Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 10:31 pm BST

PDB ID	:	8BU6
Title	:	Structure of DDB1 bound to DS55-engaged CDK12-cyclin K
Authors	:	Kozicka, Z.; Kempf, G.; Focht, V.; Thoma, N.H.
Deposited on	:	2022-11-30
Resolution	:	3.45 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 (i) 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 (i)) were used in the production of this report:

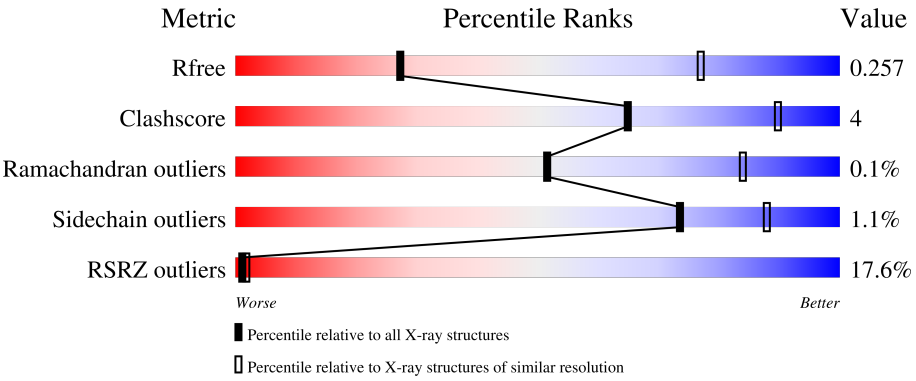
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	840	18% 85% 13% ·
1	D	840	16% 88% 10% ·
1	G	840	18% 88% 11% ·
2	B	344	17% 78% 15% · 6%
2	E	344	19% 79% 15% · 6%

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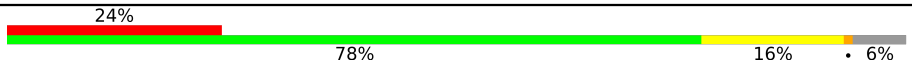
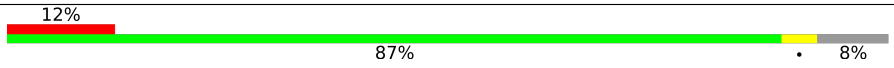
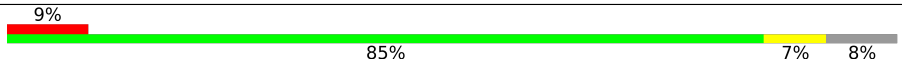
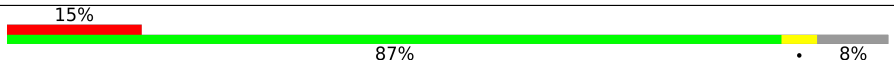
Mol	Chain	Length	Quality of chain
2	H	344	
3	C	271	
3	F	271	
3	I	271	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 67260 atoms, of which 33551 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	G	826	Total	C	H	N	O	S	6449	0	0
			12936	4105	6449	1094	1252	36			
1	D	827	Total	C	H	N	O	S	6462	0	0
			12957	4111	6462	1095	1253	36			
1	A	826	Total	C	H	N	O	S	6452	0	0
			12938	4106	6452	1093	1251	36			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	GLY	-	expression tag	UNP Q16531
G	-2	GLY	-	expression tag	UNP Q16531
G	-1	GLY	-	expression tag	UNP Q16531
G	0	ARG	-	expression tag	UNP Q16531
G	700	GLY	-	linker	UNP Q16531
G	701	ASN	-	linker	UNP Q16531
G	702	GLY	-	linker	UNP Q16531
G	703	ASN	-	linker	UNP Q16531
G	704	SER	-	linker	UNP Q16531
G	705	GLY	-	linker	UNP Q16531
G	706	GLU	-	linker	UNP Q16531
G	707	ILE	-	linker	UNP Q16531
G	708	GLN	-	linker	UNP Q16531
D	-3	GLY	-	expression tag	UNP Q16531
D	-2	GLY	-	expression tag	UNP Q16531
D	-1	GLY	-	expression tag	UNP Q16531
D	0	ARG	-	expression tag	UNP Q16531
D	700	GLY	-	linker	UNP Q16531
D	701	ASN	-	linker	UNP Q16531
D	702	GLY	-	linker	UNP Q16531
D	703	ASN	-	linker	UNP Q16531
D	704	SER	-	linker	UNP Q16531
D	705	GLY	-	linker	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
D	706	GLU	-	linker	UNP Q16531
D	707	ILE	-	linker	UNP Q16531
D	708	GLN	-	linker	UNP Q16531
A	-3	GLY	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531
A	700	GLY	-	linker	UNP Q16531
A	701	ASN	-	linker	UNP Q16531
A	702	GLY	-	linker	UNP Q16531
A	703	ASN	-	linker	UNP Q16531
A	704	SER	-	linker	UNP Q16531
A	705	GLY	-	linker	UNP Q16531
A	706	GLU	-	linker	UNP Q16531
A	707	ILE	-	linker	UNP Q16531
A	708	GLN	-	linker	UNP Q16531

- Molecule 2 is a protein called Cyclin-dependent kinase 12.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	H	324	Total	C	H	N	O	P	S	2657	0	0
			5297	1692	2657	446	485	1	16			
2	E	324	Total	C	H	N	O	P	S	2658	0	0
			5298	1692	2658	446	485	1	16			
2	B	325	Total	C	H	N	O	P	S	2663	0	0
			5309	1695	2663	447	486	1	17			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	709	GLY	-	expression tag	UNP Q9NYV4
H	710	GLY	-	expression tag	UNP Q9NYV4
H	711	GLY	-	expression tag	UNP Q9NYV4
H	965	ARG	LYS	engineered mutation	UNP Q9NYV4
H	1052	GLN	-	expression tag	UNP Q9NYV4
E	709	GLY	-	expression tag	UNP Q9NYV4
E	710	GLY	-	expression tag	UNP Q9NYV4
E	711	GLY	-	expression tag	UNP Q9NYV4
E	965	ARG	LYS	engineered mutation	UNP Q9NYV4
E	1052	GLN	-	expression tag	UNP Q9NYV4
B	709	GLY	-	expression tag	UNP Q9NYV4
B	710	GLY	-	expression tag	UNP Q9NYV4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	711	GLY	-	expression tag	UNP Q9NYV4
B	965	ARG	LYS	engineered mutation	UNP Q9NYV4
B	1052	GLN	-	expression tag	UNP Q9NYV4

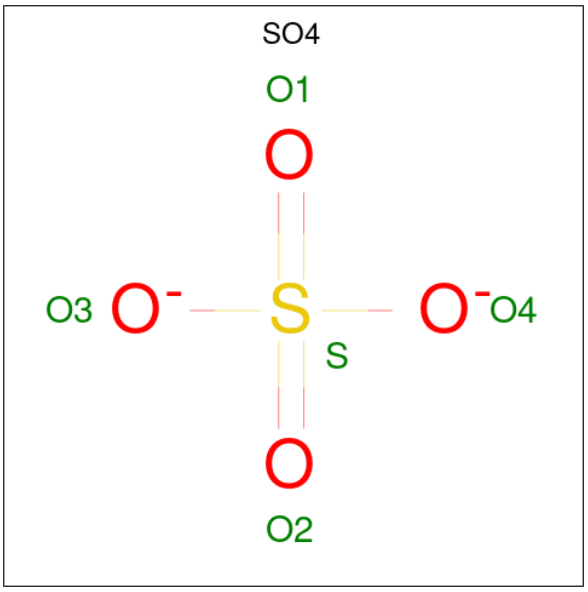
- Molecule 3 is a protein called Cyclin-K.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	I	248	Total	C	H	N	O	S	2048	0	0
			4111	1341	2048	346	363	13			
3	F	248	Total	C	H	N	O	S	2048	0	0
			4111	1341	2048	346	363	13			
3	C	248	Total	C	H	N	O	S	2048	0	0
			4111	1341	2048	346	363	13			

There are 12 discrepancies between the modelled and reference sequences:

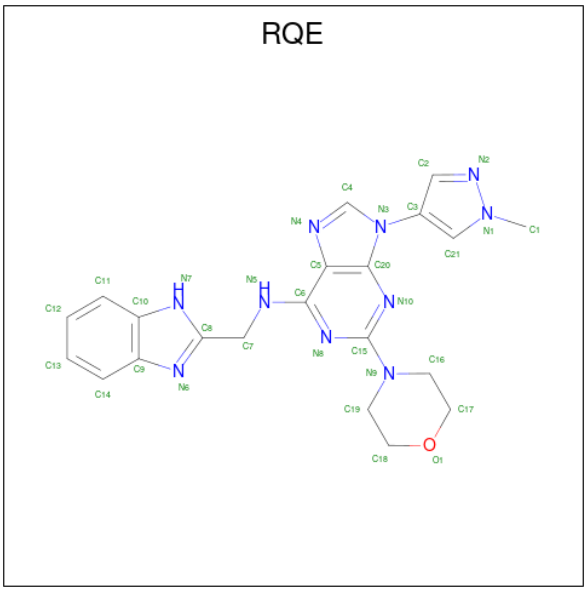
Chain	Residue	Modelled	Actual	Comment	Reference
I	-3	GLY	-	expression tag	UNP O75909
I	-2	GLY	-	expression tag	UNP O75909
I	-1	GLY	-	expression tag	UNP O75909
I	0	ARG	-	expression tag	UNP O75909
F	-3	GLY	-	expression tag	UNP O75909
F	-2	GLY	-	expression tag	UNP O75909
F	-1	GLY	-	expression tag	UNP O75909
F	0	ARG	-	expression tag	UNP O75909
C	-3	GLY	-	expression tag	UNP O75909
C	-2	GLY	-	expression tag	UNP O75909
C	-1	GLY	-	expression tag	UNP O75909
C	0	ARG	-	expression tag	UNP O75909

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0

- Molecule 5 is {N}-(1 {H}-benzimidazol-2-ylmethyl)-9-(1-methylpyrazol-4-yl)-2-morpholin-4-yl-purin-6-amine (three-letter code: RQE) (formula: $C_{21}H_{22}N_{10}O$) (labeled as "Ligand of Interest" by depositor).



