Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2022 – 04:09 pm BST

PDB ID	:	7QI1
Title	:	Crystal structure of human 14-3-3 protein beta in complex with CFTR peptide pS753pS768 and PPI stabilizer CY007424
Authors	:	Stevers, L.M.; Ottmann, C.
Deposited on	:	2021-12-14
Resolution	:	1.76 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:

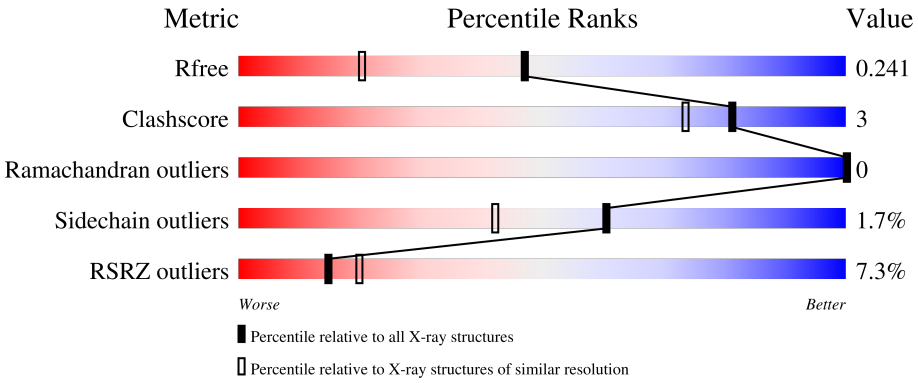
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 <=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	237	3% 92% 6% ·
1	B	237	8% 91% 7% ·
1	C	237	6% 90% 8% ·
1	D	237	8% 93% 5% ·
2	E	28	7% 39% 18% 43%

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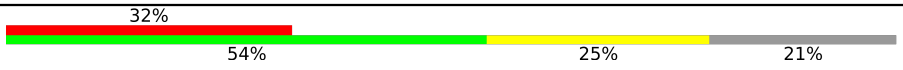
Mol	Chain	Length	Quality of chain
2	F	28	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8367 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 14-3-3 protein theta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	6	0
			1885	1182	316	378	9			
1	B	232	Total	C	N	O	S	0	4	0
			1850	1161	313	366	10			
1	C	234	Total	C	N	O	S	0	2	0
			1856	1162	310	373	11			
1	D	233	Total	C	N	O	S	0	2	0
			1854	1163	309	371	11			

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P27348
A	-3	ALA	-	expression tag	UNP P27348
A	-2	MET	-	expression tag	UNP P27348
A	-1	GLY	-	expression tag	UNP P27348
A	0	SER	-	expression tag	UNP P27348
A	1	MET	-	expression tag	UNP P27348
A	2	THR	-	expression tag	UNP P27348
A	4	ASP	GLU	conflict	UNP P27348
A	6	SER	THR	conflict	UNP P27348
A	9	VAL	ILE	conflict	UNP P27348
A	26	ALA	THR	conflict	UNP P27348
A	27	ALA	CYS	conflict	UNP P27348
A	36	HIS	ALA	conflict	UNP P27348
A	56	ALA	GLY	conflict	UNP P27348
A	60	SER	ALA	conflict	UNP P27348
A	72	GLU	ASP	conflict	UNP P27348
A	73	ARG	THR	conflict	UNP P27348
A	74	ASN	SER	conflict	UNP P27348
A	75	GLU	ASP	conflict	UNP P27348
A	78	GLN	LEU	conflict	UNP P27348
A	80	MET	LEU	conflict	UNP P27348

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Chain	Residue	Modelled	Actual	Comment	Reference
A	81	GLY	ILE	conflict	UNP P27348
A	83	GLU	ASP	conflict	UNP P27348
A	88	ILE	VAL	conflict	UNP P27348
A	90	ALA	SER	conflict	UNP P27348
A	93	GLN	ARG	conflict	UNP P27348
A	94	ASP	SER	conflict	UNP P27348
A	97	ASN	THR	conflict	UNP P27348
A	98	ASP	THR	conflict	UNP P27348
A	109	PRO	ALA	conflict	UNP P27348
A	113	GLN	ASN	conflict	UNP P27348
A	132	SER	ALA	conflict	UNP P27348
A	136	SER	CYS	conflict	UNP P27348
A	139	ASN	ASP	conflict	UNP P27348
A	140	LYS	ARG	conflict	UNP P27348
A	141	GLN	LYS	conflict	UNP P27348
A	142	THR	GLN	conflict	UNP P27348
A	144	VAL	ILE	conflict	UNP P27348
A	145	SER	ASP	conflict	UNP P27348
A	149	GLN	GLY	conflict	UNP P27348
A	156	GLU	ASP	conflict	UNP P27348
A	186	SER	ASN	conflict	UNP P27348
A	189	LYS	LEU	conflict	UNP P27348
A	192	SER	THR	conflict	UNP P27348
A	211	GLU	ASP	conflict	UNP P27348
B	-4	GLY	-	expression tag	UNP P27348
B	-3	ALA	-	expression tag	UNP P27348
B	-2	MET	-	expression tag	UNP P27348
B	-1	GLY	-	expression tag	UNP P27348
B	0	SER	-	expression tag	UNP P27348
B	1	MET	-	expression tag	UNP P27348
B	2	THR	-	expression tag	UNP P27348
B	4	ASP	GLU	conflict	UNP P27348
B	6	SER	THR	conflict	UNP P27348
B	9	VAL	ILE	conflict	UNP P27348
B	26	ALA	THR	conflict	UNP P27348
B	27	ALA	CYS	conflict	UNP P27348
B	36	HIS	ALA	conflict	UNP P27348
B	56	ALA	GLY	conflict	UNP P27348
B	60	SER	ALA	conflict	UNP P27348
B	72	GLU	ASP	conflict	UNP P27348
B	73	ARG	THR	conflict	UNP P27348
B	74	ASN	SER	conflict	UNP P27348

