



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:17 PM UTC

PDB ID : 3TD3 / pdb_00003td3
Title : Crystal structure of OmpA-like domain from *Acinetobacter baumannii* in complex with glycine
Authors : Park, J.S.; Lee, W.C.; Song, J.H.; Kim, H.Y.
Deposited on : 2011-08-10
Resolution : 1.59 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

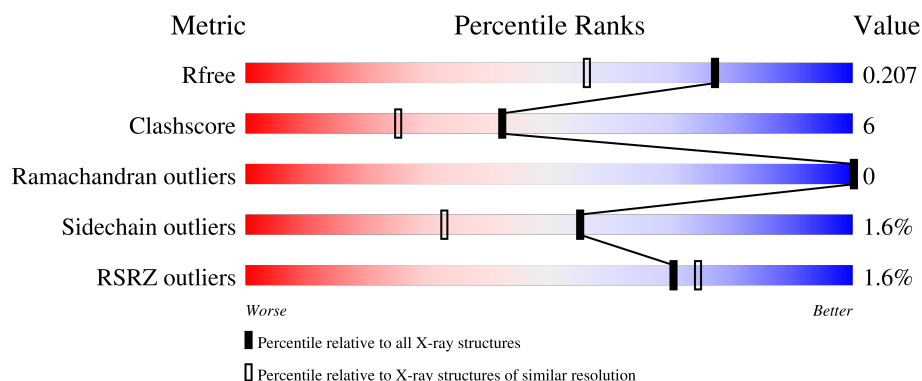
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

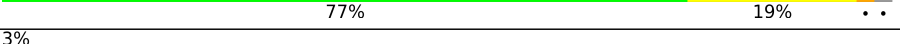
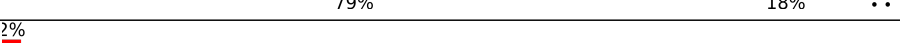
The reported resolution of this entry is 1.59 Å.

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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	123	
1	B	123	
1	C	123	
1	D	123	
1	E	123	

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Mol	Chain	Length	Quality of chain
1	F	123	% 85% 14% ..
1	G	123	% 75% 22% ...
1	H	123	2% 81% 16% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8836 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 Outer membrane protein omp38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	120	Total	C	N	O	S	0	0	0
			954	586	176	189	3			
1	B	120	Total	C	N	O	S	0	0	0
			954	586	176	189	3			
1	C	120	Total	C	N	O	S	0	0	0
			954	586	176	189	3			
1	D	122	Total	C	N	O	S	0	0	0
			970	595	180	192	3			
1	E	120	Total	C	N	O	S	0	0	0
			954	586	176	189	3			
1	F	122	Total	C	N	O	S	0	0	0
			970	595	180	192	3			
1	G	122	Total	C	N	O	S	0	0	0
			970	595	180	192	3			
1	H	121	Total	C	N	O	S	0	0	0
			964	592	179	190	3			

There are 32 discrepancies between the modelled and reference sequences:

