



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:39 AM UTC

PDB ID : 4G88 / pdb_00004g88
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 : 2012-07-22
Resolution : 1.70 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

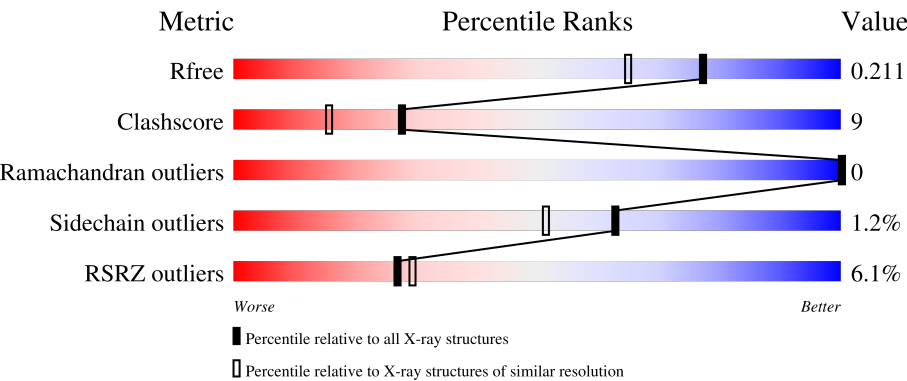
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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.



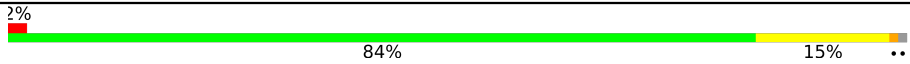
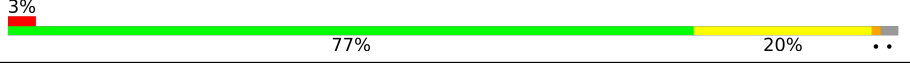
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	3% 78% 20% ..
1	B	123	2% 86% 13% .
1	C	123	17% 77% 18% ..
1	D	123	16% 71% 29%
1	E	123	2% 79% 19% .

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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
3	SRT	G	402	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8558 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	122	Total	C	N	O	S	0	0	0
			970	595	180	192	3			
1	C	120	Total	C	N	O	S	0	0	0
			954	586	176	189	3			
1	D	123	Total	C	N	O	S	0	0	0
			974	597	181	193	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	123	Total	C	N	O	S	0	0	0
			974	597	181	193	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:

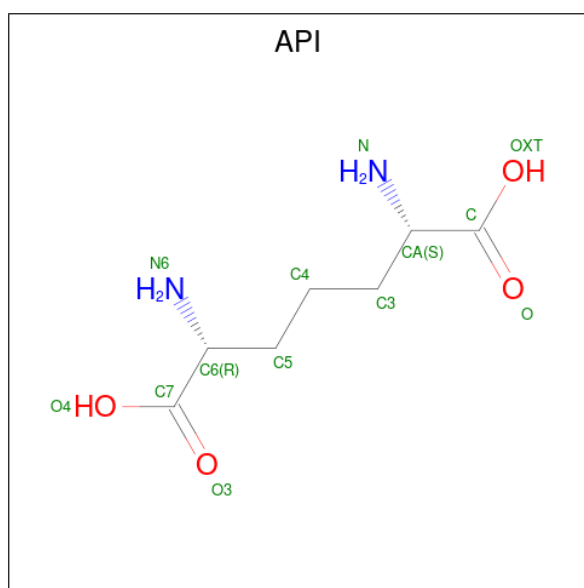
Chain	Residue	Modelled	Actual	Comment	Reference
A	217	GLY	-	expression tag	UNP Q6RYW5
A	218	SER	-	expression tag	UNP Q6RYW5
A	219	HIS	-	expression tag	UNP Q6RYW5
A	220	MET	-	expression tag	UNP Q6RYW5
B	217	GLY	-	expression tag	UNP Q6RYW5
B	218	SER	-	expression tag	UNP Q6RYW5
B	219	HIS	-	expression tag	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: $C_7H_{14}N_2O_4$).



