



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:36 PM UTC

PDB ID : 6ET1 / pdb_00006et1
Title : Crystal structure of PqsBC from Pseudomonas aeruginosa (crystal form 2)
Authors : Witzgall, F.; Blankenfeldt, W.
Deposited on : 2017-10-25
Resolution : 2.65 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:

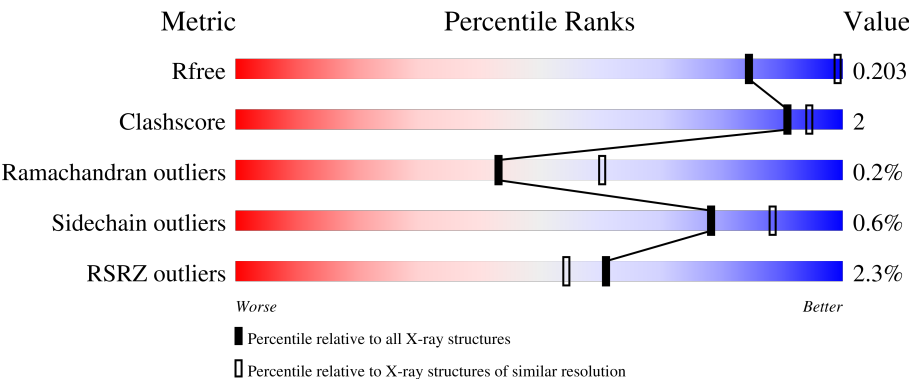
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	365	3% 91% 5%
1	C	365	5% 91% 5%
1	E	365	3% 92% . .
1	G	365	2% 93% . .
2	B	283	% 96% ...