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Chain	Residue	Modelled	Actual	Comment	Reference
B	75	GLU	ASP	conflict	UNP P27348
B	78	GLN	LEU	conflict	UNP P27348
B	80	MET	LEU	conflict	UNP P27348
B	81	GLY	ILE	conflict	UNP P27348
B	83	GLU	ASP	conflict	UNP P27348
B	88	ILE	VAL	conflict	UNP P27348
B	90	ALA	SER	conflict	UNP P27348
B	93	GLN	ARG	conflict	UNP P27348
B	94	ASP	SER	conflict	UNP P27348
B	97	ASN	THR	conflict	UNP P27348
B	98	ASP	THR	conflict	UNP P27348
B	109	PRO	ALA	conflict	UNP P27348
B	113	GLN	ASN	conflict	UNP P27348
B	132	SER	ALA	conflict	UNP P27348
B	136	SER	CYS	conflict	UNP P27348
B	139	ASN	ASP	conflict	UNP P27348
B	140	LYS	ARG	conflict	UNP P27348
B	141	GLN	LYS	conflict	UNP P27348
B	142	THR	GLN	conflict	UNP P27348
B	144	VAL	ILE	conflict	UNP P27348
B	145	SER	ASP	conflict	UNP P27348
B	149	GLN	GLY	conflict	UNP P27348
B	156	GLU	ASP	conflict	UNP P27348
B	186	SER	ASN	conflict	UNP P27348
B	189	LYS	LEU	conflict	UNP P27348
B	192	SER	THR	conflict	UNP P27348
B	211	GLU	ASP	conflict	UNP P27348
C	-4	GLY	-	expression tag	UNP P27348
C	-3	ALA	-	expression tag	UNP P27348
C	-2	MET	-	expression tag	UNP P27348
C	-1	GLY	-	expression tag	UNP P27348
C	0	SER	-	expression tag	UNP P27348
C	1	MET	-	expression tag	UNP P27348
C	2	THR	-	expression tag	UNP P27348
C	4	ASP	GLU	conflict	UNP P27348
C	6	SER	THR	conflict	UNP P27348
C	9	VAL	ILE	conflict	UNP P27348
C	26	ALA	THR	conflict	UNP P27348
C	27	ALA	CYS	conflict	UNP P27348
C	36	HIS	ALA	conflict	UNP P27348
C	56	ALA	GLY	conflict	UNP P27348
C	60	SER	ALA	conflict	UNP P27348

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Chain	Residue	Modelled	Actual	Comment	Reference
C	72	GLU	ASP	conflict	UNP P27348
C	73	ARG	THR	conflict	UNP P27348
C	74	ASN	SER	conflict	UNP P27348
C	75	GLU	ASP	conflict	UNP P27348
C	78	GLN	LEU	conflict	UNP P27348
C	80	MET	LEU	conflict	UNP P27348
C	81	GLY	ILE	conflict	UNP P27348
C	83	GLU	ASP	conflict	UNP P27348
C	88	ILE	VAL	conflict	UNP P27348
C	90	ALA	SER	conflict	UNP P27348
C	93	GLN	ARG	conflict	UNP P27348
C	94	ASP	SER	conflict	UNP P27348
C	97	ASN	THR	conflict	UNP P27348
C	98	ASP	THR	conflict	UNP P27348
C	109	PRO	ALA	conflict	UNP P27348
C	113	GLN	ASN	conflict	UNP P27348
C	132	SER	ALA	conflict	UNP P27348
C	136	SER	CYS	conflict	UNP P27348
C	139	ASN	ASP	conflict	UNP P27348
C	140	LYS	ARG	conflict	UNP P27348
C	141	GLN	LYS	conflict	UNP P27348
C	142	THR	GLN	conflict	UNP P27348
C	144	VAL	ILE	conflict	UNP P27348
C	145	SER	ASP	conflict	UNP P27348
C	149	GLN	GLY	conflict	UNP P27348
C	156	GLU	ASP	conflict	UNP P27348
C	186	SER	ASN	conflict	UNP P27348
C	189	LYS	LEU	conflict	UNP P27348
C	192	SER	THR	conflict	UNP P27348
C	211	GLU	ASP	conflict	UNP P27348
D	-4	GLY	-	expression tag	UNP P27348
D	-3	ALA	-	expression tag	UNP P27348
D	-2	MET	-	expression tag	UNP P27348
D	-1	GLY	-	expression tag	UNP P27348
D	0	SER	-	expression tag	UNP P27348
D	1	MET	-	expression tag	UNP P27348
D	2	THR	-	expression tag	UNP P27348
D	4	ASP	GLU	conflict	UNP P27348
D	6	SER	THR	conflict	UNP P27348
D	9	VAL	ILE	conflict	UNP P27348
D	26	ALA	THR	conflict	UNP P27348
D	27	ALA	CYS	conflict	UNP P27348

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Chain	Residue	Modelled	Actual	Comment	Reference
D	36	HIS	ALA	conflict	UNP P27348
D	56	ALA	GLY	conflict	UNP P27348
D	60	SER	ALA	conflict	UNP P27348
D	72	GLU	ASP	conflict	UNP P27348
D	73	ARG	THR	conflict	UNP P27348
D	74	ASN	SER	conflict	UNP P27348
D	75	GLU	ASP	conflict	UNP P27348
D	78	GLN	LEU	conflict	UNP P27348
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D	94	ASP	SER	conflict	UNP P27348
D	97	ASN	THR	conflict	UNP P27348
D	98	ASP	THR	conflict	UNP P27348
D	109	PRO	ALA	conflict	UNP P27348
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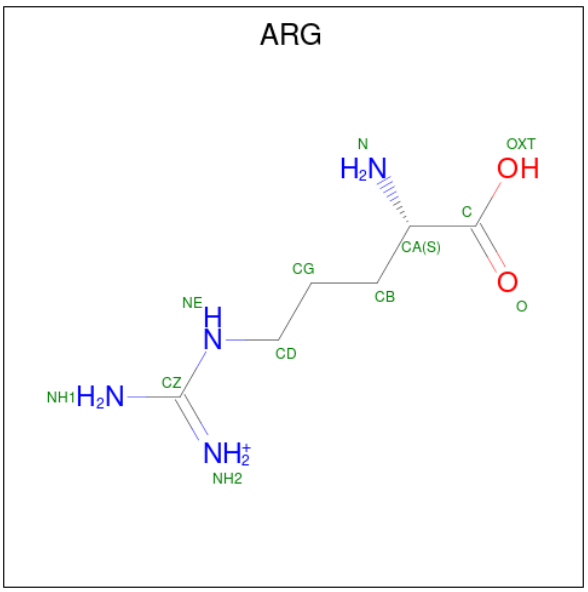
D	132	SER	ALA	conflict	UNP P27348
D	136	SER	CYS	conflict	UNP P27348
D	139	ASN	ASP	conflict	UNP P27348
D	140	LYS	ARG	conflict	UNP P27348
D	141	GLN	LYS	conflict	UNP P27348
D	142	THR	GLN	conflict	UNP P27348
D	144	VAL	ILE	conflict	UNP P27348
D	145	SER	ASP	conflict	UNP P27348
D	149	GLN	GLY	conflict	UNP P27348
D	156	GLU	ASP	conflict	UNP P27348
D	186	SER	ASN	conflict	UNP P27348
D	189	LYS	LEU	conflict	UNP P27348
D	192	SER	THR	conflict	UNP P27348
D	211	GLU	ASP	conflict	UNP P27348

