



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 04:35 PM UTC

PDB ID : 4G4Z / pdb_00004g4z
Title : Crystal structure of OmpA peptidoglycan-binding domain from *Acinetobacter baumannii*
Authors : Lee, W.C.; Song, J.H.; Park, J.S.; Kim, H.Y.
Deposited on : 2012-07-16
Resolution : 1.80 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

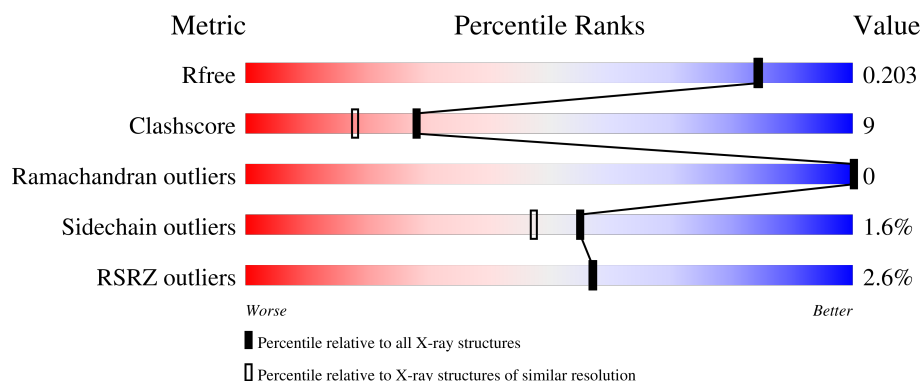
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	2% 79% 19% .
1	B	123	2% 73% 24% ..
1	C	123	4% 78% 17% ..
1	D	123	5% 79% 19% ..
1	E	123	2% 79% 19% ..

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Mol	Chain	Length	Quality of chain
1	F	123	2% 80% 18% ..
1	G	123	% 74% 23% ..
1	H	123	2% 80% 17% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8701 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	121	Total	C	N	O	S	0	0	0
			964	592	179	190	3			
1	C	119	Total	C	N	O	S	0	0	0
			946	581	175	188	2			
1	D	122	Total	C	N	O	S	0	0	0
			970	595	180	192	3			
1	E	121	Total	C	N	O	S	0	0	0
			964	592	179	190	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:

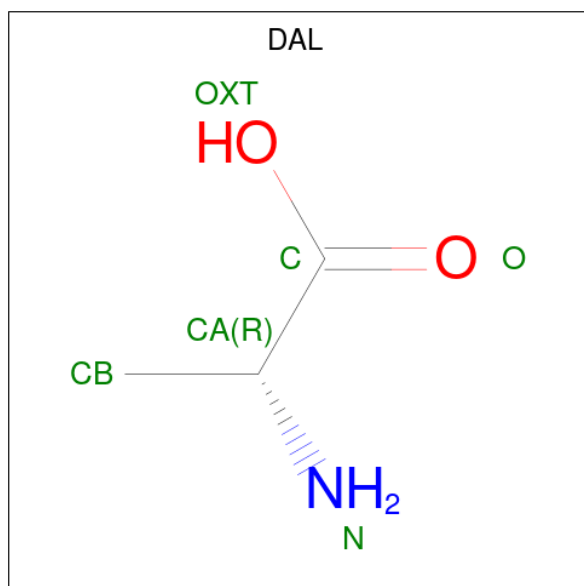
Chain	Residue	Modelled	Actual	Comment	Reference
A	217	GLY	-	expression tag	UNP Q6RYW5
A	218	SER	-	expression tag	UNP Q6RYW5
A	219	HIS	-	expression tag	UNP Q6RYW5
A	220	MET	-	expression tag	UNP Q6RYW5
B	217	GLY	-	expression tag	UNP Q6RYW5
B	218	SER	-	expression tag	UNP Q6RYW5
B	219	HIS	-	expression tag	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 D-ALANINE (CCD ID: DAL) (formula: $C_3H_7NO_2$).



