



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:52 PM UTC

PDB ID : 3TD4 / pdb_00003td4
Title : Crystal structure of OmpA-like domain from *Acinetobacter baumannii* in complex with diaminopimelate
Authors : Park, J.S.; Lee, W.C.; Song, J.H.; Kim, H.Y.
Deposited on : 2011-08-10
Resolution : 1.79 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

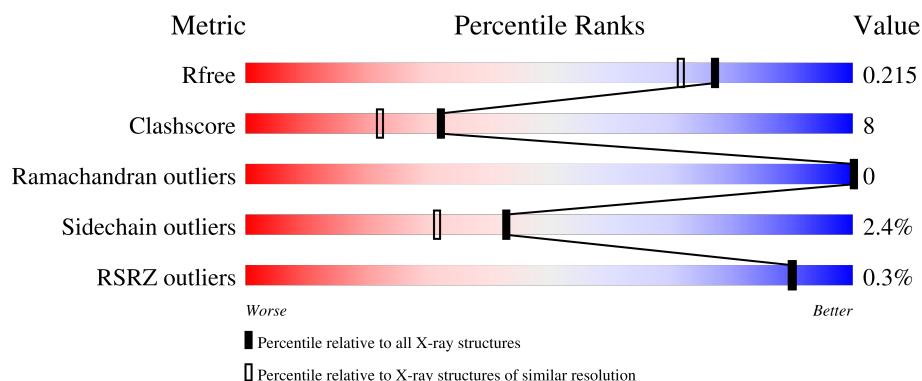
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	
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	80% 18% ..
1	G	123	76% 20% ..
1	H	123	80% 12% 6% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8457 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	122	Total	C	N	O	S	0	0	0
			970	595	180	192	3			
1	B	123	Total	C	N	O	S	0	0	0
			974	597	181	193	3			
1	C	121	Total	C	N	O	S	0	0	0
			964	592	179	190	3			
1	D	121	Total	C	N	O	S	0	0	0
			964	592	179	190	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:

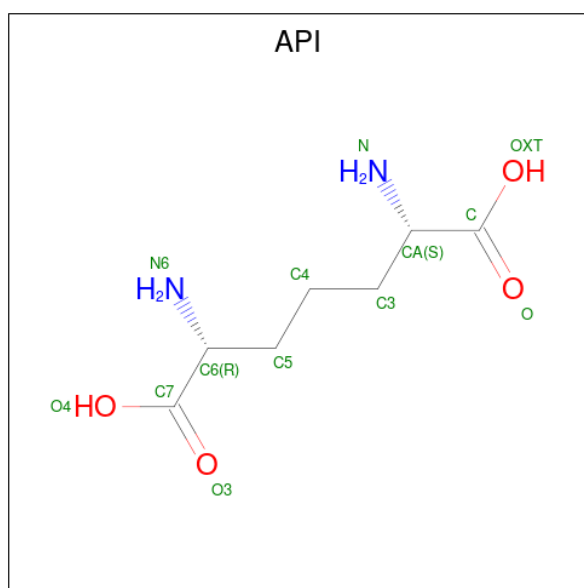
Chain	Residue	Modelled	Actual	Comment	Reference
A	217	GLY	-	expression tag	UNP Q6RYW5
A	218	SER	-	expression tag	UNP Q6RYW5
A	219	HIS	-	expression tag	UNP Q6RYW5
A	220	MET	-	expression tag	UNP Q6RYW5
B	217	GLY	-	expression tag	UNP Q6RYW5
B	218	SER	-	expression tag	UNP Q6RYW5
B	219	HIS	-	expression tag	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 2,6-DIAMINOPIMELIC ACID (CCD ID: API) (formula: $C_7H_{14}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	7	2	4		
2	B	1	Total	C	N	O	0	0
			13	7	2	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			13	7	2	4		
2	D	1	Total	C	N	O	0	0
			13	7	2	4		
2	E	1	Total	C	N	O	0	0
			13	7	2	4		
2	F	1	Total	C	N	O	0	0
			13	7	2	4		
2	G	1	Total	C	N	O	0	0
			13	7	2	4		
2	H	1	Total	C	N	O	0	0
			13	7	2	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total	O	0	0
			92	92		
3	B	69	Total	O	0	0
			69	69		
3	C	72	Total	O	0	0
			72	72		
3	D	58	Total	O	0	0
			58	58		
3	E	85	Total	O	0	0
			85	85		
3	F	85	Total	O	0	0
			85	85		
3	G	88	Total	O	0	0
			88	88		
3	H	74	Total	O	0	0
			74	74		

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.