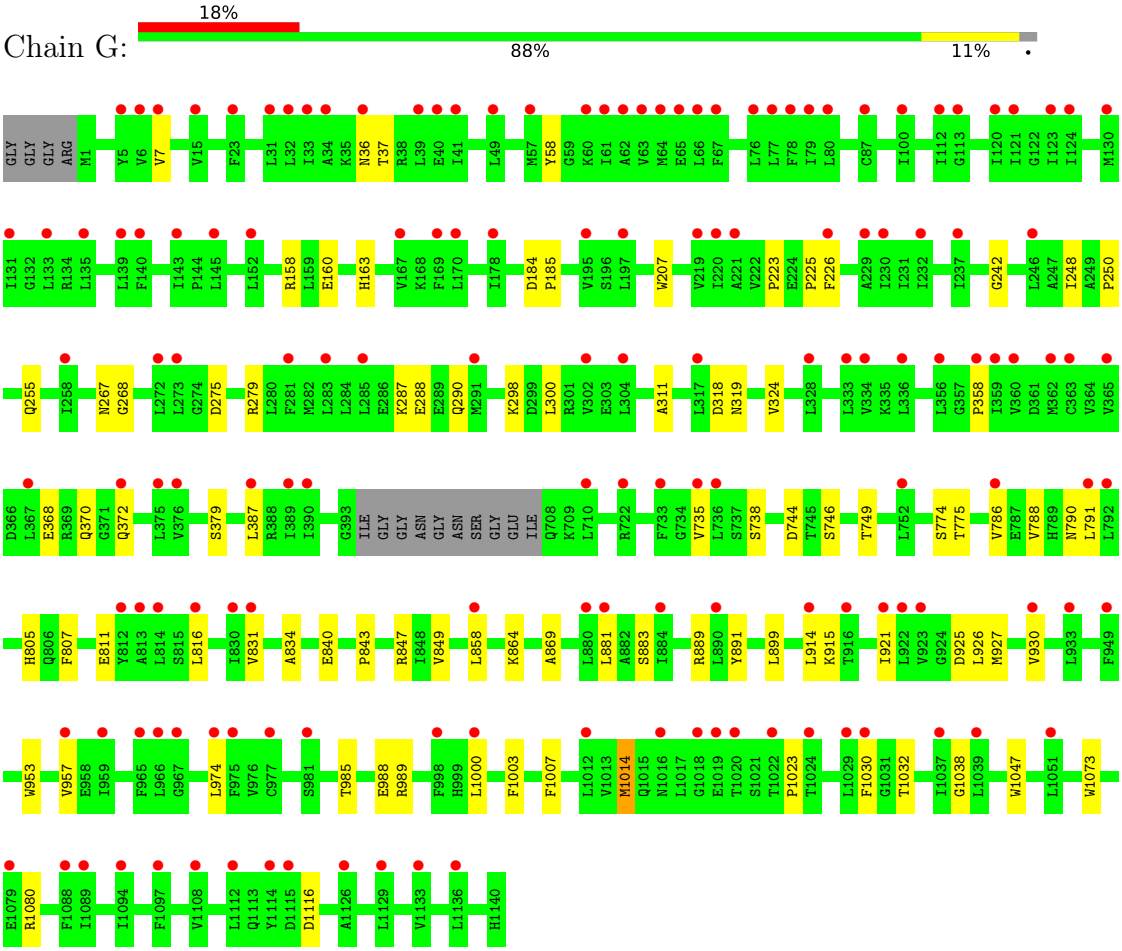
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	H	1	Total	C	H	N	O	22	0
			54	21	22	10	1		
5	E	1	Total	C	H	N	O	22	0
			54	21	22	10	1		
5	B	1	Total	C	H	N	O	22	0
			54	21	22	10	1		

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.

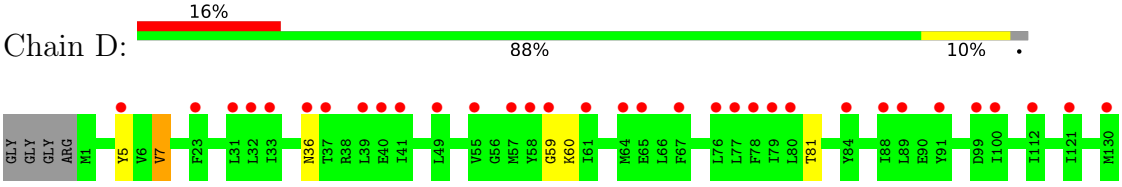
• Molecule 1: DNA damage-binding protein 1

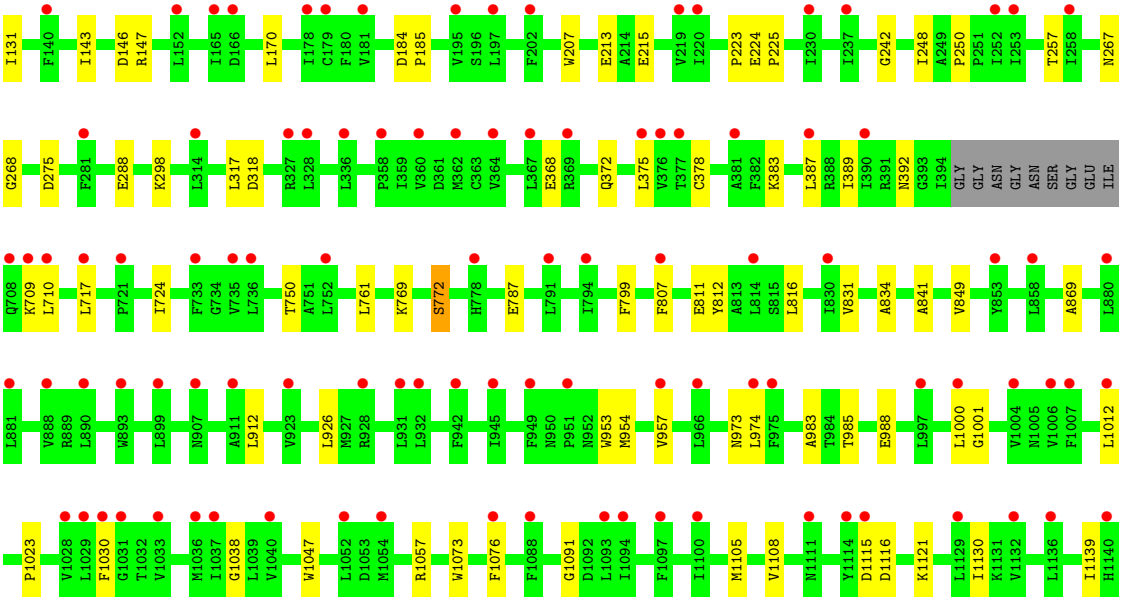
Chain G:



• Molecule 1: DNA damage-binding protein 1

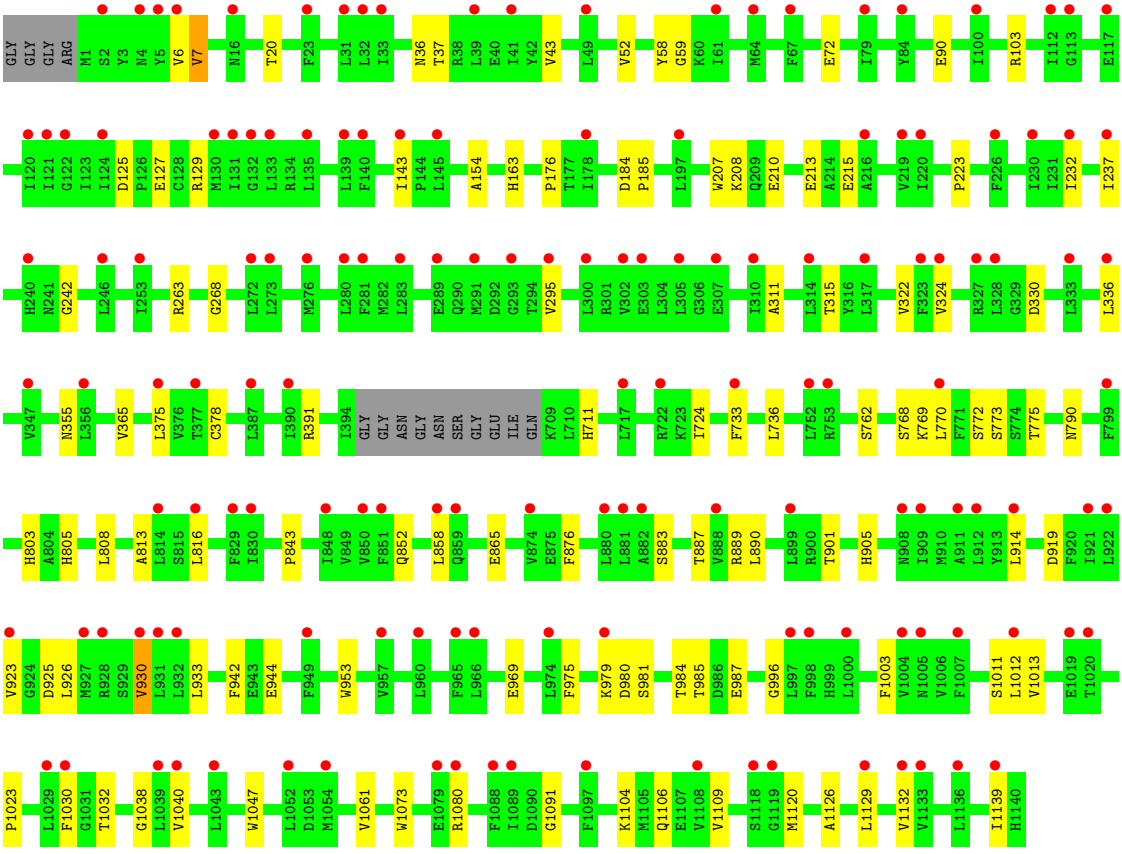
Chain D:





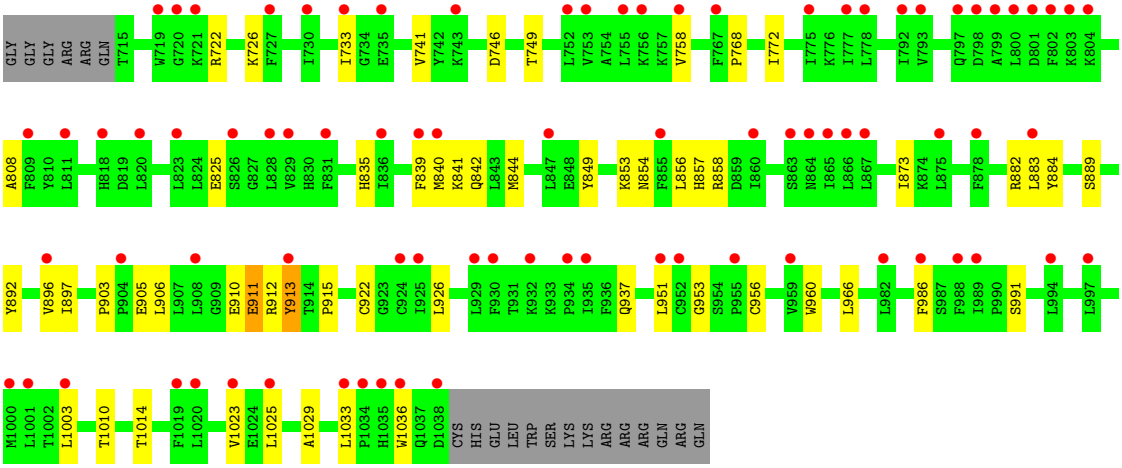
• Molecule 1: DNA damage-binding protein 1

