



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 01:24 AM EDT

PDB ID : 4G88  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

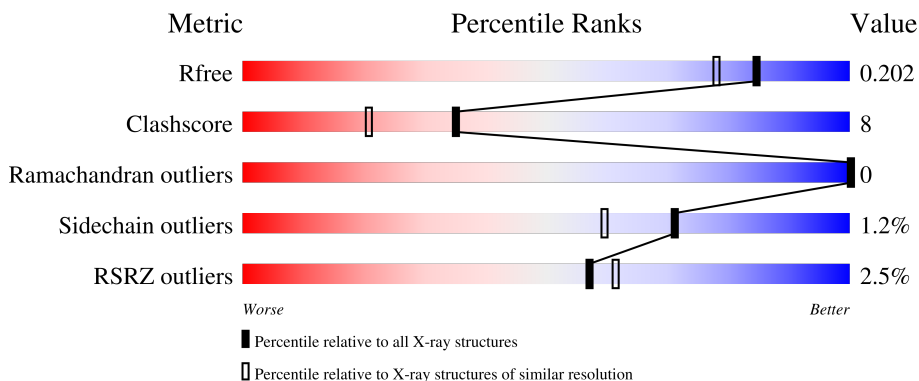
# 1 Overall quality at a glance i

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))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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  $\geq 3$ , 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	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">2% 82% 16% ..</p>
1	B	123	<div style="display: flex; align-items: center;"> <div style="width: 90%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">90% 9% .</p>
1	C	123	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">11% 80% 16% ..</p>
1	D	123	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">2% 75% 24% .</p>
1	E	123	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">2% 82% 15% .</p>

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Mol	Chain	Length	Quality of chain
1	F	123	<p>% 89% 10% ..</p>
1	G	123	<p>% 83% 17%</p>
1	H	123	<p>2% 82% 15% ..</p>

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
			Total	C	N	O	S			
1	A	122	970	595	180	192	3	0	0	0
1	B	122	970	595	180	192	3	0	0	0
1	C	120	954	586	176	189	3	0	0	0
1	D	123	974	597	181	193	3	0	0	0
1	E	120	954	586	176	189	3	0	0	0
1	F	122	970	595	180	192	3	0	0	0
1	G	123	974	597	181	193	3	0	0	0
1	H	121	964	592	179	190	3	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

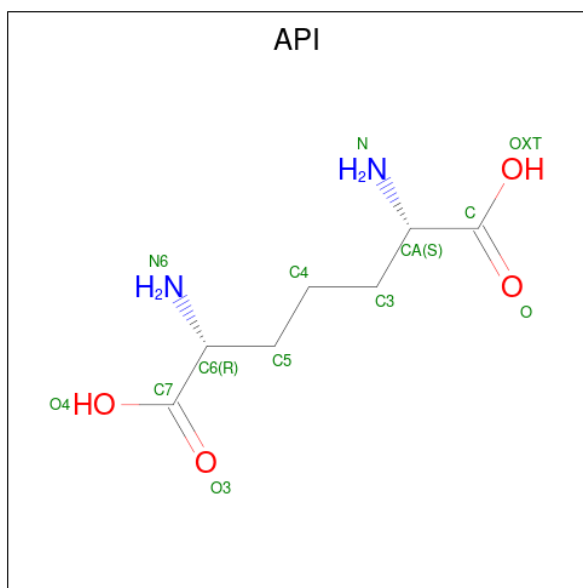
Chain	Residue	Modelled	Actual	Comment	Reference
A	217	GLY	-	expression tag	UNP Q6RYW5
A	218	SER	-	expression tag	UNP Q6RYW5
A	219	HIS	-	expression tag	UNP Q6RYW5
A	220	MET	-	expression tag	UNP Q6RYW5
B	217	GLY	-	expression tag	UNP Q6RYW5
B	218	SER	-	expression tag	UNP Q6RYW5
B	219	HIS	-	expression tag	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<sub>7</sub>H<sub>14</sub>N<sub>2</sub>O<sub>4</sub>).



