Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 01:15 PM GMT

PDB ID	:	3TD4
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

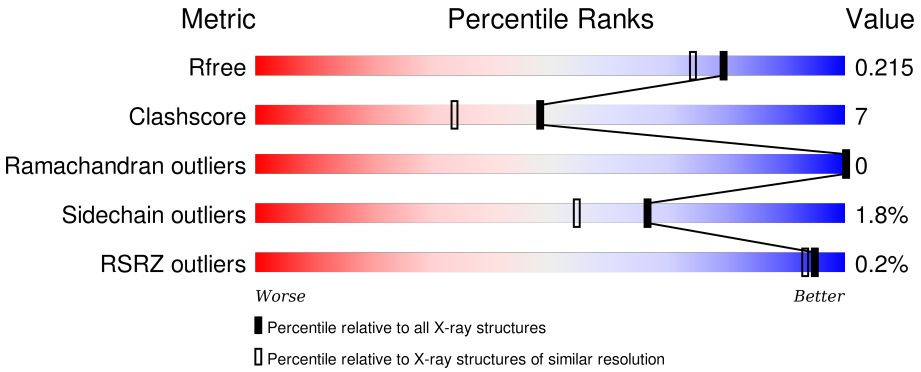
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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 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	123	80% 16%
1	B	123	81% 18%
1	C	123	2% 80% 17%
1	D	123	86% 10%
1	E	123	79% 18%

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Mol	Chain	Length	Quality of chain
1	F	123	
1	G	123	
1	H	123	

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	API	A	401	-	-	-	X
2	API	B	401	-	-	-	X
2	API	C	401	-	-	-	X
2	API	E	401	-	-	-	X
2	API	F	401	-	-	-	X
2	API	G	401	-	-	-	X
2	API	H	401	-	-	-	X

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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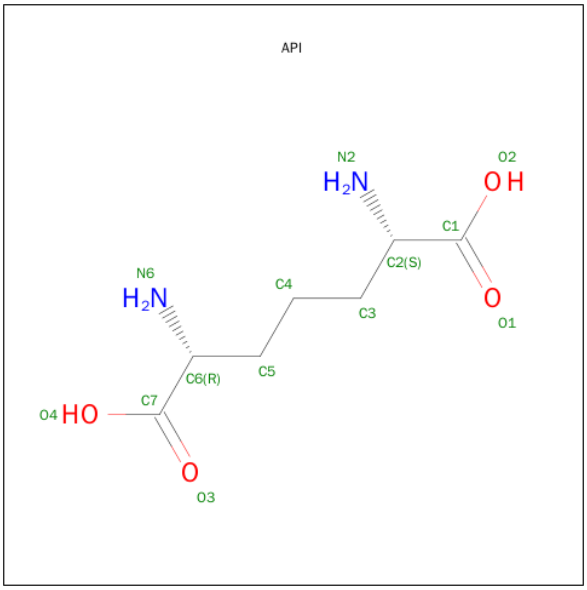
Chain	Residue	Modelled	Actual	Comment	Reference
D	218	SER	-	EXPRESSION TAG	UNP Q6RYW5
D	219	HIS	-	EXPRESSION TAG	UNP Q6RYW5
D	220	MET	-	EXPRESSION TAG	UNP Q6RYW5
E	217	GLY	-	EXPRESSION TAG	UNP Q6RYW5
E	218	SER	-	EXPRESSION TAG	UNP Q6RYW5
E	219	HIS	-	EXPRESSION TAG	UNP Q6RYW5
E	220	MET	-	EXPRESSION TAG	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 (three-letter code: API) (formula: $C_7H_{14}N_2O_4$).



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

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

- Molecule 3 is water.

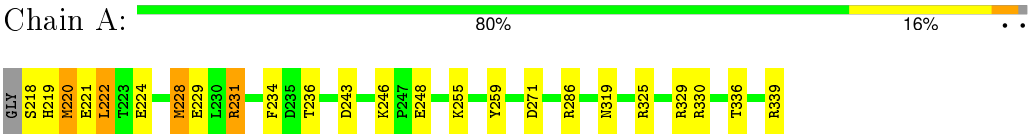
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	92	Total O 92 92	0	0
3	B	69	Total O 69 69	0	0
3	C	72	Total O 72 72	0	0
3	D	58	Total O 58 58	0	0
3	E	85	Total O 85 85	0	0
3	F	85	Total O 85 85	0	0
3	G	88	Total O 88 88	0	0
3	H	74	Total O 74 74	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

