



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:52 AM UTC

PDB ID : 7X6F / pdb_00007x6f
Title : Outer membrane lipoprotein QseG of Escherichia coli O157:H7
Authors : Matsumoto, K.; Fukuda, Y.; Inoue, T.
Deposited on : 2022-03-07
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

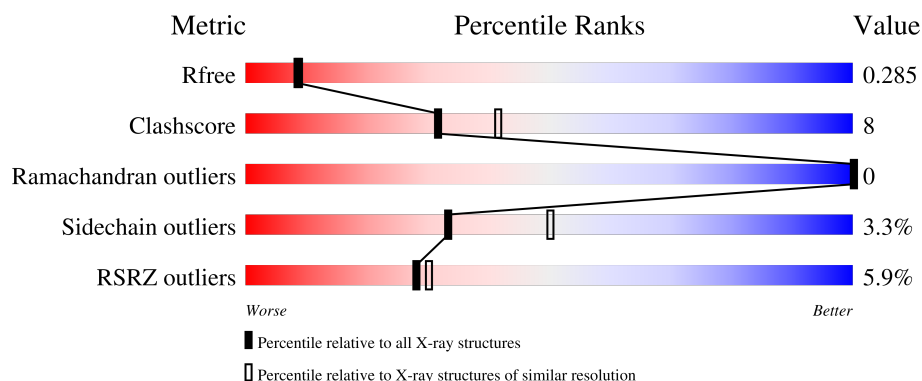
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	175	3% 65% 17% • 18%
1	B	175	2% 71% 14% • 14%
1	C	175	2% 66% 16% • 18%
1	D	175	2% 74% 13% • 14%
1	E	175	6% 65% 19% • 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	175	14% 63% 18% • 17%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7708 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 Quorum-sensing regulator protein G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	3	0
			1211	749	226	231	5			
1	B	150	Total	C	N	O	S	0	0	0
			1239	767	230	238	4			
1	C	144	Total	C	N	O	S	0	1	0
			1194	740	221	228	5			
1	D	151	Total	C	N	O	S	0	2	0
			1265	782	237	242	4			
1	E	149	Total	C	N	O	S	0	2	0
			1251	772	235	240	4			
1	F	145	Total	C	N	O	S	0	1	0
			1208	750	223	231	4			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	initiating methionine	UNP P0AD45
A	36	GLY	-	expression tag	UNP P0AD45
A	37	SER	-	expression tag	UNP P0AD45
A	38	SER	-	expression tag	UNP P0AD45
A	39	HIS	-	expression tag	UNP P0AD45
A	40	HIS	-	expression tag	UNP P0AD45
A	41	HIS	-	expression tag	UNP P0AD45
A	42	HIS	-	expression tag	UNP P0AD45
A	43	HIS	-	expression tag	UNP P0AD45
A	44	HIS	-	expression tag	UNP P0AD45
A	45	GLY	-	expression tag	UNP P0AD45
A	46	GLY	-	expression tag	UNP P0AD45
A	47	GLY	-	expression tag	UNP P0AD45
A	48	SER	-	expression tag	UNP P0AD45
A	49	GLU	-	expression tag	UNP P0AD45
A	50	ASN	-	expression tag	UNP P0AD45
A	51	LEU	-	expression tag	UNP P0AD45

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	TYR	-	expression tag	UNP P0AD45
A	53	PHE	-	expression tag	UNP P0AD45
A	54	GLN	-	expression tag	UNP P0AD45
A	55	GLY	-	expression tag	UNP P0AD45
B	35	MET	-	initiating methionine	UNP P0AD45
B	36	GLY	-	expression tag	UNP P0AD45
B	37	SER	-	expression tag	UNP P0AD45
B	38	SER	-	expression tag	UNP P0AD45
B	39	HIS	-	expression tag	UNP P0AD45
B	40	HIS	-	expression tag	UNP P0AD45
B	41	HIS	-	expression tag	UNP P0AD45
B	42	HIS	-	expression tag	UNP P0AD45
B	43	HIS	-	expression tag	UNP P0AD45
B	44	HIS	-	expression tag	UNP P0AD45
B	45	GLY	-	expression tag	UNP P0AD45
B	46	GLY	-	expression tag	UNP P0AD45
B	47	GLY	-	expression tag	UNP P0AD45
B	48	SER	-	expression tag	UNP P0AD45
B	49	GLU	-	expression tag	UNP P0AD45
B	50	ASN	-	expression tag	UNP P0AD45
B	51	LEU	-	expression tag	UNP P0AD45
B	52	TYR	-	expression tag	UNP P0AD45
B	53	PHE	-	expression tag	UNP P0AD45
B	54	GLN	-	expression tag	UNP P0AD45
B	55	GLY	-	expression tag	UNP P0AD45
C	35	MET	-	initiating methionine	UNP P0AD45
C	36	GLY	-	expression tag	UNP P0AD45
C	37	SER	-	expression tag	UNP P0AD45
C	38	SER	-	expression tag	UNP P0AD45
C	39	HIS	-	expression tag	UNP P0AD45
C	40	HIS	-	expression tag	UNP P0AD45
C	41	HIS	-	expression tag	UNP P0AD45
C	42	HIS	-	expression tag	UNP P0AD45
C	43	HIS	-	expression tag	UNP P0AD45
C	44	HIS	-	expression tag	UNP P0AD45
C	45	GLY	-	expression tag	UNP P0AD45
C	46	GLY	-	expression tag	UNP P0AD45
C	47	GLY	-	expression tag	UNP P0AD45
C	48	SER	-	expression tag	UNP P0AD45
C	49	GLU	-	expression tag	UNP P0AD45
C	50	ASN	-	expression tag	UNP P0AD45
C	51	LEU	-	expression tag	UNP P0AD45

Continued on next page...