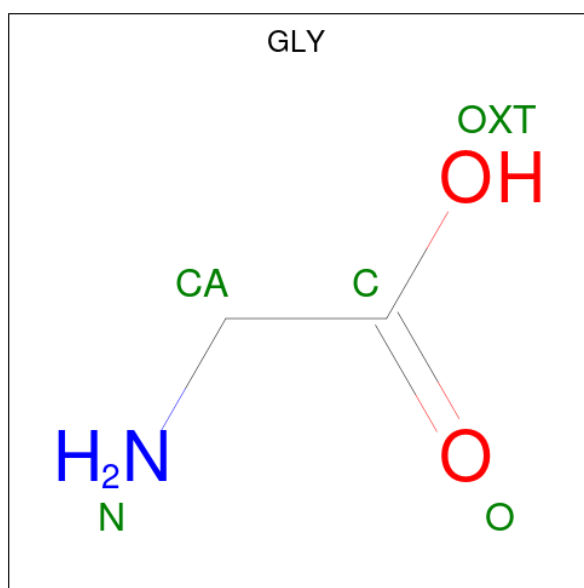
Chain	Residue	Modelled	Actual	Comment	Reference
A	217	GLY	-	expression tag	UNP Q6RYW5
A	218	SER	-	expression tag	UNP Q6RYW5
A	219	HIS	-	expression tag	UNP Q6RYW5
A	220	MET	-	expression tag	UNP Q6RYW5
B	217	GLY	-	expression tag	UNP Q6RYW5
B	218	SER	-	expression tag	UNP Q6RYW5
B	219	HIS	-	expression tag	UNP Q6RYW5
B	220	MET	-	expression tag	UNP Q6RYW5
C	217	GLY	-	expression tag	UNP Q6RYW5
C	218	SER	-	expression tag	UNP Q6RYW5
C	219	HIS	-	expression tag	UNP Q6RYW5
C	220	MET	-	expression tag	UNP Q6RYW5
D	217	GLY	-	expression tag	UNP Q6RYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	218	SER	-	expression tag	UNP Q6RYW5
D	219	HIS	-	expression tag	UNP Q6RYW5
D	220	MET	-	expression tag	UNP Q6RYW5
E	217	GLY	-	expression tag	UNP Q6RYW5
E	218	SER	-	expression tag	UNP Q6RYW5
E	219	HIS	-	expression tag	UNP Q6RYW5
E	220	MET	-	expression tag	UNP Q6RYW5
F	217	GLY	-	expression tag	UNP Q6RYW5
F	218	SER	-	expression tag	UNP Q6RYW5
F	219	HIS	-	expression tag	UNP Q6RYW5
F	220	MET	-	expression tag	UNP Q6RYW5
G	217	GLY	-	expression tag	UNP Q6RYW5
G	218	SER	-	expression tag	UNP Q6RYW5
G	219	HIS	-	expression tag	UNP Q6RYW5
G	220	MET	-	expression tag	UNP Q6RYW5
H	217	GLY	-	expression tag	UNP Q6RYW5
H	218	SER	-	expression tag	UNP Q6RYW5
H	219	HIS	-	expression tag	UNP Q6RYW5
H	220	MET	-	expression tag	UNP Q6RYW5

- Molecule 2 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	B	1	Total	C	N	O	0	0
			5	2	1	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total 5	C 2	N 1	O 2	0	0
2	D	1	Total 5	C 2	N 1	O 2	0	0
2	E	1	Total 5	C 2	N 1	O 2	0	0
2	F	1	Total 5	C 2	N 1	O 2	0	0
2	G	1	Total 5	C 2	N 1	O 2	0	0
2	H	1	Total 5	C 2	N 1	O 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	165	Total 165	O 165	0	0
3	B	135	Total 135	O 135	0	0
3	C	119	Total 119	O 119	0	0
3	D	117	Total 117	O 117	0	0
3	E	132	Total 132	O 132	0	0
3	F	137	Total 137	O 137	0	0
3	G	161	Total 161	O 161	0	0
3	H	140	Total 140	O 140	0	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: Outer membrane protein omp38

Chain A:  76% 20% ..



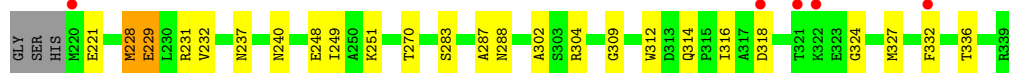
- Molecule 1: Outer membrane protein omp38

Chain B:  85% 13% .



- Molecule 1: Outer membrane protein omp38

Chain C:  4% 77% 19% ..



- Molecule 1: Outer membrane protein omp38

Chain D:  3% 79% 18% ..