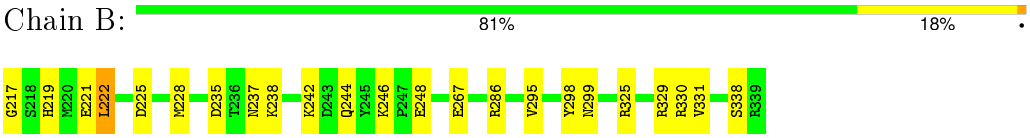
- Molecule 1: Outer membrane protein omp38

Chain A:



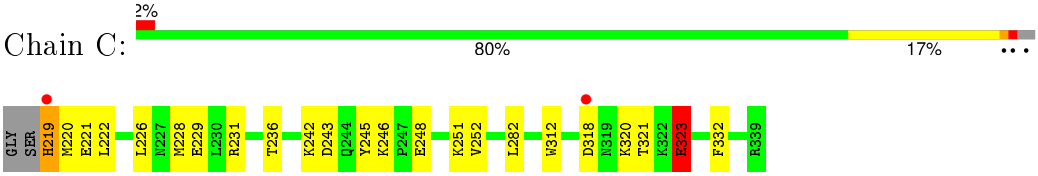
- Molecule 1: Outer membrane protein omp38

Chain B:



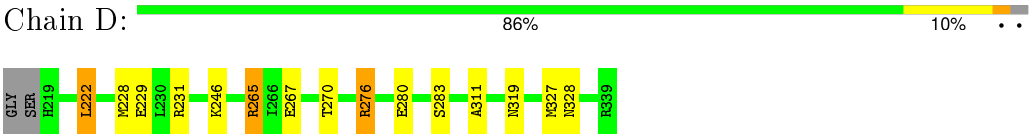
- Molecule 1: Outer membrane protein omp38

Chain C:



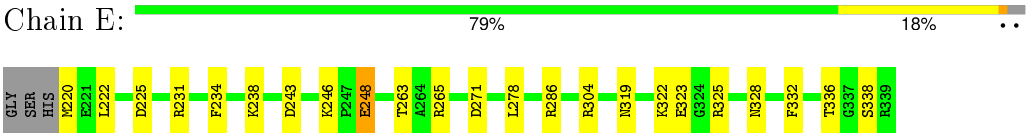
- Molecule 1: Outer membrane protein omp38

Chain D:



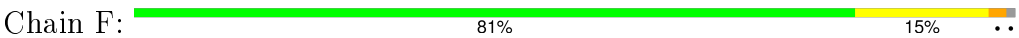
- Molecule 1: Outer membrane protein omp38

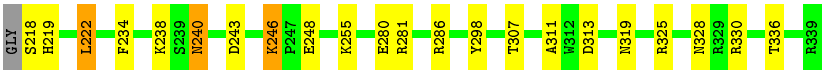
Chain E:



- Molecule 1: Outer membrane protein omp38

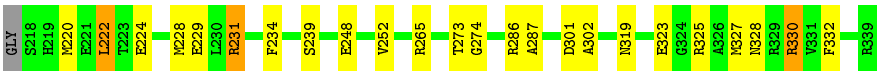
Chain F:





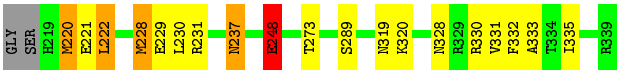
• Molecule 1: Outer membrane protein omp38

Chain G:



• Molecule 1: Outer membrane protein omp38

Chain H:



4 Data and refinement statistics (i)

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 47.43 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.1 (94.86-1.79) 99.2 (47.43-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.26%)	DCC
Wilson B-factor (Å^2)	16.7	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 50.6	EDS
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 98908 reflections (0.001%)	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.*