Continued from previous page...

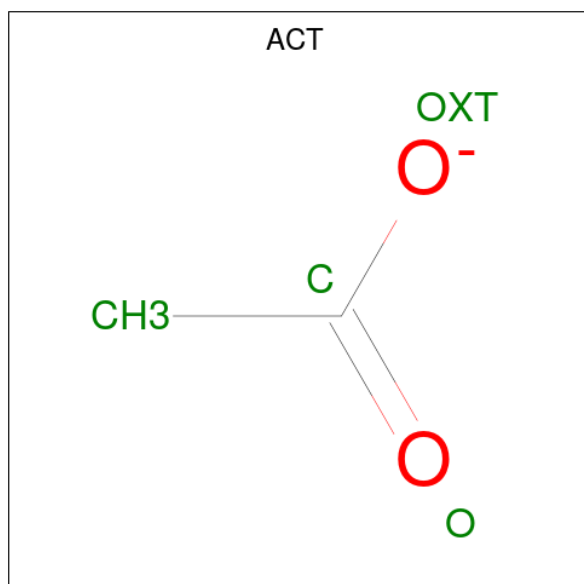
Chain	Residue	Modelled	Actual	Comment	Reference
C	52	TYR	-	expression tag	UNP P0AD45
C	53	PHE	-	expression tag	UNP P0AD45
C	54	GLN	-	expression tag	UNP P0AD45
C	55	GLY	-	expression tag	UNP P0AD45
D	35	MET	-	initiating methionine	UNP P0AD45
D	36	GLY	-	expression tag	UNP P0AD45
D	37	SER	-	expression tag	UNP P0AD45
D	38	SER	-	expression tag	UNP P0AD45
D	39	HIS	-	expression tag	UNP P0AD45
D	40	HIS	-	expression tag	UNP P0AD45
D	41	HIS	-	expression tag	UNP P0AD45
D	42	HIS	-	expression tag	UNP P0AD45
D	43	HIS	-	expression tag	UNP P0AD45
D	44	HIS	-	expression tag	UNP P0AD45
D	45	GLY	-	expression tag	UNP P0AD45
D	46	GLY	-	expression tag	UNP P0AD45
D	47	GLY	-	expression tag	UNP P0AD45
D	48	SER	-	expression tag	UNP P0AD45
D	49	GLU	-	expression tag	UNP P0AD45
D	50	ASN	-	expression tag	UNP P0AD45
D	51	LEU	-	expression tag	UNP P0AD45
D	52	TYR	-	expression tag	UNP P0AD45
D	53	PHE	-	expression tag	UNP P0AD45
D	54	GLN	-	expression tag	UNP P0AD45
D	55	GLY	-	expression tag	UNP P0AD45
E	35	MET	-	initiating methionine	UNP P0AD45
E	36	GLY	-	expression tag	UNP P0AD45
E	37	SER	-	expression tag	UNP P0AD45
E	38	SER	-	expression tag	UNP P0AD45
E	39	HIS	-	expression tag	UNP P0AD45
E	40	HIS	-	expression tag	UNP P0AD45
E	41	HIS	-	expression tag	UNP P0AD45
E	42	HIS	-	expression tag	UNP P0AD45
E	43	HIS	-	expression tag	UNP P0AD45
E	44	HIS	-	expression tag	UNP P0AD45
E	45	GLY	-	expression tag	UNP P0AD45
E	46	GLY	-	expression tag	UNP P0AD45
E	47	GLY	-	expression tag	UNP P0AD45
E	48	SER	-	expression tag	UNP P0AD45
E	49	GLU	-	expression tag	UNP P0AD45
E	50	ASN	-	expression tag	UNP P0AD45
E	51	LEU	-	expression tag	UNP P0AD45

Continued on next page...

Continued from previous page...