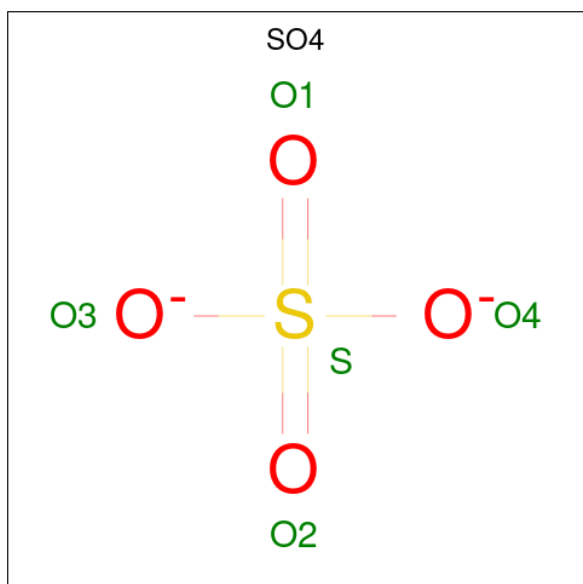
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			6	3	1	2		
2	B	1	Total	C	N	O	0	0
			6	3	1	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			6	3	1	2		
2	D	1	Total	C	N	O	0	0
			6	3	1	2		
2	E	1	Total	C	N	O	0	0
			6	3	1	2		
2	F	1	Total	C	N	O	0	0
			6	3	1	2		
2	G	1	Total	C	N	O	0	0
			6	3	1	2		
2	H	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

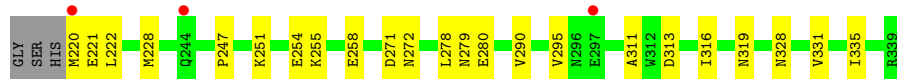
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	126	Total	O	0	0
			126	126		
4	B	104	Total	O	0	0
			104	104		
4	C	93	Total	O	0	0
			93	93		
4	D	88	Total	O	0	0
			88	88		
4	E	123	Total	O	0	0
			123	123		
4	F	135	Total	O	0	0
			135	135		
4	G	137	Total	O	0	0
			137	137		
4	H	105	Total	O	0	0
			105	105		

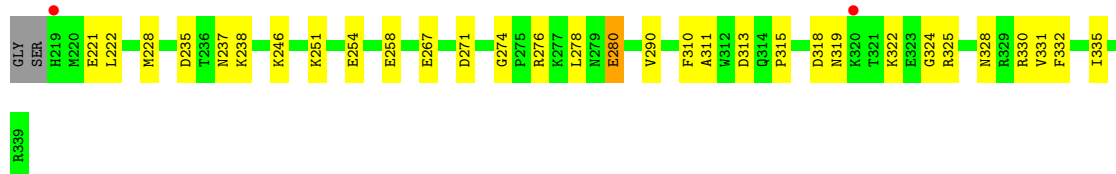
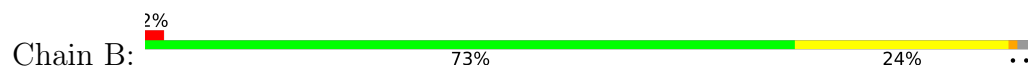
3 Residue-property plots [i](#)

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.

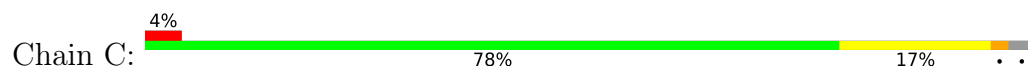
- Molecule 1: Outer membrane protein Omp38



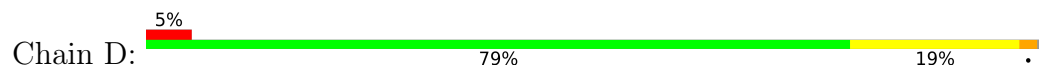
- Molecule 1: Outer membrane protein Omp38



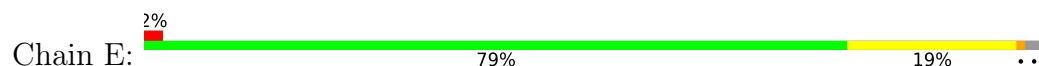
- Molecule 1: Outer membrane protein Omp38