- Molecule 2 is a protein called Cystic fibrosis transmembrane conductance regulator.

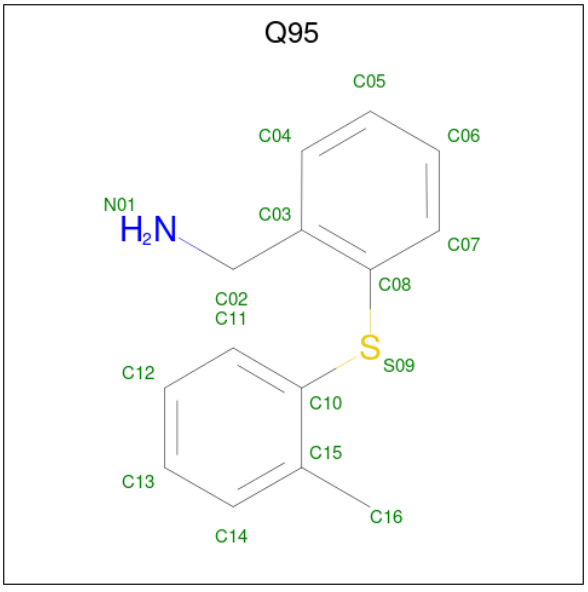
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	F	22	Total	C	N	O	P	S	0	0	0
			171	101	33	34	2	1			
2	E	16	Total	C	N	O	P	S	0	0	0
			118	67	21	27	2	1			

- Molecule 3 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



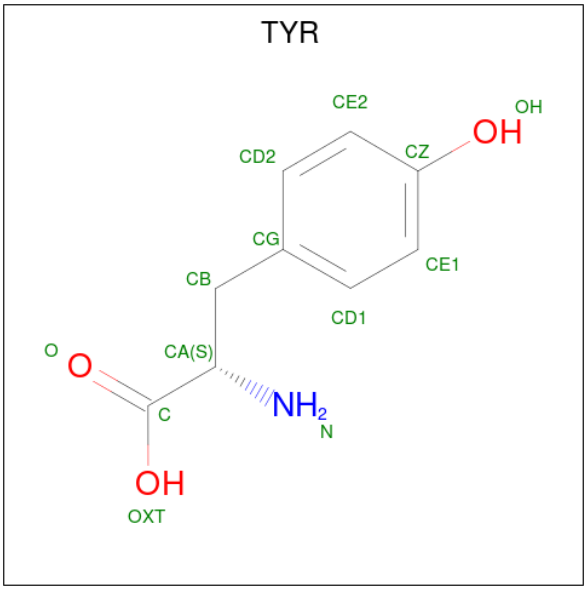
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	6	4	1		
3	B	1	Total	C	N	O	0	0
			11	6	4	1		

- Molecule 4 is [2-(2-methylphenyl)sulfanylphenyl]methanamine (three-letter code: Q95) (formula: $C_{14}H_{15}NS$) (labeled as "Ligand of Interest" by depositor).



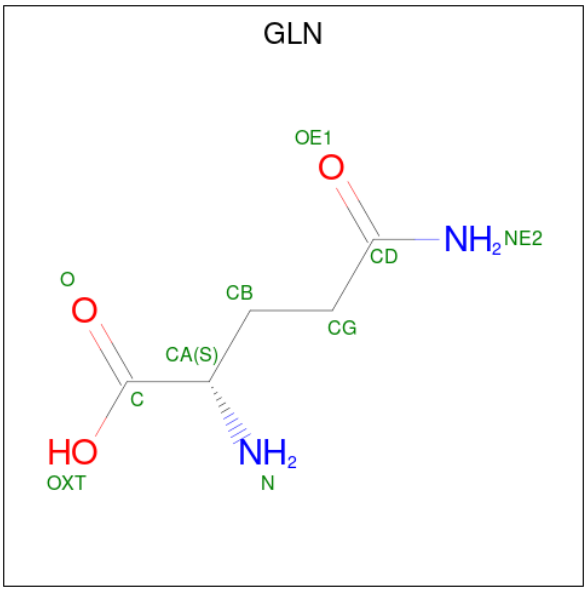
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N S 16 14 1 1	0	0
4	A	1	Total C N S 16 14 1 1	0	0

- Molecule 5 is TYROSINE (three-letter code: TYR) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C N O 12 9 1 2	0	0
5	C	1	Total C N O 12 9 1 2	0	0

- Molecule 6 is GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N O 8 5 2 1	0	0
6	C	1	Total C N O 8 5 2 1	0	0

- Molecule 7 is water.