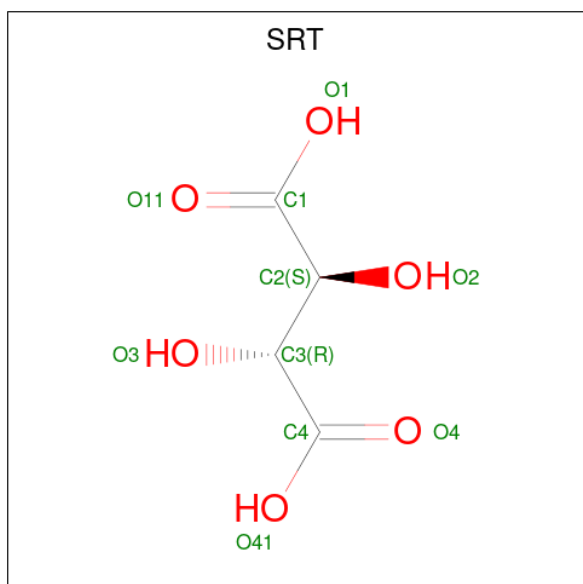
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	7	2	4		
2	B	1	Total	C	N	O	0	0
			13	7	2	4		

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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 S,R MESO-TARTARIC ACID (CCD ID: SRT) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			10	4	6		
3	G	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	111	Total	O	0	0
			111	111		

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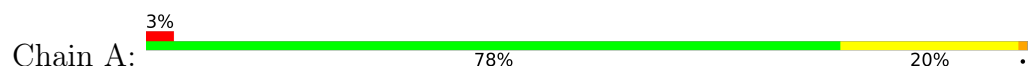
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	83	Total 83	O 83	0	0
4	C	54	Total 54	O 54	0	0
4	D	51	Total 51	O 51	0	0
4	E	83	Total 83	O 83	0	0
4	F	133	Total 133	O 133	0	0
4	G	115	Total 115	O 115	0	0
4	H	74	Total 74	O 74	0	0

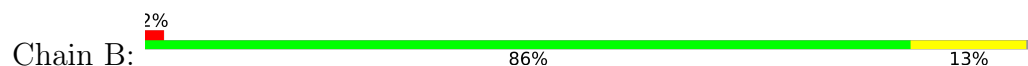
3 Residue-property plots [i](#)

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.

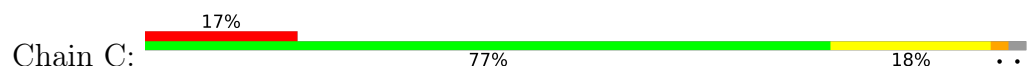
- Molecule 1: Outer membrane protein Omp38



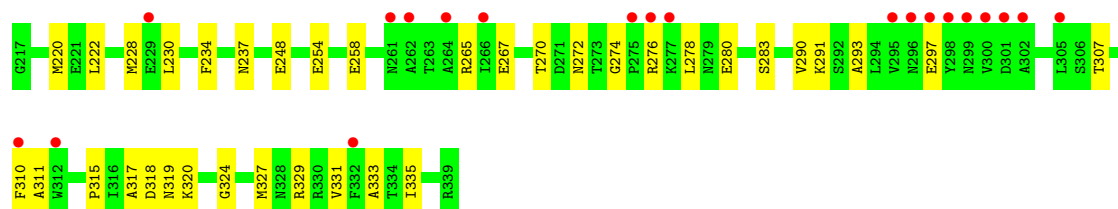
- Molecule 1: Outer membrane protein Omp38



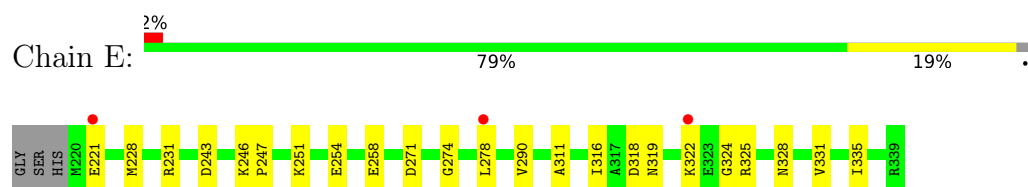
- Molecule 1: Outer membrane protein Omp38



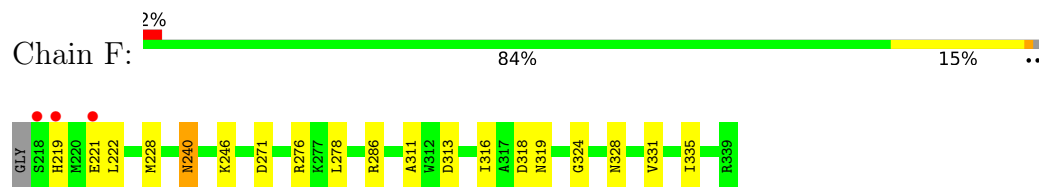
- Molecule 1: Outer membrane protein Omp38



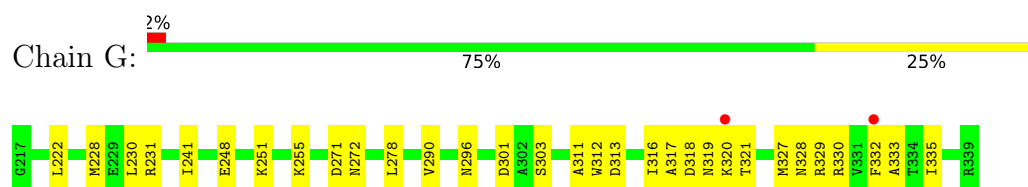
- Molecule 1: Outer membrane protein Omp38