- Molecule 1: Outer membrane protein Omp38

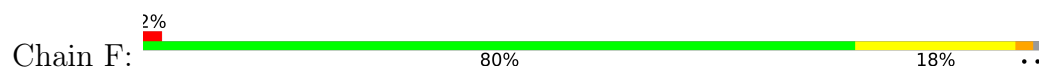


- Molecule 1: Outer membrane protein Omp38

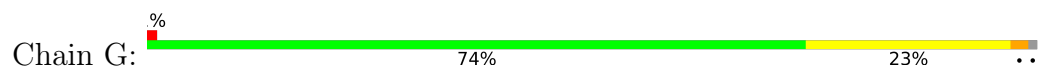




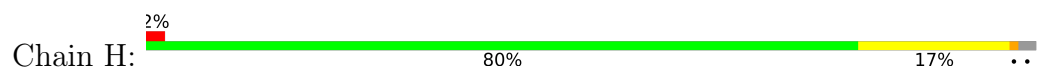
- Molecule 1: Outer membrane protein Omp38



- 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	58.34Å 98.89Å 98.28Å 90.00° 105.90° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-1.80) 99.7 (50.00-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 1.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.195 , 0.225 0.196 , 0.203	Depositor DCC
R_{free} test set	4934 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8701	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, DAL

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	0.34	0/967	0.90	7/1301 (0.5%)
1	B	0.33	0/978	0.88	6/1316 (0.5%)
1	C	0.33	0/959	0.87	2/1291 (0.2%)
1	D	0.33	0/984	0.86	5/1324 (0.4%)
1	E	0.36	0/978	0.86	4/1316 (0.3%)
1	F	0.31	0/984	0.93	7/1324 (0.5%)
1	G	0.34	0/984	0.90	6/1324 (0.5%)
1	H	0.33	0/978	0.88	5/1316 (0.4%)
All	All	0.33	0/7812	0.89	42/10512 (0.4%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	274	GLY	CA-C-N	8.03	128.05	119.78
1	F	274	GLY	C-N-CA	8.03	128.05	119.78
1	G	271	ASP	N-CA-C	-6.72	101.08	110.35
1	H	271	ASP	N-CA-C	-6.70	101.11	110.35
1	E	271	ASP	N-CA-C	-6.62	101.22	110.35
1	B	271	ASP	N-CA-C	-6.39	101.53	110.35
1	F	316	ILE	N-CA-C	-6.28	106.87	112.90
1	A	271	ASP	N-CA-C	-6.17	101.83	110.35
1	G	313	ASP	N-CA-C	6.01	119.87	112.54
1	F	271	ASP	N-CA-C	-5.97	102.11	110.35
1	B	280	GLU	N-CA-C	-5.91	104.76	111.14
1	A	272	ASN	N-CA-C	5.86	119.50	112.93
1	H	316	ILE	N-CA-C	-5.86	107.42	113.10
1	D	271	ASP	N-CA-C	-5.76	102.41	110.35
1	H	272	ASN	N-CA-C	5.66	119.27	112.93
1	G	316	ILE	N-CA-C	-5.65	107.62	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	271	ASP	N-CA-C	-5.55	102.69	110.35
1	G	274	GLY	CA-C-N	5.54	125.49	119.78
1	G	274	GLY	C-N-CA	5.54	125.49	119.78
1	A	280	GLU	N-CA-C	-5.47	105.21	111.07
1	D	259	TYR	CA-C-N	5.42	126.62	119.84
1	D	259	TYR	C-N-CA	5.42	126.62	119.84
1	A	295	VAL	N-CA-C	5.38	115.58	110.53
1	B	311	ALA	CB-CA-C	-5.37	110.37	116.54
1	B	274	GLY	CA-C-N	5.36	125.30	119.78
1	B	274	GLY	C-N-CA	5.36	125.30	119.78
1	A	313	ASP	N-CA-C	5.24	118.93	112.54
1	C	311	ALA	CB-CA-C	-5.23	110.52	116.54
1	D	311	ALA	CB-CA-C	-5.22	110.54	116.54
1	D	316	ILE	N-CA-C	-5.20	107.76	113.43
1	F	272	ASN	N-CA-C	5.19	118.74	112.93
1	H	313	ASP	N-CA-C	5.16	118.84	112.54
1	E	311	ALA	CB-CA-C	-5.16	110.61	116.54
1	A	316	ILE	N-CA-C	-5.15	108.11	113.10
1	A	311	ALA	CB-CA-C	-5.14	110.62	116.54
1	H	280	GLU	N-CA-C	-5.14	105.57	111.07
1	G	272	ASN	N-CA-C	5.12	118.67	112.93
1	E	316	ILE	N-CA-C	-5.07	108.18	113.10
1	F	311	ALA	CB-CA-C	-5.07	110.71	116.54
1	E	272	ASN	N-CA-C	5.02	118.55	112.93
1	F	280	GLU	N-CA-C	-5.01	105.72	111.14
1	B	313	ASP	N-CA-C	5.01	118.66	112.54