[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: 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	1.44	4/984 (0.4%)	1.29	6/1324 (0.5%)
1	B	1.39	5/988 (0.5%)	1.28	8/1329 (0.6%)
1	C	1.36	3/978 (0.3%)	1.16	3/1316 (0.2%)
1	D	1.23	2/978 (0.2%)	1.18	6/1316 (0.5%)
1	E	1.32	3/967 (0.3%)	1.24	6/1301 (0.5%)
1	F	1.43	5/984 (0.5%)	1.32	7/1324 (0.5%)
1	G	1.47	8/984 (0.8%)	1.35	11/1324 (0.8%)
1	H	1.38	3/978 (0.3%)	1.26	4/1316 (0.3%)
All	All	1.38	33/7841 (0.4%)	1.26	51/10550 (0.5%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	248	GLU	CD-OE2	9.68	1.36	1.25
1	C	221	GLU	CG-CD	7.83	1.63	1.51
1	B	331	VAL	CB-CG1	7.45	1.68	1.52
1	A	330	ARG	CZ-NH2	7.33	1.42	1.33
1	B	248	GLU	CD-OE1	7.16	1.33	1.25
1	G	323	GLU	CB-CG	6.68	1.64	1.52
1	D	311	ALA	CA-CB	6.62	1.66	1.52
1	A	234	PHE	CD1-CE1	6.50	1.52	1.39
1	E	323	GLU	CG-CD	6.41	1.61	1.51
1	G	252	VAL	CB-CG2	6.24	1.66	1.52
1	D	229	GLU	CB-CG	6.16	1.63	1.52
1	G	287	ALA	CA-CB	6.12	1.65	1.52
1	A	271	ASP	CB-CG	6.11	1.64	1.51
1	B	298	TYR	CD1-CE1	6.03	1.48	1.39
1	H	331	VAL	CB-CG1	6.01	1.65	1.52
1	F	234	PHE	CE1-CZ	6.01	1.48	1.37
1	F	298	TYR	CD1-CE1	6.00	1.48	1.39
1	F	298	TYR	CE2-CZ	5.93	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	311	ALA	CA-CB	5.89	1.64	1.52
1	B	295	VAL	CB-CG1	5.82	1.65	1.52
1	A	228	MET	CG-SD	5.78	1.96	1.81
1	G	224	GLU	CG-CD	-5.78	1.43	1.51
1	H	289	SER	CA-CB	5.71	1.61	1.52
1	H	248	GLU	CB-CG	-5.60	1.41	1.52
1	C	312	TRP	CE3-CZ3	5.51	1.47	1.38
1	G	239	SER	CA-CB	5.50	1.61	1.52
1	C	323	GLU	CB-CG	5.46	1.62	1.52
1	G	234	PHE	CD1-CE1	5.41	1.50	1.39
1	E	248	GLU	CD-OE1	5.24	1.31	1.25
1	G	302	ALA	CA-CB	5.24	1.63	1.52
1	E	234	PHE	CE1-CZ	5.22	1.47	1.37
1	G	265	ARG	CG-CD	5.20	1.65	1.51
1	B	267	GLU	CB-CG	5.12	1.61	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	330	ARG	NE-CZ-NH2	-11.75	114.42	120.30
1	G	327	MET	CG-SD-CE	-11.08	82.47	100.20
1	G	301	ASP	CB-CG-OD1	10.13	127.41	118.30
1	D	276	ARG	NE-CZ-NH2	9.46	125.03	120.30
1	A	231	ARG	NE-CZ-NH2	9.39	124.99	120.30
1	A	286	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	F	286	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	F	330	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	B	330	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	H	228	MET	CG-SD-CE	8.74	114.18	100.20
1	F	286	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	B	286	ARG	NE-CZ-NH1	8.65	124.63	120.30
1	B	286	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	D	276	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	G	330	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	A	220	MET	CG-SD-CE	-7.66	87.95	100.20
1	G	220	MET	CG-SD-CE	-7.60	88.03	100.20
1	B	228	MET	CG-SD-CE	7.27	111.83	100.20
1	E	304	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	330	ARG	NE-CZ-NH1	-7.22	116.69	120.30
1	B	330	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	D	327	MET	CG-SD-CE	-6.91	89.14	100.20
1	G	286	ARG	NE-CZ-NH2	-6.78	116.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	286	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	D	222	LEU	CA-CB-CG	6.57	130.41	115.30
1	B	329	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	282	LEU	CB-CG-CD2	-6.34	100.22	111.00
1	E	286	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	G	301	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	E	286	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	F	281	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	E	332	PHE	CB-CG-CD2	-6.15	116.50	120.80
1	A	224	GLU	OE1-CD-OE2	-5.89	116.23	123.30
1	A	222	LEU	CB-CG-CD1	-5.86	101.05	111.00
1	H	228	MET	CA-CB-CG	5.85	123.24	113.30
1	F	222	LEU	CA-CB-CG	5.58	128.14	115.30
1	C	226	LEU	CB-CG-CD2	-5.41	101.81	111.00
1	G	231	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	F	313	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	D	327	MET	CB-CG-SD	-5.12	97.05	112.40
1	F	307	THR	CA-CB-OG1	5.11	119.72	109.00
1	B	222	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	H	289	SER	CB-CA-C	5.09	119.77	110.10
1	G	265	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	E	265	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	C	242	LYS	CD-CE-NZ	-5.08	100.02	111.70
1	D	246	LYS	CD-CE-NZ	-5.08	100.03	111.70
1	E	238	LYS	CD-CE-NZ	-5.05	100.08	111.70
1	G	231	ARG	NE-CZ-NH2	5.03	122.81	120.30
1	B	325	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	G	228	MET	CG-SD-CE	5.01	108.22	100.20

There are no chirality outliers.

