLN	CD-NE2	5.21	1.45	1.32
1	A	275	ALA	CA-C	-5.21	1.39	1.52
1	A	33	SER	CA-CB	-5.18	1.45	1.52
1	A	35	ASP	CG-OD1	5.17	1.37	1.25
1	A	10	THR	CA-C	-5.17	1.39	1.52
1	A	91	ASP	CG-OD1	-5.17	1.13	1.25
1	A	198	TYR	CE1-CZ	-5.16	1.31	1.38
1	A	44	ASP	CG-OD1	5.15	1.37	1.25
1	A	52	PHE	C-O	-5.12	1.13	1.23
1	A	159	PHE	CD1-CE1	-5.12	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	LEU	CA-CB	-5.12	1.42	1.53
1	A	44	ASP	CA-CB	5.12	1.65	1.53
1	A	128	LYS	CB-CG	5.11	1.66	1.52
1	A	73	LEU	N-CA	5.09	1.56	1.46
1	A	102	ALA	CA-C	-5.08	1.39	1.52
1	A	45	PHE	CG-CD1	5.08	1.46	1.38
1	A	80	ALA	C-O	-5.08	1.13	1.23
1	A	189	GLN	C-O	-5.07	1.13	1.23
1	A	250	ALA	N-CA	-5.05	1.36	1.46
1	A	183	VAL	N-CA	5.03	1.56	1.46
1	A	2	ALA	N-CA	5.02	1.56	1.46
1	A	15	PHE	CG-CD1	-5.02	1.31	1.38
1	A	79	ARG	CZ-NH1	5.02	1.39	1.33
1	A	175	TRP	CD2-CE2	5.02	1.47	1.41