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	16	0
1	B	964	0	952	23	0
1	C	946	0	936	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	970	0	957	23	0
1	E	964	0	952	16	0
1	F	970	0	957	19	0
1	G	970	0	957	31	0
1	H	964	0	952	15	0
2	A	6	0	6	1	0
2	B	6	0	6	0	0
2	C	6	0	6	0	0
2	D	6	0	6	1	0
2	E	6	0	6	0	0
2	F	6	0	6	0	0
2	G	6	0	6	0	0
2	H	6	0	6	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
4	A	126	0	0	0	0
4	B	104	0	0	2	0
4	C	93	0	0	2	0
4	D	88	0	0	1	0
4	E	123	0	0	4	0
4	F	135	0	0	2	0
4	G	137	0	0	1	0
4	H	105	0	0	1	0
All	All	8701	0	7656	138	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 (138) 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:255:LYS:HE3	1:C:222:LEU:HD21	1.54	0.86
1:A:221:GLU:HG2	1:C:231:ARG:HH22	1.42	0.85
1:D:279:ASN:HD21	2:D:401:DAL:H	1.27	0.83
1:G:251:LYS:HE3	1:G:255:LYS:HE2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:ASP:OD1	1:D:273:THR:HG22	1.84	0.77
1:B:246:LYS:HE3	4:B:604:HOH:O	1.85	0.75
1:C:318:ASP:OD2	1:C:320:LYS:HB2	1.89	0.73
1:B:228:MET:CE	1:D:220:MET:HE1	2.21	0.71
1:A:279:ASN:HD21	2:A:401:DAL:H	1.35	0.71
1:E:322:LYS:HA	4:E:522:HOH:O	1.94	0.67
1:G:228:MET:HB2	1:G:335:ILE:HB	1.78	0.66
1:G:248:GLU:HG3	4:G:521:HOH:O	1.95	0.65
1:D:319:ASN:ND2	1:D:328:ASN:HD22	1.95	0.64
1:E:325:ARG:HB2	4:E:522:HOH:O	1.98	0.64
1:E:228:MET:HE1	1:E:255:LYS:HB2	1.79	0.63
1:C:330:ARG:HD2	1:C:332:PHE:CE1	2.34	0.62
1:B:228:MET:HE2	1:D:220:MET:HE1	1.81	0.62
1:E:327:MET:HE3	4:E:507:HOH:O	1.99	0.62
1:D:330:ARG:HD2	1:D:332:PHE:CE1	2.35	0.61
1:B:235:ASP:HB2	1:B:238:LYS:HD2	1.82	0.61
1:A:228:MET:HE1	1:A:255:LYS:HB2	1.82	0.60
1:G:261:ASN:C	1:G:261:ASN:HD22	2.10	0.60
1:A:220:MET:HE1	1:C:248:GLU:O	2.02	0.60
1:D:228:MET:HB2	1:D:335:ILE:HB	1.84	0.60
1:F:240:ASN:HD22	1:F:240:ASN:H	1.50	0.59
1:H:228:MET:HB2	1:H:335:ILE:HB	1.83	0.58
1:G:229:GLU:HG3	1:G:332:PHE:CE1	2.37	0.58
1:H:230:LEU:HB3	1:H:333:ALA:HB3	1.86	0.58
1:G:317:ALA:HB2	1:G:327:MET:HE3	1.85	0.57
1:G:229:GLU:CD	1:G:332:PHE:HE1	2.13	0.57
1:E:278:LEU:HD23	1:E:278:LEU:C	2.31	0.56
1:F:219:HIS:HB2	1:G:248:GLU:OE1	2.06	0.56
1:B:319:ASN:ND2	1:B:328:ASN:HD22	2.04	0.55
1:C:276:ARG:O	1:C:280:GLU:HG3	2.07	0.55
1:F:255:LYS:HE2	1:G:222:LEU:HD21	1.88	0.55
1:A:221:GLU:CG	1:C:231:ARG:HH22	2.15	0.55