There are no planarity outliers.

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	970	0	957	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	974	0	960	13	0
1	C	964	0	952	31	0
1	D	964	0	952	10	0
1	E	954	0	945	14	0
1	F	970	0	957	15	0
1	G	970	0	957	15	0
1	H	964	0	952	20	0
2	A	13	0	12	0	0
2	B	13	0	12	3	0
2	C	13	0	12	1	0
2	D	13	0	12	0	0
2	E	13	0	12	0	0
2	F	13	0	12	0	0
2	G	13	0	12	3	0
2	H	13	0	12	1	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	1	0
All	All	8457	0	7728	114	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 7.

All (114) 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
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:B:217:GLY:N	1:E:263:THR:HG1	1.76	0.84
1:A:221:GLU:HG2	1:C:231:ARG:NH2	1.94	0.82
1:A:248:GLU:HG2	1:C:220:MET:HB2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	0.72
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:B:237:ASN:ND2	2:B:401:API:H2	2.09	0.68
1:E:278:LEU:HD12	3:E:427:HOH:O	1.94	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:G:273:THR:OG1	2:G:401:API:H31	1.98	0.63
1:H:231:ARG:HB2	3:H:620:HOH:O	1.99	0.62
1:B:237:ASN:HD21	2:B:401:API:H2	1.65	0.62
1:C:222:LEU:C	1:C:222:LEU:HD12	2.20	0.62
1:A:220:MET:HE1	1:C:252:VAL:HG23	1.82	0.61
1:B:225:ASP:OD1	1:B:338:SER:OG	2.18	0.61
1:A:219:HIS:CD2	1:C:245:TYR:HE1	2.19	0.61
1:A:219:HIS:HB2	1:C:248:GLU:OE1	1.99	0.61
1:G:229:GLU:OE1	3:G:486:HOH:O	2.16	0.60
1:F:218:SER:CB	3:F:211:HOH:O	2.47	0.60
1:C:243:ASP:HA	1:C:246:LYS:HD3	1.84	0.59
1:A:221:GLU:HG2	1:C:231:ARG:HH22	1.67	0.59
1:A:219:HIS:HB3	1:C:231:ARG:O	2.03	0.59
1:A:221:GLU:CG	1:C:231:ARG:NH2	2.64	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:A:228:MET:HE1	1:A:255:LYS:HB2	1.86	0.56
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
1:C:231:ARG:HG2	1:C:332:PHE:CD1	2.41	0.54
1:F:243:ASP:HA	1:F:246:LYS:HD2	1.88	0.54
1:D:276:ARG:CD	1:D:280:GLU:OE2	2.50	0.54
1:A:222:LEU:HD13	1:C:228:MET:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:274:GLY:HA3	2:G:401:API:HN22	1.73	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:H:229:GLU:CD	1:H:332:PHE:CE1	2.80	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:F:240:ASN:ND2	1:F:240:ASN:H	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:G:332:PHE:CD1	3:G:415:HOH:O	2.54	0.51
1:A:231:ARG:HH11	1:C:219:HIS:HB3	1.73	0.49
1:C:236:THR:CG2	2:C:401:API:H32	2.43	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:E:231:ARG:HH22	1:H:221:GLU:CD	2.16	0.47
1:D:270:THR:HG23	1:D:283:SER:HB3	1.96	0.47
1:E:319:ASN:ND2	1:E:328:ASN:HD22	2.13	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: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
1:H:319:ASN:ND2	1:H:328:ASN:HD22	2.15	0.45
1:F:280:GLU:HG2	3:F:596:HOH:O	2.16	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:F:319:ASN:ND2	1:F:328:ASN:HD22	2.15	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:G:274:GLY:CA	2:G:401:API:HN22	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:322:LYS:HG2	1:E:325:ARG:NH2	2.35	0.42
1:A:243:ASP:HA	1:A:246:LYS:HE2	2.01	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:A:231:ARG:NE	3:A:358:HOH:O	2.30	0.41
1:H:220:MET:HE3	1:H:220:MET:C	2.41	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:B:237:ASN:ND2	2:B:401:API:C2	2.80	0.41
1:F:218:SER:HB2	3:F:211:HOH:O	2.16	0.41
1:A:259:TYR:CE1	1:A:339:ARG:HG2	2.56	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:H:237:ASN:HD22	1:H:237:ASN:HA	1.69	0.40
1:A:221:GLU:CD	1:C:231:ARG:HH22	2.25	0.40
1:H:273:THR:OG1	2:H:401:API:H31	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	105/105 (100%)	105 (100%)	0	100	100
1	B	105/105 (100%)	103 (98%)	2 (2%)	65	52
1	C	104/105 (99%)	101 (97%)	3 (3%)	50	34
1	D	104/105 (99%)	102 (98%)	2 (2%)	65	52
1	E	103/105 (98%)	103 (100%)	0	100	100
1	F	105/105 (100%)	102 (97%)	3 (3%)	50	34
1	G	105/105 (100%)	104 (99%)	1 (1%)	82	77
1	H	104/105 (99%)	100 (96%)	4 (4%)	40	22
All	All	835/840 (99%)	820 (98%)	15 (2%)	66	54