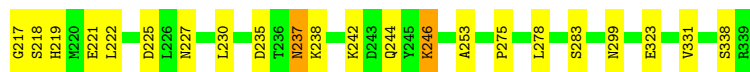
- Molecule 1: Outer membrane protein omp38

Chain A:  76% 20% ..



- Molecule 1: Outer membrane protein omp38

Chain B:  82% 16% .



- Molecule 1: Outer membrane protein omp38

Chain C:  79% 15% ..



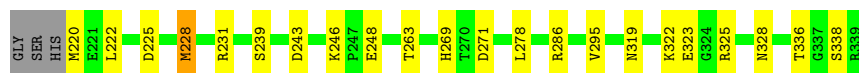
- Molecule 1: Outer membrane protein omp38

Chain D:  82% 14% ..



- Molecule 1: Outer membrane protein omp38

Chain E:  80% 17% ..



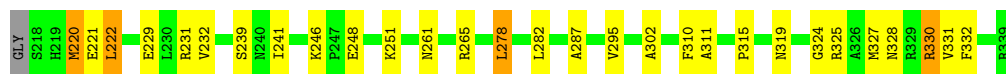
- Molecule 1: Outer membrane protein omp38

Chain F:  80% 18% ..



- Molecule 1: Outer membrane protein omp38

Chain G:  76% 20% ..



- Molecule 1: Outer membrane protein omp38

Chain H:  80% 12% 6% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.87Å 98.22Å 98.44Å 90.00° 105.51° 90.00°	Depositor
Resolution (Å)	94.86 – 1.79 94.85 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.1 (94.86-1.79) 99.1 (94.85-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.179 , 0.214 0.178 , 0.215	Depositor DCC
R_{free} test set	4939 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8457	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 5.68% 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: API

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	1.70	9/984 (0.9%)	1.46	3/1324 (0.2%)
1	B	1.60	5/988 (0.5%)	1.45	5/1329 (0.4%)
1	C	1.56	4/978 (0.4%)	1.39	3/1316 (0.2%)
1	D	1.45	4/978 (0.4%)	1.35	6/1316 (0.5%)
1	E	1.61	4/967 (0.4%)	1.42	3/1301 (0.2%)
1	F	1.65	8/984 (0.8%)	1.49	3/1324 (0.2%)
1	G	1.75	16/984 (1.6%)	1.49	6/1324 (0.5%)
1	H	1.61	5/978 (0.5%)	1.43	7/1316 (0.5%)
All	All	1.62	55/7841 (0.7%)	1.44	36/10550 (0.3%)