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	283	93% 5% •
2	F	283	% 94% • •
2	H	283	% 94% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 38956 atoms, of which 18998 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 PqsC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	348	Total	C	H	N	O	S	0	1	0
			5273	1696	2604	454	501	18			
1	C	346	Total	C	H	N	O	S	0	3	0
			5285	1694	2614	462	496	19			
1	E	350	Total	C	H	N	O	S	0	0	0
			5334	1708	2639	466	503	18			
1	G	354	Total	C	H	N	O	S	0	3	0
			5344	1724	2632	460	509	19			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP Q9I4X1
A	-15	GLY	-	expression tag	UNP Q9I4X1
A	-14	HIS	-	expression tag	UNP Q9I4X1
A	-13	HIS	-	expression tag	UNP Q9I4X1
A	-12	HIS	-	expression tag	UNP Q9I4X1
A	-11	HIS	-	expression tag	UNP Q9I4X1
A	-10	HIS	-	expression tag	UNP Q9I4X1
A	-9	HIS	-	expression tag	UNP Q9I4X1
A	-8	ALA	-	expression tag	UNP Q9I4X1
A	-7	GLU	-	expression tag	UNP Q9I4X1
A	-6	ASN	-	expression tag	UNP Q9I4X1
A	-5	LEU	-	expression tag	UNP Q9I4X1
A	-4	TYR	-	expression tag	UNP Q9I4X1
A	-3	PHE	-	expression tag	UNP Q9I4X1
A	-2	GLN	-	expression tag	UNP Q9I4X1
A	-1	GLY	-	expression tag	UNP Q9I4X1
A	0	HIS	-	expression tag	UNP Q9I4X1
C	-16	MET	-	initiating methionine	UNP Q9I4X1
C	-15	GLY	-	expression tag	UNP Q9I4X1
C	-14	HIS	-	expression tag	UNP Q9I4X1
C	-13	HIS	-	expression tag	UNP Q9I4X1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP Q9I4X1
C	-11	HIS	-	expression tag	UNP Q9I4X1
C	-10	HIS	-	expression tag	UNP Q9I4X1
C	-9	HIS	-	expression tag	UNP Q9I4X1
C	-8	ALA	-	expression tag	UNP Q9I4X1
C	-7	GLU	-	expression tag	UNP Q9I4X1
C	-6	ASN	-	expression tag	UNP Q9I4X1
C	-5	LEU	-	expression tag	UNP Q9I4X1
C	-4	TYR	-	expression tag	UNP Q9I4X1
C	-3	PHE	-	expression tag	UNP Q9I4X1
C	-2	GLN	-	expression tag	UNP Q9I4X1
C	-1	GLY	-	expression tag	UNP Q9I4X1
C	0	HIS	-	expression tag	UNP Q9I4X1
E	-16	MET	-	initiating methionine	UNP Q9I4X1
E	-15	GLY	-	expression tag	UNP Q9I4X1
E	-14	HIS	-	expression tag	UNP Q9I4X1
E	-13	HIS	-	expression tag	UNP Q9I4X1
E	-12	HIS	-	expression tag	UNP Q9I4X1
E	-11	HIS	-	expression tag	UNP Q9I4X1
E	-10	HIS	-	expression tag	UNP Q9I4X1
E	-9	HIS	-	expression tag	UNP Q9I4X1
E	-8	ALA	-	expression tag	UNP Q9I4X1
E	-7	GLU	-	expression tag	UNP Q9I4X1
E	-6	ASN	-	expression tag	UNP Q9I4X1
E	-5	LEU	-	expression tag	UNP Q9I4X1
E	-4	TYR	-	expression tag	UNP Q9I4X1
E	-3	PHE	-	expression tag	UNP Q9I4X1
E	-2	GLN	-	expression tag	UNP Q9I4X1
E	-1	GLY	-	expression tag	UNP Q9I4X1
E	0	HIS	-	expression tag	UNP Q9I4X1
G	-16	MET	-	initiating methionine	UNP Q9I4X1
G	-15	GLY	-	expression tag	UNP Q9I4X1
G	-14	HIS	-	expression tag	UNP Q9I4X1
G	-13	HIS	-	expression tag	UNP Q9I4X1
G	-12	HIS	-	expression tag	UNP Q9I4X1
G	-11	HIS	-	expression tag	UNP Q9I4X1
G	-10	HIS	-	expression tag	UNP Q9I4X1
G	-9	HIS	-	expression tag	UNP Q9I4X1
G	-8	ALA	-	expression tag	UNP Q9I4X1
G	-7	GLU	-	expression tag	UNP Q9I4X1
G	-6	ASN	-	expression tag	UNP Q9I4X1
G	-5	LEU	-	expression tag	UNP Q9I4X1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	TYR	-	expression tag	UNP Q9I4X1
G	-3	PHE	-	expression tag	UNP Q9I4X1
G	-2	GLN	-	expression tag	UNP Q9I4X1
G	-1	GLY	-	expression tag	UNP Q9I4X1
G	0	HIS	-	expression tag	UNP Q9I4X1

- Molecule 2 is a protein called PqsB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	280	Total	C	H	N	O	S	0	4	0
			4294	1353	2150	379	404	8			
2	D	278	Total	C	H	N	O	S	0	2	0
			4227	1335	2113	373	398	8			
2	F	279	Total	C	H	N	O	S	0	4	0
			4269	1346	2137	378	400	8			
2	H	278	Total	C	H	N	O	S	0	0	0
			4211	1329	2109	373	392	8			

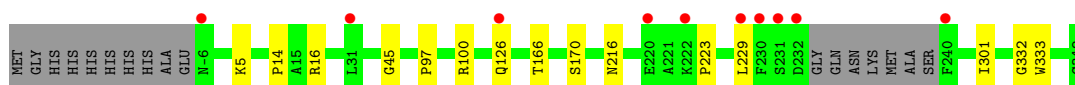
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	89	Total	O	0	0
			89	89		
3	B	108	Total	O	0	0
			108	108		
3	C	45	Total	O	0	0
			45	45		
3	D	100	Total	O	0	0
			100	100		
3	E	134	Total	O	0	0
			134	134		
3	F	122	Total	O	0	0
			122	122		
3	G	60	Total	O	0	0
			60	60		
3	H	61	Total	O	0	0
			61	61		