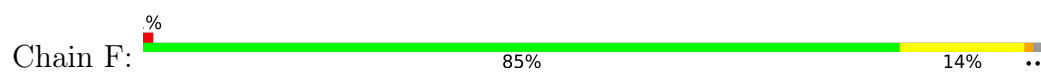


- Molecule 1: Outer membrane protein omp38

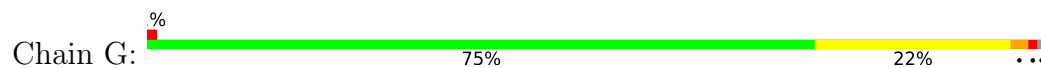
Chain E:  2% 76% 20% ..



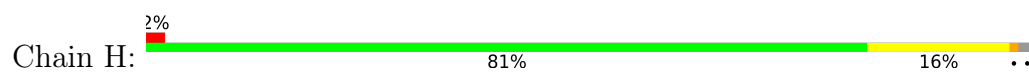
- Molecule 1: Outer membrane protein omp38



- Molecule 1: Outer membrane protein omp38



- Molecule 1: Outer membrane protein omp38



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.11Å 98.75Å 98.32Å 90.00° 105.84° 90.00°	Depositor
Resolution (Å)	94.59 – 1.59 94.59 – 1.59	Depositor EDS
% Data completeness (in resolution range)	99.4 (94.59-1.59) 99.4 (94.59-1.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.181 , 0.219 (Not available) , 0.207	Depositor DCC
R_{free} test set	7075 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8836	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.78	7/967 (0.7%)	1.51	3/1301 (0.2%)
1	B	1.58	4/967 (0.4%)	1.42	3/1301 (0.2%)
1	C	1.59	9/967 (0.9%)	1.47	4/1301 (0.3%)
1	D	1.55	7/984 (0.7%)	1.33	4/1324 (0.3%)
1	E	1.81	10/967 (1.0%)	1.54	7/1301 (0.5%)
1	F	1.58	3/984 (0.3%)	1.46	4/1324 (0.3%)
1	G	1.73	16/984 (1.6%)	1.48	4/1324 (0.3%)
1	H	1.69	9/978 (0.9%)	1.45	2/1316 (0.2%)
All	All	1.67	65/7798 (0.8%)	1.46	31/10492 (0.3%)