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	311	ALA	CA-CB	7.62	1.66	1.53
1	G	287	ALA	CA-CB	7.56	1.65	1.53
1	A	330	ARG	CZ-NH2	7.02	1.42	1.33
1	G	261	ASN	C-O	-6.73	1.15	1.24
1	E	295	VAL	N-CA	6.61	1.54	1.46
1	F	311	ALA	CA-CB	6.54	1.64	1.52
1	C	336	THR	CA-C	-6.46	1.44	1.52
1	G	265	ARG	C-O	6.38	1.31	1.24
1	G	220	MET	N-CA	6.36	1.53	1.46
1	F	249	ILE	N-CA	6.31	1.54	1.46
1	F	337	GLY	N-CA	6.28	1.51	1.45
1	A	232	VAL	N-CA	-6.25	1.38	1.46
1	A	326	ALA	CA-C	6.24	1.60	1.52
1	H	329	ARG	CD-NE	6.20	1.54	1.46
1	A	228	MET	CG-SD	6.17	1.96	1.80
1	G	302	ALA	CA-CB	6.12	1.63	1.53
1	G	295	VAL	CA-CB	-6.09	1.47	1.54
1	G	331	VAL	CA-CB	-6.08	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	228	MET	SD-CE	-6.01	1.64	1.79
1	B	246	LYS	N-CA	5.97	1.52	1.46
1	D	223	THR	N-CA	5.91	1.53	1.45
1	G	241	ILE	CA-CB	-5.86	1.47	1.54
1	F	338	SER	N-CA	5.86	1.53	1.45
1	G	315	PRO	N-CA	-5.83	1.39	1.47
1	F	248	GLU	CD-OE2	5.76	1.36	1.25
1	E	269	HIS	CA-C	-5.72	1.45	1.52
1	B	253	ALA	CA-CB	5.70	1.62	1.53
1	A	307	THR	N-CA	5.69	1.53	1.45
1	H	268	GLY	N-CA	5.61	1.50	1.44
1	F	224	GLU	CA-CB	-5.54	1.43	1.53
1	G	324	GLY	CA-C	5.53	1.59	1.51
1	G	330	ARG	C-O	5.48	1.30	1.23
1	G	282	LEU	CA-C	5.45	1.59	1.52
1	B	230	LEU	CA-C	5.43	1.59	1.52
1	F	327	MET	N-CA	5.43	1.53	1.46
1	B	275	PRO	N-CA	-5.38	1.40	1.46
1	C	244	GLN	C-O	-5.37	1.17	1.24
1	C	241	ILE	CA-CB	5.37	1.59	1.53
1	F	253	ALA	CA-CB	5.37	1.61	1.53
1	C	228	MET	CB-CG	-5.37	1.36	1.52
1	D	223	THR	C-O	5.35	1.30	1.23
1	A	300	VAL	CA-CB	5.35	1.60	1.54
1	G	251	LYS	N-CA	5.34	1.52	1.46
1	B	227	ASN	C-O	5.31	1.29	1.24
1	E	286	ARG	CA-C	5.21	1.59	1.52
1	H	289	SER	CA-CB	5.18	1.61	1.53
1	G	261	ASN	CG-OD1	5.13	1.33	1.23
1	G	221	GLU	N-CA	5.11	1.52	1.45
1	G	239	SER	CA-CB	5.09	1.61	1.53
1	D	300	VAL	CA-CB	5.08	1.60	1.54
1	H	327	MET	N-CA	5.07	1.52	1.46
1	A	290	VAL	CA-C	5.06	1.59	1.52
1	H	220	MET	CB-CG	-5.04	1.37	1.52
1	A	287	ALA	CA-C	5.02	1.59	1.52
1	A	271	ASP	CB-CG	5.01	1.64	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	274	GLY	CA-C-N	8.61	128.63	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	274	GLY	C-N-CA	8.61	128.63	119.76
1	G	327	MET	CG-SD-CE	-8.38	82.47	100.90
1	B	283	SER	N-CA-C	-8.07	102.56	111.36
1	B	237	ASN	N-CA-C	6.77	121.30	113.38
1	F	307	THR	CA-CB-OG1	6.75	119.72	109.60
1	D	276	ARG	NE-CZ-NH2	6.47	125.03	119.20
1	A	231	ARG	NE-CZ-NH2	6.44	124.99	119.20
1	H	274	GLY	CA-C-N	-6.43	114.01	120.31
1	H	274	GLY	C-N-CA	-6.43	114.01	120.31
1	C	314	GLN	CA-C-N	-6.41	113.37	119.85
1	C	314	GLN	C-N-CA	-6.41	113.37	119.85
1	E	239	SER	N-CA-C	-6.09	104.36	112.94
1	H	228	MET	CG-SD-CE	6.04	114.18	100.90
1	A	220	MET	CG-SD-CE	-5.89	87.95	100.90
1	G	220	MET	CG-SD-CE	-5.85	88.03	100.90
1	D	276	ARG	CB-CG-CD	5.59	124.15	111.30
1	B	331	VAL	N-CA-C	-5.53	100.36	108.11
1	G	232	VAL	N-CA-C	-5.48	100.23	108.12
1	H	312	TRP	N-CA-C	-5.44	105.95	112.59
1	D	327	MET	CG-SD-CE	-5.35	89.14	100.90
1	G	246	LYS	CA-C-N	-5.34	113.40	119.28
1	G	246	LYS	C-N-CA	-5.34	113.40	119.28
1	E	323	GLU	CA-C-N	5.32	125.85	120.00
1	E	323	GLU	C-N-CA	5.32	125.85	120.00
1	H	330	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	D	239	SER	N-CA-C	-5.25	105.16	112.30
1	H	289	SER	CB-CA-C	5.25	119.77	110.85
1	D	276	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	D	327	MET	CB-CG-SD	-5.22	97.05	112.70
1	B	218	SER	N-CA-C	-5.21	106.89	113.20
1	B	323	GLU	N-CA-C	-5.14	105.67	111.28
1	G	278	LEU	N-CA-C	-5.12	105.60	111.07
1	H	230	LEU	N-CA-C	-5.07	100.90	109.07
1	C	248	GLU	CA-CB-CG	-5.06	103.97	114.10
1	A	337	GLY	N-CA-C	-5.01	103.44	110.75