1:C:228:MET:HB2	1:C:335:ILE:HB	1.89	0.55
1:B:330:ARG:HD2	1:B:332:PHE:CE1	2.41	0.55
1:F:221:GLU:HG3	1:G:231:ARG:HH22	1.72	0.55
1:G:261:ASN:C	1:G:261:ASN:ND2	2.64	0.55
1:B:335:ILE:N	1:B:335:ILE:HD12	2.22	0.55
1:G:317:ALA:CB	1:G:327:MET:HE3	2.37	0.55
1:D:293:ALA:O	1:D:297:GLU:HB2	2.07	0.54
1:G:241:ILE:HD11	1:G:290:VAL:HA	1.90	0.54
1:F:231:ARG:HH12	1:G:221:GLU:CD	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:ASN:HD22	1:G:262:ALA:N	2.07	0.53
1:H:222:LEU:HD22	1:H:222:LEU:C	2.33	0.53
1:G:319:ASN:ND2	1:G:328:ASN:HD22	2.07	0.53
1:C:322:LYS:NZ	1:C:322:LYS:HB3	2.24	0.53
1:E:335:ILE:HD12	1:E:335:ILE:N	2.24	0.52
1:B:254:GLU:O	1:B:258:GLU:HG3	2.10	0.52
1:E:243:ASP:OD1	1:E:246:LYS:HE3	2.09	0.52
1:H:327:MET:HA	1:H:327:MET:HE2	1.92	0.52
1:H:318:ASP:O	1:H:324:GLY:HA3	2.10	0.52
1:H:327:MET:HE3	4:H:529:HOH:O	2.10	0.52
1:G:261:ASN:HD21	1:G:338:SER:H	1.57	0.51
1:D:335:ILE:HD12	1:D:335:ILE:N	2.26	0.50
1:B:322:LYS:HG2	1:B:325:ARG:NH2	2.27	0.50
1:D:276:ARG:HD2	1:D:280:GLU:OE2	2.11	0.50
1:A:247:PRO:O	1:A:251:LYS:HG3	2.12	0.50
1:B:315:PRO:HB3	4:B:526:HOH:O	2.12	0.50
1:F:222:LEU:HD13	1:G:228:MET:HG2	1.94	0.50
1:A:221:GLU:HG2	1:C:231:ARG:NH2	2.21	0.49
1:B:278:LEU:C	1:B:278:LEU:HD23	2.38	0.49
1:B:228:MET:HE1	1:D:220:MET:HE1	1.93	0.49
1:B:228:MET:HB2	1:B:335:ILE:HB	1.93	0.48
1:B:251:LYS:HB3	1:D:220:MET:HE3	1.94	0.48
1:H:330:ARG:HD2	1:H:332:PHE:CE1	2.47	0.48
1:G:301:ASP:OD2	1:G:303:SER:OG	2.29	0.48
1:H:290:VAL:HG21	1:H:331:VAL:HG11	1.95	0.48
1:C:322:LYS:HB3	1:C:322:LYS:HZ3	1.78	0.47
1:F:221:GLU:HB2	1:G:229:GLU:HB3	1.95	0.47
1:H:319:ASN:HD22	1:H:325:ARG:HG2	1.79	0.47
1:A:222:LEU:HD21	1:C:255:LYS:HE3	1.96	0.47
1:G:230:LEU:HD22	1:G:252:VAL:HG21	1.97	0.47
1:C:251:LYS:HE3	1:C:255:LYS:HE2	1.95	0.47
1:F:276:ARG:O	1:F:280:GLU:HG3	2.15	0.47
1:F:278:LEU:C	1:F:278:LEU:HD23	2.39	0.47
1:E:319:ASN:ND2	1:E:328:ASN:HD22	2.12	0.47
1:C:248:GLU:HG3	4:C:537:HOH:O	2.15	0.47
1:B:228:MET:HG2	1:D:222:LEU:HB2	1.95	0.46
1:C:221:GLU:N	4:C:593:HOH:O	2.47	0.46
1:D:220:MET:O	1:D:220:MET:HG3	2.15	0.46
1:G:335:ILE:HD12	1:G:335:ILE:N	2.30	0.46
1:A:220:MET:HE1	1:C:251:LYS:HB3	1.96	0.46
1:B:222:LEU:HD13	1:D:228:MET:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:ASP:OD2	1:C:303:SER:OG	2.30	0.46