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	228	MET	SD-CE	-14.88	1.42	1.79
1	B	267	GLU	N-CA	8.43	1.56	1.46
1	C	228	MET	SD-CE	-7.75	1.60	1.79
1	A	228	MET	SD-CE	-7.75	1.60	1.79
1	G	228	MET	SD-CE	-7.19	1.61	1.79
1	H	331	VAL	CA-CB	-7.10	1.45	1.54
1	G	327	MET	CB-CG	7.03	1.73	1.52
1	C	249	ILE	CA-CB	-7.02	1.45	1.54
1	G	330	ARG	C-O	6.88	1.32	1.23
1	C	228	MET	CB-CG	-6.77	1.32	1.52
1	H	306	SER	N-CA	6.58	1.53	1.45
1	A	330	ARG	CZ-NH2	6.50	1.42	1.33
1	E	286	ARG	CZ-NH2	6.20	1.41	1.33
1	G	338	SER	N-CA	6.17	1.53	1.45
1	H	336	THR	CA-C	-6.03	1.45	1.52
1	G	247	PRO	C-O	5.99	1.31	1.24
1	D	324	GLY	N-CA	5.98	1.53	1.45
1	G	223	THR	N-CA	5.94	1.53	1.45
1	C	309	GLY	CA-C	5.93	1.56	1.52
1	H	228	MET	SD-CE	-5.89	1.64	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	258	GLU	N-CA	5.84	1.53	1.46
1	E	267	GLU	N-CA	5.82	1.53	1.46
1	H	266	ILE	CA-CB	5.78	1.60	1.54
1	H	328	ASN	C-O	5.69	1.31	1.24
1	D	228	MET	SD-CE	-5.68	1.65	1.79
1	H	232	VAL	C-O	-5.63	1.18	1.24
1	D	300	VAL	CA-CB	5.62	1.60	1.54
1	A	334	THR	N-CA	5.58	1.52	1.46
1	A	252	VAL	CA-CB	5.57	1.60	1.54
1	A	233	PHE	N-CA	5.56	1.52	1.45
1	A	256	LEU	N-CA	-5.56	1.39	1.46
1	G	293	ALA	C-O	5.56	1.30	1.24
1	D	230	LEU	N-CA	5.55	1.52	1.46
1	E	293	ALA	C-O	-5.54	1.17	1.24
1	C	287	ALA	N-CA	5.53	1.52	1.46
1	E	283	SER	N-CA	5.53	1.53	1.46
1	D	221	GLU	CB-CG	5.51	1.69	1.52
1	E	311	ALA	N-CA	5.51	1.53	1.46
1	C	240	ASN	CA-C	5.48	1.60	1.52
1	G	323	GLU	N-CA	-5.41	1.39	1.46
1	H	336	THR	N-CA	5.40	1.52	1.46
1	D	286	ARG	N-CA	5.40	1.52	1.46
1	D	282	LEU	N-CA	5.38	1.52	1.46
1	C	232	VAL	N-CA	5.37	1.52	1.46
1	G	279	ASN	N-CA	5.37	1.53	1.46
1	E	280	GLU	N-CA	5.32	1.52	1.46
1	G	241	ILE	CA-CB	-5.28	1.47	1.54
1	A	287	ALA	N-CA	5.26	1.52	1.46
1	G	268	GLY	N-CA	5.25	1.50	1.44
1	G	233	PHE	N-CA	5.24	1.52	1.45
1	F	318	ASP	CA-CB	5.23	1.60	1.53
1	E	278	LEU	CA-C	5.21	1.59	1.52
1	G	223	THR	CA-CB	-5.20	1.43	1.54
1	G	316	ILE	N-CA	5.20	1.52	1.46
1	E	228	MET	CG-SD	5.19	1.93	1.80
1	F	311	ALA	CA-CB	5.16	1.62	1.53
1	B	253	ALA	CA-CB	5.14	1.61	1.53
1	B	330	ARG	N-CA	5.14	1.52	1.46
1	G	327	MET	CA-CB	5.13	1.61	1.53
1	H	250	ALA	CA-CB	5.10	1.61	1.53
1	G	266	ILE	CA-CB	-5.09	1.48	1.54
1	C	304	ARG	CB-CG	-5.08	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	331	VAL	CA-CB	-5.06	1.48	1.54
1	C	316	ILE	CA-CB	5.01	1.60	1.54
1	B	305	LEU	C-O	-5.01	1.18	1.24