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	970	0	957	35	0
1	B	974	0	960	12	0
1	C	964	0	952	33	0
1	D	964	0	952	14	0
1	E	954	0	945	15	0
1	F	970	0	957	16	0
1	G	970	0	957	15	0
1	H	964	0	952	22	0
2	A	13	0	7	0	0
2	B	13	0	7	1	0
2	C	13	0	7	0	0
2	D	13	0	7	0	0
2	E	13	0	7	0	0
2	F	13	0	7	0	0
2	G	13	0	7	0	0
2	H	13	0	7	0	0
3	A	92	0	0	3	0
3	B	69	0	0	3	0
3	C	72	0	0	3	0
3	D	58	0	0	0	0
3	E	85	0	0	1	0
3	F	85	0	0	4	0
3	G	88	0	0	3	0
3	H	74	0	0	2	0
All	All	8457	0	7688	124	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 8.

All (124) 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:B:299:ASN:HB2	3:B:521:HOH:O	1.40	1.20
1:F:246:LYS:HE2	3:F:116:HOH:O	1.45	1.11
1:A:231:ARG:NH1	1:C:219:HIS:CB	2.24	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:229:GLU:HG3	1:H:332:PHE:CE1	2.02	0.94
1:A:231:ARG:NH1	1:C:219:HIS:HB2	1.83	0.93
1:D:276:ARG:HD2	1:D:280:GLU:OE2	1.75	0.86
1:A:231:ARG:NH1	1:C:219:HIS:HB3	1.89	0.84
1:A:221:GLU:HG2	1:C:231:ARG:NH2	1.94	0.82
1:B:217:GLY:N	1:E:263:THR:HG1	1.79	0.81
1:A:248:GLU:HG2	1:C:220:MET:HB2	1.63	0.79
1:A:231:ARG:HH12	1:C:219:HIS:CB	1.97	0.77
1:H:229:GLU:CD	1:H:332:PHE:HE1	1.92	0.77
1:A:228:MET:HE1	1:A:255:LYS:HB2	1.70	0.72
1:A:231:ARG:HH12	1:C:219:HIS:HB2	1.53	0.72
1:F:240:ASN:HD22	1:F:240:ASN:H	1.38	0.72
1:H:229:GLU:CG	1:H:332:PHE:HE1	2.04	0.71
1:F:255:LYS:HE2	1:G:222:LEU:HD21	1.73	0.70
1:H:229:GLU:HG3	1:H:332:PHE:HE1	1.55	0.69
1:H:229:GLU:CG	1:H:332:PHE:CE1	2.73	0.69
1:B:235:ASP:HB2	1:B:238:LYS:HD2	1.74	0.68
1:E:278:LEU:HD12	3:E:427:HOH:O	1.94	0.67
1:C:222:LEU:HD12	1:C:222:LEU:C	2.20	0.67
1:E:231:ARG:NH2	1:H:221:GLU:OE1	2.28	0.66
1:D:319:ASN:ND2	1:D:328:ASN:HD22	1.93	0.66
1:C:231:ARG:HG2	1:C:332:PHE:CE1	2.31	0.65
1:D:276:ARG:HD3	1:D:280:GLU:HG3	1.79	0.64
1:H:231:ARG:HB2	3:H:620:HOH:O	1.99	0.62
1:B:225:ASP:OD1	1:B:338:SER:OG	2.18	0.61
1:A:219:HIS:HB2	1:C:248:GLU:OE1	1.99	0.61
1:A:219:HIS:CD2	1:C:245:TYR:HE1	2.19	0.61
1:F:218:SER:CB	3:F:211:HOH:O	2.47	0.60
1:G:229:GLU:OE1	3:G:486:HOH:O	2.16	0.60
1:C:243:ASP:HA	1:C:246:LYS:HD3	1.84	0.59
1:A:219:HIS:HB3	1:C:231:ARG:O	2.03	0.59
1:A:221:GLU:HG2	1:C:231:ARG:HH22	1.67	0.59
1:A:221:GLU:CG	1:C:231:ARG:NH2	2.64	0.58
1:H:229:GLU:CD	1:H:332:PHE:CE1	2.80	0.58
1:B:222:LEU:HD13	1:D:228:MET:HG2	1.86	0.57