1:C:312:TRP:C	1:C:312:TRP:CD1	2.94	0.46
1:H:318:ASP:OD1	1:H:320:LYS:HE2	2.16	0.46
1:A:319:ASN:ND2	1:A:328:ASN:HD22	2.14	0.46
1:D:278:LEU:C	1:D:278:LEU:HD23	2.41	0.45
1:F:221:GLU:CD	1:G:231:ARG:HH22	2.23	0.45
1:F:218:SER:HA	4:F:580:HOH:O	2.16	0.45
1:H:278:LEU:C	1:H:278:LEU:HD23	2.42	0.45
1:F:231:ARG:NH1	1:G:221:GLU:OE1	2.49	0.44
1:B:276:ARG:O	1:B:280:GLU:HG3	2.18	0.44
1:F:221:GLU:CG	1:G:231:ARG:HH22	2.31	0.44
1:G:229:GLU:CG	1:G:332:PHE:HE1	2.32	0.43
1:F:335:ILE:N	1:F:335:ILE:HD12	2.33	0.43
1:E:299:ASN:HB3	4:E:536:HOH:O	2.19	0.42
1:C:254:GLU:O	1:C:258:GLU:HG3	2.19	0.42
1:D:255:LYS:HA	1:D:255:LYS:HD3	1.88	0.42
1:H:335:ILE:HD12	1:H:335:ILE:N	2.35	0.42
1:A:254:GLU:HG2	1:A:258:GLU:OE2	2.19	0.42
1:C:261:ASN:OD1	1:C:261:ASN:C	2.63	0.42
1:E:238:LYS:HB3	1:E:240:ASN:OD1	2.20	0.42
1:E:231:ARG:HH22	1:H:221:GLU:CD	2.27	0.42
1:B:290:VAL:HG21	1:B:331:VAL:HG11	2.01	0.42
1:G:255:LYS:HA	1:G:255:LYS:HD3	1.86	0.42
1:D:276:ARG:O	1:D:280:GLU:HG3	2.20	0.42
1:D:288:ASN:HD22	1:D:307:THR:HG21	1.85	0.42
1:E:222:LEU:HD13	1:H:228:MET:HG2	2.01	0.41
1:A:278:LEU:HD23	1:A:278:LEU:C	2.45	0.41
1:G:251:LYS:HE3	1:G:255:LYS:CE	2.43	0.41
1:B:318:ASP:O	1:B:324:GLY:HA3	2.19	0.41
1:B:228:MET:HE3	1:D:222:LEU:HD13	2.02	0.41
1:C:231:ARG:HG2	1:C:332:PHE:CE1	2.55	0.41
1:C:255:LYS:HD3	1:C:258:GLU:OE1	2.21	0.41
1:D:290:VAL:HG21	1:D:331:VAL:HG11	2.01	0.41
1:G:229:GLU:OE2	1:G:231:ARG:NH2	2.53	0.41
1:F:315:PRO:HB3	4:F:527:HOH:O	2.20	0.41
1:E:318:ASP:O	1:E:324:GLY:HA3	2.21	0.41
1:F:251:LYS:HG2	1:G:220:MET:HE1	2.00	0.41
1:F:270:THR:HG23	1:F:283:SER:HB3	2.03	0.41
1:F:322:LYS:HE3	1:F:322:LYS:HB2	1.86	0.41
1:B:267:GLU:HB3	1:B:310:PHE:CE2	2.55	0.41
1:E:221:GLU:OE1	1:E:221:GLU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HD13	1:C:228:MET:CG	2.50	0.41
1:B:267:GLU:HB3	1:B:310:PHE:HE2	1.85	0.41
1:E:221:GLU:OE1	1:E:222:LEU:N	2.54	0.41
1:D:321:THR:HB	4:D:556:HOH:O	2.21	0.40
1:F:319:ASN:ND2	1:F:328:ASN:HD22	2.18	0.40
1:B:222:LEU:HD13	1:D:228:MET:CG	2.52	0.40
1:A:290:VAL:HG21	1:A:331:VAL:HG11	2.02	0.40
1:C:335:ILE:HD12	1:C:335:ILE:N	2.37	0.40
1:G:267:GLU:HB3	1:G:310:PHE:CE2	2.57	0.40
1:A:335:ILE:HD12	1:A:335:ILE:N	2.36	0.40
1:E:231:ARG:NH2	1:H:221:GLU:OE1	2.48	0.40