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	223	THR	OG1-CB-CG2	7.30	123.90	109.30
1	C	302	ALA	N-CA-C	7.26	120.06	111.71
1	E	286	ARG	O-C-N	7.15	129.43	122.07
1	G	220	MET	CG-SD-CE	-7.07	85.35	100.90
1	H	330	ARG	NE-CZ-NH2	-6.65	113.22	119.20
1	G	327	MET	CB-CG-SD	-6.55	93.05	112.70
1	D	327	MET	CB-CG-SD	-6.20	94.10	112.70
1	E	321	THR	N-CA-CB	-6.14	100.59	111.08
1	C	237	ASN	N-CA-C	5.92	120.30	113.38
1	B	308	GLN	CA-C-N	-5.87	118.05	122.33
1	B	308	GLN	C-N-CA	-5.87	118.05	122.33
1	A	330	ARG	NE-CZ-NH1	-5.82	115.68	121.50
1	E	286	ARG	NE-CZ-NH2	-5.73	114.05	119.20
1	E	286	ARG	CA-C-O	-5.70	114.83	120.82
1	A	253	ALA	O-C-N	5.69	128.15	122.12
1	D	276	ARG	N-CA-C	5.68	117.94	111.02
1	E	318	ASP	N-CA-C	5.61	117.83	109.59
1	F	330	ARG	NE-CZ-NH2	-5.55	114.20	119.20
1	D	294	LEU	N-CA-C	5.43	117.20	111.28
1	C	229	GLU	CA-CB-CG	-5.29	103.51	114.10
1	C	288	ASN	N-CA-C	5.29	117.79	111.71
1	H	228	MET	CA-CB-CG	5.28	124.67	114.10
1	B	242	LYS	CD-CE-NZ	-5.27	95.05	111.90
1	A	282	LEU	N-CA-C	-5.18	105.71	111.36
1	G	323	GLU	CB-CG-CD	-5.11	103.92	112.60
1	F	308	GLN	CA-C-N	-5.10	117.66	122.66
1	F	308	GLN	C-N-CA	-5.10	117.66	122.66
1	E	274	GLY	CA-C-N	5.05	125.49	120.14
1	E	274	GLY	C-N-CA	5.05	125.49	120.14
1	G	255	LYS	CD-CE-NZ	-5.04	95.77	111.90
1	F	307	THR	CA-CB-OG1	5.02	117.13	109.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	954	0	945	18	0
1	B	954	0	945	6	0
1	C	954	0	945	17	0
1	D	970	0	957	13	0
1	E	954	0	945	19	0
1	F	970	0	957	12	0
1	G	970	0	957	19	0
1	H	964	0	952	9	0
2	A	5	0	2	1	0
2	B	5	0	2	0	0
2	C	5	0	2	0	0
2	D	5	0	2	1	0
2	E	5	0	2	0	0
2	F	5	0	2	0	0
2	G	5	0	2	0	0
2	H	5	0	2	0	0
3	A	165	0	0	3	0
3	B	135	0	0	0	0
3	C	119	0	0	4	0
3	D	117	0	0	1	0
3	E	132	0	0	4	0
3	F	137	0	0	1	1
3	G	161	0	0	0	0
3	H	140	0	0	1	1
All	All	8836	0	7619	96	1

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 6.