1:C:222:LEU:HD11	3:C:540:HOH:O	2.04	0.57
1:A:218:SER:HB3	1:F:336:THR:OG1	2.04	0.57
1:E:225:ASP:OD1	1:E:338:SER:OG	2.15	0.57
1:B:299:ASN:CB	3:B:521:HOH:O	2.19	0.55
1:B:217:GLY:HA2	1:E:336:THR:OG1	2.07	0.55
1:A:219:HIS:CD2	1:C:245:TYR:CE1	2.95	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ARG:HG2	1:C:332:PHE:CD1	2.41	0.54
1:D:276:ARG:CD	1:D:280:GLU:OE2	2.50	0.54
1:F:243:ASP:HA	1:F:246:LYS:HD2	1.88	0.54
1:A:220:MET:HE1	1:C:252:VAL:HG23	1.89	0.53
1:A:222:LEU:HD13	1:C:228:MET:HG2	1.90	0.53
1:C:301:ASP:OD2	1:C:303:SER:OG	2.24	0.53
1:C:219:HIS:N	3:C:580:HOH:O	2.42	0.52
1:D:265:ARG:HD3	1:D:267:GLU:OE2	2.08	0.52
1:E:248:GLU:HG2	1:H:220:MET:HB2	1.92	0.52
1:A:221:GLU:CG	1:C:231:ARG:HH22	2.21	0.52
1:G:231:ARG:HG2	1:G:332:PHE:CD2	2.45	0.52
1:B:244:GLN:HA	3:B:430:HOH:O	2.10	0.52
1:E:231:ARG:HH22	1:H:221:GLU:CD	2.16	0.52
1:F:240:ASN:H	1:F:240:ASN:ND2	2.05	0.52
1:G:231:ARG:HG2	1:G:332:PHE:CE2	2.46	0.51
1:G:319:ASN:ND2	1:G:328:ASN:HD22	2.08	0.51
1:H:327:MET:HE3	3:H:138:HOH:O	2.11	0.51
1:G:332:PHE:CD1	3:G:415:HOH:O	2.54	0.51
1:A:220:MET:HE2	1:C:228:MET:HE2	1.93	0.50
1:A:231:ARG:HH11	1:C:219:HIS:HB3	1.73	0.49
1:F:251:LYS:HG2	1:G:220:MET:HE1	1.94	0.49
1:E:222:LEU:HD13	1:H:228:MET:HG2	1.94	0.49
1:A:319:ASN:HD22	1:A:325:ARG:HG2	1.77	0.49
1:E:220:MET:HB2	1:H:248:GLU:HG3	1.95	0.48
1:A:231:ARG:CZ	1:C:219:HIS:HB2	2.41	0.48
1:A:336:THR:OG1	1:F:218:SER:HB3	2.12	0.48
1:F:218:SER:HB2	1:G:248:GLU:OE2	2.14	0.48
1:A:218:SER:CB	3:A:83:HOH:O	2.62	0.47
1:D:270:THR:HG23	1:D:283:SER:HB3	1.96	0.47
1:D:327:MET:HB3	1:D:327:MET:HE3	1.52	0.47
1:A:228:MET:HE1	1:A:255:LYS:CB	2.43	0.46
1:C:318:ASP:OD1	1:C:320:LYS:HE3	2.15	0.46
1:C:321:THR:HB	1:C:323:GLU:OE2	2.16	0.46
1:E:319:ASN:ND2	1:E:328:ASN:HD22	2.13	0.46
1:H:220:MET:C	1:H:220:MET:HE3	2.40	0.46
1:H:228:MET:HB2	1:H:335:ILE:HB	1.98	0.46
1:D:276:ARG:HD3	1:D:280:GLU:CG	2.46	0.46
1:A:236:THR:HG22	1:A:329:ARG:CZ	2.46	0.46
1:A:218:SER:HB2	3:A:83:HOH:O	2.15	0.46
1:H:220:MET:HE1	1:H:222:LEU:HD12	1.98	0.46
1:F:319:ASN:HD22	1:F:325:ARG:HG2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:MET:HE2	1:H:220:MET:SD	2.55	0.45
1:F:280:GLU:HG2	3:F:596:HOH:O	2.16	0.45
1:H:319:ASN:ND2	1:H:328:ASN:HD22	2.15	0.45
1:A:221:GLU:CD	1:C:231:ARG:HH22	2.25	0.45
1:B:235:ASP:OD2	1:B:242:LYS:NZ	2.49	0.45