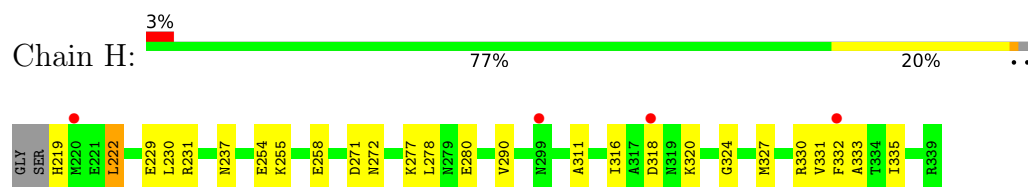
- Molecule 1: Outer membrane protein Omp38



- 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	58.52Å 99.30Å 98.12Å 90.00° 105.95° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70 50.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-1.70) 99.9 (50.00-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.234 0.211 , 0.211	Depositor DCC
R_{free} test set	5927 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.1	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	0.94	EDS
Total number of atoms	8558	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 4.97% 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: SRT, 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	0.35	0/984	0.91	5/1324 (0.4%)
1	B	0.33	0/984	0.89	4/1324 (0.3%)
1	C	0.33	0/967	0.84	0/1301
1	D	0.32	0/988	0.81	3/1329 (0.2%)
1	E	0.33	0/967	0.88	5/1301 (0.4%)
1	F	0.33	0/984	0.89	5/1324 (0.4%)
1	G	0.36	0/988	0.90	6/1329 (0.5%)
1	H	0.33	0/978	0.90	5/1316 (0.4%)
All	All	0.34	0/7840	0.88	33/10548 (0.3%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	271	ASP	N-CA-C	-6.75	101.03	110.35
1	H	316	ILE	N-CA-C	-6.70	106.60	113.10
1	G	271	ASP	N-CA-C	-6.58	101.26	110.35
1	F	271	ASP	N-CA-C	-6.26	101.71	110.35
1	B	271	ASP	N-CA-C	-5.94	102.15	110.35
1	H	272	ASN	N-CA-C	5.92	119.56	112.93
1	A	271	ASP	N-CA-C	-5.88	101.24	110.36
1	E	271	ASP	N-CA-C	-5.80	102.34	110.35
1	F	316	ILE	N-CA-C	-5.65	107.62	113.10
1	A	316	ILE	N-CA-C	-5.54	107.73	113.10
1	G	316	ILE	N-CA-C	-5.47	107.47	113.43
1	G	313	ASP	N-CA-C	5.41	119.14	112.54
1	A	313	ASP	N-CA-C	5.40	119.13	112.54
1	E	274	GLY	CA-C-N	5.39	125.30	119.85
1	E	274	GLY	C-N-CA	5.39	125.30	119.85
1	B	274	GLY	CA-C-N	5.38	125.32	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	GLY	C-N-CA	5.38	125.32	119.78
1	G	296	ASN	N-CA-C	5.37	118.30	111.69
1	G	272	ASN	N-CA-C	5.36	118.94	112.93
1	A	272	ASN	N-CA-C	5.33	118.91	112.93
1	F	311	ALA	CB-CA-C	-5.32	110.42	116.54
1	F	276	ARG	N-CA-C	5.28	117.46	111.02
1	H	280	GLU	N-CA-C	-5.26	105.46	111.14
1	E	316	ILE	N-CA-C	-5.25	108.01	113.10
1	F	313	ASP	N-CA-C	5.23	118.92	112.54
1	G	311	ALA	CB-CA-C	-5.23	110.53	116.54
1	D	311	ALA	CB-CA-C	-5.19	110.57	116.54
1	D	274	GLY	CA-C-N	5.19	125.10	119.76
1	D	274	GLY	C-N-CA	5.19	125.10	119.76
1	E	311	ALA	CB-CA-C	-5.17	110.59	116.54
1	A	280	GLU	N-CA-C	-5.10	105.64	111.14
1	B	311	ALA	CB-CA-C	-5.03	110.75	116.54
1	H	311	ALA	CB-CA-C	-5.03	110.76	116.54