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	221	GLU
1	B	246	LYS
1	C	219	HIS
1	C	229	GLU
1	C	323	GLU

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Mol	Chain	Res	Type
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	222	LEU
1	H	237	ASN
1	H	248	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	HIS
1	A	314	GLN
1	A	319	ASN
1	B	319	ASN
1	C	237	ASN
1	C	308	GLN
1	C	314	GLN
1	D	288	ASN
1	D	308	GLN
1	D	314	GLN
1	D	319	ASN
1	E	237	ASN
1	E	319	ASN
1	F	240	ASN
1	F	319	ASN
1	G	308	GLN
1	G	319	ASN
1	H	219	HIS
1	H	237	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 (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates 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	A	401	-	6,12,12	0.68	0	3,15,15	0.95	0
2	API	B	401	-	6,12,12	0.54	0	3,15,15	0.53	0
2	API	C	401	-	6,12,12	0.69	0	3,15,15	0.88	0
2	API	D	401	-	6,12,12	0.55	0	3,15,15	0.54	0
2	API	E	401	-	6,12,12	0.61	0	3,15,15	2.07	1 (33%)
2	API	F	401	-	6,12,12	0.54	0	3,15,15	1.51	0
2	API	G	401	-	6,12,12	0.74	0	3,15,15	2.72	1 (33%)
2	API	H	401	-	6,12,12	0.63	0	3,15,15	3.51	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	API	A	401	-	-	0/6/14/14	0/0/0/0
2	API	B	401	-	-	0/6/14/14	0/0/0/0
2	API	C	401	-	-	0/6/14/14	0/0/0/0
2	API	D	401	-	-	0/6/14/14	0/0/0/0
2	API	E	401	-	-	0/6/14/14	0/0/0/0
2	API	F	401	-	-	0/6/14/14	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	API	G	401	-	-	0/6/14/14	0/0/0/0
2	API	H	401	-	-	0/6/14/14	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	API	C3-C2-N2	-2.80	102.58	110.52
2	G	401	API	C3-C2-N2	4.55	123.46	110.52
2	H	401	API	C3-C2-N2	5.88	127.23	110.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	API	3	0
2	C	401	API	1	0
2	G	401	API	3	0
2	H	401	API	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	122/123 (99%)	-0.26	0 100 100	7, 13, 28, 36	0
1	B	123/123 (100%)	-0.36	0 100 100	9, 16, 26, 35	0
1	C	121/123 (98%)	-0.29	2 (1%) 73 69	9, 15, 29, 43	0
1	D	121/123 (98%)	-0.21	0 100 100	11, 19, 30, 39	0
1	E	120/123 (97%)	-0.26	0 100 100	7, 15, 27, 31	0
1	F	122/123 (99%)	-0.35	0 100 100	8, 15, 24, 32	0
1	G	122/123 (99%)	-0.27	0 100 100	6, 14, 24, 36	0
1	H	121/123 (98%)	-0.29	0 100 100	6, 14, 26, 34	0
All	All	972/984 (98%)	-0.29	2 (0%) 95 93	6, 15, 28, 43	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	318	ASP	3.2
1	C	219	HIS	2.2

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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	API	G	401	13/13	0.94	0.14	5.37	9,13,41,44	0
2	API	C	401	13/13	0.93	0.14	5.03	14,18,41,43	0
2	API	F	401	13/13	0.93	0.13	3.61	8,14,46,47	0
2	API	A	401	13/13	0.93	0.12	3.27	6,14,40,43	0
2	API	H	401	13/13	0.93	0.12	2.22	6,14,39,40	0
2	API	B	401	13/13	0.95	0.12	2.06	13,17,42,47	0
2	API	E	401	13/13	0.94	0.14	2.01	11,15,38,39	0
2	API	D	401	13/13	0.95	0.12	1.46	15,19,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.