Chain A:



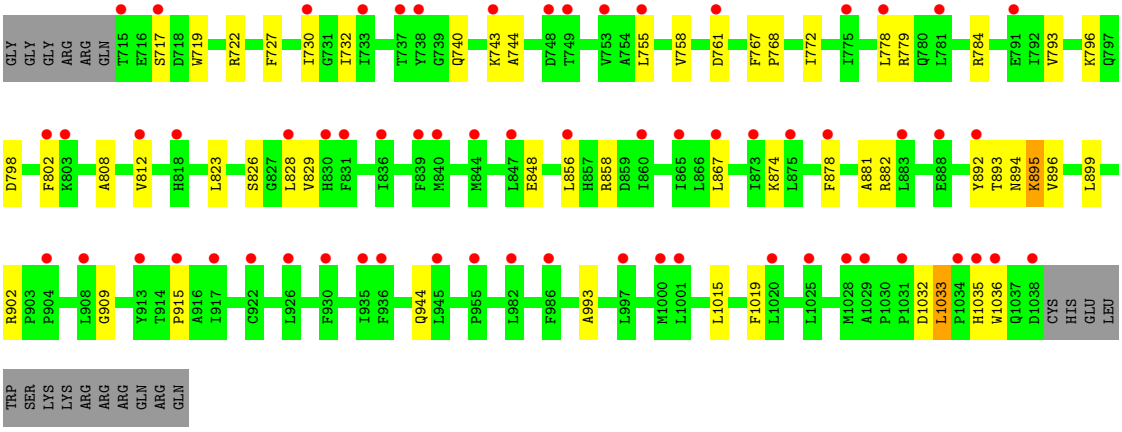
• Molecule 2: Cyclin-dependent kinase 12

Chain H:



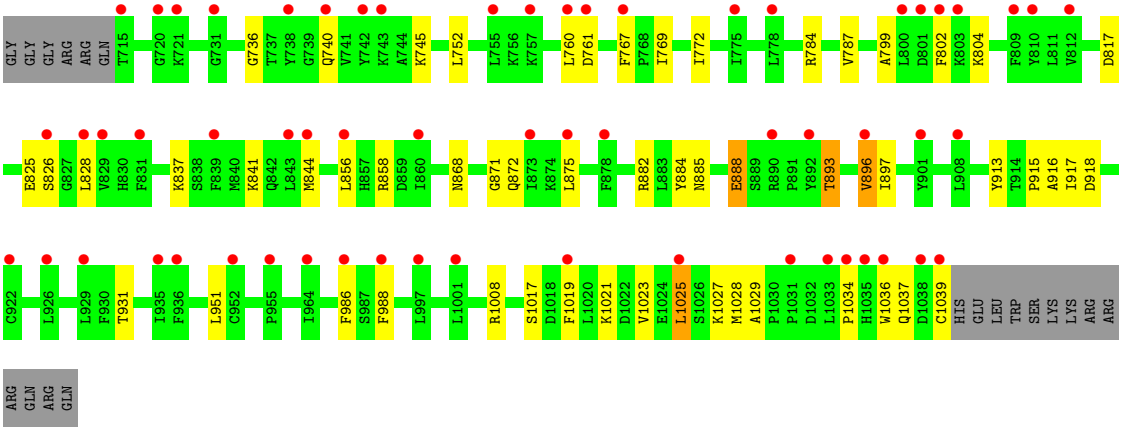
• Molecule 2: Cyclin-dependent kinase 12

Chain E:



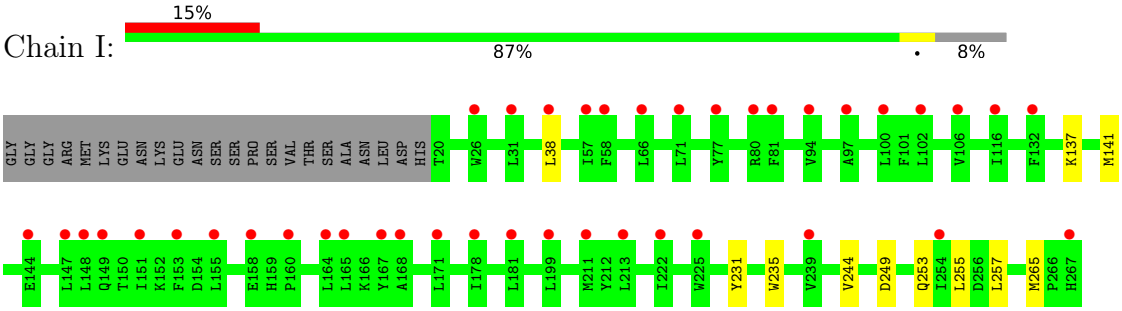
• Molecule 2: Cyclin-dependent kinase 12

Chain B:



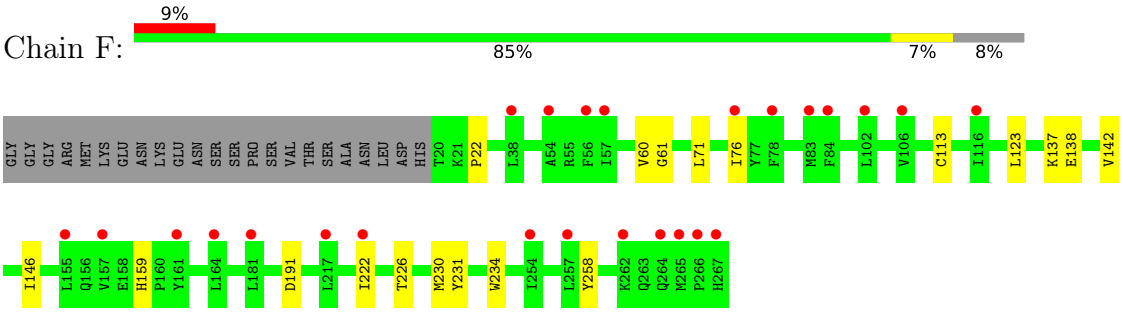
• Molecule 3: Cyclin-K

Chain I:



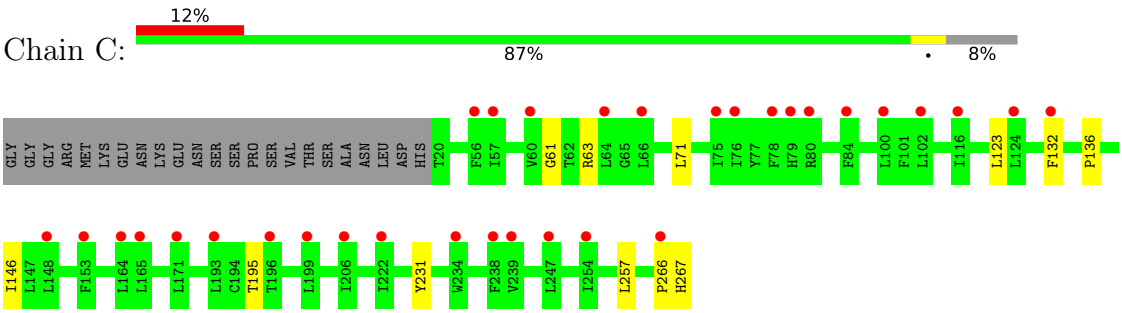
• Molecule 3: Cyclin-K

Chain F:



• Molecule 3: Cyclin-K

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	249.27Å 249.27Å 220.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.68 – 3.45 215.88 – 3.45	Depositor EDS
% Data completeness (in resolution range)	73.8 (60.68-3.45) 73.9 (215.88-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.218 , 0.249 0.233 , 0.257	Depositor DCC
R_{free} test set	3856 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	139.6	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 101.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.067 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	67260	wwPDB-VP
Average B, all atoms (Å^2)	165.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: SO4, TPO, RQE

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	0.33	0/6603	0.60	0/8930
1	D	0.33	0/6612	0.60	0/8942
1	G	0.33	0/6604	0.61	0/8931
2	B	0.39	1/2693 (0.0%)	0.62	1/3630 (0.0%)
2	E	0.34	0/2687	0.61	0/3622
2	H	0.34	0/2687	0.60	0/3622
3	C	0.33	0/2120	0.56	0/2868
3	F	0.34	0/2120	0.56	0/2868
3	I	0.33	0/2120	0.56	0/2868
All	All	0.34	1/34246 (0.0%)	0.60	1/46281 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	888	GLU	CG-CD	-6.75	1.41	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	888	GLU	CG-CD-OE2	-5.71	106.88	118.30

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	6486	6452	6454	67	0
1	D	6495	6462	6464	48	1
1	G	6487	6449	6451	48	0
2	B	2646	2663	2663	33	1
2	E	2640	2658	2658	30	0
2	H	2640	2657	2657	34	0
3	C	2063	2048	2048	7	0
3	F	2063	2048	2048	11	0
3	I	2063	2048	2048	5	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
4	F	10	0	0	0	0
4	G	5	0	0	0	0
4	I	5	0	0	0	0
5	B	32	22	0	0	0
5	E	32	22	0	0	0
5	H	32	22	0	0	0
All	All	33709	33551	33491	274	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 4.