All (96) 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)
3:A:557:HOH:O	1:F:218:SER:HB2	1.67	0.93
1:G:229:GLU:CD	1:G:332:PHE:HE1	1.77	0.92
1:D:244:GLN:NE2	1:E:265:ARG:NH2	2.22	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ASP:HB2	1:B:238:LYS:HD2	1.61	0.83
1:E:321:THR:HG21	3:E:421:HOH:O	1.80	0.80
1:C:327:MET:HE1	3:C:822:HOH:O	1.81	0.79
1:A:231:ARG:NH2	1:C:221:GLU:OE1	2.14	0.78
1:G:229:GLU:OE1	1:G:332:PHE:HE1	1.67	0.76
1:A:228:MET:HE1	1:A:255:LYS:HB2	1.68	0.75
1:E:321:THR:CG2	1:E:324:GLY:H	2.00	0.74
1:A:220:MET:HE2	1:C:228:MET:CE	2.20	0.72
1:G:229:GLU:CD	1:G:332:PHE:CE1	2.65	0.71
1:D:244:GLN:HE22	1:E:265:ARG:NH2	1.87	0.70
1:A:279:ASN:HD21	2:A:101:GLY:N	1.91	0.69
1:D:278:LEU:HD12	3:D:536:HOH:O	1.92	0.68
1:G:229:GLU:OE2	1:G:231:ARG:NE	2.26	0.68
1:C:229:GLU:OE2	1:C:231:ARG:NH1	2.28	0.67
1:E:321:THR:HG23	1:E:324:GLY:H	1.61	0.64
1:C:231:ARG:HG2	1:C:332:PHE:CE2	2.32	0.64
1:E:228:MET:HE1	1:E:255:LYS:HB2	1.81	0.61
1:G:229:GLU:OE1	1:G:332:PHE:CE1	2.54	0.60
1:G:229:GLU:HG3	1:G:332:PHE:CE1	2.38	0.59
1:C:336:THR:HG22	3:C:501:HOH:O	2.02	0.58
1:F:221:GLU:HG2	1:G:229:GLU:HB3	1.85	0.58
1:A:228:MET:HE1	1:A:255:LYS:CB	2.33	0.58
1:B:225:ASP:OD1	1:B:338:SER:OG	2.22	0.57
1:C:314:GLN:NE2	3:C:1181:HOH:O	2.34	0.57
1:A:220:MET:HE2	1:C:228:MET:HE1	1.85	0.57
1:E:222:LEU:HD13	1:H:228:MET:HG2	1.86	0.56
1:H:277:LYS:HE2	3:H:906:HOH:O	2.06	0.56
1:C:231:ARG:HG2	1:C:332:PHE:CD2	2.41	0.55
1:E:299:ASN:HB3	3:E:354:HOH:O	2.06	0.55
1:E:321:THR:HG23	1:E:323:GLU:HG2	1.89	0.54
1:D:244:GLN:HE22	1:E:265:ARG:HH22	1.55	0.54
1:H:230:LEU:HB3	1:H:333:ALA:HB3	1.89	0.53
1:E:319:ASN:HD22	1:E:325:ARG:HG2	1.74	0.53
1:G:319:ASN:HD22	1:G:325:ARG:HG2	1.74	0.52
1:D:279:ASN:HD21	2:D:401:GLY:N	2.07	0.52
1:E:229:GLU:O	1:H:220:MET:HA	2.09	0.52
1:F:238:LYS:HE3	3:F:1312:HOH:O	2.10	0.51
1:D:319:ASN:ND2	1:D:328:ASN:HD22	2.08	0.51
1:F:219:HIS:HB2	1:G:248:GLU:OE1	2.11	0.51
1:A:319:ASN:HD22	1:A:325:ARG:HG2	1.76	0.51
1:A:319:ASN:ND2	1:A:328:ASN:HD22	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:319:ASN:ND2	1:E:328:ASN:HD22	2.09	0.50
1:E:228:MET:HB3	1:E:335:ILE:HB	1.94	0.49
1:G:319:ASN:ND2	1:G:328:ASN:HD22	2.08	0.49
1:B:319:ASN:ND2	1:B:328:ASN:HD22	2.11	0.49
1:G:229:GLU:CG	1:G:332:PHE:CE1	2.95	0.49
1:A:220:MET:N	3:A:538:HOH:O	2.46	0.49
1:A:270:THR:HG21	1:A:279:ASN:HD22	1.78	0.49
1:D:261:ASN:C	1:D:261:ASN:OD1	2.55	0.49
1:C:318:ASP:O	1:C:324:GLY:HA3	2.13	0.48
1:G:229:GLU:CG	1:G:332:PHE:HE1	2.25	0.48
1:G:278:LEU:C	1:G:278:LEU:HD23	2.38	0.48
1:H:318:ASP:O	1:H:324:GLY:HA3	2.14	0.48
1:F:278:LEU:C	1:F:278:LEU:HD23	2.38	0.48
1:G:228:MET:HB2	1:G:335:ILE:HB	1.96	0.48
1:E:321:THR:CG2	1:E:323:GLU:HG2	2.45	0.47
1:F:222:LEU:HD13	1:G:228:MET:HG2	1.96	0.47
1:E:321:THR:HG22	1:E:324:GLY:H	1.75	0.47
1:F:255:LYS:HE2	1:G:222:LEU:HD21	1.96	0.46
1:B:235:ASP:CB	1:B:238:LYS:HD2	2.39	0.46
1:A:247:PRO:O	1:A:251:LYS:HG3	2.16	0.46
1:E:228:MET:HB2	1:E:228:MET:HE2	1.71	0.46
1:F:327:MET:HB3	1:F:327:MET:HE2	1.79	0.45
1:G:318:ASP:OD2	1:G:320:LYS:HB2	2.17	0.45
1:C:270:THR:HG23	1:C:283:SER:HB3	1.99	0.45
1:G:251:LYS:HE3	1:G:255:LYS:HD3	1.99	0.45
1:A:220:MET:HE1	1:C:251:LYS:HB3	1.99	0.45
1:B:222:LEU:HD13	1:D:228:MET:HG2	1.98	0.44
1:D:319:ASN:HD22	1:D:325:ARG:HG2	1.82	0.44
1:A:243:ASP:HA	1:A:246:LYS:HG3	2.00	0.43
1:C:327:MET:CE	3:C:822:HOH:O	2.51	0.43
1:H:231:ARG:HB3	1:H:332:PHE:CE1	2.52	0.43
1:H:319:ASN:HD22	1:H:325:ARG:HG2	1.84	0.43
1:D:228:MET:HB2	1:D:335:ILE:HB	2.00	0.43
1:F:319:ASN:ND2	1:F:328:ASN:HD22	2.16	0.43
1:C:312:TRP:C	1:C:312:TRP:CD1	2.97	0.43
3:E:1008:HOH:O	1:H:219:HIS:HD2	2.02	0.43
1:A:222:LEU:HD13	1:C:228:MET:HG2	2.01	0.42
1:E:220:MET:N	3:E:362:HOH:O	2.52	0.42
1:E:231:ARG:O	1:H:219:HIS:HB3	2.19	0.42
1:C:327:MET:HA	1:C:327:MET:HE2	2.02	0.42
3:A:557:HOH:O	1:F:218:SER:CB	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:ASP:HA	1:D:246:LYS:HE2	2.02	0.41
1:D:230:LEU:HB3	1:D:333:ALA:HB3	2.02	0.41
1:G:322:LYS:HE3	1:G:322:LYS:HB3	1.89	0.41
1:A:220:MET:HE1	1:C:248:GLU:O	2.21	0.41
1:B:278:LEU:C	1:B:278:LEU:HD23	2.46	0.41
1:A:221:GLU:OE1	1:A:223:THR:HG23	2.20	0.41
1:A:278:LEU:HD23	1:A:278:LEU:C	2.45	0.41
1:D:255:LYS:HD3	1:D:255:LYS:HA	1.92	0.41
1:F:318:ASP:O	1:F:324:GLY:HA3	2.21	0.41
1:F:319:ASN:HD22	1:F:325:ARG:HG2	1.86	0.41
1:A:228:MET:HB3	1:A:335:ILE:HB	2.03	0.41