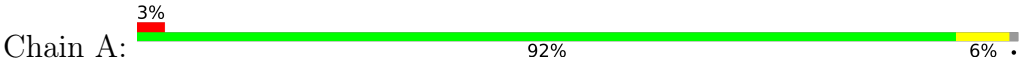
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	142	Total O 142 142	0	0
7	B	162	Total O 162 162	0	0
7	F	13	Total O 13 13	0	0
7	E	9	Total O 9 9	0	0
7	C	108	Total O 108 108	0	0
7	D	105	Total O 105 105	0	0

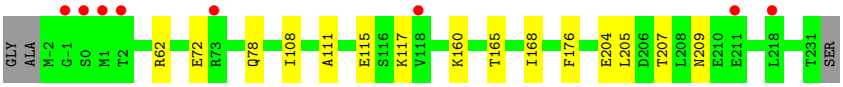
3 Residue-property plots (i)

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: 14-3-3 protein theta

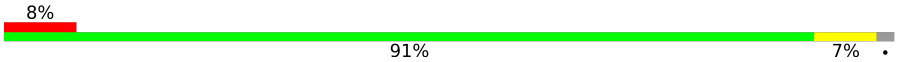
Chain A:





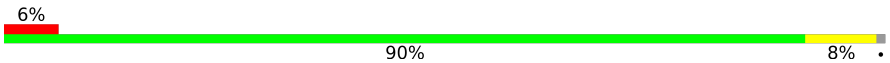
• Molecule 1: 14-3-3 protein theta

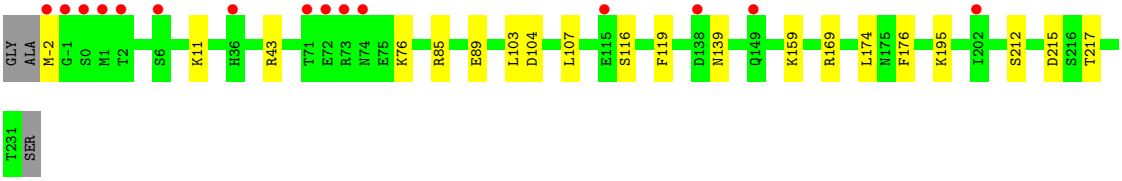
Chain B:



• Molecule 1: 14-3-3 protein theta

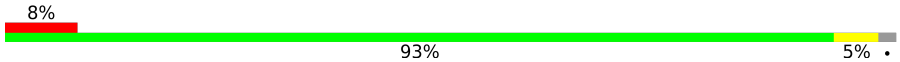
Chain C:

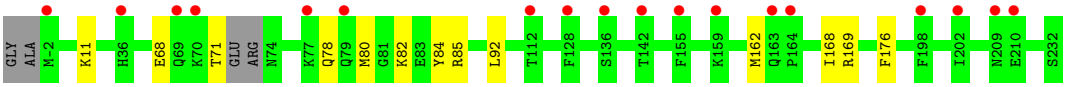




• Molecule 1: 14-3-3 protein theta

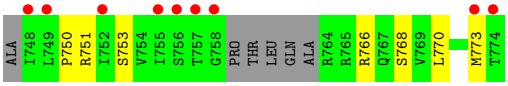
Chain D:





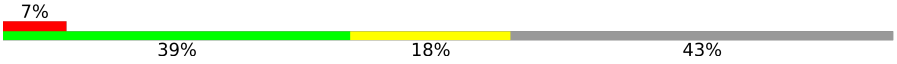
• Molecule 2: Cystic fibrosis transmembrane conductance regulator

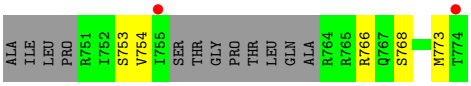
Chain F:



• Molecule 2: Cystic fibrosis transmembrane conductance regulator

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.37Å 111.46Å 130.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.28 – 1.76 56.28 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.9 (56.28-1.76) 99.9 (56.28-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.195 , 0.241 0.195 , 0.241	Depositor DCC
R_{free} test set	5010 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8367	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7486e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SEP, Q95

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	0.37	0/1927	0.50	0/2599
1	B	0.37	0/1885	0.50	0/2539
1	C	0.34	0/1889	0.48	0/2548
1	D	0.33	0/1886	0.47	0/2540
2	E	0.37	0/94	0.59	0/122
2	F	0.39	0/148	0.55	0/194
All	All	0.35	0/7829	0.49	0/10542

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

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	1885	0	1852	8	0
1	B	1850	0	1820	12	0
1	C	1856	0	1815	12	0
1	D	1854	0	1823	8	0
2	E	118	0	97	3	0
2	F	171	0	167	3	0
3	A	11	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	12	0	0
4	A	32	0	0	0	0
5	C	12	0	9	0	0
5	F	12	0	8	1	0
6	C	16	0	10	1	0
7	A	142	0	0	1	0
7	B	162	0	0	5	0
7	C	108	0	0	3	0
7	D	105	0	0	1	0
7	E	9	0	0	0	0
7	F	13	0	0	0	0
All	All	8367	0	7625	40	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 3.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ASP:HA	1:B:218[A]:LEU:HD12	1.73	0.69
1:C:-2:MET:N	7:C:403:HOH:O	2.29	0.64
1:B:143:THR:HG21	7:B:544:HOH:O	1.99	0.62
1:B:185:ASN:ND2	7:B:402:HOH:O	2.30	0.58
1:A:108:ILE:HG23	1:A:117:LYS:HE3	1.87	0.56
1:A:111:ALA:HB3	1:A:117:LYS:HD2	1.89	0.54
1:B:40:ASN:ND2	2:E:773:MET:O	2.30	0.53
1:D:92:LEU:HD21	7:D:309:HOH:O	2.09	0.52
1:D:82:LYS:HG3	1:D:85:ARG:NH2	2.26	0.50
1:C:215:ASP:OD2	1:C:215:ASP:N	2.34	0.49
1:A:207:THR:HB	2:F:770:LEU:O	2.13	0.49
1:C:11:LYS:HE2	1:D:84:TYR:CE1	2.49	0.48
1:A:115:GLU:HG3	1:A:168:ILE:HD12	1.96	0.47
1:D:71:THR:O	1:D:78:GLN:NE2	2.47	0.47
2:E:754:VAL:HG22	1:C:174:LEU:HD23	1.97	0.47
1:D:162:MET:O	1:D:169:ARG:NH1	2.47	0.45
1:C:76:LYS:HA	1:C:76:LYS:HE2	1.98	0.45
1:C:85:ARG:O	1:C:89:GLU:HG3	2.16	0.45
1:B:43:ARG:HH22	2:E:773:MET:HG2	1.81	0.45
1:C:11:LYS:NZ	7:C:406:HOH:O	2.41	0.45
1:D:68:GLU:OE1	1:D:85:ARG:NE	2.33	0.44
1:B:79:GLN:NE2	7:B:410:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LEU:HA	1:B:107:LEU:HB2	2.00	0.44
1:C:159:LYS:NZ	1:C:169:ARG:HH21	2.16	0.44
1:D:80:MET:HE2	1:D:80:MET:HB2	1.87	0.43
1:B:5:LYS:HB3	1:B:5:LYS:HE3	1.68	0.43
1:C:43:ARG:HD2	1:C:119:PHE:CD2	2.53	0.43
1:B:5:LYS:HD2	1:B:42:GLU:OE2	2.19	0.43
1:A:72:GLU:O	1:A:78[A]:GLN:NE2	2.52	0.43
1:C:139:ASN:ND2	7:C:401:HOH:O	2.24	0.43
1:C:217:THR:HG21	6:C:302:GLN:NE2	2.33	0.42
1:B:142:THR:HG23	7:B:449:HOH:O	2.20	0.42
1:A:165:THR:OG1	1:A:204:GLU:OE2	2.21	0.42
1:B:165:THR:HG22	1:B:216:SER:OG	2.19	0.42
1:B:36:HIS:HB2	7:B:516:HOH:O	2.20	0.41
2:F:750:PRO:HB3	5:F:801:TYR:HB3	2.02	0.41
1:A:160:LYS:HD3	1:A:160:LYS:C	2.42	0.40
1:A:62[A]:ARG:NH1	7:A:415:HOH:O	2.55	0.40
2:F:773:MET:HG3	1:D:168:ILE:HD11	2.04	0.40
1:C:103:LEU:HA	1:C:107:LEU:HB2	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	238/237 (100%)	234 (98%)	4 (2%)	0	100	100
1	B	232/237 (98%)	228 (98%)	4 (2%)	0	100	100
1	C	234/237 (99%)	230 (98%)	4 (2%)	0	100	100
1	D	231/237 (98%)	226 (98%)	5 (2%)	0	100	100
2	E	10/28 (36%)	9 (90%)	1 (10%)	0	100	100
2	F	16/28 (57%)	14 (88%)	2 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	961/1004 (96%)	941 (98%)	20 (2%)	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	204/208 (98%)	201 (98%)	3 (2%)	65 49
1	B	199/208 (96%)	198 (100%)	1 (0%)	88 83
1	C	201/208 (97%)	196 (98%)	5 (2%)	47 25
1	D	201/208 (97%)	199 (99%)	2 (1%)	76 63
2	E	9/23 (39%)	8 (89%)	1 (11%)	6 1
2	F	16/23 (70%)	14 (88%)	2 (12%)	4 0
All	All	830/878 (94%)	816 (98%)	14 (2%)	60 42