All (274) 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)
2:B:858:ARG:NH2	2:B:893:TPO:O1P	2.04	0.89
2:E:829:VAL:HG12	2:E:1033:LEU:HD12	1.55	0.88
2:B:828:LEU:HB3	2:B:1034:PRO:HG3	1.68	0.76
2:H:835:HIS:HD2	2:H:1029:ALA:HB1	1.49	0.75
1:A:7:VAL:HG13	1:A:1091:GLY:HA3	1.71	0.73
2:B:784:ARG:HH21	2:B:872:GLN:HG3	1.56	0.70
1:D:985:THR:HB	1:D:988:GLU:HG2	1.73	0.69
2:E:823:LEU:HB3	2:E:829:VAL:HG11	1.74	0.68
1:A:7:VAL:HG21	1:A:1139:ILE:HD11	1.74	0.68
1:D:983:ALA:HB3	1:D:988:GLU:HG3	1.78	0.66
1:A:773:SER:O	1:A:775:THR:N	2.28	0.64
2:E:826:SER:HB2	2:E:828:LEU:HD12	1.78	0.64
2:H:906:LEU:HD21	2:H:913:TYR:CD2	2.33	0.63
1:A:1109:VAL:HG12	1:A:1129:LEU:HD12	1.82	0.62
2:H:906:LEU:HD21	2:H:913:TYR:HD2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:856:LEU:HG	2:H:884:TYR:HB2	1.81	0.62
1:D:387:LEU:HG	1:D:717:LEU:HD11	1.83	0.61
2:H:910:GLU:O	2:H:912:ARG:N	2.31	0.60
1:A:768:SER:HB3	1:A:808:LEU:HD11	1.82	0.60
1:A:773:SER:C	1:A:775:THR:H	2.05	0.60
1:D:912:LEU:HD11	1:D:926:LEU:HD13	1.84	0.59
1:G:925:ASP:OD1	1:G:926:LEU:N	2.36	0.59
3:F:191:ASP:OD2	3:F:258:TYR:OH	2.12	0.59
2:H:841:LYS:HD2	2:H:1023:VAL:HB	1.85	0.58
1:D:1115:ASP:OD2	1:D:1121:LYS:NZ	2.37	0.57
1:A:1109:VAL:HG11	1:A:1126:ALA:HA	1.86	0.57
2:B:931:THR:HG22	2:B:988:PHE:HZ	1.69	0.57
1:A:43:VAL:HG23	1:A:52:VAL:HG21	1.86	0.57
1:G:883:SER:HB3	1:G:914:LEU:HD11	1.87	0.56
1:D:7:VAL:HG13	1:D:1091:GLY:HA3	1.87	0.56
1:G:775:THR:O	1:G:775:THR:HG22	2.06	0.56
1:A:883:SER:HB3	1:A:914:LEU:HD11	1.87	0.55
1:G:207:TRP:HB3	1:G:242:GLY:HA2	1.89	0.55
2:E:1032:ASP:C	2:E:1033:LEU:HD13	2.26	0.55
2:H:856:LEU:HD21	2:H:915:PRO:HG3	1.87	0.55
1:D:213:GLU:HG2	1:D:215:GLU:H	1.72	0.55
2:B:951:LEU:HD21	2:B:986:PHE:HE2	1.70	0.55
2:H:839:PHE:HA	2:H:873:ILE:HD13	1.88	0.54
3:F:113:CYS:HB3	3:F:137:LYS:HE3	1.89	0.54
1:A:770:LEU:HD21	1:A:865:GLU:HB2	1.90	0.54
2:B:856:LEU:HD22	2:B:915:PRO:HA	1.89	0.54
1:A:223:PRO:HG3	1:A:263:ARG:HH11	1.72	0.54
1:G:387:LEU:HD11	1:G:735:VAL:HG21	1.90	0.53
2:B:841:LYS:HD2	2:B:1023:VAL:HB	1.90	0.53
2:H:951:LEU:HD21	2:H:986:PHE:HE2	1.73	0.53
1:G:318:ASP:OD1	1:G:319:ASN:N	2.41	0.53
1:A:1023:PRO:HB3	1:A:1047:TRP:CE2	2.44	0.53
2:E:1033:LEU:HD22	2:E:1033:LEU:H	1.74	0.52
1:D:60:LYS:O	1:D:81:THR:HA	2.09	0.52
1:D:207:TRP:HB3	1:D:242:GLY:HA2	1.92	0.52
1:A:925:ASP:OD1	1:A:926:LEU:N	2.43	0.52
2:B:841:LYS:HD3	2:B:1025:LEU:HD13	1.91	0.52
1:G:248:ILE:HG12	1:G:250:PRO:HD3	1.90	0.52
1:A:843:PRO:HD3	2:B:1036:TRP:CD1	2.45	0.52
2:H:892:TYR:HB2	2:H:911:GLU:O	2.10	0.52
1:G:255:GLN:HB2	1:G:279:ARG:HH22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:842:GLN:CG	2:H:1025:LEU:HD11	2.41	0.51
2:E:732:ILE:HG23	2:E:732:ILE:O	2.11	0.51
2:H:858:ARG:HE	2:H:896:VAL:HG11	1.76	0.50
3:C:132:PHE:HB3	3:C:136:PRO:HB3	1.94	0.50
1:D:926:LEU:O	1:D:953:TRP:HA	2.11	0.50
1:D:1105:MET:SD	1:D:1130:ILE:HD11	2.51	0.50
1:A:979:LYS:O	1:A:981:SER:N	2.37	0.50
2:B:817:ASP:HB2	2:B:868:ASN:HA	1.92	0.50
1:D:709:LYS:HG2	1:D:710:LEU:N	2.27	0.50
3:F:222:ILE:O	3:F:226:THR:HG23	2.12	0.50
1:A:985:THR:HG22	1:A:987:GLU:H	1.76	0.49
1:A:736:LEU:HG	1:A:816:LEU:HD22	1.93	0.49
1:D:974:LEU:HD11	1:D:1000:LEU:HD22	1.94	0.49
1:G:816:LEU:HD13	1:G:831:VAL:HG22	1.95	0.49
2:H:858:ARG:HB3	2:H:896:VAL:HG11	1.93	0.49
1:A:887:THR:HA	1:A:905:HIS:O	2.12	0.49
2:E:1033:LEU:HD22	2:E:1033:LEU:N	2.27	0.49
1:A:36:ASN:O	1:A:37:THR:OG1	2.23	0.49
1:G:881:LEU:HD21	1:G:921:ILE:HG21	1.95	0.49
2:H:857:HIS:O	2:H:858:ARG:HB2	2.13	0.48
2:B:769:ILE:HA	2:B:772:ILE:HD12	1.95	0.48
1:G:58:TYR:HB3	1:G:1073:TRP:HB2	1.95	0.48
1:G:1023:PRO:HB3	1:G:1047:TRP:CE2	2.47	0.48
2:B:826:SER:HB2	2:B:828:LEU:HD12	1.94	0.48
1:D:224:GLU:N	1:D:225:PRO:HD2	2.29	0.48
1:D:834:ALA:HB2	1:D:869:ALA:HA	1.96	0.48
2:E:796:LYS:HE3	2:E:798:ASP:HB3	1.96	0.48
2:H:844:MET:HE3	2:H:922:CYS:HB3	1.95	0.48
2:E:758:VAL:O	2:E:808:ALA:HB1	2.13	0.48
1:A:213:GLU:HG2	1:A:215:GLU:H	1.78	0.48
2:E:717:SER:OG	3:F:22:PRO:HB3	2.14	0.48
2:E:856:LEU:HD11	2:E:915:PRO:HG3	1.96	0.48
1:D:372:GLN:NE2	1:D:392:ASN:O	2.47	0.47
1:A:762:SER:O	1:A:803:HIS:HA	2.14	0.47
2:H:768:PRO:O	2:H:772:ILE:HG13	2.14	0.47
1:D:389:ILE:HG12	1:D:799:PHE:CZ	2.49	0.47
1:A:90:GLU:HB2	1:A:103:ARG:HD2	1.95	0.47
2:E:758:VAL:HG11	2:E:767:PHE:CZ	2.49	0.47
1:D:1116:ASP:OD1	1:D:1116:ASP:O	2.32	0.47
2:B:799:ALA:HB1	2:B:804:LYS:HD2	1.95	0.47
1:A:223:PRO:HD2	1:A:268:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:917:ILE:HG13	2:B:918:ASP:N	2.30	0.47
2:H:842:GLN:HG2	2:H:1025:LEU:HD11	1.96	0.47
1:A:43:VAL:HG23	1:A:52:VAL:CG2	2.45	0.47
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.97	0.47
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.45	0.47
1:A:207:TRP:HB3	1:A:242:GLY:HA2	1.97	0.47
1:A:1061:VAL:HG11	1:A:1104:LYS:HB3	1.97	0.47
1:G:864:LYS:NZ	1:G:899:LEU:O	2.35	0.47
1:D:288:GLU:HB2	1:D:298:LYS:HB2	1.97	0.46
1:G:36:ASN:O	1:G:37:THR:OG1	2.27	0.46
2:B:916:ALA:HB1	2:B:1008:ARG:HD2	1.97	0.46
1:G:184:ASP:HB2	1:G:185:PRO:CD	2.45	0.46
2:H:897:ILE:HD12	2:H:903:PRO:HD3	1.96	0.46
2:E:722:ARG:HB3	2:E:793:VAL:HG12	1.96	0.46
2:E:1033:LEU:HD13	2:E:1033:LEU:N	2.30	0.46
2:H:858:ARG:HH11	2:H:882:ARG:HB2	1.79	0.46
1:D:841:ALA:O	2:E:1036:TRP:HB3	2.14	0.46
1:A:365:VAL:HG11	1:A:733:PHE:CZ	2.51	0.46
2:H:960:TRP:CZ2	2:H:966:LEU:HD11	2.51	0.46
2:E:993:ALA:HB2	2:E:1019:PHE:CE1	2.51	0.46
2:H:854:ASN:O	2:H:883:LEU:HD12	2.14	0.46
3:I:38:LEU:HB2	1:D:750:THR:HG21	1.98	0.46
2:E:802:PHE:HB3	3:F:146:ILE:HD11	1.97	0.46
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.50	0.46
1:A:736:LEU:HD13	1:A:813:ALA:HB1	1.98	0.46
2:B:745:LYS:HB2	2:B:752:LEU:HD23	1.98	0.46
1:G:368:GLU:OE1	1:G:370:GLN:NE2	2.49	0.46
2:E:858:ARG:NH1	2:E:882:ARG:HG3	2.30	0.46
1:G:974:LEU:HD11	1:G:1000:LEU:HD22	1.98	0.45
2:H:733:ILE:HD11	2:H:741:VAL:CG1	2.46	0.45
1:D:769:LYS:O	1:D:772:SER:HB2	2.16	0.45
1:G:311:ALA:HB2	1:G:324:VAL:HG13	1.97	0.45
1:G:791:LEU:HD23	1:G:858:LEU:HD21	1.98	0.45
1:A:1047:TRP:HZ3	1:A:1132:VAL:HG13	1.80	0.45
2:B:736:GLY:H	2:B:740:GLN:HA	1.81	0.45
3:C:63:ARG:HE	3:C:123:LEU:HD21	1.81	0.45
2:H:746:ASP:HB3	2:H:749:THR:O	2.16	0.45
1:D:7:VAL:HG21	1:D:1139:ILE:HD11	1.98	0.45
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.52	0.45