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	23	0
1	B	970	0	957	11	0
1	C	954	0	945	29	0
1	D	974	0	960	29	0
1	E	954	0	945	17	0
1	F	970	0	957	12	0
1	G	974	0	960	25	0
1	H	964	0	952	20	0
2	A	13	0	7	0	0
2	B	13	0	7	0	0
2	C	13	0	7	4	0
2	D	13	0	7	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	D	10	0	4	1	0
3	G	10	0	4	2	0
4	A	111	0	0	1	0
4	B	83	0	0	0	0
4	C	54	0	0	1	0
4	D	51	0	0	1	0
4	E	83	0	0	1	0
4	F	133	0	0	1	0
4	G	115	0	0	2	0
4	H	74	0	0	1	0
All	All	8558	0	7697	140	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 (140) 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:E:221:GLU:HG2	1:H:231:ARG:HH22	1.46	0.80
1:E:221:GLU:HG3	1:H:231:ARG:HH12	1.49	0.74
1:F:246:LYS:HE3	4:F:630:HOH:O	1.88	0.73
1:C:323:GLU:H	1:C:323:GLU:CD	2.00	0.70
1:E:221:GLU:CG	1:H:231:ARG:HH12	2.08	0.67
1:C:318:ASP:OD2	1:C:320:LYS:HB2	1.94	0.67
1:A:219:HIS:HB2	1:C:248:GLU:OE1	1.97	0.65
1:B:318:ASP:OD2	1:B:320:LYS:HB2	1.97	0.64
1:A:220:MET:HE1	1:C:251:LYS:HG2	1.80	0.64
1:A:228:MET:HE1	1:A:255:LYS:HB2	1.79	0.63
1:F:240:ASN:HD22	1:F:240:ASN:H	1.47	0.62
1:C:236:THR:HG23	2:C:401:API:H51	1.82	0.61
1:H:318:ASP:OD1	1:H:320:LYS:HE2	2.00	0.61
1:C:228:MET:HB2	1:C:335:ILE:HB	1.81	0.61
1:D:228:MET:HB2	1:D:335:ILE:HB	1.82	0.61
1:C:276:ARG:O	1:C:280:GLU:HG3	2.01	0.61
1:G:329:ARG:HH22	3:G:402:SRT:H2	1.67	0.60
1:D:293:ALA:O	1:D:297:GLU:HB3	2.01	0.60
1:G:320:LYS:HG3	1:G:321:THR:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:318:ASP:CG	1:G:320:LYS:HG2	2.27	0.58
1:H:330:ARG:HD2	1:H:332:PHE:CE1	2.38	0.58
1:C:330:ARG:HD2	1:C:332:PHE:CE1	2.39	0.58
1:G:228:MET:HB2	1:G:335:ILE:HB	1.86	0.57
1:D:317:ALA:HB2	1:D:327:MET:HE3	1.86	0.57
1:G:330:ARG:HD2	1:G:332:PHE:CE2	2.39	0.57
1:C:222:LEU:C	1:C:222:LEU:HD22	2.28	0.57
1:C:318:ASP:OD1	1:C:320:LYS:HE2	2.05	0.56
1:C:321:THR:HB	1:C:323:GLU:OE2	2.04	0.56
1:F:228:MET:HE3	1:G:222:LEU:HD22	1.88	0.56
1:D:254:GLU:O	1:D:258:GLU:HG3	2.05	0.56
1:A:220:MET:HE1	1:C:251:LYS:CG	2.36	0.55
1:E:221:GLU:HG2	1:H:231:ARG:NH2	2.18	0.55
1:E:319:ASN:ND2	1:E:328:ASN:HD22	2.05	0.55
1:A:221:GLU:CG	1:C:231:ARG:HH22	2.20	0.55
1:A:254:GLU:O	1:A:258:GLU:HG3	2.07	0.55
1:H:222:LEU:HD22	1:H:222:LEU:C	2.31	0.54
1:E:228:MET:HB2	1:E:335:ILE:HB	1.90	0.54
1:E:247:PRO:O	1:E:251:LYS:HG3	2.08	0.54
1:G:251:LYS:HE3	1:G:255:LYS:HE2	1.89	0.54
1:G:319:ASN:ND2	1:G:328:ASN:HD22	2.06	0.53
1:D:276:ARG:O	1:D:280:GLU:HG3	2.08	0.53
1:G:317:ALA:CB	1:G:327:MET:HE3	2.39	0.53
1:B:335:ILE:N	1:B:335:ILE:HD12	2.24	0.52
1:D:278:LEU:C	1:D:278:LEU:HD23	2.34	0.52