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	PHE
1	A	205	LEU
1	A	209	ASN
1	B	176	PHE
2	F	751	ARG
2	F	766	ARG
2	E	766	ARG
1	C	104	ASP
1	C	116	SER
1	C	176	PHE
1	C	195	LYS
1	C	212	SER
1	D	11	LYS
1	D	176	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	110	ASN
1	A	149	GLN
1	B	36	HIS
1	B	79	GLN
1	C	69	GLN
1	D	78	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	SEP	E	768	2	8,9,10	1.34	1 (12%)	8,12,14	0.84	0
2	SEP	E	753	2	8,9,10	1.35	1 (12%)	8,12,14	0.77	0
2	SEP	F	753	2	8,9,10	1.43	1 (12%)	8,12,14	1.11	1 (12%)
2	SEP	F	768	2	8,9,10	1.33	1 (12%)	8,12,14	1.08	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	SEP	E	768	2	-	0/5/8/10	-
2	SEP	E	753	2	-	0/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	F	753	2	-	0/5/8/10	-
2	SEP	F	768	2	-	0/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	753	SEP	P-O1P	3.11	1.60	1.50
2	F	768	SEP	P-O1P	2.87	1.59	1.50
2	E	768	SEP	P-O1P	2.81	1.59	1.50
2	E	753	SEP	P-O1P	2.80	1.59	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	753	SEP	O3P-P-O2P	2.22	116.13	107.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	TYR	F	801	6,4	11,12,13	0.61	0	12,15,17	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	TYR	C	303	4	11,12,13	0.56	0	12,15,17	1.41	1 (8%)
3	ARG	A	301	6,4	9,10,11	2.51	3 (33%)	5,11,13	0.76	0
3	ARG	B	301	6,4	9,10,11	2.38	2 (22%)	5,11,13	0.47	0
4	Q95	A	302	5,3	17,17,17	1.00	2 (11%)	22,22,22	1.12	2 (9%)
6	GLN	C	302	3	6,7,9	0.56	0	2,7,11	0.53	0
6	GLN	C	301	5,3	6,7,9	0.44	0	2,7,11	0.25	0
4	Q95	A	303	5,3	17,17,17	1.10	2 (11%)	22,22,22	0.86	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
5	TYR	F	801	6,4	-	1/5/6/8	0/1/1/1
5	TYR	C	303	4	-	0/5/6/8	0/1/1/1
3	ARG	A	301	6,4	-	0/8/9/11	-
3	ARG	B	301	6,4	-	0/8/9/11	-
4	Q95	A	302	5,3	-	2/6/6/6	0/2/2/2
6	GLN	C	302	3	-	3/5/6/9	-
6	GLN	C	301	5,3	-	0/5/6/9	-
4	Q95	A	303	5,3	-	1/6/6/6	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	ARG	CZ-NE	6.33	1.45	1.33
3	A	301	ARG	CZ-NE	6.31	1.45	1.33
3	A	301	ARG	CZ-NH2	3.33	1.45	1.32
4	A	303	Q95	C08-S09	3.03	1.82	1.78
3	B	301	ARG	CZ-NH1	2.72	1.46	1.34
4	A	302	Q95	C10-S09	2.71	1.82	1.78
4	A	303	Q95	C10-S09	2.45	1.82	1.78
4	A	302	Q95	C08-S09	2.40	1.81	1.78
3	A	301	ARG	CZ-NH1	-2.14	1.26	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	303	TYR	CG-CB-CA	-3.65	106.70	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	302	Q95	C16-C15-C10	-2.33	118.81	121.87
4	A	302	Q95	C14-C15-C10	2.07	119.97	117.63

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	801	TYR	O-C-CA-CB
6	C	302	GLN	N-CA-CB-CG
6	C	302	GLN	C-CA-CB-CG
6	C	302	GLN	NE2-CD-CG-CB
4	A	303	Q95	C07-C08-S09-C10
4	A	302	Q95	C07-C08-S09-C10
4	A	302	Q95	N01-C02-C03-C08