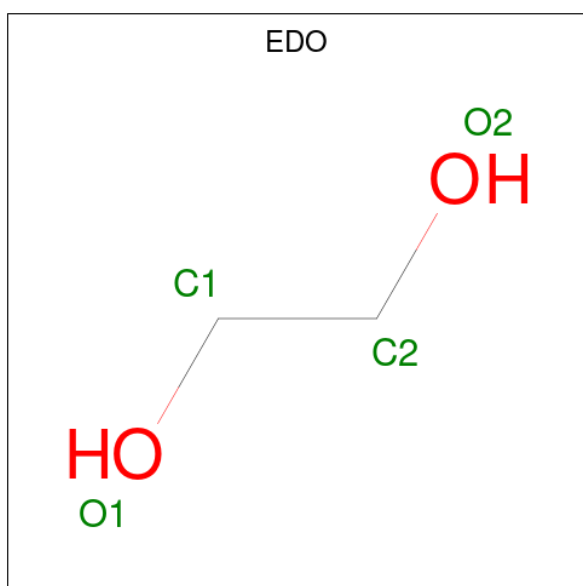
Chain	Residue	Modelled	Actual	Comment	Reference
E	52	TYR	-	expression tag	UNP P0AD45
E	53	PHE	-	expression tag	UNP P0AD45
E	54	GLN	-	expression tag	UNP P0AD45
E	55	GLY	-	expression tag	UNP P0AD45
F	35	MET	-	initiating methionine	UNP P0AD45
F	36	GLY	-	expression tag	UNP P0AD45
F	37	SER	-	expression tag	UNP P0AD45
F	38	SER	-	expression tag	UNP P0AD45
F	39	HIS	-	expression tag	UNP P0AD45
F	40	HIS	-	expression tag	UNP P0AD45
F	41	HIS	-	expression tag	UNP P0AD45
F	42	HIS	-	expression tag	UNP P0AD45
F	43	HIS	-	expression tag	UNP P0AD45
F	44	HIS	-	expression tag	UNP P0AD45
F	45	GLY	-	expression tag	UNP P0AD45
F	46	GLY	-	expression tag	UNP P0AD45
F	47	GLY	-	expression tag	UNP P0AD45
F	48	SER	-	expression tag	UNP P0AD45
F	49	GLU	-	expression tag	UNP P0AD45
F	50	ASN	-	expression tag	UNP P0AD45
F	51	LEU	-	expression tag	UNP P0AD45
F	52	TYR	-	expression tag	UNP P0AD45
F	53	PHE	-	expression tag	UNP P0AD45
F	54	GLN	-	expression tag	UNP P0AD45
F	55	GLY	-	expression tag	UNP P0AD45

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



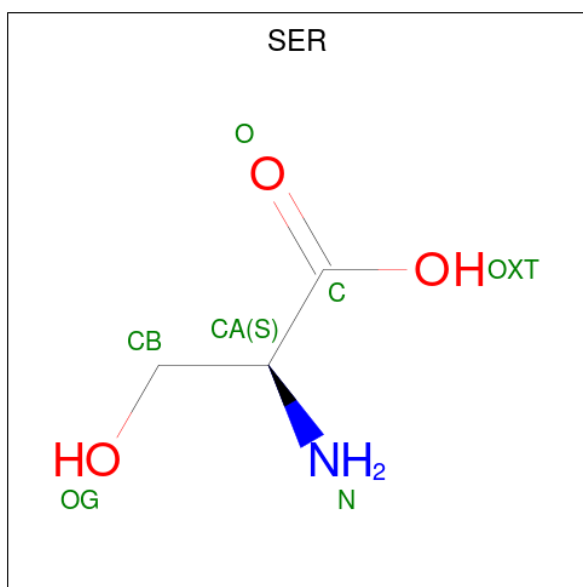
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



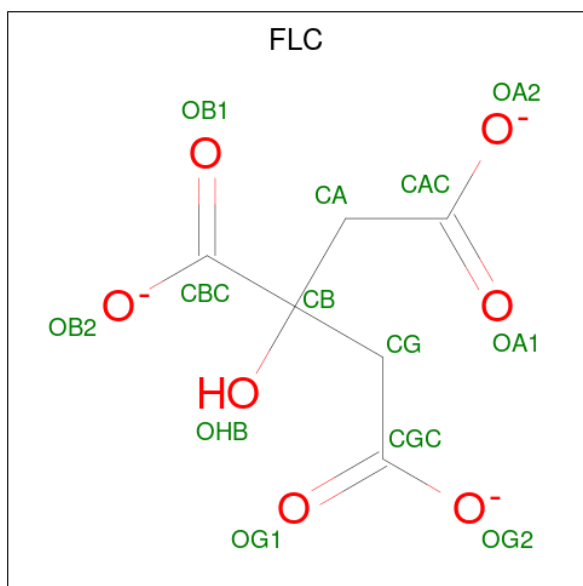
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	1
			8	4	4		

- Molecule 4 is SERINE (CCD ID: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 5 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			13	6	7		
5	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total 1	Mg 1	0	0