All (1) 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)
3:F:187:HOH:O	3:H:1473:HOH:O[2_556]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	118/123 (96%)	116 (98%)	2 (2%)	0	100	100
1	B	118/123 (96%)	117 (99%)	1 (1%)	0	100	100
1	C	118/123 (96%)	117 (99%)	1 (1%)	0	100	100
1	D	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
1	E	118/123 (96%)	117 (99%)	1 (1%)	0	100	100
1	F	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
1	G	120/123 (98%)	119 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	119/123 (97%)	118 (99%)	1 (1%)	0	100	100
All	All	951/984 (97%)	942 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	97/105 (92%)	97 (100%)	0	100	100
1	B	31/105 (30%)	29 (94%)	2 (6%)	15	3
1	C	48/105 (46%)	48 (100%)	0	100	100
1	D	54/105 (51%)	51 (94%)	3 (6%)	19	4
1	E	103/105 (98%)	101 (98%)	2 (2%)	50	27
1	F	105/105 (100%)	105 (100%)	0	100	100
1	G	105/105 (100%)	103 (98%)	2 (2%)	50	27
1	H	96/105 (91%)	95 (99%)	1 (1%)	68	50
All	All	639/840 (76%)	629 (98%)	10 (2%)	55	33

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	221	GLU
1	B	277	LYS
1	D	218	SER
1	D	221	GLU
1	D	222	LEU
1	E	277	LYS
1	E	321	THR
1	G	255	LYS
1	G	327	MET
1	H	222	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	GLN
1	A	279	ASN
1	A	314	GLN
1	B	319	ASN
1	D	244	GLN
1	D	288	ASN
1	D	314	GLN
1	D	319	ASN
1	E	237	ASN
1	E	319	ASN
1	F	296	ASN
1	F	319	ASN
1	G	319	ASN
1	H	219	HIS
1	H	319	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](#)