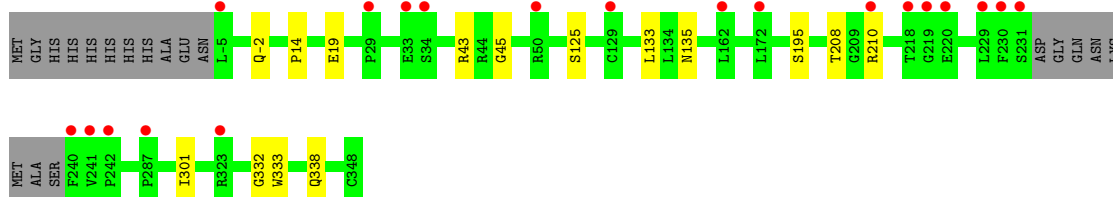
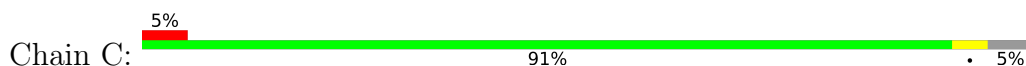
3 Residue-property plots [i](#)

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: PqsC



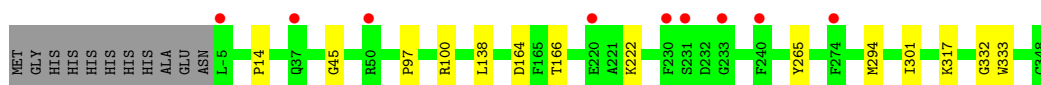
- Molecule 1: PqsC



- Molecule 1: PqsC

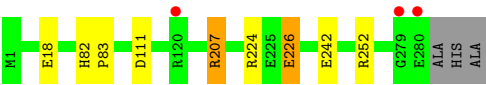


- Molecule 1: PqsC



- Molecule 2: PqsB

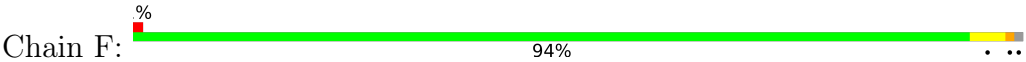




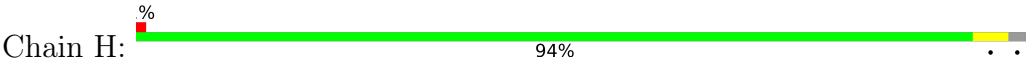
● Molecule 2: PqsB



● Molecule 2: PqsB



● Molecule 2: PqsB



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.48Å 230.92Å 134.25Å 90.00° 113.92° 90.00°	Depositor
Resolution (Å)	48.11 – 2.65 48.11 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.11-2.65) 99.3 (48.11-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.181 , 0.203 0.182 , 0.203	Depositor DCC
R_{free} test set	5978 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	38956	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.12	0/2732	0.29	0/3713
1	C	0.11	0/2740	0.28	0/3721
1	E	0.13	0/2756	0.31	0/3742
1	G	0.12	0/2784	0.28	0/3780
2	B	0.13	0/2189	0.33	0/2972
2	D	0.12	0/2154	0.31	0/2928
2	F	0.13	0/2180	0.32	0/2960
2	H	0.12	0/2135	0.31	0/2900
All	All	0.12	0/19670	0.30	0/26716

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	2669	2604	2606	9	0
1	C	2671	2614	2616	8	0
1	E	2695	2639	2641	11	0
1	G	2712	2632	2629	7	0
2	B	2144	2150	2151	8	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2114	2113	2114	9	0
2	F	2132	2137	2129	8	0
2	H	2102	2109	2108	8	1
3	A	89	0	0	4	0
3	B	108	0	0	2	0
3	C	45	0	0	2	0
3	D	100	0	0	3	0
3	E	134	0	0	3	0
3	F	122	0	0	4	0
3	G	60	0	0	1	0
3	H	61	0	0	0	0
All	All	19958	18998	18994	64	1

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 2.