1:G:330:ARG:HD2	1:G:332:PHE:CE2	2.52	0.45
1:B:237:ASN:ND2	2:B:401:API:CA	2.80	0.45
1:F:319:ASN:ND2	1:F:328:ASN:HD22	2.15	0.44
1:A:220:MET:HB2	1:A:220:MET:HE3	1.80	0.44
1:G:229:GLU:OE2	1:G:231:ARG:NH2	2.49	0.44
1:H:230:LEU:HB3	1:H:333:ALA:HB3	2.00	0.44
1:A:229:GLU:O	1:C:220:MET:HA	2.18	0.43
1:C:323:GLU:H	1:C:323:GLU:CD	2.24	0.43
1:A:278:LEU:HD23	1:A:278:LEU:C	2.43	0.43
1:H:320:LYS:HB2	1:H:320:LYS:HE2	1.71	0.43
1:F:238:LYS:HB3	1:F:240:ASN:ND2	2.33	0.43
1:C:251:LYS:CE	3:C:374:HOH:O	2.65	0.43
1:D:278:LEU:C	1:D:278:LEU:HD23	2.43	0.43
1:H:278:LEU:C	1:H:278:LEU:HD23	2.43	0.43
1:B:219:HIS:HB3	1:D:231:ARG:O	2.18	0.42
1:E:243:ASP:HA	1:E:246:LYS:HG2	2.01	0.42
1:E:319:ASN:HD22	1:E:325:ARG:HG2	1.83	0.42
1:A:243:ASP:HA	1:A:246:LYS:HE2	2.01	0.42
1:E:322:LYS:HG2	1:E:325:ARG:NH2	2.35	0.42
1:A:221:GLU:HG2	1:C:231:ARG:HH21	1.81	0.41
1:E:271:ASP:HB2	1:E:319:ASN:ND2	2.35	0.41
1:G:278:LEU:HD23	1:G:278:LEU:C	2.45	0.41
1:A:231:ARG:NE	3:A:358:HOH:O	2.30	0.41
1:D:220:MET:HE3	1:D:220:MET:HB3	1.84	0.41
1:G:319:ASN:HD22	1:G:325:ARG:HG2	1.86	0.41
1:F:219:HIS:HB2	1:G:248:GLU:OE1	2.20	0.41
1:A:259:TYR:CE1	1:A:339:ARG:HG2	2.56	0.41
1:D:261:ASN:OD1	1:D:261:ASN:C	2.64	0.41
1:F:218:SER:HB2	3:F:211:HOH:O	2.16	0.41
1:B:278:LEU:C	1:B:278:LEU:HD23	2.46	0.41
1:D:319:ASN:HD21	1:D:328:ASN:HD22	1.66	0.41
1:G:248:GLU:HG3	3:G:541:HOH:O	2.21	0.40
1:G:310:PHE:O	1:G:311:ALA:C	2.64	0.40
1:H:237:ASN:HD22	1:H:237:ASN:HA	1.69	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	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
1	B	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
1	C	119/123 (97%)	118 (99%)	1 (1%)	0	100	100
1	D	119/123 (97%)	118 (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
1	H	119/123 (97%)	118 (99%)	1 (1%)	0	100	100
All	All	956/984 (97%)	947 (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	105/105 (100%)	104 (99%)	1 (1%)	68	64
1	B	105/105 (100%)	103 (98%)	2 (2%)	50	41
1	C	104/105 (99%)	99 (95%)	5 (5%)	23	11
1	D	104/105 (99%)	101 (97%)	3 (3%)	37	25
1	E	103/105 (98%)	103 (100%)	0	100	100
1	F	105/105 (100%)	102 (97%)	3 (3%)	37	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	105/105 (100%)	104 (99%)	1 (1%)	68	64
1	H	104/105 (99%)	99 (95%)	5 (5%)	23	11
All	All	835/840 (99%)	815 (98%)	20 (2%)	43	31