1:A:1080:ARG:HD3	2:B:825:GLU:HA	1.98	0.45
1:D:1030:PHE:CZ	1:D:1038:GLY:HA3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1007:PHE:CD1	1:G:1030:PHE:HB3	2.51	0.45
1:A:890:LEU:HB2	1:A:942:PHE:HZ	1.81	0.45
2:E:719:TRP:CZ3	2:E:779:ARG:HD2	2.51	0.45
3:F:222:ILE:HD12	3:F:234:TRP:CZ2	2.51	0.45
1:G:926:LEU:O	1:G:953:TRP:HA	2.16	0.45
1:A:773:SER:C	1:A:775:THR:N	2.69	0.45
1:A:984:THR:HG22	1:A:984:THR:O	2.16	0.45
2:B:1017:SER:O	2:B:1021:LYS:CB	2.65	0.45
1:G:226:PHE:CE2	1:G:287:LYS:HG2	2.52	0.44
2:H:1025:LEU:HD12	2:H:1025:LEU:HA	1.85	0.44
1:D:375:LEU:HB2	1:D:1012:LEU:HD21	1.99	0.44
2:B:871:GLY:HA3	2:B:1028:MET:HG2	1.99	0.44
1:A:923:VAL:O	1:A:930:VAL:HA	2.17	0.44
2:B:885:ASN:ND2	2:B:888:GLU:HB3	2.33	0.44
1:A:311:ALA:HB2	1:A:324:VAL:HG13	2.00	0.44
1:A:858:LEU:HD12	1:A:858:LEU:O	2.18	0.44
1:G:915:LYS:HE3	1:G:957:VAL:O	2.18	0.44
1:D:807:PHE:HB3	1:D:811:GLU:OE1	2.17	0.44
3:F:61:GLY:HA3	3:F:71:LEU:CD2	2.47	0.44
1:A:852:GLN:O	1:A:858:LEU:HA	2.17	0.44
2:E:848:GLU:OE1	2:E:1015:LEU:HD12	2.17	0.44
1:A:889:ARG:HD3	1:A:901:THR:HG23	1.99	0.44
1:G:223:PRO:HD2	1:G:268:GLY:HA3	2.00	0.44
1:G:225:PRO:HG2	1:G:267:ASN:HB2	2.00	0.44
1:G:889:ARG:HD2	1:G:891:TYR:CZ	2.53	0.44
1:A:330:ASP:HA	1:A:355:ASN:HB3	1.99	0.44
1:A:953:TRP:O	1:A:969:GLU:HA	2.18	0.43
1:G:749:THR:HG21	1:G:786:VAL:HG21	1.98	0.43
2:H:849:TYR:O	2:H:853:LYS:HG2	2.17	0.43
1:D:146:ASP:OD1	1:D:147:ARG:N	2.51	0.43
1:A:769:LYS:O	1:A:772:SER:HB3	2.18	0.43
1:A:1047:TRP:CZ3	1:A:1132:VAL:HG13	2.53	0.43
1:G:1116:ASP:OD1	1:G:1116:ASP:O	2.35	0.43
2:H:758:VAL:O	2:H:808:ALA:HB1	2.19	0.43
1:A:58:TYR:HB3	1:A:1073:TRP:HB2	2.01	0.43
2:B:802:PHE:HB3	3:C:146:ILE:HD11	2.00	0.43
2:E:778:LEU:HD21	2:E:878:PHE:CD1	2.53	0.43
1:A:1011:SER:OG	1:A:1013:VAL:HG22	2.18	0.43
2:B:787:VAL:HB	2:B:875:LEU:O	2.18	0.43
3:C:195:THR:CG2	3:C:257:LEU:HD11	2.48	0.43
1:G:774:SER:O	1:G:775:THR:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:PRO:HG2	1:D:267:ASN:O	2.19	0.43
3:F:138:GLU:O	3:F:142:VAL:HG13	2.19	0.43
1:A:1003:PHE:O	1:A:1032:THR:HA	2.19	0.43
1:G:914:LEU:O	1:G:915:LYS:HG2	2.19	0.43
3:F:60:VAL:HG22	3:F:123:LEU:HD12	2.01	0.43
2:B:858:ARG:HE	2:B:896:VAL:HG11	1.84	0.43
1:G:744:ASP:OD1	1:G:746:SER:N	2.47	0.43
1:D:131:ILE:HB	1:D:143:ILE:HB	2.01	0.43
1:A:20:THR:HG23	1:A:315:THR:OG1	2.19	0.43
1:A:322:VAL:HG21	1:A:336:LEU:HD11	2.01	0.43
2:B:858:ARG:O	2:B:897:ILE:HG12	2.19	0.43
2:E:856:LEU:O	2:E:881:ALA:HA	2.19	0.43
1:D:816:LEU:HD13	1:D:831:VAL:HG22	2.01	0.42
3:F:226:THR:HG21	3:F:234:TRP:HB2	1.99	0.42
3:C:266:PRO:O	3:C:267:HIS:C	2.57	0.42
1:D:787:GLU:HB2	1:D:812:TYR:CZ	2.54	0.42
1:G:248:ILE:HD12	1:G:300:LEU:O	2.19	0.42
1:D:317:LEU:O	1:D:318:ASP:HB2	2.19	0.42
1:A:375:LEU:HB2	1:A:1012:LEU:HD21	2.00	0.42
2:H:889:SER:HB2	2:H:912:ARG:HD3	2.01	0.42
1:A:125:ASP:OD2	1:A:176:PRO:HB3	2.20	0.42
2:B:885:ASN:CG	2:B:888:GLU:HB3	2.40	0.42
1:G:834:ALA:HB2	1:G:869:ALA:HA	2.01	0.42
3:I:255:LEU:HD22	3:I:265:MET:SD	2.60	0.42
1:D:36:ASN:ND2	1:D:1001:GLY:O	2.52	0.42
2:E:755:LEU:HD23	2:E:812:VAL:HA	2.00	0.42
1:G:738:SER:HA	1:G:788:VAL:O	2.19	0.42
2:H:722:ARG:HE	2:H:726:LYS:HG3	1.85	0.42
2:E:899:LEU:O	2:E:944:GLN:NE2	2.52	0.42
1:A:59:GLY:HA2	1:A:1073:TRP:CE3	2.55	0.42
1:A:378:CYS:SG	1:A:724:ILE:HB	2.59	0.42
1:A:391:ARG:NH2	1:A:711:HIS:ND1	2.67	0.42
3:C:195:THR:HG21	3:C:257:LEU:HD11	2.02	0.42
2:H:953:GLY:O	2:H:1003:LEU:HD11	2.20	0.42
1:A:790:ASN:HA	1:A:805:HIS:O	2.20	0.42
1:A:975:PHE:HA	1:A:996:GLY:O	2.19	0.42
2:E:895:LYS:HB3	2:E:902:ARG:NH1	2.34	0.42
1:A:933:LEU:HD23	1:A:944:GLU:HA	2.02	0.42
2:H:858:ARG:O	2:H:897:ILE:HG12	2.20	0.42
1:A:985:THR:HG22	1:A:987:GLU:N	2.34	0.42
1:A:1106:GLN:HA	1:A:1109:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1010:THR:O	2:H:1014:THR:HG23	2.20	0.41
1:A:127:GLU:HB2	1:A:129:ARG:HG3	2.01	0.41
1:D:954:MET:HE2	1:D:957:VAL:HG12	2.02	0.41
1:D:378:CYS:SG	1:D:724:ILE:HB	2.61	0.41
2:E:894:ASN:HD21	2:E:909:GLY:HA2	1.84	0.41
1:D:59:GLY:HA2	1:D:1073:TRP:CZ3	2.54	0.41
1:D:257:THR:O	1:D:275:ASP:HB2	2.20	0.41
1:D:275:ASP:OD1	1:D:275:ASP:C	2.59	0.41
1:A:876:PHE:CZ	1:A:919:ASP:HA	2.56	0.41
1:D:184:ASP:HB2	1:D:185:PRO:CD	2.50	0.41
1:A:72:GLU:OE2	1:A:103:ARG:NH2	2.54	0.41
1:G:1080:ARG:O	2:H:937:GLN:NE2	2.45	0.41
1:D:1057:ARG:HD3	1:D:1108:VAL:O	2.21	0.41
1:G:807:PHE:HB3	1:G:811:GLU:OE1	2.20	0.41
1:D:5:TYR:CE1	1:D:1091:GLY:HA2	2.56	0.41
2:B:1036:TRP:CG	2:B:1037:GLN:N	2.89	0.41
1:G:1080:ARG:HD3	2:H:825:GLU:HA	2.01	0.41
2:H:840:MET:HG3	2:H:926:LEU:HD13	2.02	0.41
1:D:223:PRO:HD2	1:D:268:GLY:HA3	2.03	0.41
1:D:761:LEU:HA	1:D:761:LEU:HD23	1.84	0.41
1:D:983:ALA:CB	1:D:988:GLU:HG3	2.50	0.41
2:E:727:PHE:HB3	2:E:744:ALA:HB1	2.02	0.41
2:E:730:ILE:HD12	2:E:743:LYS:HG2	2.02	0.41
2:E:784:ARG:O	2:E:874:LYS:HE2	2.20	0.41
1:A:208:LYS:NZ	1:A:210:GLU:OE2	2.54	0.41
2:B:760:LEU:HD21	2:B:767:PHE:HD1	1.86	0.41
2:B:858:ARG:HH11	2:B:882:ARG:HB2	1.86	0.41
2:B:1027:LYS:HE2	2:B:1029:ALA:HB2	2.02	0.41
1:G:275:ASP:OD1	1:G:275:ASP:C	2.59	0.41
1:G:1030:PHE:CZ	1:G:1038:GLY:HA3	2.56	0.41
1:G:158:ARG:HH12	1:G:160:GLU:HG2	1.86	0.40
1:G:288:GLU:HB2	1:G:298:LYS:HB2	2.03	0.40
1:G:358:PRO:O	1:G:379:SER:HA	2.21	0.40
1:G:840:GLU:OE1	1:G:843:PRO:HA	2.20	0.40
1:G:985:THR:OG1	1:G:988:GLU:HG3	2.21	0.40
1:D:248:ILE:HG12	1:D:250:PRO:HD3	2.03	0.40
1:D:973:ASN:HB3	1:D:1076:PHE:CE1	2.55	0.40
3:F:76:ILE:HD12	3:F:159:HIS:CE1	2.56	0.40
1:G:372:GLN:HG3	1:G:1014:MET:HA	2.02	0.40
1:G:1003:PHE:O	1:G:1032:THR:HA	2.22	0.40
3:I:137:LYS:O	3:I:141:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:GLY:HA3	3:C:71:LEU:HD21	2.02	0.40
3:I:235:TRP:CH2	3:I:244:VAL:HG22	2.56	0.40
1:G:58:TYR:HB3	1:G:1073:TRP:CB	2.51	0.40
1:G:790:ASN:HA	1:G:805:HIS:O	2.21	0.40
3:I:249:ASP:O	3:I:253:GLN:HG3	2.22	0.40
1:D:170:LEU:HD23	1:D:170:LEU:HA	1.92	0.40
1:A:6:VAL:HG22	1:A:1040:VAL:HG22	2.04	0.40
1:A:232:ILE:HD13	1:A:237:ILE:HG23	2.03	0.40
1:D:1023:PRO:HB3	1:D:1047:TRP:CE2	2.56	0.40
2:E:768:PRO:O	2:E:772:ILE:HG13	2.21	0.40
2:B:837:LYS:HE2	2:B:1019:PHE:CE1	2.56	0.40
2:B:844:MET:HE2	2:B:844:MET:HA	2.03	0.40
2:B:856:LEU:HD11	2:B:884:TYR:HB2	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)
1:D:368:GLU:O	2:B:888:GLU:OE2[4_565]	2.17	0.03