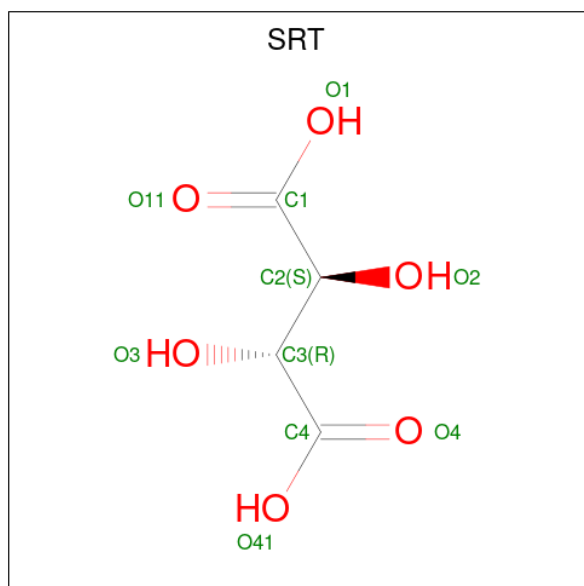
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	13	7	2	4	0	0
2	B	1	13	7	2	4	0	0

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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 (three-letter code: SRT) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



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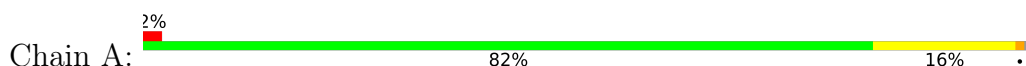
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	83	Total 83	O 83	0	0
4	C	54	Total 54	O 54	0	0
4	D	51	Total 51	O 51	0	0
4	E	83	Total 83	O 83	0	0
4	F	133	Total 133	O 133	0	0
4	G	115	Total 115	O 115	0	0
4	H	74	Total 74	O 74	0	0

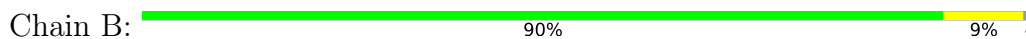
### 3 Residue-property plots [i](#)

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.

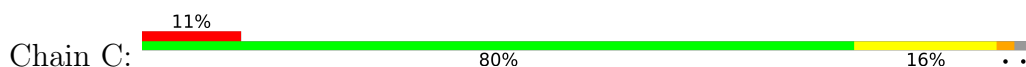
- Molecule 1: Outer membrane protein Omp38



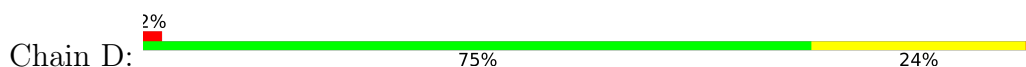
- Molecule 1: Outer membrane protein Omp38



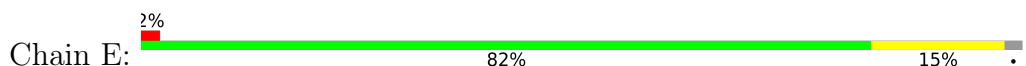
- Molecule 1: Outer membrane protein Omp38



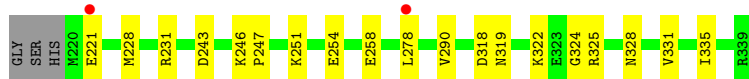
- Molecule 1: Outer membrane protein Omp38



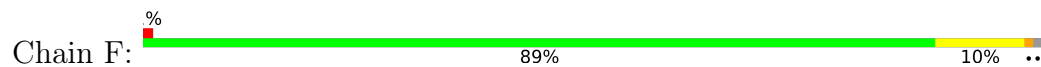
- Molecule 1: Outer membrane protein Omp38



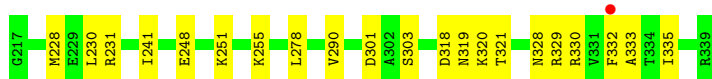
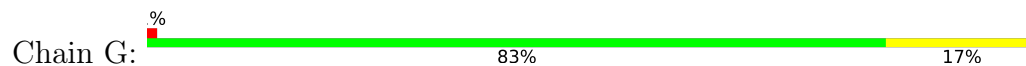




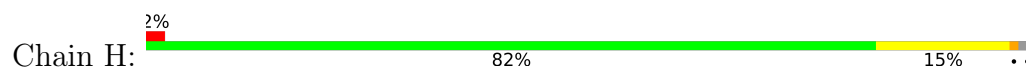
- Molecule 1: Outer membrane protein Omp38