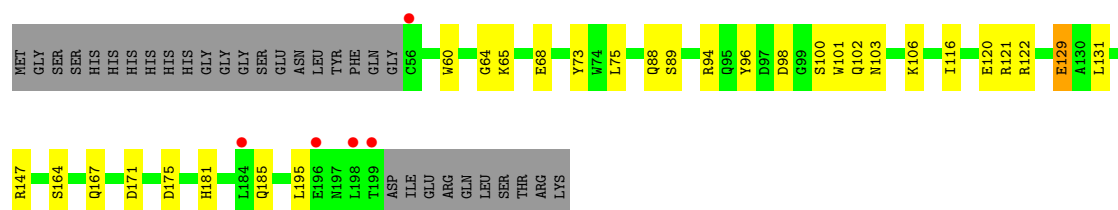
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	52	Total 52	O 52	0	0
7	B	60	Total 60	O 60	0	0
7	C	59	Total 59	O 59	0	3
7	D	46	Total 46	O 46	0	1
7	E	35	Total 35	O 35	0	0
7	F	27	Total 27	O 27	0	0

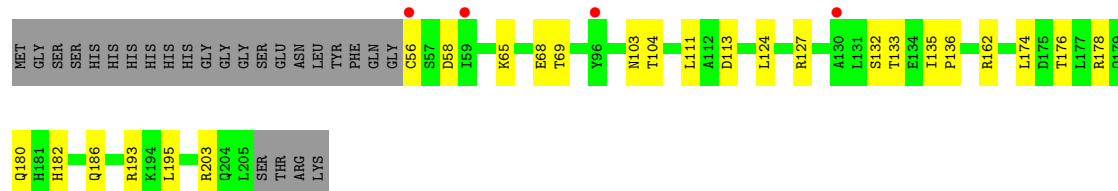
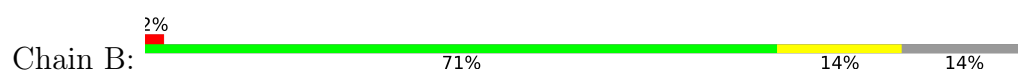
3 Residue-property plots [i](#)

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.

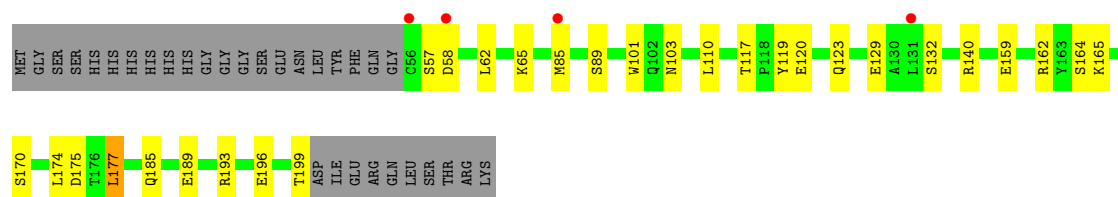
• Molecule 1: Quorum-sensing regulator protein G



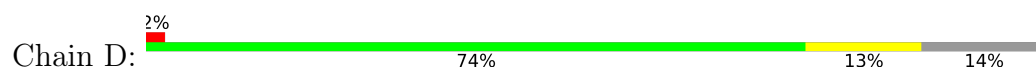
• Molecule 1: Quorum-sensing regulator protein G



• Molecule 1: Quorum-sensing regulator protein G

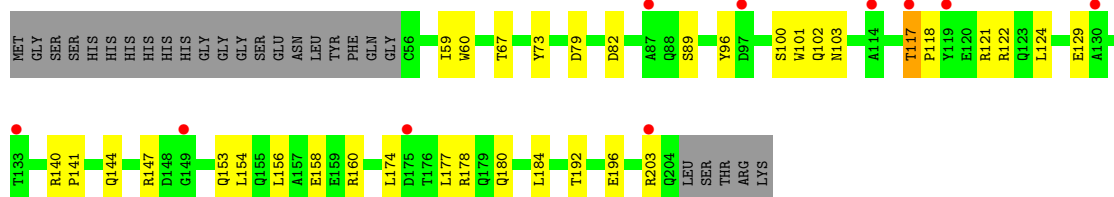


• Molecule 1: Quorum-sensing regulator protein G

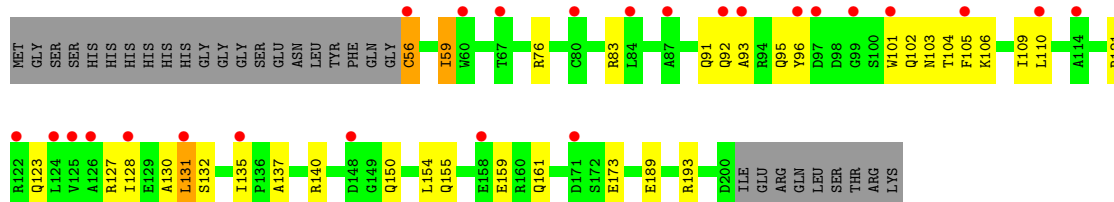




• Molecule 1: Quorum-sensing regulator protein G



• Molecule 1: Quorum-sensing regulator protein G



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.96Å 149.78Å 88.30Å 90.00° 94.65° 90.00°	Depositor
Resolution (Å)	39.80 – 2.30 39.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.80-2.30) 98.8 (39.80-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267, PHENIX 1.19.2	Depositor
R, R_{free}	0.221 , 0.274 (Not available) , 0.285	Depositor DCC
R_{free} test set	2466 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7708	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.77% 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: EDO, ACT, FLC, MG