1:G:278:LEU:C	1:G:278:LEU:HD23	2.35	0.52
1:F:222:LEU:HD13	1:G:228:MET:HG2	1.90	0.52
1:C:299:ASN:CG	1:C:299:ASN:O	2.54	0.51
1:C:335:ILE:HD12	1:C:335:ILE:N	2.26	0.51
1:D:329:ARG:HH22	3:D:402:SRT:H2	1.74	0.51
1:A:319:ASN:ND2	1:A:328:ASN:HD22	2.09	0.51
1:G:241:ILE:HD11	1:G:290:VAL:HA	1.92	0.51
1:G:317:ALA:HB2	1:G:327:MET:HE3	1.93	0.50
1:G:301:ASP:OD2	1:G:303:SER:OG	2.27	0.50
1:B:228:MET:HB2	1:B:335:ILE:HB	1.92	0.50
1:H:254:GLU:O	1:H:258:GLU:HG3	2.11	0.50
1:A:228:MET:HE1	1:A:255:LYS:CB	2.42	0.49
1:D:335:ILE:HD12	1:D:335:ILE:N	2.26	0.49
1:H:335:ILE:HD12	1:H:335:ILE:N	2.27	0.49
1:G:335:ILE:HD12	1:G:335:ILE:N	2.28	0.49
1:E:335:ILE:HD12	1:E:335:ILE:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:318:ASP:O	1:H:324:GLY:HA3	2.13	0.49
1:D:265:ARG:HH21	1:D:265:ARG:HG3	1.78	0.48
1:H:278:LEU:C	1:H:278:LEU:HD23	2.39	0.48
1:G:329:ARG:NH2	3:G:402:SRT:H2	2.27	0.48
1:A:244:GLN:HB3	4:A:603:HOH:O	2.13	0.48
1:A:278:LEU:HD23	1:A:278:LEU:C	2.37	0.48
1:A:221:GLU:HG3	1:C:231:ARG:HH22	1.79	0.48
1:D:318:ASP:O	1:D:324:GLY:HA3	2.14	0.48
1:F:335:ILE:N	1:F:335:ILE:HD12	2.29	0.48
1:A:219:HIS:HB2	1:C:248:GLU:CD	2.38	0.47
1:D:291:LYS:HD2	1:D:307:THR:HG23	1.96	0.47
1:A:330:ARG:HD2	1:A:332:PHE:CE1	2.50	0.47
1:B:228:MET:HG2	1:D:222:LEU:HB2	1.96	0.47
1:A:318:ASP:CG	1:A:320:LYS:HZ2	2.22	0.47
1:D:272:ASN:H	1:D:319:ASN:ND2	2.13	0.47
1:B:219:HIS:HB2	1:D:248:GLU:OE2	2.15	0.47
1:D:267:GLU:HB3	1:D:310:PHE:HE2	1.80	0.46
1:D:276:ARG:O	1:D:276:ARG:HD3	2.16	0.46
1:D:317:ALA:CB	1:D:327:MET:HE3	2.45	0.46
1:F:278:LEU:C	1:F:278:LEU:HD23	2.40	0.46
1:E:290:VAL:HG21	1:E:331:VAL:HG11	1.97	0.46
1:G:255:LYS:HA	1:G:255:LYS:HD3	1.79	0.46
1:B:318:ASP:O	1:B:324:GLY:HA3	2.15	0.46
1:H:277:LYS:HE3	4:H:535:HOH:O	2.15	0.46
1:C:290:VAL:HG21	1:C:331:VAL:HG11	1.97	0.46
1:H:290:VAL:HG21	1:H:331:VAL:HG11	1.98	0.46
1:H:229:GLU:OE1	1:H:231:ARG:NH1	2.49	0.45
1:D:290:VAL:HG21	1:D:331:VAL:HG11	1.97	0.45
1:D:315:PRO:HB3	4:D:520:HOH:O	2.15	0.45
1:D:318:ASP:CG	1:D:320:LYS:HZ1	2.23	0.45
1:C:301:ASP:OD2	1:C:303:SER:OG	2.27	0.45
1:B:251:LYS:HG2	1:D:220:MET:HE1	1.99	0.45
1:D:234:PHE:CE2	1:D:331:VAL:HG23	2.51	0.45
1:C:220:MET:N	4:C:547:HOH:O	2.50	0.45
1:D:318:ASP:OD1	1:D:320:LYS:HB2	2.16	0.45
1:A:335:ILE:HD12	1:A:335:ILE:N	2.32	0.45
1:H:327:MET:HA	1:H:327:MET:HE2	1.98	0.45
1:E:322:LYS:HD2	1:E:325:ARG:HH21	1.82	0.44
1:B:220:MET:HB2	1:D:248:GLU:HG2	1.98	0.44
1:C:270:THR:HB	2:C:401:API:O3	2.17	0.44
1:E:278:LEU:HD11	4:E:579:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:HIS:HB2	1:G:248:GLU:OE1	2.17	0.44