All (64) 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:C:-2:GLN:O	3:C:401:HOH:O	1.96	0.83
1:A:126[A]:GLN:NE2	3:A:402:HOH:O	2.12	0.80
2:F:204:GLU:OE2	2:F:207:ARG:NH2	2.15	0.79
1:A:223:PRO:O	3:A:401:HOH:O	2.01	0.77
1:E:165:PHE:O	3:E:401:HOH:O	2.07	0.72
1:C:195:SER:O	3:C:402:HOH:O	2.07	0.71
2:F:57:ASP:OD1	2:F:92:ARG:NH2	2.23	0.71
2:B:242:GLU:OE2	1:E:-6:ASN:ND2	2.24	0.70
1:G:222:LYS:O	3:G:401:HOH:O	2.14	0.65
2:D:204:GLU:OE2	3:D:301:HOH:O	2.16	0.63
2:B:224:ARG:NE	2:B:226[A]:GLU:OE1	2.26	0.62
2:F:120:ARG:NH1	3:F:305:HOH:O	2.32	0.62
2:F:133:LEU:O	3:F:301:HOH:O	2.16	0.61
1:A:97:PRO:O	1:A:100:ARG:NH1	2.36	0.59
2:H:210:PHE:CD2	2:H:224:ARG:HD2	2.38	0.58
2:F:126:ARG:NE	3:F:304:HOH:O	2.30	0.57
2:B:111:ASP:OD1	3:B:301:HOH:O	2.18	0.54
1:G:97:PRO:O	1:G:100:ARG:NH1	2.41	0.53
1:A:170:SER:O	3:A:403:HOH:O	2.18	0.52
1:E:169:THR:OG1	3:E:402:HOH:O	2.14	0.52
1:E:119:ARG:NE	3:E:414:HOH:O	2.41	0.52
2:F:126:ARG:NH2	3:F:309:HOH:O	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:LEU:O	1:C:338:GLN:NE2	2.45	0.50
2:D:35:MET:HE2	2:D:80:ILE:HD11	1.94	0.50
1:E:332:GLY:N	1:E:333:TRP:HA	2.26	0.49
2:F:24:GLU:OE2	2:F:236:ARG:NE	2.37	0.49
2:H:224:ARG:NE	2:H:226:GLU:OE2	2.46	0.48
1:C:208:THR:OG1	1:C:210[B]:ARG:NE	2.46	0.48
1:G:332:GLY:N	1:G:333:TRP:HA	2.27	0.48
1:A:332:GLY:N	1:A:333:TRP:HA	2.27	0.48
2:D:102:SER:OG	2:D:271:GLU:OE1	2.30	0.48
1:E:125:SER:OG	1:E:135:ASN:OD1	2.28	0.47
1:C:332:GLY:N	1:C:333:TRP:HA	2.29	0.47
1:C:125:SER:OG	1:C:135:ASN:OD1	2.33	0.46
2:B:224:ARG:NH1	1:E:-3:PHE:HE2	2.14	0.45
2:H:102:SER:OG	2:H:271:GLU:OE1	2.29	0.45
1:A:14:PRO:HG2	1:A:45:GLY:HA3	1.98	0.45
1:G:14:PRO:HG2	1:G:45:GLY:HA3	1.98	0.45
2:D:113:LEU:C	2:D:113:LEU:HD23	2.41	0.45
2:B:207:ARG:NH1	2:B:224:ARG:HD2	2.32	0.45
1:C:19:GLU:OE2	1:C:43:ARG:NE	2.50	0.45
1:E:166:THR:O	1:E:216:ASN:ND2	2.43	0.44
2:B:224:ARG:HD3	1:E:-3:PHE:CE2	2.52	0.44
2:B:82:HIS:HB2	2:B:83:PRO:HD3	2.01	0.43
2:H:82:HIS:HB2	2:H:83:PRO:HD3	2.01	0.42
1:A:166:THR:O	1:A:216:ASN:ND2	2.48	0.42
2:B:252:ARG:NH1	3:B:314:HOH:O	2.52	0.42
1:G:164:ASP:OD1	1:G:166[B]:THR:HG22	2.20	0.42
2:D:82:HIS:HB2	2:D:83:PRO:HD3	2.00	0.42
1:A:5:LYS:NZ	3:A:413:HOH:O	2.53	0.42
1:A:229:LEU:O	1:A:229:LEU:HD23	2.20	0.42
2:D:31[B]:ASP:OD1	3:D:302:HOH:O	2.21	0.42
1:C:14:PRO:HG2	1:C:45:GLY:HA3	2.02	0.41
2:D:67:ASP:HB2	2:D:73:ARG:O	2.20	0.41
2:D:224:ARG:NH2	3:D:315:HOH:O	2.52	0.41
2:H:206:VAL:HG12	2:H:210:PHE:CE2	2.56	0.41
2:F:224:ARG:NE	2:F:226:GLU:OE2	2.52	0.41
2:H:113:LEU:C	2:H:113:LEU:HD23	2.45	0.41
1:E:22:ASP:OD2	1:E:24:VAL:HG23	2.20	0.41
1:G:265:TYR:OH	1:G:317:LYS:HD3	2.21	0.41
2:D:77:ALA:HA	2:D:78:PRO:C	2.46	0.40
1:E:55:GLU:OE1	1:E:55:GLU:N	2.51	0.40
1:G:138:LEU:HD23	2:H:113:LEU:HD12	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:84:LEU:HA	2:H:87:VAL:HG22	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:GLU:OE2	2:H:236:ARG:HH12[4_445]	1.58	0.02