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	0.38	0/1231	0.57	0/1665
1	B	0.36	0/1259	0.49	0/1703
1	C	0.40	0/1214	0.57	0/1643
1	D	0.37	0/1285	0.57	0/1736
1	E	0.29	0/1271	0.52	0/1718
1	F	0.27	0/1230	0.50	0/1666
All	All	0.35	0/7490	0.54	0/10131

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	1211	0	1196	19	0
1	B	1239	0	1224	19	0
1	C	1194	0	1180	20	0
1	D	1265	0	1253	16	0
1	E	1251	0	1232	22	0
1	F	1208	0	1184	30	0
2	A	4	0	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	3	1	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
3	A	4	0	6	1	0
3	C	8	0	12	2	0
4	B	6	0	4	1	0
5	C	13	0	5	2	0
5	D	13	0	5	2	0
6	C	1	0	0	0	0
7	A	52	0	0	3	0
7	B	60	0	0	7	0
7	C	59	0	0	5	0
7	D	46	0	0	4	0
7	E	35	0	0	2	0
7	F	27	0	0	0	0
All	All	7708	0	7313	120	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 (120) 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:196:GLU:HA	1:C:199:THR:HG22	1.59	0.84
1:A:101:TRP:HE1	3:A:302:EDO:H22	1.43	0.83
1:F:91:GLN:O	1:F:95:GLN:NE2	2.15	0.80
1:B:56:CYS:N	7:B:403:HOH:O	2.17	0.78
1:C:65:LYS:H	5:C:303:FLC:HA2	1.48	0.78
1:E:117:THR:HG22	1:E:118:PRO:HD2	1.69	0.74
1:F:101[A]:TRP:HA	1:F:131:LEU:HD13	1.71	0.72
1:F:101[B]:TRP:HA	1:F:131:LEU:HD13	1.70	0.72
1:F:96:TYR:HB3	1:F:103:ASN:HB3	1.72	0.71
1:A:65:LYS:H	1:A:65:LYS:HD3	1.56	0.70
1:D:140:ARG:NE	7:D:402:HOH:O	2.23	0.70
1:D:83:ARG:NH2	7:D:403:HOH:O	2.24	0.70
1:F:137:ALA:HA	1:F:140:ARG:HD2	1.74	0.69
1:E:178:ARG:NH2	1:F:173:GLU:OE2	2.26	0.69
1:A:68:GLU:OE2	1:A:102:GLN:NE2	2.23	0.69
1:D:123:GLN:OE1	7:D:401:HOH:O	2.10	0.69
1:B:162:ARG:NH2	7:B:404:HOH:O	2.26	0.68
1:B:203:ARG:O	4:B:301:SER:N	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASP:CG	1:A:103:ASN:HD22	2.04	0.65
1:B:68:GLU:OE1	7:B:402:HOH:O	2.14	0.65
1:C:177:LEU:HD21	1:D:178:ARG:HG2	1.78	0.64
1:C:159:GLU:OE2	7:C:401:HOH:O	2.15	0.63
1:B:103:ASN:ND2	7:B:405:HOH:O	2.32	0.61
1:E:154:LEU:O	1:E:158:GLU:HG3	2.00	0.61
1:F:56:CYS:HA	1:F:76:ARG:HH12	1.67	0.60
1:C:140:ARG:NH2	7:C:402:HOH:O	2.21	0.60
1:E:122:ARG:HA	1:E:154:LEU:HD11	1.84	0.60
1:C:132:SER:O	1:C:140:ARG:NH1	2.34	0.59
1:F:189:GLU:O	1:F:193:ARG:HG3	2.02	0.59
1:A:129:GLU:OE1	1:A:147:ARG:NH1	2.37	0.57
1:B:65:LYS:HA	1:B:68:GLU:HG2	1.86	0.57
1:E:82:ASP:OD2	7:E:301:HOH:O	2.17	0.57
1:C:185:GLN:O	1:C:189:GLU:HG2	2.05	0.57
1:D:176:THR:O	1:D:180:GLN:HG3	2.05	0.57
1:C:119:TYR:HB3	7:C:407:HOH:O	2.04	0.56
1:A:94:ARG:O	7:A:401:HOH:O	2.17	0.56
1:B:127:ARG:NH2	7:B:401:HOH:O	2.11	0.56
1:B:174:LEU:HD23	1:B:178:ARG:HH22	1.71	0.56
1:F:92:GLN:HA	1:F:95:GLN:HE21	1.70	0.56
1:F:121:ARG:NH1	1:F:150:GLN:OE1	2.39	0.56
1:B:132:SER:HA	1:B:135:ILE:HD12	1.87	0.55
1:C:162:ARG:HA	1:C:165:LYS:HE3	1.88	0.55
1:F:105:PHE:O	1:F:109:ILE:HG13	2.07	0.55
1:E:122:ARG:HB2	1:E:154:LEU:HD21	1.88	0.54
1:C:189:GLU:O	1:C:193:ARG:HG3	2.08	0.54
1:D:198:LEU:O	1:D:202:GLU:HG2	2.08	0.54
1:A:181:HIS:O	1:A:185:GLN:HB2	2.09	0.53
1:D:65[B]:LYS:N	5:D:302:FLC:OB1	2.42	0.53
1:B:133:THR:HG22	2:B:302:ACT:H1	1.90	0.53
1:F:102:GLN:O	1:F:106:LYS:HG3	2.09	0.53
1:D:65[B]:LYS:HA	1:D:68:GLU:HG2	1.92	0.51
1:F:56:CYS:HA	1:F:76:ARG:NH1	2.25	0.51
1:F:155:GLN:O	1:F:159:GLU:HG2	2.10	0.51
1:B:193:ARG:HD2	7:B:410:HOH:O	2.09	0.51
1:E:192:THR:O	1:E:196:GLU:HG2	2.10	0.51
1:D:65[A]:LYS:N	5:D:302:FLC:OB1	2.42	0.51
1:E:60:TRP:HB3	1:E:96:TYR:OH	2.10	0.51
1:F:104:THR:HG22	1:F:128:ILE:HD13	1.93	0.50
1:C:58:ASP:O	1:C:62:LEU:HG	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:SER:OG	1:E:103:ASN:OD1	2.29	0.50