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	822/840 (98%)	800 (97%)	21 (3%)	1 (0%)	51 84
1	D	823/840 (98%)	805 (98%)	17 (2%)	1 (0%)	51 84
1	G	822/840 (98%)	801 (97%)	21 (3%)	0	100 100
2	B	322/344 (94%)	314 (98%)	8 (2%)	0	100 100
2	E	321/344 (93%)	309 (96%)	11 (3%)	1 (0%)	41 75
2	H	321/344 (93%)	311 (97%)	9 (3%)	1 (0%)	41 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	246/271 (91%)	242 (98%)	4 (2%)	0	100 100
3	F	246/271 (91%)	242 (98%)	4 (2%)	0	100 100
3	I	246/271 (91%)	242 (98%)	4 (2%)	0	100 100
All	All	4169/4365 (96%)	4066 (98%)	99 (2%)	4 (0%)	51 84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	895	LYS
2	H	911	GLU
1	D	772	SER
1	A	980	ASP

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	721/728 (99%)	716 (99%)	5 (1%)	84 93
1	D	722/728 (99%)	719 (100%)	3 (0%)	91 97
1	G	721/728 (99%)	712 (99%)	9 (1%)	71 87
2	B	292/308 (95%)	287 (98%)	5 (2%)	60 82
2	E	291/308 (94%)	284 (98%)	7 (2%)	49 76
2	H	291/308 (94%)	285 (98%)	6 (2%)	53 78
3	C	223/242 (92%)	222 (100%)	1 (0%)	91 97
3	F	223/242 (92%)	221 (99%)	2 (1%)	78 91
3	I	223/242 (92%)	221 (99%)	2 (1%)	78 91
All	All	3707/3834 (97%)	3667 (99%)	40 (1%)	73 88

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	7	VAL
1	G	163	HIS
1	G	290	GLN
1	G	847	ARG
1	G	849	VAL
1	G	927	MET
1	G	930	VAL
1	G	989	ARG
1	G	1014	MET
2	H	905	GLU
2	H	913	TYR
2	H	956	CYS
2	H	991	SER
2	H	1033	LEU
2	H	1036	TRP
3	I	231	TYR
3	I	257	LEU
1	D	7	VAL
1	D	383	LYS
1	D	849	VAL
2	E	740	GLN
2	E	761	ASP
2	E	867	LEU
2	E	892	TYR
2	E	896	VAL
2	E	1033	LEU
2	E	1035	HIS
3	F	230	MET
3	F	231	TYR
1	A	7	VAL
1	A	163	HIS
1	A	295	VAL
1	A	930	VAL
1	A	1120	MET
2	B	761	ASP
2	B	896	VAL
2	B	913	TYR
2	B	1025	LEU
2	B	1039	CYS
3	C	231	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	835	HIS
2	E	864	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

3 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	TPO	E	893	2	8,10,11	1.89	2 (25%)	10,14,16	1.07	0
2	TPO	H	893	2	8,10,11	1.04	0	10,14,16	0.94	0
2	TPO	B	893	2	8,10,11	1.67	1 (12%)	10,14,16	1.23	1 (10%)

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	TPO	E	893	2	-	5/9/11/13	-
2	TPO	H	893	2	-	0/9/11/13	-
2	TPO	B	893	2	-	1/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	893	TPO	P-O1P	3.50	1.61	1.50
2	B	893	TPO	P-O1P	3.36	1.61	1.50
2	E	893	TPO	CB-CA	2.34	1.59	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	893	TPO	CG2-CB-CA	-2.67	107.90	113.16

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	893	TPO	N-CA-CB-CG2
2	E	893	TPO	N-CA-CB-OG1
2	E	893	TPO	C-CA-CB-CG2
2	E	893	TPO	O-C-CA-CB
2	E	893	TPO	CG2-CB-OG1-P
2	B	893	TPO	C-CA-CB-CG2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	893	TPO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
4	SO4	C	301	-	4,4,4	0.14	0	6,6,6	0.11	0
4	SO4	A	1201	-	4,4,4	0.14	0	6,6,6	0.26	0
5	RQE	H	1101	-	30,37,37	1.04	2 (6%)	27,53,53	1.00	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	I	301	-	4,4,4	0.16	0	6,6,6	0.23	0
5	RQE	E	1101	-	30,37,37	0.97	2 (6%)	27,53,53	1.00	2 (7%)
4	SO4	F	302	-	4,4,4	0.13	0	6,6,6	0.08	0
5	RQE	B	1101	-	30,37,37	0.94	1 (3%)	27,53,53	1.10	3 (11%)
4	SO4	G	1201	-	4,4,4	0.17	0	6,6,6	0.16	0
4	SO4	F	301	-	4,4,4	0.13	0	6,6,6	0.29	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	RQE	E	1101	-	-	7/7/21/21	0/6/6/6
5	RQE	H	1101	-	-	5/7/21/21	0/6/6/6
5	RQE	B	1101	-	-	7/7/21/21	0/6/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1101	RQE	C3-N3	-3.21	1.40	1.44
5	B	1101	RQE	C6-N8	2.31	1.36	1.32
5	E	1101	RQE	C3-N3	-2.16	1.41	1.44
5	H	1101	RQE	C4-N4	-2.09	1.31	1.34
5	E	1101	RQE	C6-N8	2.07	1.35	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1101	RQE	C5-C6-N8	-2.98	118.33	120.81
5	H	1101	RQE	C5-C6-N8	-2.80	118.48	120.81
5	B	1101	RQE	N8-C15-N9	2.39	120.05	117.11
5	B	1101	RQE	C12-C11-C10	-2.31	116.76	120.08
5	H	1101	RQE	C12-C11-C10	-2.21	116.91	120.08
5	B	1101	RQE	C5-C6-N8	-2.19	118.99	120.81
5	E	1101	RQE	C12-C11-C10	-2.17	116.97	120.08

There are no chirality outliers.

All (19) torsion outliers are listed below:

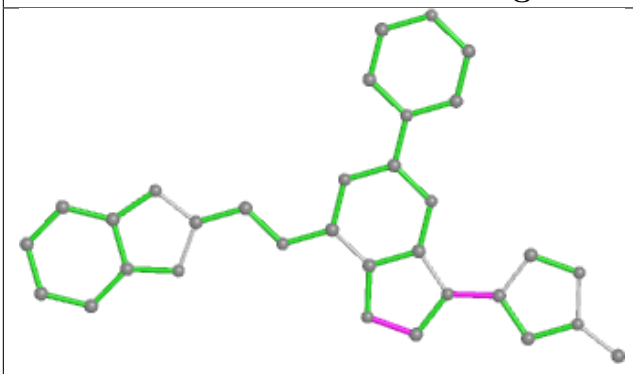
Mol	Chain	Res	Type	Atoms
5	H	1101	RQE	C8-C7-N5-C6
5	H	1101	RQE	N10-C15-N9-C16
5	H	1101	RQE	N10-C15-N9-C19
5	H	1101	RQE	N8-C15-N9-C16
5	H	1101	RQE	N8-C15-N9-C19
5	E	1101	RQE	C8-C7-N5-C6
5	E	1101	RQE	N10-C15-N9-C16
5	E	1101	RQE	N10-C15-N9-C19
5	E	1101	RQE	N8-C15-N9-C16
5	E	1101	RQE	N8-C15-N9-C19
5	B	1101	RQE	C8-C7-N5-C6
5	B	1101	RQE	N10-C15-N9-C19
5	B	1101	RQE	N8-C15-N9-C16
5	B	1101	RQE	N8-C15-N9-C19
5	B	1101	RQE	N10-C15-N9-C16
5	B	1101	RQE	N8-C6-N5-C7
5	E	1101	RQE	C5-C6-N5-C7
5	E	1101	RQE	N8-C6-N5-C7
5	B	1101	RQE	C5-C6-N5-C7

There are no ring outliers.

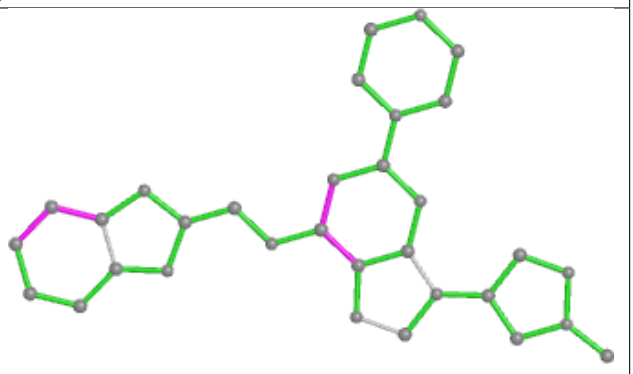
No monomer is involved in short contacts.

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.