1:A:222:LEU:HD13	1:C:228:MET:HG2	1.98	0.44
1:B:228:MET:HG2	1:D:222:LEU:CB	2.47	0.44
1:E:228:MET:HG2	1:H:222:LEU:HB2	2.00	0.44
1:B:290:VAL:HG21	1:B:331:VAL:HG11	2.00	0.44
1:C:318:ASP:O	1:C:324:GLY:HA3	2.17	0.44
1:D:276:ARG:HD2	1:D:280:GLU:OE2	2.16	0.44
1:F:221:GLU:HG3	1:G:231:ARG:HH22	1.82	0.43
1:G:251:LYS:HE3	1:G:255:LYS:CE	2.48	0.43
1:D:230:LEU:HB3	1:D:333:ALA:HB3	1.99	0.43
1:C:279:ASN:OD1	2:C:401:API:N6	2.52	0.42
1:A:220:MET:SD	1:C:248:GLU:HG2	2.60	0.42
1:G:248:GLU:HG3	4:G:520:HOH:O	2.19	0.42
1:H:255:LYS:HD3	1:H:258:GLU:OE1	2.20	0.42
1:A:247:PRO:O	1:A:251:LYS:HG3	2.20	0.42
1:C:221:GLU:O	1:C:221:GLU:HG3	2.19	0.42
1:A:221:GLU:HG2	1:C:231:ARG:HH12	1.84	0.42
1:D:270:THR:HG23	1:D:283:SER:HB3	2.02	0.42
1:E:318:ASP:O	1:E:324:GLY:HA3	2.20	0.41
1:G:312:TRP:CD1	1:G:312:TRP:C	2.98	0.41
1:A:219:HIS:HB3	1:C:231:ARG:O	2.20	0.41
1:D:270:THR:HB	2:D:401:API:O4	2.20	0.41
1:E:243:ASP:HA	1:E:246:LYS:HG2	2.02	0.41
1:F:219:HIS:HB3	1:G:231:ARG:O	2.20	0.41
1:H:230:LEU:HB3	1:H:333:ALA:HB3	2.03	0.41
1:F:318:ASP:O	1:F:324:GLY:HA3	2.21	0.41
1:F:319:ASN:ND2	1:F:328:ASN:HD22	2.18	0.41
1:A:228:MET:HB3	1:A:335:ILE:HB	2.02	0.41
1:A:264:ALA:HB2	1:A:335:ILE:HG13	2.02	0.41
1:F:286:ARG:HB3	1:F:331:VAL:HG23	2.03	0.41
1:G:230:LEU:HB3	1:G:333:ALA:HB3	2.03	0.41
1:H:255:LYS:HD3	1:H:255:LYS:HA	1.89	0.41
1:E:231:ARG:O	1:H:219:HIS:HB3	2.21	0.40
1:E:254:GLU:O	1:E:258:GLU:HG3	2.21	0.40
1:C:236:THR:CG2	2:C:401:API:H51	2.51	0.40
1:G:255:LYS:NZ	4:G:589:HOH:O	2.53	0.40
1:A:246:LYS:HB2	1:A:247:PRO:HD3	2.03	0.40
1:E:246:LYS:HB2	1:E:247:PRO:HD3	2.04	0.40
1:B:312:TRP:C	1:B:312:TRP:CD1	2.99	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%)	118 (98%)	2 (2%)	0	100	100
1	B	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
1	C	118/123 (96%)	116 (98%)	2 (2%)	0	100	100
1	D	121/123 (98%)	118 (98%)	3 (2%)	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	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
1	H	119/123 (97%)	118 (99%)	1 (1%)	0	100	100
All	All	957/984 (97%)	945 (99%)	12 (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	58
1	B	105/105 (100%)	103 (98%)	2 (2%)	50	34
1	C	103/105 (98%)	100 (97%)	3 (3%)	37	20
1	D	105/105 (100%)	104 (99%)	1 (1%)	68	58
1	E	103/105 (98%)	103 (100%)	0	100	100
1	F	105/105 (100%)	104 (99%)	1 (1%)	68	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	105/105 (100%)	105 (100%)	0	100	100
1	H	104/105 (99%)	102 (98%)	2 (2%)	50	34
All	All	835/840 (99%)	825 (99%)	10 (1%)	63	51