There are no symmetry-related clashes.

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%)	117 (99%)	1 (1%)	0	100	100
1	B	119/123 (97%)	118 (99%)	1 (1%)	0	100	100
1	C	117/123 (95%)	116 (99%)	1 (1%)	0	100	100
1	D	120/123 (98%)	120 (100%)	0	0	100	100
1	E	119/123 (97%)	118 (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
1	H	119/123 (97%)	118 (99%)	1 (1%)	0	100	100
All	All	952/984 (97%)	945 (99%)	7 (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	103/105 (98%)	103 (100%)	0	100	100
1	B	104/105 (99%)	102 (98%)	2 (2%)	50	41
1	C	102/105 (97%)	100 (98%)	2 (2%)	48	38
1	D	105/105 (100%)	104 (99%)	1 (1%)	68	64
1	E	104/105 (99%)	102 (98%)	2 (2%)	50	41
1	F	105/105 (100%)	103 (98%)	2 (2%)	50	41
1	G	105/105 (100%)	102 (97%)	3 (3%)	37	25
1	H	104/105 (99%)	103 (99%)	1 (1%)	68	64
All	All	832/840 (99%)	819 (98%)	13 (2%)	55	47

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	221	GLU
1	B	237	ASN
1	C	221	GLU
1	C	322	LYS
1	D	220	MET
1	E	221	GLU
1	E	237	ASN
1	F	237	ASN
1	F	240	ASN
1	G	221	GLU
1	G	222	LEU
1	G	261	ASN
1	H	222	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	ASN

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Mol	Chain	Res	Type
1	A	308	GLN
1	A	314	GLN
1	A	319	ASN
1	B	296	ASN
1	B	319	ASN
1	C	244	GLN
1	C	308	GLN
1	C	314	GLN
1	D	244	GLN
1	D	279	ASN
1	D	288	ASN
1	D	296	ASN
1	D	299	ASN
1	D	308	GLN
1	D	314	GLN
1	D	319	ASN
1	E	299	ASN
1	E	319	ASN
1	F	219	HIS
1	F	237	ASN
1	F	240	ASN
1	F	296	ASN
1	F	319	ASN
1	G	261	ASN
1	G	319	ASN
1	H	237	ASN
1	H	299	ASN
1	H	308	GLN
1	H	319	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 oligosaccharides in this entry.

5.6 Ligand geometry

16 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	DAL	F	401	-	5,5,5	0.38	0	6,6,6	0.53	0
2	DAL	A	401	-	5,5,5	0.68	0	6,6,6	0.72	0
3	SO4	F	402	-	4,4,4	0.37	0	6,6,6	0.09	0
3	SO4	B	402	-	4,4,4	0.36	0	6,6,6	0.07	0
2	DAL	G	401	-	5,5,5	1.00	1 (20%)	6,6,6	0.72	0
3	SO4	A	402	-	4,4,4	0.36	0	6,6,6	0.10	0
3	SO4	C	402	-	4,4,4	0.37	0	6,6,6	0.08	0
2	DAL	B	401	-	5,5,5	0.37	0	6,6,6	0.53	0
3	SO4	G	402	-	4,4,4	0.37	0	6,6,6	0.10	0
3	SO4	D	402	-	4,4,4	0.36	0	6,6,6	0.08	0
3	SO4	H	402	-	4,4,4	0.37	0	6,6,6	0.06	0
2	DAL	E	401	-	5,5,5	0.48	0	6,6,6	0.67	0
3	SO4	E	402	-	4,4,4	0.38	0	6,6,6	0.06	0
2	DAL	D	401	-	5,5,5	0.33	0	6,6,6	0.59	0
2	DAL	C	401	-	5,5,5	0.92	0	6,6,6	0.72	0
2	DAL	H	401	-	5,5,5	0.40	0	6,6,6	0.54	0