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	345/365 (94%)	333 (96%)	11 (3%)	1 (0%)	36	52
1	C	345/365 (94%)	333 (96%)	11 (3%)	1 (0%)	36	52
1	E	346/365 (95%)	332 (96%)	13 (4%)	1 (0%)	36	52
1	G	355/365 (97%)	342 (96%)	12 (3%)	1 (0%)	36	52
2	B	281/283 (99%)	275 (98%)	6 (2%)	0	100	100
2	D	277/283 (98%)	271 (98%)	6 (2%)	0	100	100
2	F	280/283 (99%)	275 (98%)	5 (2%)	0	100	100
2	H	275/283 (97%)	269 (98%)	6 (2%)	0	100	100
All	All	2504/2592 (97%)	2430 (97%)	70 (3%)	4 (0%)	43	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	ILE
1	C	301	ILE
1	E	301	ILE
1	G	301	ILE

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	279/300 (93%)	278 (100%)	1 (0%)	84	93
1	C	279/300 (93%)	279 (100%)	0	100	100
1	E	283/300 (94%)	282 (100%)	1 (0%)	84	93
1	G	281/300 (94%)	280 (100%)	1 (0%)	84	93
2	B	224/222 (101%)	221 (99%)	3 (1%)	61	77
2	D	220/222 (99%)	217 (99%)	3 (1%)	59	76
2	F	222/222 (100%)	219 (99%)	3 (1%)	59	76
2	H	216/222 (97%)	216 (100%)	0	100	100
All	All	2004/2088 (96%)	1992 (99%)	12 (1%)	78	88