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

Mol	Chain	Res	Type
1	A	244	GLN
1	B	221	GLU
1	B	237	ASN
1	C	221	GLU
1	C	222	LEU
1	C	323	GLU
1	D	237	ASN
1	F	240	ASN
1	H	222	LEU
1	H	237	ASN

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	219	HIS
1	A	227	ASN
1	A	244	GLN
1	A	296	ASN
1	A	319	ASN
1	B	237	ASN
1	B	314	GLN
1	B	319	ASN
1	C	244	GLN
1	C	296	ASN
1	C	308	GLN
1	C	314	GLN
1	D	237	ASN
1	D	244	GLN
1	D	288	ASN
1	D	296	ASN
1	D	308	GLN
1	D	314	GLN
1	D	319	ASN

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Mol	Chain	Res	Type
1	E	299	ASN
1	E	319	ASN
1	F	240	ASN
1	F	296	ASN
1	F	319	ASN
1	G	319	ASN
1	H	219	HIS
1	H	237	ASN
1	H	299	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](#)

10 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	1.85	4 (40%)	9,15,15	1.08	1 (11%)
2	API	A	401	-	10,12,12	1.45	2 (20%)	9,15,15	1.22	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	API	G	401	-	10,12,12	0.60	0	9,15,15	1.08	1 (11%)
2	API	E	401	-	10,12,12	1.35	2 (20%)	9,15,15	1.23	2 (22%)
2	API	F	401	-	10,12,12	0.66	0	9,15,15	1.15	1 (11%)
3	SRT	D	402	-	9,9,9	1.19	0	12,12,12	1.89	1 (8%)
2	API	C	401	-	10,12,12	1.33	2 (20%)	9,15,15	1.19	0
2	API	H	401	-	10,12,12	1.43	2 (20%)	9,15,15	1.06	1 (11%)
3	SRT	G	402	-	9,9,9	1.04	0	12,12,12	2.68	5 (41%)
2	API	B	401	-	10,12,12	1.89	4 (40%)	9,15,15	1.04	1 (11%)

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	-	-	2/14/14/14	-
2	API	A	401	-	-	0/14/14/14	-
2	API	G	401	-	-	0/14/14/14	-
2	API	E	401	-	-	2/14/14/14	-
2	API	F	401	-	-	0/14/14/14	-
3	SRT	D	402	-	-	9/12/12/12	-
2	API	C	401	-	-	2/14/14/14	-
2	API	H	401	-	-	2/14/14/14	-
3	SRT	G	402	-	-	9/12/12/12	-
2	API	B	401	-	-	2/14/14/14	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	API	O3-C7	3.23	1.31	1.22
2	A	401	API	O-C	3.03	1.31	1.22
2	H	401	API	O3-C7	2.97	1.30	1.22
2	C	401	API	O-C	2.95	1.30	1.22
2	H	401	API	O4-C7	-2.92	1.21	1.30
2	B	401	API	O-C	2.92	1.30	1.22
2	D	401	API	O-C	2.91	1.30	1.22
2	A	401	API	OXT-C	-2.91	1.21	1.30
2	E	401	API	O3-C7	2.87	1.30	1.22
2	D	401	API	O3-C7	2.83	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	API	OXT-C	-2.78	1.21	1.30
2	D	401	API	OXT-C	-2.75	1.21	1.30
2	C	401	API	OXT-C	-2.69	1.22	1.30
2	D	401	API	O4-C7	-2.67	1.22	1.30
2	B	401	API	O4-C7	-2.65	1.22	1.30
2	E	401	API	O4-C7	-2.64	1.22	1.30

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	402	SRT	O3-C3-C2	-6.83	96.26	110.17
3	D	402	SRT	O3-C3-C2	-5.36	99.25	110.17
3	G	402	SRT	O2-C2-C3	3.71	117.71	110.17
2	E	401	API	C5-C6-N6	2.83	117.51	110.12
3	G	402	SRT	O1-C1-C2	2.64	120.64	113.31
2	D	401	API	C5-C6-N6	2.60	116.89	110.12
3	G	402	SRT	O2-C2-C1	2.39	115.81	110.69
2	H	401	API	C5-C6-N6	2.39	116.34	110.12
2	A	401	API	C5-C6-N6	2.35	116.26	110.12
2	F	401	API	C3-CA-N	2.30	116.10	110.12
2	A	401	API	C3-CA-N	2.28	116.06	110.12
2	E	401	API	C3-CA-N	2.18	115.81	110.12
2	G	401	API	C5-C6-N6	2.09	115.56	110.12
3	G	402	SRT	O41-C4-C3	2.04	118.99	113.31
2	B	401	API	C3-CA-N	2.01	115.36	110.12