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	DAL	F	401	-	-	0/4/4/4	-
2	DAL	A	401	-	-	0/4/4/4	-
2	DAL	G	401	-	-	0/4/4/4	-
2	DAL	B	401	-	-	0/4/4/4	-
2	DAL	E	401	-	-	0/4/4/4	-
2	DAL	D	401	-	-	0/4/4/4	-
2	DAL	C	401	-	-	0/4/4/4	-
2	DAL	H	401	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	DAL	CA-C	2.12	1.56	1.54

There are no bond angle outliers.

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	401	DAL	1	0
2	D	401	DAL	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%)	-0.15	3 (2%) 58 58	6, 12, 27, 33	0
1	B	121/123 (98%)	0.03	2 (1%) 69 69	8, 15, 27, 37	0
1	C	119/123 (96%)	0.06	5 (4%) 40 40	8, 15, 30, 40	0
1	D	122/123 (99%)	0.40	6 (4%) 35 33	11, 20, 32, 36	0
1	E	121/123 (98%)	0.03	3 (2%) 58 58	8, 14, 27, 40	0
1	F	122/123 (99%)	-0.23	3 (2%) 58 58	6, 12, 23, 33	0
1	G	122/123 (99%)	-0.20	1 (0%) 82 83	6, 12, 23, 30	0
1	H	121/123 (98%)	-0.10	2 (1%) 69 69	6, 14, 25, 36	0
All	All	968/984 (98%)	-0.02	25 (2%) 57 57	6, 15, 28, 40	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	219	HIS	4.8
1	D	299	ASN	4.0
1	E	221	GLU	3.7
1	F	219	HIS	3.4
1	B	219	HIS	3.3
1	A	297	GLU	3.2
1	H	332	PHE	2.9
1	D	273	THR	2.8
1	C	318	ASP	2.7
1	D	332	PHE	2.6
1	D	300	VAL	2.5
1	D	318	ASP	2.4
1	A	244	GLN	2.3
1	C	221	GLU	2.2
1	F	221	GLU	2.2
1	C	327	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	220	MET	2.1
1	F	218	SER	2.1
1	E	323	GLU	2.1
1	B	320	LYS	2.1
1	G	299	ASN	2.1
1	C	320	LYS	2.0
1	H	318	ASP	2.0
1	D	297	GLU	2.0
1	C	316	ILE	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(Å ²)	Q<0.9
3	SO4	D	402	5/5	0.63	0.21	96,96,96,96	0
3	SO4	C	402	5/5	0.64	0.25	100,100,100,100	0
3	SO4	H	402	5/5	0.66	0.24	80,80,81,81	0
3	SO4	G	402	5/5	0.69	0.25	81,81,82,82	0
3	SO4	B	402	5/5	0.77	0.18	87,87,87,87	0
3	SO4	E	402	5/5	0.81	0.17	52,52,54,54	0
3	SO4	F	402	5/5	0.84	0.14	59,59,59,60	0
2	DAL	D	401	6/6	0.93	0.08	14,16,16,17	0
2	DAL	B	401	6/6	0.93	0.09	15,17,17,17	0
2	DAL	E	401	6/6	0.95	0.06	13,13,14,15	0
2	DAL	C	401	6/6	0.95	0.07	15,15,16,17	0
3	SO4	A	402	5/5	0.96	0.10	28,29,30,30	0
2	DAL	H	401	6/6	0.97	0.05	8,10,11,11	0
2	DAL	A	401	6/6	0.97	0.05	7,8,9,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DAL	F	401	6/6	0.97	0.06	11,11,12,12	0
2	DAL	G	401	6/6	0.98	0.05	8,9,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.