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	LEU
1	B	221	GLU
1	B	246	LYS
1	C	229	GLU
1	C	246	LYS
1	C	247	PRO
1	C	320	LYS
1	C	323	GLU
1	D	221	GLU
1	D	222	LEU
1	D	265	ARG
1	F	222	LEU
1	F	240	ASN
1	F	246	LYS
1	G	222	LEU
1	H	220	MET
1	H	221	GLU
1	H	222	LEU
1	H	237	ASN
1	H	248	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	HIS
1	A	237	ASN
1	A	314	GLN
1	A	319	ASN
1	B	296	ASN
1	B	319	ASN
1	D	288	ASN
1	D	308	GLN
1	D	314	GLN

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Mol	Chain	Res	Type
1	D	319	ASN
1	E	244	GLN
1	E	319	ASN
1	F	219	HIS
1	F	240	ASN
1	F	299	ASN
1	F	319	ASN
1	G	308	GLN
1	G	319	ASN
1	H	227	ASN
1	H	237	ASN
1	H	308	GLN
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	API	D	401	-	10,12,12	0.94	1 (10%)	9,15,15	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	API	H	401	-	10,12,12	1.33	1 (10%)	9,15,15	3.42	5 (55%)
2	API	G	401	-	10,12,12	1.60	2 (20%)	9,15,15	3.03	2 (22%)
2	API	B	401	-	10,12,12	1.34	2 (20%)	9,15,15	1.21	1 (11%)
2	API	C	401	-	10,12,12	1.15	0	9,15,15	1.48	1 (11%)
2	API	A	401	-	10,12,12	1.27	1 (10%)	9,15,15	0.94	0
2	API	E	401	-	10,12,12	1.25	1 (10%)	9,15,15	1.38	2 (22%)
2	API	F	401	-	10,12,12	1.42	1 (10%)	9,15,15	1.33	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	API	D	401	-	-	3/14/14/14	-
2	API	H	401	-	-	3/14/14/14	-
2	API	G	401	-	-	2/14/14/14	-
2	API	B	401	-	-	4/14/14/14	-
2	API	C	401	-	-	5/14/14/14	-
2	API	A	401	-	-	4/14/14/14	-
2	API	E	401	-	-	1/14/14/14	-
2	API	F	401	-	-	2/14/14/14	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	API	O3-C7	3.19	1.31	1.22
2	G	401	API	O4-C7	-3.19	1.20	1.30
2	H	401	API	C3-CA	3.10	1.59	1.53
2	E	401	API	O4-C7	-2.76	1.21	1.30
2	G	401	API	C3-CA	2.58	1.58	1.53
2	B	401	API	O3-C7	2.51	1.29	1.22
2	D	401	API	OXT-C	-2.33	1.23	1.30
2	B	401	API	OXT-C	-2.22	1.23	1.30
2	A	401	API	C3-CA	2.10	1.57	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	API	C3-CA-C	-7.00	91.89	110.45
2	H	401	API	C3-CA-N	6.56	127.23	110.12
2	H	401	API	C3-CA-C	-6.36	93.59	110.45
2	G	401	API	C3-CA-N	5.12	123.46	110.12
2	C	401	API	C3-CA-C	-3.23	101.89	110.45
2	E	401	API	C3-CA-N	-2.89	102.58	110.12
2	H	401	API	OXT-C-O	2.60	129.97	124.08
2	B	401	API	C3-CA-C	-2.49	103.85	110.45
2	E	401	API	C5-C4-C3	-2.27	103.11	113.28
2	H	401	API	C4-C5-C6	2.22	120.40	113.22
2	H	401	API	C5-C6-C7	-2.13	104.80	110.45