1:C:89:SER:OG	1:C:110:LEU:O	2.30	0.49
1:F:101[A]:TRP:CA	1:F:131:LEU:HD13	2.40	0.49
1:B:104:THR:HG21	1:B:127:ARG:HB3	1.93	0.49
1:C:123:GLN:NE2	7:C:407:HOH:O	2.45	0.49
1:B:111:LEU:HD12	1:B:124:LEU:HD21	1.95	0.48
1:E:101:TRP:CE2	1:E:102:GLN:HG3	2.48	0.48
1:A:88:GLN:NE2	7:A:412:HOH:O	2.47	0.48
1:D:90:ARG:HH12	1:D:116:ILE:HG22	1.79	0.48
1:A:121[B]:ARG:NH2	7:A:404:HOH:O	2.31	0.48
1:F:103:ASN:HD22	1:F:103:ASN:N	2.12	0.48
1:F:135:ILE:H	1:F:140:ARG:NH2	2.12	0.47
1:F:135:ILE:O	1:F:140:ARG:NE	2.38	0.47
1:F:93:ALA:HA	1:F:110:LEU:HD13	1.96	0.47
1:A:167:GLN:O	1:A:171:ASP:HB2	2.15	0.47
1:C:101:TRP:HE1	3:C:302[B]:EDO:H21	1.79	0.47
1:E:180:GLN:O	1:E:184:LEU:HG	2.14	0.47
1:D:65[A]:LYS:HA	1:D:68:GLU:HG2	1.96	0.47
1:E:129:GLU:CD	1:E:147:ARG:HD2	2.41	0.46
1:D:60:TRP:O	1:D:106:LYS:NZ	2.46	0.46
1:A:64:GLY:O	1:A:68:GLU:HG3	2.17	0.45
1:A:98:ASP:CG	1:A:103:ASN:ND2	2.73	0.44
1:D:175:ASP:OD1	1:D:178:ARG:NH1	2.50	0.44
1:A:195:LEU:HD21	1:B:195:LEU:HA	2.00	0.44
1:E:79:ASP:OD1	7:E:302:HOH:O	2.21	0.44
1:E:156:LEU:HD23	1:E:156:LEU:HA	1.88	0.44
1:E:156:LEU:O	1:E:160:ARG:HG3	2.18	0.43
1:F:83:ARG:HG2	1:F:83:ARG:HH11	1.83	0.43
1:F:83:ARG:HG2	1:F:83:ARG:NH1	2.33	0.43
1:B:69:THR:HA	1:B:136:PRO:HG2	2.00	0.43
1:C:101:TRP:HE1	3:C:302[A]:EDO:H22	1.82	0.43
1:B:182:HIS:O	1:B:186:GLN:HG3	2.19	0.43
1:B:174:LEU:HD23	1:B:178:ARG:NH2	2.34	0.43
1:A:60:TRP:HB3	1:A:96:TYR:OH	2.19	0.43
1:E:140:ARG:HB3	1:E:141:PRO:HD3	2.01	0.43
1:A:131:LEU:C	1:A:131:LEU:HD12	2.44	0.42
1:B:176:THR:O	1:B:180:GLN:HG3	2.20	0.42
1:F:130:ALA:C	1:F:132:SER:H	2.27	0.42
1:B:113:ASP:HB2	7:B:443:HOH:O	2.18	0.42
1:C:65:LYS:N	5:C:303:FLC:HA2	2.25	0.42
1:D:108:GLY:HA2	1:D:124:LEU:HD13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101[B]:TRP:CD1	1:F:101[B]:TRP:C	2.97	0.42
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.93	0.42
1:C:165:LYS:HE2	1:C:165:LYS:HB2	1.77	0.41
1:E:174:LEU:HD22	1:F:173:GLU:HG2	2.02	0.41
1:A:73:TYR:OH	1:A:106:LYS:HE2	2.19	0.41
1:C:103:ASN:ND2	7:C:409:HOH:O	2.54	0.41
1:E:59:ILE:HG13	1:E:73:TYR:CE1	2.56	0.41
1:C:117:THR:OG1	1:C:120:GLU:HG3	2.20	0.41
1:C:170:SER:O	1:C:174:LEU:HG	2.20	0.41
1:D:94:ARG:HH21	1:E:153:GLN:HE21	1.69	0.41
1:D:160:ARG:NH1	7:D:405:HOH:O	2.38	0.41
1:E:174:LEU:CD2	1:F:173:GLU:HG2	2.51	0.41
1:F:96:TYR:HD1	1:F:103:ASN:OD1	2.03	0.41
1:A:116:ILE:HB	1:A:120:GLU:HB2	2.02	0.41
1:F:59:ILE:HD13	1:F:76:ARG:NH1	2.36	0.40
1:F:59:ILE:HG12	1:F:76:ARG:HD2	2.03	0.40
1:F:123:GLN:C	1:F:127:ARG:HD3	2.46	0.40
1:E:121:ARG:O	1:E:124:LEU:HG	2.21	0.40
1:A:100[B]:SER:OG	1:A:102:GLN:OE1	2.36	0.40
1:E:100:SER:HB2	1:E:102:GLN:OE1	2.21	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	145/175 (83%)	142 (98%)	3 (2%)	0	100	100
1	B	148/175 (85%)	146 (99%)	2 (1%)	0	100	100
1	C	143/175 (82%)	140 (98%)	3 (2%)	0	100	100
1	D	151/175 (86%)	146 (97%)	5 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	149/175 (85%)	146 (98%)	3 (2%)	0	100	100
1	F	144/175 (82%)	136 (94%)	8 (6%)	0	100	100
All	All	880/1050 (84%)	856 (97%)	24 (3%)	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	131/154 (85%)	126 (96%)	5 (4%)	29	44
1	B	134/154 (87%)	133 (99%)	1 (1%)	76	87
1	C	129/154 (84%)	122 (95%)	7 (5%)	20	29
1	D	137/154 (89%)	134 (98%)	3 (2%)	45	65
1	E	135/154 (88%)	128 (95%)	7 (5%)	21	31
1	F	130/154 (84%)	125 (96%)	5 (4%)	29	44
All	All	796/924 (86%)	768 (96%)	28 (4%)	33	48