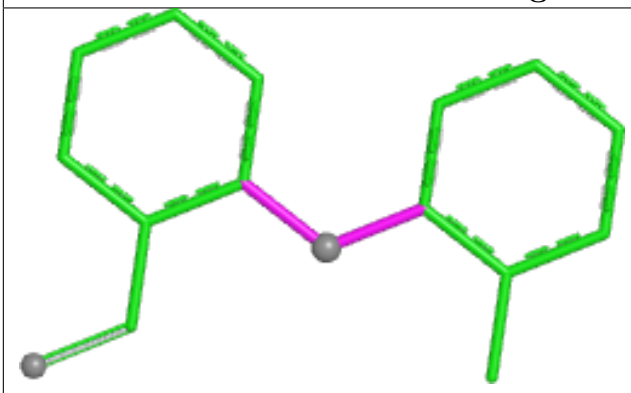
There are no ring outliers.

2 monomers are involved in 2 short contacts:

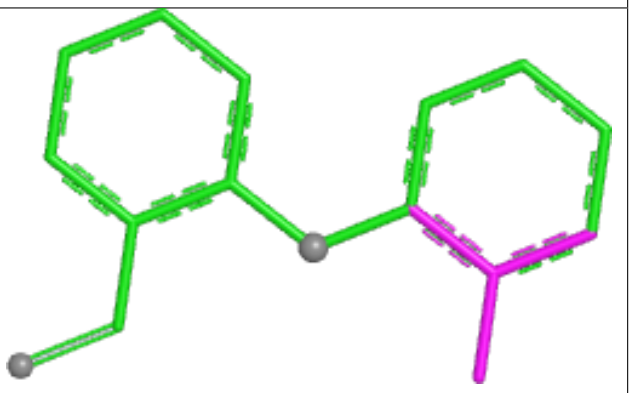
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	801	TYR	1	0
6	C	302	GLN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