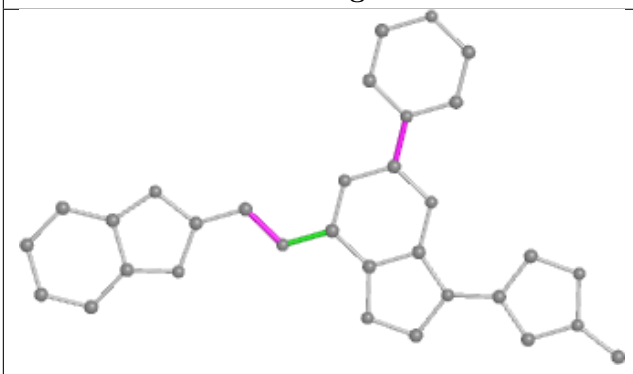
Ligand RQE H 1101



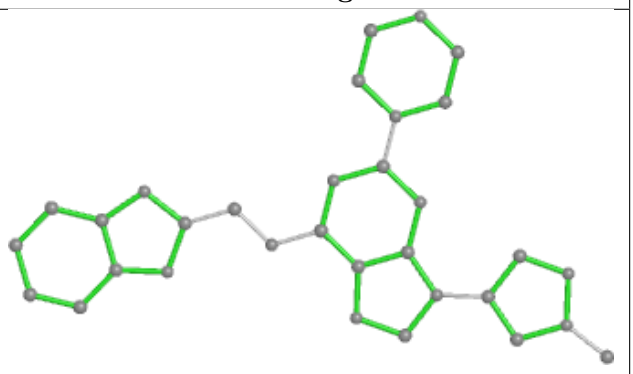
Bond lengths



Bond angles

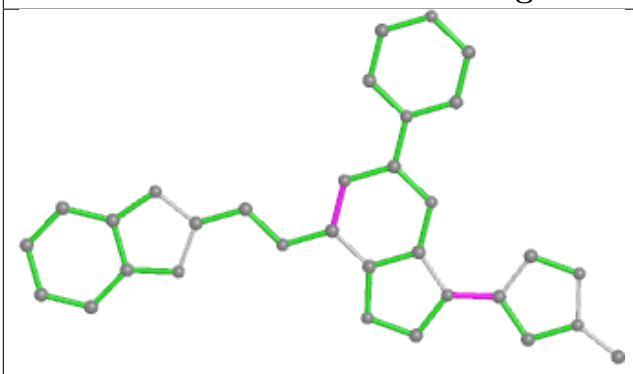


Torsions

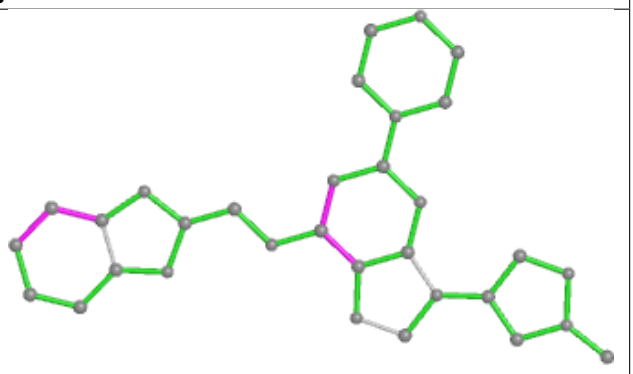


Rings

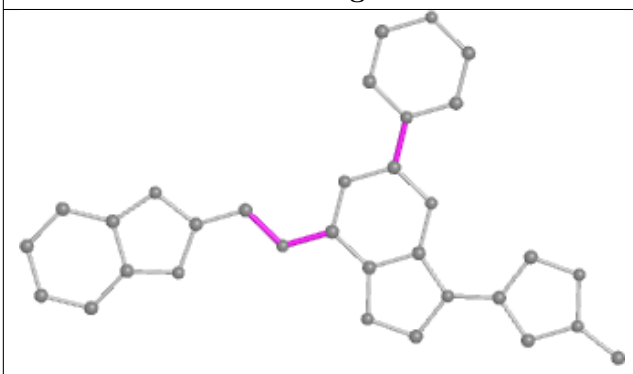
Ligand RQE E 1101



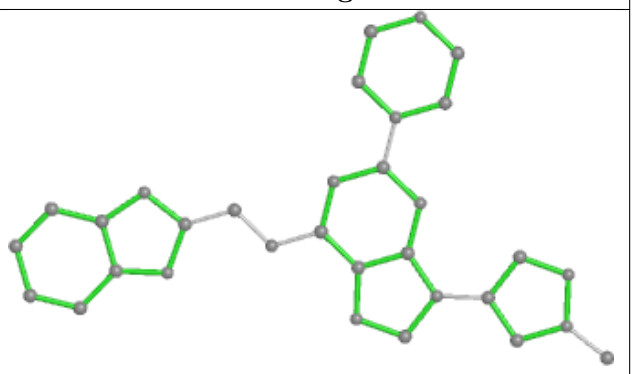
Bond lengths



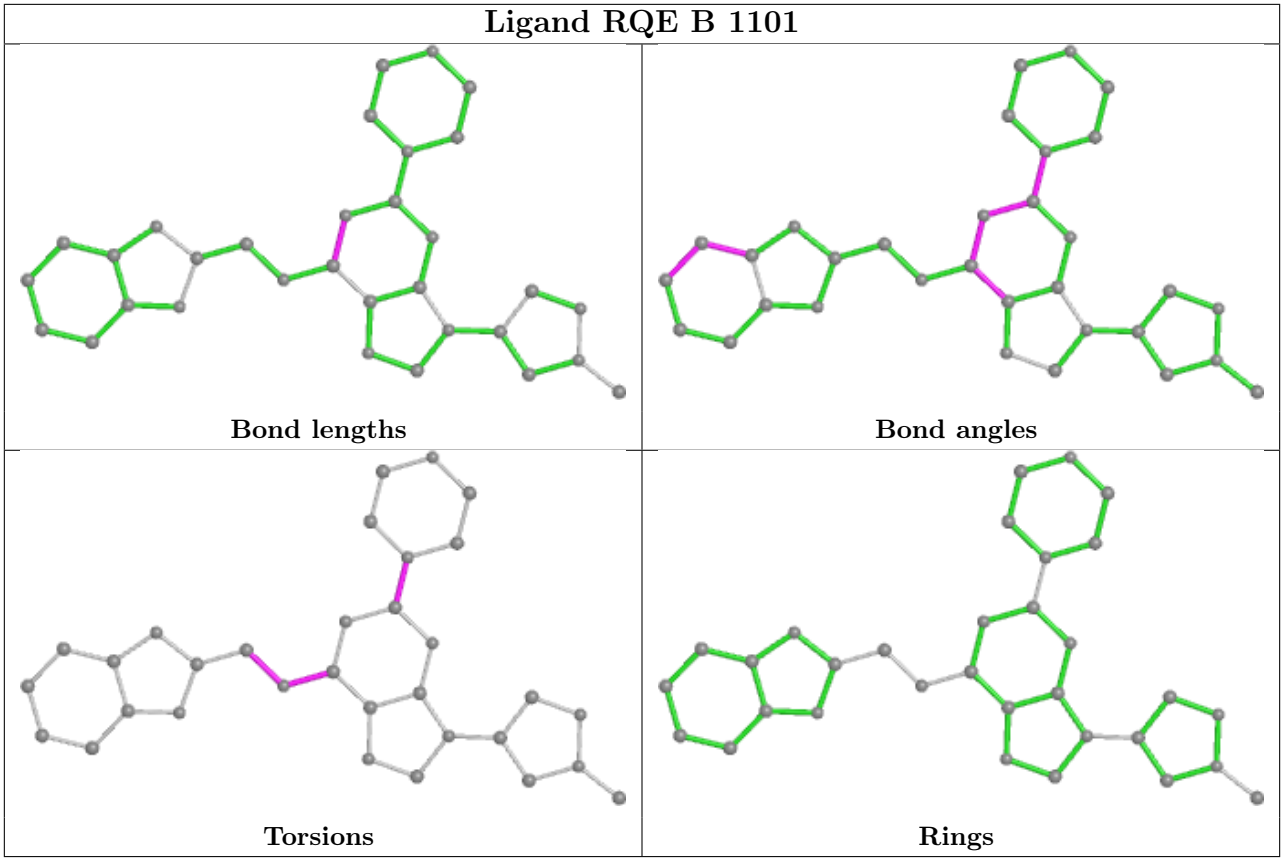
Bond angles



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	826/840 (98%)	0.87	147 (17%)	1	2	112, 150, 228, 315	0
1	D	827/840 (98%)	0.86	133 (16%)	1	2	103, 142, 218, 327	0
1	G	826/840 (98%)	0.90	152 (18%)	1	2	103, 147, 223, 337	0
2	B	324/344 (94%)	1.11	60 (18%)	1	2	95, 131, 210, 287	0
2	E	323/344 (93%)	1.08	64 (19%)	1	1	109, 143, 221, 270	0
2	H	323/344 (93%)	1.17	83 (25%)	0	0	113, 153, 218, 284	0
3	C	248/271 (91%)	0.94	32 (12%)	3	5	102, 129, 176, 242	0
3	F	248/271 (91%)	0.91	25 (10%)	7	9	96, 120, 170, 227	0
3	I	248/271 (91%)	0.89	41 (16%)	1	2	111, 143, 192, 247	0
All	All	4193/4365 (96%)	0.94	737 (17%)	1	2	95, 143, 220, 337	0