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	SER
1	A	122	ARG
1	A	129	GLU
1	A	164	SER
1	A	175	ASP
1	B	58	ASP
1	C	57	SER
1	C	85[A]	MET
1	C	85[B]	MET
1	C	129	GLU
1	C	164	SER
1	C	175	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	177	LEU
1	D	59	ILE
1	D	67	THR
1	D	138	GLN
1	E	67	THR
1	E	89	SER
1	E	117	THR
1	E	144	GLN
1	E	177	LEU
1	E	203[A]	ARG
1	E	203[B]	ARG
1	F	56	CYS
1	F	59	ILE
1	F	131	LEU
1	F	154	LEU
1	F	161	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	153	GLN
1	A	179	GLN
1	A	186	GLN
1	A	187	GLN
1	B	103	ASN
1	B	153	GLN
1	B	186	GLN
1	C	88	GLN
1	C	92	GLN
1	C	95	GLN
1	C	103	ASN
1	C	179	GLN
1	D	155	GLN
1	E	103	ASN
1	E	155	GLN
1	E	161	GLN
1	F	95	GLN
1	F	103	ASN
1	F	179	GLN
1	F	180	GLN
1	F	181	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	185	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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	ACT	C	301	6	3,3,3	1.44	1 (33%)	3,3,3	0.51	0
3	EDO	C	302[B]	-	3,3,3	0.66	0	2,2,2	0.05	0
2	ACT	A	301	-	3,3,3	1.49	1 (33%)	3,3,3	0.53	0
5	FLC	D	302	-	12,12,12	1.05	0	17,17,17	1.55	3 (17%)
5	FLC	C	303	-	12,12,12	1.02	0	17,17,17	1.52	3 (17%)
2	ACT	D	301	-	3,3,3	0.68	0	3,3,3	0.73	0
4	SER	B	301	-	4,5,6	0.69	0	1,5,7	0.28	0
3	EDO	C	302[A]	-	3,3,3	0.48	0	2,2,2	0.44	0
3	EDO	A	302	-	3,3,3	0.65	0	2,2,2	0.04	0
2	ACT	B	302	-	3,3,3	1.24	1 (33%)	3,3,3	0.59	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
3	EDO	C	302[B]	-	-	1/1/1/1	-
5	FLC	D	302	-	-	3/16/16/16	-
5	FLC	C	303	-	-	7/16/16/16	-
4	SER	B	301	-	-	0/2/4/6	-
3	EDO	C	302[A]	-	-	1/1/1/1	-
3	EDO	A	302	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	ACT	CH3-C	2.55	1.59	1.49
2	C	301	ACT	CH3-C	2.46	1.58	1.49
2	B	302	ACT	CH3-C	2.09	1.57	1.49