8 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
2	GLY	E	501	-	4,4,4	1.83	1 (25%)	3,4,4	1.81	1 (33%)
2	GLY	G	701	-	4,4,4	1.13	0	3,4,4	0.36	0
2	GLY	C	340	-	4,4,4	1.60	1 (25%)	3,4,4	1.14	0
2	GLY	F	601	-	4,4,4	1.00	0	3,4,4	2.39	2 (66%)
2	GLY	A	101	-	4,4,4	0.72	0	3,4,4	1.08	0
2	GLY	D	401	-	4,4,4	1.55	1 (25%)	3,4,4	0.61	0
2	GLY	B	201	-	4,4,4	1.72	1 (25%)	3,4,4	0.57	0
2	GLY	H	801	-	4,4,4	1.44	1 (25%)	3,4,4	1.68	1 (33%)

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	GLY	E	501	-	-	0/2/2/2	-
2	GLY	G	701	-	-	0/2/2/2	-
2	GLY	C	340	-	-	0/2/2/2	-
2	GLY	F	601	-	-	0/2/2/2	-
2	GLY	A	101	-	-	0/2/2/2	-
2	GLY	D	401	-	-	0/2/2/2	-
2	GLY	B	201	-	-	0/2/2/2	-
2	GLY	H	801	-	-	0/2/2/2	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	GLY	OXT-C	-3.17	1.20	1.30
2	C	340	GLY	OXT-C	-2.99	1.20	1.30
2	E	501	GLY	OXT-C	-2.84	1.21	1.30
2	D	401	GLY	OXT-C	-2.82	1.21	1.30
2	H	801	GLY	OXT-C	-2.50	1.22	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	GLY	OXT-C-O	-2.92	115.82	123.33
2	F	601	GLY	OXT-C-CA	2.85	124.70	113.38
2	H	801	GLY	OXT-C-O	-2.54	116.79	123.33
2	E	501	GLY	O-C-CA	-2.21	113.10	122.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	101	GLY	1	0
2	D	401	GLY	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	120/123 (97%)	-0.24	0	100	100	6, 13, 27, 37	0
1	B	120/123 (97%)	-0.20	0	100	100	8, 14, 26, 35	0
1	C	120/123 (97%)	-0.04	5 (4%)	40	42	7, 14, 34, 45	0
1	D	122/123 (99%)	0.07	4 (3%)	49	52	9, 18, 29, 38	0
1	E	120/123 (97%)	-0.16	2 (1%)	69	72	8, 13, 24, 30	0
1	F	122/123 (99%)	-0.31	1 (0%)	82	86	7, 12, 22, 34	0
1	G	122/123 (99%)	-0.34	1 (0%)	82	86	6, 12, 24, 33	0
1	H	121/123 (98%)	-0.28	2 (1%)	69	72	5, 12, 23, 34	0
All	All	967/984 (98%)	-0.19	15 (1%)	70	74	5, 14, 28, 45	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	318	ASP	3.5
1	F	219	HIS	3.2
1	C	220	MET	2.8
1	C	332	PHE	2.6
1	H	332	PHE	2.5
1	C	321	THR	2.5
1	D	332	PHE	2.4
1	H	318	ASP	2.4
1	D	299	ASN	2.4
1	D	298	TYR	2.4
1	E	221	GLU	2.4
1	C	322	LYS	2.1
1	E	278	LEU	2.1
1	G	332	PHE	2.0
1	D	300	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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
2	GLY	B	201	5/5	0.95	0.07	12,13,16,17	0
2	GLY	F	601	5/5	0.95	0.07	10,11,12,13	0
2	GLY	C	340	5/5	0.96	0.07	14,16,16,20	0
2	GLY	E	501	5/5	0.97	0.05	11,11,14,14	0
2	GLY	D	401	5/5	0.97	0.06	16,16,16,17	0
2	GLY	A	101	5/5	0.98	0.04	8,8,10,10	0
2	GLY	G	701	5/5	0.98	0.03	6,7,9,9	0
2	GLY	H	801	5/5	0.98	0.05	8,8,9,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.