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
2	B	207	ARG
2	B	226[A]	GLU
2	B	226[B]	GLU
2	D	1	MET
2	D	224	ARG
2	D	230	GLN
1	E	294	MET
2	F	1	MET
2	F	92	ARG
2	F	207	ARG
1	G	294	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	291	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	195	ASN
1	C	109	ASN
2	D	91	ASN
2	D	171	GLN
2	D	195	ASN
2	F	171	GLN
2	H	195	ASN
2	H	230	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	CSO	F	16	2	3,6,7	0.70	0	1,6,8	0.07	0
2	CSO	D	16	2	3,6,7	0.70	0	1,6,8	0.00	0
2	CSO	B	16	2	3,6,7	0.74	0	1,6,8	0.08	0
2	CSO	H	16	2	3,6,7	0.70	0	1,6,8	0.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSO	F	16	2	-	1/1/5/7	-
2	CSO	D	16	2	-	1/1/5/7	-
2	CSO	B	16	2	-	1/1/5/7	-
2	CSO	H	16	2	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	16	CSO	N-CA-CB-SG
2	D	16	CSO	N-CA-CB-SG
2	F	16	CSO	N-CA-CB-SG
2	H	16	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	348/365 (95%)	-0.00	10 (2%)	53	46	32, 65, 110, 156	1 (0%)
1	C	346/365 (94%)	0.45	20 (5%)	29	22	47, 95, 128, 156	3 (0%)
1	E	350/365 (95%)	-0.15	10 (2%)	53	46	33, 53, 96, 153	0
1	G	354/365 (96%)	0.03	9 (2%)	58	52	31, 70, 112, 143	2 (0%)
2	B	279/283 (98%)	-0.34	3 (1%)	78	75	22, 49, 82, 120	4 (1%)
2	D	277/283 (97%)	-0.09	1 (0%)	88	87	31, 67, 103, 147	2 (0%)
2	F	278/283 (98%)	-0.42	2 (0%)	84	82	24, 45, 73, 99	3 (1%)
2	H	277/283 (97%)	-0.12	3 (1%)	78	75	46, 66, 100, 149	0
All	All	2509/2592 (96%)	-0.06	58 (2%)	61	54	22, 64, 111, 156	15 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	231	SER	8.9
1	A	232	ASP	7.7
1	A	240	PHE	6.2
1	C	240	PHE	5.9
1	E	240	PHE	5.9
2	B	280	GLU	5.7
1	C	241	VAL	5.5
1	E	230	PHE	5.3
1	E	241	VAL	4.4
1	C	220	GLU	4.4
2	D	278	ALA	4.3
1	A	230	PHE	4.3
2	F	279	GLY	4.2
1	A	-6	ASN	4.1
1	C	230	PHE	4.0
2	H	278	ALA	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	220	GLU	3.6
1	C	231	SER	3.4
1	G	231	SER	3.3
1	A	220	GLU	3.2
1	C	33	GLU	3.2
1	E	-9	HIS	3.2
1	E	-8	ALA	3.1
1	E	-7	GLU	3.1
1	C	242	PRO	2.9
1	C	-5	LEU	2.9
1	G	220	GLU	2.9
2	B	279	GLY	2.9
1	A	31	LEU	2.9
1	C	50[A]	ARG	2.8
1	C	172	LEU	2.8
1	C	229	LEU	2.8
2	F	54	GLU	2.7
2	B	120	ARG	2.6
1	A	222	LYS	2.6
1	A	126[A]	GLN	2.6
1	A	231	SER	2.5
2	H	168	ASP	2.5
1	C	210[A]	ARG	2.4
1	E	229	LEU	2.4
1	G	240	PHE	2.4
1	E	-6	ASN	2.4
1	C	34	SER	2.3
1	C	323	ARG	2.3
1	G	-5	LEU	2.3
1	C	287	PRO	2.3
1	G	50	ARG	2.2
1	C	218	THR	2.2
1	A	229	LEU	2.2
1	C	219	GLY	2.2
1	G	230	PHE	2.2
2	H	126	ARG	2.2
1	G	233	GLY	2.1
1	C	162	LEU	2.1
1	G	274[A]	PHE	2.1
1	C	129	CYS	2.1
1	C	29	PRO	2.0
1	G	37	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CSO	D	16	7/8	0.94	0.09	44,52,62,70	0
2	CSO	H	16	7/8	0.94	0.08	63,67,80,86	0
2	CSO	F	16	7/8	0.96	0.08	41,48,58,65	0
2	CSO	B	16	7/8	0.96	0.09	53,62,75,84	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.