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	302	FLC	OB2-CBC-CB	4.07	120.95	113.14
5	C	303	FLC	OB2-CBC-CB	3.69	120.22	113.14
5	C	303	FLC	OG2-CGC-CG	2.32	121.71	114.35
5	C	303	FLC	OA2-CAC-CA	2.13	121.09	114.35
5	D	302	FLC	OG2-CGC-CG	2.07	120.91	114.35
5	D	302	FLC	OA2-CAC-OA1	-2.06	118.03	123.33

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	303	FLC	CAC-CA-CB-CBC
5	C	303	FLC	CAC-CA-CB-OHB
5	D	302	FLC	CAC-CA-CB-CBC
5	D	302	FLC	CAC-CA-CB-OHB
5	C	303	FLC	CAC-CA-CB-CG
5	D	302	FLC	CAC-CA-CB-CG
3	A	302	EDO	O1-C1-C2-O2
5	C	303	FLC	OHB-CB-CG-CGC
3	C	302[A]	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	302[B]	EDO	O1-C1-C2-O2
5	C	303	FLC	CA-CB-CG-CGC
5	C	303	FLC	CG-CB-CBC-OB1
5	C	303	FLC	CG-CB-CBC-OB2

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302[B]	EDO	1	0
5	D	302	FLC	2	0
5	C	303	FLC	2	0
4	B	301	SER	1	0
3	C	302[A]	EDO	1	0
3	A	302	EDO	1	0
2	B	302	ACT	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, 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	144/175 (82%)	0.55	5 (3%)	47	49	14, 42, 77, 95	3 (2%)
1	B	150/175 (85%)	0.58	4 (2%)	56	58	29, 49, 70, 83	0
1	C	144/175 (82%)	0.62	4 (2%)	55	57	18, 42, 71, 86	1 (0%)
1	D	151/175 (86%)	0.59	4 (2%)	57	59	23, 46, 68, 79	2 (1%)
1	E	149/175 (85%)	0.78	10 (6%)	24	26	28, 55, 73, 88	2 (1%)
1	F	145/175 (82%)	1.26	25 (17%)	4	4	40, 68, 104, 111	1 (0%)
All	All	883/1050 (84%)	0.73	52 (5%)	28	30	14, 50, 86, 111	9 (1%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	101[A]	TRP	4.2
1	F	131	LEU	4.0
1	E	203[A]	ARG	3.9
1	F	126	ALA	3.6
1	D	87	ALA	3.3
1	F	128	ILE	3.2
1	F	171	ASP	3.1
1	E	130	ALA	3.1
1	E	97	ASP	3.0
1	F	96	TYR	3.0
1	F	125	VAL	2.9
1	A	56	CYS	2.8
1	A	198	LEU	2.8
1	F	87	ALA	2.7
1	B	56	CYS	2.7
1	F	56	CYS	2.7
1	A	196	GLU	2.6
1	F	60	TRP	2.6
1	C	56	CYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	93	ALA	2.5
1	F	114	ALA	2.5
1	F	97	ASP	2.5
1	E	119	TYR	2.5
1	E	87	ALA	2.5
1	F	158	GLU	2.5
1	E	117	THR	2.4
1	E	114	ALA	2.4
1	A	199	THR	2.4
1	F	135	ILE	2.4
1	B	96	TYR	2.4
1	F	84	LEU	2.4
1	E	175	ASP	2.3
1	C	85[A]	MET	2.3
1	B	130	ALA	2.3
1	D	114	ALA	2.3
1	D	137	ALA	2.3
1	F	122	ARG	2.3
1	F	148	ASP	2.3
1	A	184	LEU	2.2
1	C	131	LEU	2.2
1	B	59	ILE	2.2
1	C	58	ASP	2.2
1	D	119	TYR	2.1
1	F	110	LEU	2.1
1	F	80	CYS	2.1
1	E	133	THR	2.1
1	F	124	LEU	2.1
1	F	105	PHE	2.1
1	E	149	GLY	2.1
1	F	99	GLY	2.1
1	F	67	THR	2.0
1	F	92	GLN	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
5	FLC	C	303	13/13	0.64	0.14	65,79,87,95	0
5	FLC	D	302	13/13	0.64	0.14	61,70,76,79	0
2	ACT	B	302	4/4	0.68	0.18	46,63,67,69	0
2	ACT	A	301	4/4	0.72	0.19	43,45,53,58	0
4	SER	B	301	6/7	0.79	0.14	70,72,79,80	0
2	ACT	C	301	4/4	0.81	0.18	43,46,50,54	0
2	ACT	D	301	4/4	0.84	0.11	35,56,57,64	0
3	EDO	C	302[B]	4/4	0.86	0.23	25,28,36,38	4
3	EDO	C	302[A]	4/4	0.86	0.23	33,35,36,38	4
3	EDO	A	302	4/4	0.89	0.14	33,40,40,55	0
6	MG	C	304	1/1	0.93	0.07	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.