- Molecule 1: Outer membrane protein Omp38



- Molecule 1: Outer membrane protein Omp38



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.52Å 99.30Å 98.12Å 90.00° 105.95° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70 43.37 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-1.70) 99.9 (43.37-1.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 1.70Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.210 , 0.234 0.205 , 0.202	Depositor DCC
$R_{free}$ test set	5927 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.6	Xtrriage
Anisotropy	0.330	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8558	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.31	0/984	0.61	0/1324
1	B	0.29	0/984	0.59	0/1324
1	C	0.29	0/967	0.58	0/1301
1	D	0.28	0/988	0.53	0/1329
1	E	0.30	0/967	0.59	0/1301
1	F	0.29	0/984	0.61	0/1324
1	G	0.32	0/988	0.61	0/1329
1	H	0.29	0/978	0.60	0/1316
All	All	0.30	0/7840	0.59	0/10548

There are no bond length outliers.

There are no bond angle outliers.

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	20	0
1	B	970	0	957	9	0
1	C	954	0	945	26	0
1	D	974	0	960	26	0
1	E	954	0	945	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	970	0	957	11	0
1	G	974	0	960	21	0
1	H	964	0	952	19	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
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	127	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 (127) 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: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:C:323:GLU:H	1:C:323:GLU:CD	2.00	0.65
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:330:ARG:HD2	1:G:332:PHE:CE2	2.39	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:D:254:GLU:O	1:D:258:GLU:HG3	2.05	0.56
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: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:318:ASP:CG	1:G:320:LYS:HG2	2.27	0.54
1:G:319:ASN:ND2	1:G:328:ASN:HD22	2.06	0.53
1:C:222:LEU:C	1:C:222:LEU:HD22	2.28	0.53
1:D:276:ARG:O	1:D:280:GLU:HG3	2.08	0.53
1:B:335:ILE:N	1:B:335:ILE:HD12	2.24	0.52
1:F:222:LEU:HD13	1:G:228:MET:HG2	1.90	0.52
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: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:H:222:LEU:HD22	1:H:222:LEU:C	2.31	0.50
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLU:HG3	1:C:231:ARG:HH22	1.79	0.48
1:D:278:LEU:C	1:D:278:LEU:HD23	2.34	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:D:291:LYS:HD2	1:D:307:THR:HG23	1.96	0.47
1:G:278:LEU:C	1:G:278:LEU:HD23	2.35	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:D:272:ASN:H	1:D:319:ASN:ND2	2.13	0.47
1:C:299:ASN:CG	1:C:299:ASN:O	2.54	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: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:A:228:MET:HE1	1:A:255:LYS:HB2	1.97	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: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
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:H:278:LEU:C	1:H:278:LEU:HD23	2.39	0.44
1:A:278:LEU:HD23	1:A:278:LEU:C	2.37	0.43
1:F:221:GLU:HG3	1:G:231:ARG:HH22	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:HIS:HB2	1:C:248:GLU:CD	2.38	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:A:318:ASP:CG	1:A:320:LYS:HZ2	2.22	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:F:278:LEU:C	1:F:278:LEU:HD23	2.40	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:D:318:ASP:CG	1:D:320:LYS:HZ2	2.23	0.40
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

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%)	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 [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%)	104 (99%)	1 (1%)	76	67
1	B	105/105 (100%)	103 (98%)	2 (2%)	57	41
1	C	103/105 (98%)	101 (98%)	2 (2%)	57	41
1	D	105/105 (100%)	103 (98%)	2 (2%)	57	41
1	E	103/105 (98%)	103 (100%)	0	100	100
1	F	105/105 (100%)	104 (99%)	1 (1%)	76	67

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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%)	57	41
All	All	835/840 (99%)	825 (99%)	10 (1%)	71	59

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	D	222	LEU
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 (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	GLN
1	A	308	GLN
1	A	319	ASN
1	B	237	ASN
1	B	296	ASN
1	B	319	ASN
1	C	308	GLN
1	C	314	GLN
1	D	237	ASN
1	D	244	GLN
1	D	288	ASN
1	D	308	GLN
1	D	314	GLN
1	D	319	ASN
1	E	299	ASN
1	E	319	ASN
1	F	240	ASN
1	F	319	ASN
1	G	308	GLN