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	401	API	C4-C3-CA-C
2	F	401	API	C4-C3-CA-N
2	G	401	API	C4-C3-CA-N
2	H	401	API	C4-C3-CA-N
2	C	401	API	OXT-C-CA-N
2	H	401	API	C3-C4-C5-C6
2	B	401	API	OXT-C-CA-N
2	C	401	API	C3-C4-C5-C6
2	C	401	API	CA-C3-C4-C5
2	B	401	API	O-C-CA-N
2	C	401	API	O-C-CA-N
2	D	401	API	O-C-CA-N
2	D	401	API	CA-C3-C4-C5
2	G	401	API	C4-C3-CA-C
2	H	401	API	C4-C3-CA-C
2	D	401	API	OXT-C-CA-N
2	B	401	API	CA-C3-C4-C5
2	E	401	API	C4-C3-CA-N
2	A	401	API	OXT-C-CA-N
2	A	401	API	C3-C4-C5-C6
2	A	401	API	O-C-CA-N
2	A	401	API	CA-C3-C4-C5
2	B	401	API	C3-C4-C5-C6
2	C	401	API	O-C-CA-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	API	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	122/123 (99%)	-0.36	0 100 100	7, 13, 28, 36	0
1	B	123/123 (100%)	-0.28	0 100 100	9, 16, 26, 35	0
1	C	121/123 (98%)	-0.29	2 (1%) 69 69	9, 15, 29, 43	0
1	D	121/123 (98%)	-0.13	1 (0%) 82 83	11, 19, 30, 39	0
1	E	120/123 (97%)	-0.36	0 100 100	7, 15, 27, 31	0
1	F	122/123 (99%)	-0.40	0 100 100	8, 15, 24, 32	0
1	G	122/123 (99%)	-0.32	0 100 100	6, 14, 24, 36	0
1	H	121/123 (98%)	-0.37	0 100 100	6, 14, 26, 34	0
All	All	972/984 (98%)	-0.32	3 (0%) 90 90	6, 15, 28, 43	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	219	HIS	2.6
1	C	318	ASP	2.3
1	D	332	PHE	2.3

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	API	B	401	13/13	0.93	0.11	13,17,42,47	0
2	API	C	401	13/13	0.93	0.10	14,18,41,43	0
2	API	D	401	13/13	0.93	0.11	15,19,49,49	0
2	API	E	401	13/13	0.93	0.10	11,15,38,39	0
2	API	F	401	13/13	0.94	0.10	8,14,46,47	0
2	API	H	401	13/13	0.94	0.10	6,14,39,40	0
2	API	G	401	13/13	0.95	0.10	9,13,41,44	0
2	API	A	401	13/13	0.96	0.10	6,14,40,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.