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	ALA	CA-C-N	13.21	146.27	117.20
1	A	233	ARG	NE-CZ-NH1	11.74	126.17	120.30
1	A	1	ALA	N-CA-C	11.37	141.70	111.00
1	A	86	TYR	CB-CG-CD2	11.37	127.82	121.00
1	A	233	ARG	NE-CZ-NH2	-10.89	114.86	120.30
1	A	1	ALA	O-C-N	-10.58	105.78	122.70
1	A	34	VAL	CG1-CB-CG2	-10.21	94.57	110.90
1	A	177	ARG	NE-CZ-NH2	-10.19	115.21	120.30
1	A	91	ASP	CB-CG-OD2	9.65	126.98	118.30
1	A	1	ALA	CB-CA-C	-8.99	96.61	110.10
1	A	86	TYR	CB-CG-CD1	-8.65	115.81	121.00
1	A	1	ALA	CA-C-O	-8.22	102.84	120.10
1	A	281	VAL	CG1-CB-CG2	-7.92	98.22	110.90
1	A	269	VAL	CG1-CB-CG2	-7.17	99.44	110.90
1	A	182	ASP	CB-CG-OD2	7.04	124.64	118.30
1	A	54	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	1	ALA	N-CA-CB	-6.67	100.76	110.10
1	A	151	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	10	THR	OG1-CB-CG2	-6.54	94.96	110.00
1	A	68	LEU	CB-CG-CD2	6.53	122.11	111.00
1	A	280	LEU	CB-CG-CD1	6.52	122.08	111.00
1	A	222	LEU	CB-CG-CD2	6.48	122.02	111.00
1	A	202	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	227	ASP	CB-CG-OD2	6.29	123.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	52	PHE	CB-CG-CD2	6.23	125.16	120.80
1	A	151	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	176	ASP	CB-CG-OD1	-5.97	112.93	118.30
1	A	28	LYS	CD-CE-NZ	5.91	125.28	111.70
1	A	224	VAL	CG1-CB-CG2	-5.72	101.75	110.90
1	A	91	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	A	176	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	47	SER	N-CA-CB	5.67	119.01	110.50
1	A	124	PHE	CZ-CE2-CD2	-5.62	113.36	120.10
1	A	68	LEU	CB-CG-CD1	-5.61	101.47	111.00
1	A	60	TYR	CZ-CE2-CD2	5.47	124.73	119.80
1	A	177	ARG	NH1-CZ-NH2	5.42	125.36	119.40
1	A	49	LEU	CA-CB-CG	5.42	127.77	115.30
1	A	39	SER	CB-CA-C	-5.40	99.84	110.10
1	A	132	GLU	OE1-CD-OE2	5.32	129.68	123.30
1	A	97	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	7	VAL	CG1-CB-CG2	-5.13	102.69	110.90
1	A	192	PRO	N-CD-CG	-5.07	95.59	103.20
1	A	127	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	1	ALA	C-N-CA	5.06	134.36	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	ALA	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	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	2133	0	2184	43	4
2	A	1	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	0	0	0
All	All	2144	0	2184	43	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (43) 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:146:ALA:CA	1:A:146:ALA:CB	1.76	1.61
1:A:161:LYS:CE	1:A:161:LYS:CD	1.75	1.60
1:A:234:LYS:CD	1:A:234:LYS:CE	1.80	1.57
1:A:166:LYS:CE	1:A:166:LYS:CD	1.75	1.56
1:A:1:ALA:N	1:A:1:ALA:CA	1.68	1.52
1:A:179:LYS:CE	1:A:179:LYS:NZ	1.68	1.52
1:A:274:LYS:NZ	1:A:274:LYS:CE	1.72	1.50
1:A:61:LYS:CE	1:A:61:LYS:NZ	1.76	1.49
1:A:206:MET:SD	1:A:206:MET:CE	2.11	1.38
1:A:1:ALA:O	1:A:1:ALA:C	1.73	1.26
1:A:1:ALA:CB	2:A:1289:NI:NI	1.21	1.15
1:A:1:ALA:CB	1:A:1:ALA:CA	2.43	0.97
1:A:1:ALA:HB2	2:A:1289:NI:NI	0.99	0.87
1:A:1:ALA:O	1:A:1:ALA:CA	2.24	0.86
1:A:1:ALA:N	1:A:1:ALA:HA	1.97	0.75
1:A:139:ILE:HD12	1:A:139:ILE:H	1.56	0.69
1:A:234:LYS:CE	1:A:234:LYS:CG	2.75	0.62
1:A:186:ASN:O	1:A:190:ARG:HG2	2.01	0.61
1:A:137:ALA:O	1:A:197:ILE:HG22	2.02	0.60
1:A:161:LYS:CG	1:A:161:LYS:CE	2.77	0.58
1:A:229:ILE:HB	1:A:230:PRO:CD	2.35	0.57
1:A:145:ASN:HD22	1:A:175:TRP:HZ2	1.53	0.56
1:A:202:ASP:OD2	1:A:232:ALA:HB3	2.06	0.55
1:A:75:MET:N	1:A:76:PRO:CD	2.70	0.55
1:A:184:ALA:HB3	1:A:211:ALA:HB2	1.90	0.53
1:A:183:VAL:O	1:A:187:VAL:HG23	2.09	0.53
1:A:166:LYS:CG	1:A:166:LYS:CE	2.81	0.52
1:A:184:ALA:HB1	1:A:211:ALA:HB3	1.93	0.51
1:A:177:ARG:HG2	1:A:207:GLY:CA	2.41	0.51
1:A:226:THR:O	1:A:227:ASP:HB2	2.11	0.50
1:A:139:ILE:HD12	1:A:139:ILE:N	2.23	0.49
1:A:75:MET:HB2	1:A:76:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LYS:NZ	1:A:274:LYS:CD	2.69	0.48
1:A:138:ILE:O	1:A:170:SER:HA	2.14	0.46
1:A:206:MET:CG	1:A:206:MET:CE	2.93	0.46
1:A:1:ALA:C	1:A:1:ALA:CB	2.78	0.45
1:A:134:GLY:HA3	1:A:195:LYS:HD3	2.00	0.44
1:A:3:GLU:HG3	1:A:4:TYR:CD1	2.52	0.43
1:A:146:ALA:N	1:A:146:ALA:CB	2.67	0.43
1:A:184:ALA:CB	1:A:211:ALA:CB	2.96	0.43
1:A:71:VAL:HG12	1:A:98:ASN:HD22	1.84	0.43
1:A:202:ASP:OD2	1:A:232:ALA:CB	2.68	0.42
1:A:176:ASP:HB3	1:A:179:LYS:HB3	2.03	0.41

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ALA:CB	1:A:1:ALA:CB[6_566]	1.19	1.01
1:A:1:ALA:CA	1:A:1:ALA:CB[12_665]	1.33	0.87
1:A:1:ALA:C	1:A:1:ALA:CB[12_665]	2.00	0.20
1:A:1:ALA:N	1:A:1:ALA:CB[12_665]	2.10	0.10

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	286/288 (99%)	267 (93%)	16 (6%)	3 (1%)	19 58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	TRP
1	A	227	ASP

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Mol	Chain	Res	Type
1	A	91	ASP

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	222/222 (100%)	211 (95%)	11 (5%)	30 67

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	97	ASP
1	A	127	ASP
1	A	128	LYS
1	A	177	ARG
1	A	185	THR
1	A	195	LYS
1	A	197	ILE
1	A	202	ASP
1	A	241	MET
1	A	282	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	105	ASN
1	A	145	ASN
1	A	186	ASN
1	A	210	GLN

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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	288/288 (100%)	-0.26	8 (2%) 56 32	6, 32, 68, 247	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	ASN	3.3
1	A	193	ASN	2.7
1	A	1	ALA	2.4
1	A	163	SER	2.4
1	A	240	GLN	2.4
1	A	144	GLY	2.2
1	A	218	THR	2.1
1	A	210	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
2	NI	A	1289	1/1	0.85	0.28	-	22,22,22,22	1

6.5 Other polymers (i)

There are no such residues in this entry.