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Mol	Chain	Res	Type
1	G	319	ASN
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 monosaccharides 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	$\# Z  > 2$
3	SRT	G	402	-	9,9,9	1.02	0	12,12,12	2.74	5 (41%)
2	API	A	401	-	10,12,12	1.42	2 (20%)	13,15,15	1.44	4 (30%)
2	API	F	401	-	10,12,12	0.67	0	13,15,15	0.98	1 (7%)
2	API	E	401	-	10,12,12	1.32	2 (20%)	13,15,15	1.54	4 (30%)
2	API	C	401	-	10,12,12	1.30	2 (20%)	13,15,15	1.60	3 (23%)
2	API	G	401	-	10,12,12	0.61	0	13,15,15	0.94	1 (7%)
2	API	D	401	-	10,12,12	1.79	4 (40%)	13,15,15	1.86	5 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SRT	D	402	-	9,9,9	1.16	0	12,12,12	1.94	1 (8%)
2	API	H	401	-	10,12,12	1.39	2 (20%)	13,15,15	1.44	3 (23%)
2	API	B	401	-	10,12,12	1.83	4 (40%)	13,15,15	1.81	4 (30%)

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
3	SRT	G	402	-	-	9/12/12/12	-
2	API	A	401	-	-	0/14/14/14	-
2	API	F	401	-	-	0/14/14/14	-
2	API	E	401	-	-	2/14/14/14	-
2	API	C	401	-	-	2/14/14/14	-
2	API	G	401	-	-	0/14/14/14	-
2	API	D	401	-	-	2/14/14/14	-
3	SRT	D	402	-	-	10/12/12/12	-
2	API	H	401	-	-	2/14/14/14	-
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	3.12	1.31	1.22
2	A	401	API	O-C	2.93	1.31	1.22
2	H	401	API	O3-C7	2.87	1.30	1.22
2	C	401	API	O-C	2.86	1.30	1.22
2	B	401	API	O-C	2.82	1.30	1.22
2	H	401	API	O4-C7	-2.81	1.21	1.30
2	D	401	API	O-C	2.81	1.30	1.22
2	A	401	API	OXT-C	-2.80	1.21	1.30
2	E	401	API	O3-C7	2.78	1.30	1.22
2	D	401	API	O3-C7	2.74	1.30	1.22
2	B	401	API	OXT-C	-2.68	1.21	1.30
2	D	401	API	OXT-C	-2.64	1.21	1.30
2	C	401	API	OXT-C	-2.58	1.22	1.30
2	D	401	API	O4-C7	-2.57	1.22	1.30
2	B	401	API	O4-C7	-2.55	1.22	1.30
2	E	401	API	O4-C7	-2.54	1.22	1.30

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	402	SRT	O3-C3-C2	-7.03	96.26	110.23
3	D	402	SRT	O3-C3-C2	-5.53	99.25	110.23
3	G	402	SRT	O2-C2-C3	3.77	117.71	110.23
2	C	401	API	OXT-C-CA	3.28	124.56	113.38
2	D	401	API	O4-C7-C6	3.14	124.06	113.38
2	C	401	API	O-C-CA	-3.07	111.29	122.14
2	B	401	API	OXT-C-CA	3.02	123.66	113.38
2	D	401	API	OXT-C-CA	3.00	123.59	113.38
2	H	401	API	O4-C7-C6	2.99	123.57	113.38
2	E	401	API	O4-C7-C6	2.99	123.56	113.38
2	B	401	API	O-C-CA	-2.88	111.99	122.14
2	D	401	API	O3-C7-C6	-2.86	112.05	122.14
2	B	401	API	O4-C7-C6	2.85	123.09	113.38
2	E	401	API	O3-C7-C6	-2.82	112.18	122.14
2	D	401	API	O-C-CA	-2.81	112.24	122.14
2	E	401	API	C5-C6-N6	2.80	117.51	110.17
2	H	401	API	O3-C7-C6	-2.75	112.43	122.14
3	G	402	SRT	O1-C1-C2	2.73	120.64	113.27
2	B	401	API	O3-C7-C6	-2.70	112.60	122.14
2	A	401	API	OXT-C-CA	2.69	122.54	113.38
2	D	401	API	C5-C6-N6	2.56	116.89	110.17
2	A	401	API	O-C-CA	-2.46	113.47	122.14
3	G	402	SRT	O2-C2-C1	2.45	115.81	110.66
2	H	401	API	C5-C6-N6	2.35	116.34	110.17
2	A	401	API	C5-C6-N6	2.32	116.26	110.17
2	F	401	API	C3-CA-N	2.26	116.10	110.17
2	A	401	API	C3-CA-N	2.25	116.06	110.17
2	E	401	API	C3-CA-N	2.15	115.81	110.17
3	G	402	SRT	O41-C4-C3	2.12	118.99	113.27
2	G	401	API	C5-C6-N6	2.06	115.56	110.17
2	C	401	API	C4-C5-C6	-2.01	106.87	113.35