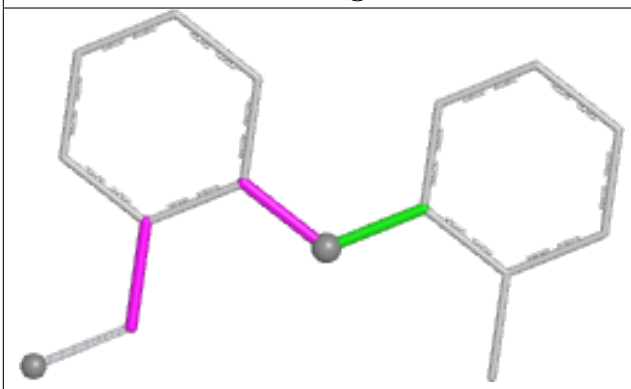
Ligand Q95 A 302



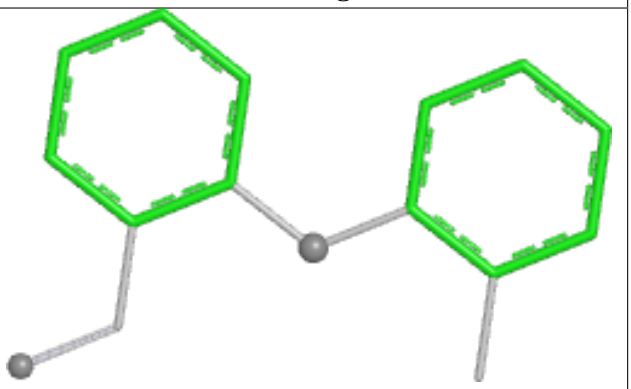
Bond lengths



Bond angles

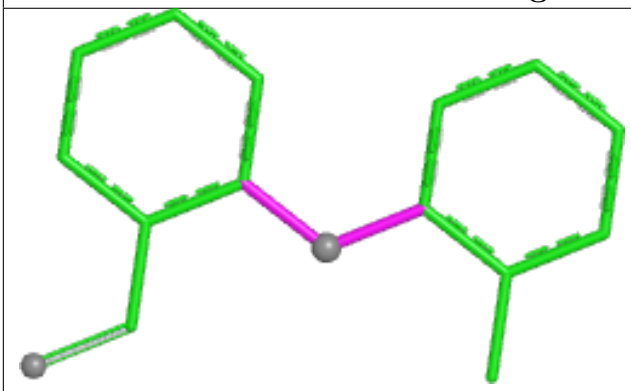


Torsions

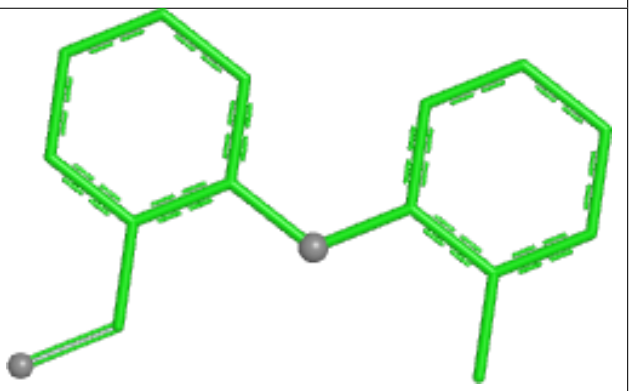


Rings

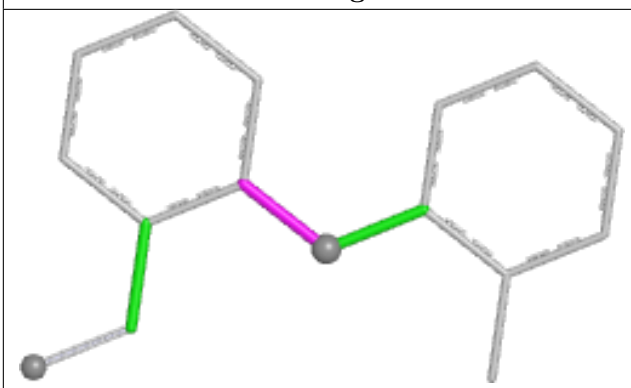
Ligand Q95 A 303



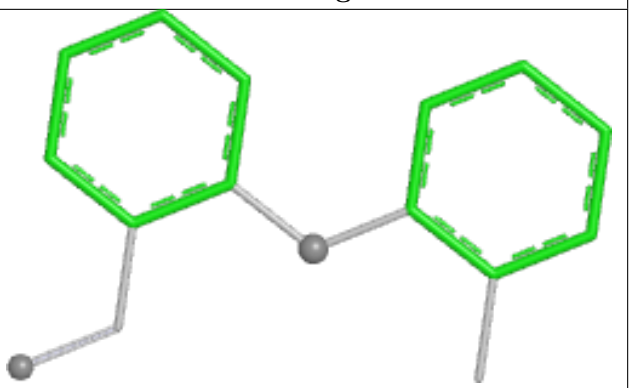
Bond lengths



Bond angles



Torsions



Rings

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	234/237 (98%)	0.67	8 (3%)	45	51	18, 30, 53, 73	0
1	B	232/237 (97%)	0.76	19 (8%)	11	15	20, 31, 55, 78	0
1	C	234/237 (98%)	0.68	15 (6%)	19	25	23, 35, 57, 83	0
1	D	233/237 (98%)	0.81	18 (7%)	13	18	21, 37, 61, 68	0
2	E	14/28 (50%)	1.18	2 (14%)	2	3	25, 40, 58, 64	0
2	F	20/28 (71%)	2.02	9 (45%)	0	0	25, 36, 65, 66	0
All	All	967/1004 (96%)	0.76	71 (7%)	15	20	18, 33, 60, 83	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	748	ILE	12.4
1	B	213	TYR	8.6
1	C	71	THR	5.1
1	B	70	LYS	5.1
1	C	-2	MET	4.9
1	D	-2	MET	4.6
1	A	-1	GLY	4.4
1	B	232	SER	4.3
1	D	79	GLN	4.2
1	C	73	ARG	4.2
1	C	72	GLU	4.2
2	F	774	THR	4.2
1	D	69	GLN	4.1
1	A	1	MET	3.9
1	B	71	THR	3.8
1	A	73	ARG	3.8
2	F	757	THR	3.7
1	C	1	MET	3.7
1	D	202	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	2	THR	3.5
1	C	74	ASN	3.5
2	E	774	THR	3.5
1	D	198	PHE	3.4
2	E	755	ILE	3.4
1	D	163	GLN	3.3
1	A	0	SER	3.3
1	B	211	GLU	3.2
1	B	36	HIS	3.2
1	D	142	THR	3.1
1	B	-2	MET	3.0
1	C	2	THR	3.0
1	D	70	LYS	2.9
2	F	749	LEU	2.9
1	B	72	GLU	2.9
2	F	752	ILE	2.9
1	B	160	LYS	2.8
2	F	758	GLY	2.8
1	D	159	LYS	2.7
1	C	138	ASP	2.7
1	C	0	SER	2.7
2	F	773	MET	2.7
1	C	6	SER	2.7
1	B	214	LYS	2.6
1	B	185	ASN	2.6
1	D	77	LYS	2.6
1	D	36	HIS	2.5
1	B	218[A]	LEU	2.5
1	A	218	LEU	2.5
1	C	202	ILE	2.5
1	B	210	GLU	2.5
1	A	211	GLU	2.4
1	B	76	LYS	2.4
1	B	203	ALA	2.4
1	C	-1	GLY	2.4
1	B	209	ASN	2.4
1	D	155	PHE	2.4
1	D	136	SER	2.4
1	C	149	GLN	2.3
1	D	209	ASN	2.3
1	D	112	THR	2.3
1	C	36	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	212	SER	2.3
1	B	40	ASN	2.2
2	F	756	SER	2.1
1	D	128	PHE	2.1
1	B	194	ALA	2.1
1	D	210	GLU	2.1
2	F	755	ILE	2.1
1	D	164	PRO	2.0
1	C	115	GLU	2.0
1	A	118	VAL	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SEP	F	768	10/11	0.96	0.10	21,24,26,28	0
2	SEP	E	753	10/11	0.96	0.11	23,26,37,43	0
2	SEP	F	753	10/11	0.97	0.12	19,21,26,26	0
2	SEP	E	768	10/11	0.98	0.12	21,22,26,29	0

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	TYR	C	303	12/13	0.75	0.21	35,40,43,46	0
4	Q95	A	303	16/16	0.78	0.27	27,36,43,47	0
6	GLN	C	301	8/10	0.79	0.17	34,37,45,51	0
3	ARG	B	301	11/12	0.82	0.25	37,46,48,51	0