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	402	SRT	O1-C1-C2-C3
3	D	402	SRT	O11-C1-C2-C3
3	D	402	SRT	C1-C2-C3-O3
3	D	402	SRT	O2-C2-C3-O3
3	G	402	SRT	C1-C2-C3-O3
3	G	402	SRT	O2-C2-C3-O3
3	G	402	SRT	O1-C1-C2-O2
3	G	402	SRT	O11-C1-C2-O2
3	G	402	SRT	O1-C1-C2-C3
3	G	402	SRT	O11-C1-C2-C3
3	D	402	SRT	O2-C2-C3-C4
3	D	402	SRT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	G	402	SRT	O2-C2-C3-C4
3	D	402	SRT	O1-C1-C2-O2
3	D	402	SRT	O11-C1-C2-O2
3	G	402	SRT	C1-C2-C3-C4
2	B	401	API	C5-C6-C7-O3
2	H	401	API	C5-C6-C7-O4
2	D	401	API	C5-C6-C7-O3
2	E	401	API	C5-C6-C7-O3
2	E	401	API	C5-C6-C7-O4
2	H	401	API	C5-C6-C7-O3
2	D	401	API	C5-C6-C7-O4
2	C	401	API	C5-C6-C7-O4
2	B	401	API	C5-C6-C7-O4
2	C	401	API	C5-C6-C7-O3
3	D	402	SRT	C2-C3-C4-O4
3	G	402	SRT	C2-C3-C4-O4

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	API	1	0
3	D	402	SRT	1	0
2	C	401	API	4	0
3	G	402	SRT	2	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	122/123 (99%)	-0.06	4 (3%)	49	53	6, 12, 28, 36	0
1	B	122/123 (99%)	0.17	2 (1%)	70	75	10, 16, 27, 34	0
1	C	120/123 (97%)	0.76	21 (17%)	4	3	10, 19, 43, 52	0
1	D	123/123 (100%)	1.12	20 (16%)	4	4	13, 23, 34, 42	0
1	E	120/123 (97%)	0.19	3 (2%)	58	62	9, 15, 26, 30	0
1	F	122/123 (99%)	-0.16	3 (2%)	58	62	6, 12, 22, 33	0
1	G	123/123 (100%)	-0.12	2 (1%)	70	75	6, 12, 19, 25	0
1	H	121/123 (98%)	0.19	4 (3%)	49	53	8, 15, 27, 36	0
All	All	973/984 (98%)	0.26	59 (6%)	27	29	6, 15, 31, 52	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	300	VAL	4.8
1	C	315	PRO	4.1
1	A	219	HIS	4.1
1	D	332	PHE	3.8
1	D	302	ALA	3.7
1	D	299	ASN	3.5
1	F	219	HIS	3.5
1	C	322	LYS	3.4
1	C	274	GLY	3.4
1	C	321	THR	3.4
1	C	316	ILE	3.3
1	C	317	ALA	3.2
1	D	298	TYR	3.2
1	C	312	TRP	3.2
1	C	318	ASP	3.2
1	H	318	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	244	GLN	3.0
1	C	327	MET	3.0
1	C	324	GLY	3.0
1	D	301	ASP	2.9
1	G	332	PHE	2.9
1	D	296	ASN	2.9
1	D	264	ALA	2.8
1	D	305	LEU	2.8
1	H	332	PHE	2.7
1	E	278	LEU	2.7
1	A	218	SER	2.7
1	D	277	LYS	2.7
1	D	297	GLU	2.7
1	C	273	THR	2.7
1	D	262	ALA	2.7
1	E	221	GLU	2.6
1	G	320	LYS	2.6
1	C	320	LYS	2.5
1	D	295	VAL	2.5
1	C	220	MET	2.5
1	F	218	SER	2.5
1	D	261	ASN	2.4
1	D	266	ILE	2.4
1	C	328	ASN	2.4
1	B	218	SER	2.3
1	E	322	LYS	2.3
1	D	275	PRO	2.3
1	C	275	PRO	2.2
1	C	325	ARG	2.2
1	D	310	PHE	2.2
1	C	319	ASN	2.1
1	A	220	MET	2.1
1	C	271	ASP	2.1
1	D	229	GLU	2.1
1	B	320	LYS	2.1
1	D	312	TRP	2.1
1	H	220	MET	2.1
1	C	313	ASP	2.1
1	C	278	LEU	2.1
1	D	276	ARG	2.1
1	C	332	PHE	2.1
1	F	221	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	299	ASN	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
2	API	C	401	13/13	0.79	0.17	25,33,43,44	0
3	SRT	D	402	10/10	0.80	0.14	31,33,35,36	0
3	SRT	G	402	10/10	0.87	0.11	19,24,25,25	0
2	API	D	401	13/13	0.89	0.12	18,22,32,32	0
2	API	B	401	13/13	0.92	0.10	16,20,27,27	0
2	API	E	401	13/13	0.93	0.09	14,19,28,29	0
2	API	F	401	13/13	0.94	0.10	10,15,27,28	0
2	API	H	401	13/13	0.94	0.09	11,16,29,29	0
2	API	G	401	13/13	0.96	0.07	7,11,20,22	0
2	API	A	401	13/13	0.96	0.07	8,13,18,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.