There are no chirality outliers.

All (29) 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	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	G	402	SRT	C1-C2-C3-O3
3	D	402	SRT	O2-C2-C3-C4
3	G	402	SRT	O2-C2-C3-C4
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	C1-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	E	401	API	C5-C6-C7-O4
2	H	401	API	C5-C6-C7-O4
2	D	401	API	C5-C6-C7-O3
2	D	401	API	C5-C6-C7-O4
2	E	401	API	C5-C6-C7-O3
2	H	401	API	C5-C6-C7-O3
2	B	401	API	C5-C6-C7-O4
2	C	401	API	C5-C6-C7-O4
3	D	402	SRT	C2-C3-C4-O4
2	C	401	API	C5-C6-C7-O3
3	G	402	SRT	C2-C3-C4-O4
3	D	402	SRT	C2-C3-C4-O41

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	402	SRT	2	0
2	C	401	API	4	0
2	D	401	API	1	0
3	D	402	SRT	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	122/123 (99%)	-0.09	2 (1%) 72 76	6, 12, 28, 36	0
1	B	122/123 (99%)	-0.13	0 100 100	10, 16, 27, 34	0
1	C	120/123 (97%)	0.49	13 (10%) 5 6	10, 19, 43, 52	0
1	D	123/123 (100%)	0.48	3 (2%) 59 63	13, 23, 34, 42	0
1	E	120/123 (97%)	0.07	2 (1%) 70 74	9, 15, 26, 30	0
1	F	122/123 (99%)	0.00	1 (0%) 86 88	6, 12, 22, 33	0
1	G	123/123 (100%)	-0.17	1 (0%) 86 88	6, 12, 19, 25	0
1	H	121/123 (98%)	-0.02	2 (1%) 70 74	8, 15, 27, 36	0
All	All	973/984 (98%)	0.08	24 (2%) 57 61	6, 15, 31, 52	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	299	ASN	4.3
1	C	318	ASP	3.7
1	C	312	TRP	3.6
1	A	219	HIS	3.6
1	D	332	PHE	3.5
1	C	320	LYS	3.1
1	H	318	ASP	2.8
1	C	322	LYS	2.6
1	H	332	PHE	2.6
1	C	323	GLU	2.6
1	C	272	ASN	2.4
1	C	315	PRO	2.4
1	C	325	ARG	2.4
1	C	327	MET	2.4
1	C	220	MET	2.4
1	C	275	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	244	GLN	2.3
1	E	221	GLU	2.2
1	G	332	PHE	2.2
1	C	332	PHE	2.1
1	C	326	ALA	2.1
1	F	219	HIS	2.1
1	D	302	ALA	2.1
1	E	278	LEU	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	API	C	401	13/13	0.77	0.30	25,33,43,44	0
3	SRT	D	402	10/10	0.78	0.23	31,33,35,36	0
3	SRT	G	402	10/10	0.89	0.13	19,24,25,25	0
2	API	B	401	13/13	0.91	0.11	16,20,27,27	0
2	API	D	401	13/13	0.91	0.12	18,22,32,32	0
2	API	E	401	13/13	0.92	0.14	14,19,28,29	0
2	API	F	401	13/13	0.93	0.12	10,15,27,28	0
2	API	H	401	13/13	0.95	0.09	11,16,29,29	0
2	API	G	401	13/13	0.96	0.09	7,11,20,22	0
2	API	A	401	13/13	0.96	0.08	8,13,18,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.