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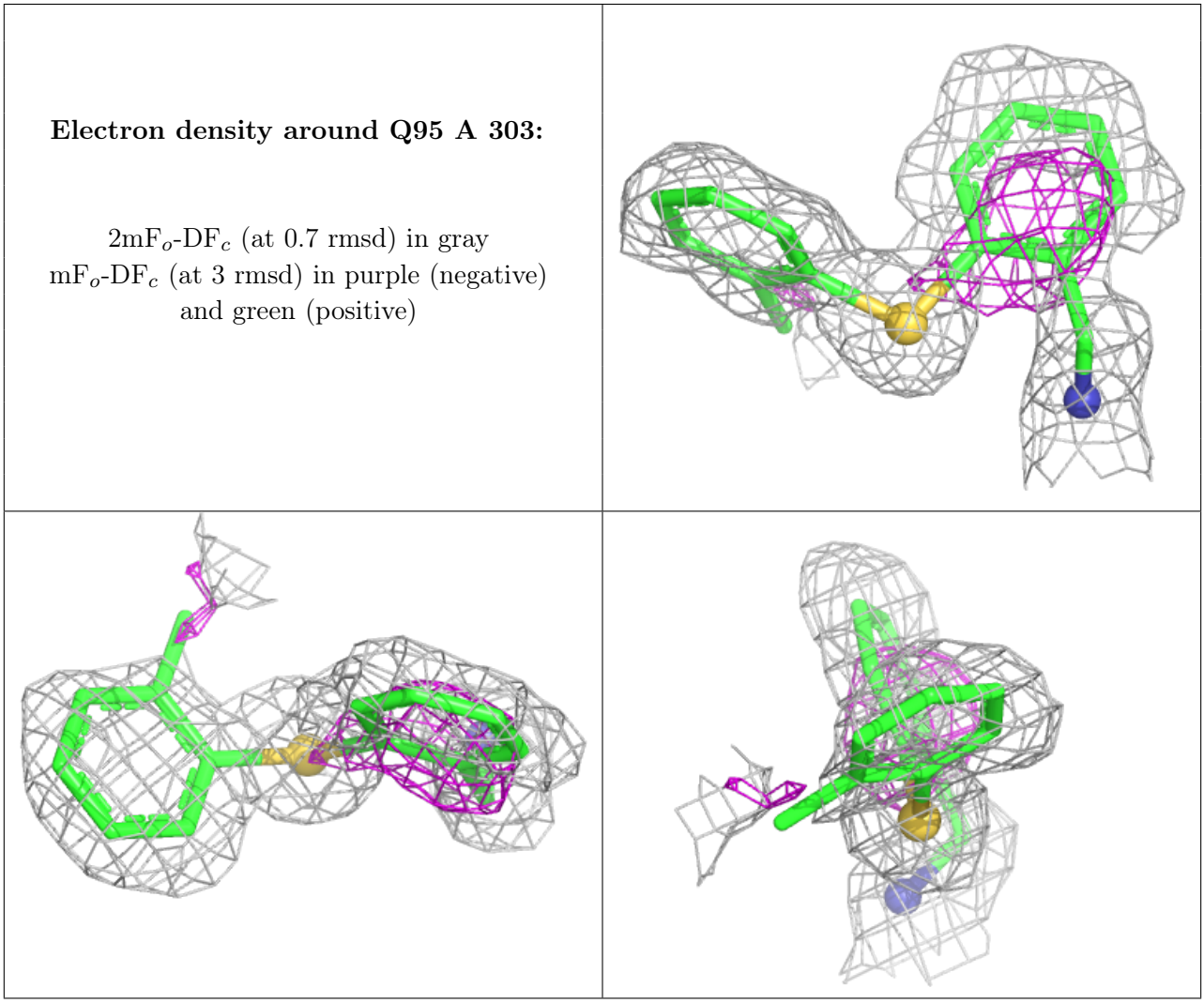
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ARG	A	301	11/12	0.86	0.13	30,39,50,52	0
5	TYR	F	801	12/13	0.88	0.19	31,34,42,47	0
4	Q95	A	302	16/16	0.90	0.14	25,28,31,31	0
6	GLN	C	302	8/10	0.90	0.18	42,47,55,59	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

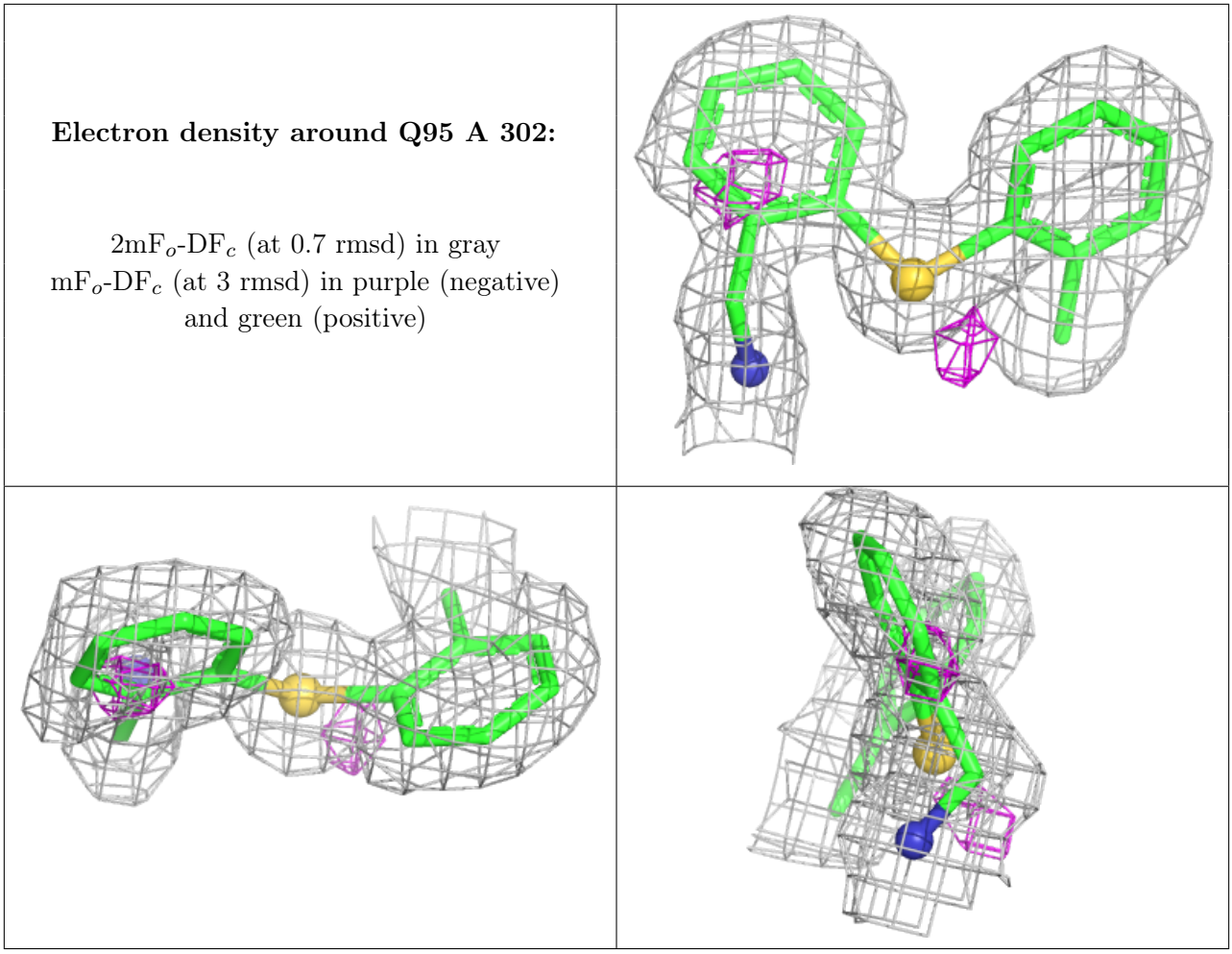
Electron density around Q95 A 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Q95 A 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.