All (737) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1034	PRO	13.2
1	G	1016	ASN	9.3
2	H	720	GLY	9.3
2	E	1035	HIS	9.0
2	B	1039	CYS	7.6
2	H	1036	TRP	7.2
1	G	1114	TYR	6.6
2	B	1035	HIS	6.0
2	E	1036	TRP	6.0
2	E	733	ILE	5.6
1	A	1129	LEU	5.6
1	A	1043	LEU	5.4
2	H	1033	LEU	5.4
2	B	1034	PRO	5.4
1	A	289	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	133	LEU	5.1
2	H	1038	ASP	5.1
2	B	802	PHE	5.0
1	G	1097	PHE	5.0
1	D	1136	LEU	4.9
2	B	738	TYR	4.9
1	G	1018	GLY	4.9
1	D	78	PHE	4.8
1	D	328	LEU	4.8
2	B	1036	TRP	4.7
2	H	828	LEU	4.7
3	F	267	HIS	4.7
1	D	708	GLN	4.7
2	H	839	PHE	4.5
1	D	55	VAL	4.5
1	D	39	LEU	4.5
1	A	327	ARG	4.5
1	D	1129	LEU	4.5
1	G	967	GLY	4.5
1	D	220	ILE	4.4
1	G	1019	GLU	4.4
1	G	23	PHE	4.4
1	A	5	TYR	4.4
1	G	140	PHE	4.4
1	G	1115	ASP	4.4
2	E	1025	LEU	4.3
1	D	1097	PHE	4.3
2	B	1031	PRO	4.3
2	H	799	ALA	4.3
2	H	803	LYS	4.2
1	D	91	TYR	4.2
1	G	39	LEU	4.2
1	A	49	LEU	4.2
1	D	195	VAL	4.2
2	H	802	PHE	4.1
2	H	775	ILE	4.1
1	D	59	GLY	4.1
1	A	307	GLU	4.1
2	B	828	LEU	4.1
1	G	57	MET	4.1
1	G	80	LEU	4.0
3	C	222	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
3	I	164	LEU	4.0
1	G	49	LEU	4.0
1	G	367	LEU	4.0
3	C	266	PRO	4.0
1	A	931	LEU	4.0
1	A	1088	PHE	4.0
2	H	735	GLU	4.0
1	A	328	LEU	3.9
2	H	798	ASP	3.9
2	H	860	ILE	3.9
1	A	1000	LEU	3.9
2	B	839	PHE	3.9
1	A	1019	GLU	3.9
1	A	31	LEU	3.9
1	A	387	LEU	3.9
1	G	273	LEU	3.9
3	I	153	PHE	3.9
1	D	1007	PHE	3.8
1	D	64	MET	3.8
1	A	131	ILE	3.8
1	A	291	MET	3.8
3	F	265	MET	3.8
3	F	266	PRO	3.8
1	A	61	ILE	3.7
1	G	64	MET	3.7
1	G	328	LEU	3.7
2	H	929	LEU	3.7
1	D	733	PHE	3.7
1	G	32	LEU	3.7
1	A	295	VAL	3.7
1	A	132	GLY	3.7
1	A	1007	PHE	3.7
3	F	262	LYS	3.7
1	D	367	LEU	3.6
2	B	803	LYS	3.6
2	H	793	VAL	3.6
1	D	179	CYS	3.6
1	D	1100	ILE	3.6
2	B	1038	ASP	3.6
1	G	1037	ILE	3.6
1	A	965	PHE	3.6
1	G	145	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	H	797	GLN	3.6
3	F	264	GLN	3.6
1	A	293	GLY	3.6
2	E	831	PHE	3.5
1	G	1129	LEU	3.5
3	I	171	LEU	3.5
1	G	359	ILE	3.5
1	A	112	ILE	3.5
2	H	865	ILE	3.5
2	H	721	LYS	3.5
1	A	122	GLY	3.5
1	G	131	ILE	3.5
1	G	966	LEU	3.5
3	I	155	LEU	3.5
1	G	195	VAL	3.5
1	A	64	MET	3.5
1	A	1040	VAL	3.5
1	G	133	LEU	3.5
1	D	1030	PHE	3.5
1	A	302	VAL	3.4
1	D	219	VAL	3.4
1	A	310	ILE	3.4
3	C	57	ILE	3.4
3	I	31	LEU	3.4
1	G	130	MET	3.4
1	D	130	MET	3.4
1	D	36	ASN	3.4
1	G	143	ILE	3.4
2	E	860	ILE	3.4
2	E	749	THR	3.4
1	A	333	LEU	3.4
2	H	800	LEU	3.4
1	G	79	ILE	3.4
1	A	230	ILE	3.4
2	H	855	PHE	3.3
1	A	932	LEU	3.3
2	E	1028	MET	3.3
1	G	67	PHE	3.3
1	A	923	VAL	3.3
3	I	167	TYR	3.3
1	A	140	PHE	3.3
1	A	356	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	922	LEU	3.3
2	H	831	PHE	3.3
1	A	733	PHE	3.3
1	D	41	ILE	3.3
2	B	775	ILE	3.3
1	G	1020	THR	3.3
1	A	966	LEU	3.3
2	B	896	VAL	3.3
1	G	356	LEU	3.3
1	D	57	MET	3.3
1	G	123	ILE	3.3
1	D	112	ILE	3.3
3	F	54	ALA	3.3
1	G	387	LEU	3.3
2	H	878	PHE	3.3
3	I	158	GLU	3.3
3	F	116	ILE	3.3
1	G	1012	LEU	3.2
2	H	913	TYR	3.2
2	E	875	LEU	3.2
1	D	1111	ASN	3.2
1	G	33	ILE	3.2
1	A	314	LEU	3.2
3	C	79	HIS	3.2
1	D	152	LEU	3.2
2	B	801	ASP	3.2
1	D	89	LEU	3.2
1	A	237	ILE	3.2
2	E	717	SER	3.2
1	A	220	ILE	3.2
2	E	955	PRO	3.2
1	G	120	ILE	3.2
1	D	1012	LEU	3.2
2	H	875	LEU	3.2
1	G	949	PHE	3.2
1	G	78	PHE	3.2
1	A	829	PHE	3.1
3	I	81	PHE	3.1
1	A	859	GLN	3.1
2	H	864	ASN	3.1
2	H	951	LEU	3.1
1	G	923	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	880	LEU	3.1
1	A	280	LEU	3.1
1	D	1115	ASP	3.1
2	H	986	PHE	3.1
1	D	387	LEU	3.1
1	A	272	LEU	3.1
2	E	867	LEU	3.1
2	B	964	ILE	3.1
2	B	955	PRO	3.1
3	I	267	HIS	3.1
1	A	305	LEU	3.1
1	D	67	PHE	3.1
1	G	36	ASN	3.1
1	A	273	LEU	3.1
1	A	717	LEU	3.1
2	B	922	CYS	3.1
2	E	781	LEU	3.1
3	C	132	PHE	3.1
1	D	237	ILE	3.0
1	G	1029	LEU	3.0
1	D	49	LEU	3.0
2	E	926	LEU	3.0
1	G	336	LEU	3.0
1	G	933	LEU	3.0
3	C	171	LEU	3.0
1	D	23	PHE	3.0
1	D	33	ILE	3.0
1	D	721	PRO	3.0
1	G	376	VAL	3.0
2	H	959	VAL	3.0
1	G	1000	LEU	3.0
1	D	710	LEU	3.0
1	A	927	MET	3.0
2	H	930	PHE	3.0
2	B	1019	PHE	3.0
3	I	132	PHE	3.0
1	G	230	ILE	3.0
3	C	124	LEU	3.0
1	G	881	LEU	3.0
1	G	220	ILE	3.0
3	I	254	ILE	3.0
1	G	733	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1108	VAL	3.0
1	A	814	LEU	3.0
2	E	730	ILE	3.0
1	G	812	TYR	3.0
2	E	930	PHE	3.0
1	A	921	ILE	2.9
2	H	756	LYS	2.9
2	E	856	LEU	2.9
2	B	826	SER	2.9
3	I	100	LEU	2.9
3	C	60	VAL	2.9
3	C	102	LEU	2.9
1	D	77	LEU	2.9
1	A	888	VAL	2.9
3	F	102	LEU	2.9
2	E	878	PHE	2.9
1	A	858	LEU	2.9
2	H	778	LEU	2.9
1	A	139	LEU	2.9
2	H	1035	HIS	2.9
2	E	904	PRO	2.9
1	D	893	TRP	2.9
1	D	31	LEU	2.9
1	D	752	LEU	2.9
2	E	715	THR	2.9
2	B	715	THR	2.9
1	G	61	ILE	2.9
1	D	100	ILE	2.9
1	D	364	VAL	2.9
1	A	120	ILE	2.9
2	E	873	ILE	2.9
3	C	76	ILE	2.9
2	E	1038	ASP	2.9
2	B	740	GLN	2.9
1	G	1030	PHE	2.9
1	A	39	LEU	2.9
2	B	831	PHE	2.9
1	G	375	LEU	2.9
1	A	1136	LEU	2.9
1	A	799	PHE	2.9
2	B	1033	LEU	2.9
3	I	222	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	853	TYR	2.8
1	G	66	LEU	2.8
1	A	912	LEU	2.8
1	D	121	ILE	2.8
3	I	239	VAL	2.8
3	F	157	VAL	2.8
1	A	323	PHE	2.8
1	A	324	VAL	2.8
1	A	1039	LEU	2.8
1	D	140	PHE	2.8
1	D	1037	ILE	2.8
2	H	924	CYS	2.8
2	H	823	LEU	2.8
1	A	880	LEU	2.8
2	B	778	LEU	2.8
3	I	165	LEU	2.8
1	G	169	PHE	2.8
1	G	1079	GLU	2.8
2	E	830	HIS	2.8
1	D	899	LEU	2.8
1	A	317	LEU	2.8
1	D	88	ILE	2.8
1	D	258	ILE	2.8
3	C	153	PHE	2.8
2	E	803	LYS	2.8
1	G	792	LEU	2.8
3	F	181	LEU	2.8
1	G	998	PHE	2.8
1	G	1133	VAL	2.8
2	H	719	TRP	2.8
1	A	722	ARG	2.8
3	F	83	MET	2.8
1	D	974	LEU	2.8
1	A	908	ASN	2.8
1	G	139	LEU	2.8
1	G	317	LEU	2.8
2	B	929	LEU	2.8
1	G	229	ALA	2.8
1	A	911	ALA	2.7
1	D	1132	VAL	2.7
1	G	41	ILE	2.7
2	H	804	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	901	TYR	2.7
1	A	914	LEU	2.7
1	A	930	VAL	2.7
3	I	77	TYR	2.7
1	A	145	LEU	2.7
1	A	974	LEU	2.7
3	C	164	LEU	2.7
2	E	1029	ALA	2.7
3	I	160	PRO	2.7
1	D	931	LEU	2.7
1	A	276	MET	2.7
2	E	844	MET	2.7
1	A	753	ARG	2.7
1	A	909	ILE	2.7
1	D	80	LEU	2.7
2	E	936	PHE	2.7
1	G	5	TYR	2.7
2	H	792	ILE	2.7
1	A	336	LEU	2.7
1	A	899	LEU	2.7
3	I	181	LEU	2.7
1	A	226	PHE	2.7
1	D	907	ASN	2.7
1	D	858	LEU	2.7
2	E	908	LEU	2.7
3	I	213	LEU	2.7
1	A	32	LEU	2.7
1	A	23	PHE	2.7
1	A	253	ILE	2.7
1	A	752	LEU	2.7
2	H	866	LEU	2.7
3	I	38	LEU	2.7
1	A	1097	PHE	2.7
1	G	831	VAL	2.7
1	D	1031	GLY	2.7
1	A	124	ILE	2.7
1	D	1029	LEU	2.6
1	A	283	LEU	2.6
2	H	1025	LEU	2.6
2	B	829	VAL	2.6
1	D	881	LEU	2.6
1	A	2	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	801	ASP	2.6
1	D	890	LEU	2.6
1	D	1093	LEU	2.6
1	A	178	ILE	2.6
1	G	63	VAL	2.6
1	D	166	ASP	2.6
1	A	1054	MET	2.6
1	G	124	ILE	2.6
2	H	988	PHE	2.6
1	G	167	VAL	2.6
1	G	1108	VAL	2.6
1	D	375	LEU	2.6
1	D	79	ILE	2.6
1	A	390	ILE	2.6
2	B	875	LEU	2.6
3	F	254	ILE	2.6
1	D	84	TYR	2.6
1	A	1030	PHE	2.6
2	E	839	PHE	2.6
1	D	360	VAL	2.6
3	F	76	ILE	2.6
2	E	892	TYR	2.6
1	G	930	VAL	2.6
1	D	376	VAL	2.6
1	G	981	SER	2.6
1	D	932	LEU	2.6
1	A	143	ILE	2.6
1	D	911	ALA	2.6
1	A	850	VAL	2.6
1	A	1133	VAL	2.6
1	G	791	LEU	2.6
1	A	848	ILE	2.6
2	E	778	LEU	2.6
1	G	360	VAL	2.6
1	D	40	GLU	2.6
1	G	283	LEU	2.6
3	C	148	LEU	2.6
2	B	809	PHE	2.6
1	G	334	VAL	2.6
2	B	873	ILE	2.6
2	H	727	PHE	2.6
2	B	721	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	1000	LEU	2.6
1	D	975	PHE	2.5
1	D	362	MET	2.5
2	H	867	LEU	2.5
1	G	258	ILE	2.5
1	D	1088	PHE	2.5
2	B	742	TYR	2.5
1	G	77	LEU	2.5
1	G	226	PHE	2.5
1	D	37	THR	2.5
1	D	1040	VAL	2.5
2	B	890	ARG	2.5
1	A	6	VAL	2.5
1	A	219	VAL	2.5
1	G	60	LYS	2.5
1	G	1126	ALA	2.5
2	H	829	VAL	2.5
1	G	304	LEU	2.5
1	A	135	LEU	2.5
3	C	56	PHE	2.5
1	A	1118	SER	2.5
1	A	770	LEU	2.5
2	H	982	LEU	2.5
1	G	1094	ILE	2.5
3	F	57	ILE	2.5
1	G	15	VAL	2.5
2	B	800	LEU	2.5
1	G	1024	THR	2.5
2	B	935	ILE	2.5
1	G	135	LEU	2.5
1	D	197	LEU	2.5
1	D	1076	PHE	2.5
1	A	281	PHE	2.5
1	A	816	LEU	2.5
1	D	5	TYR	2.5
3	C	66	LEU	2.5
2	H	904	PRO	2.5
1	G	959	ILE	2.5
3	I	57	ILE	2.5
1	A	375	LEU	2.4
1	G	281	PHE	2.4
1	A	1089	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	935	ILE	2.4
1	G	365	VAL	2.4
1	G	1039	LEU	2.4
1	A	1029	LEU	2.4
2	H	820	LEU	2.4
3	F	217	LEU	2.4
3	C	80	ARG	2.4
1	D	880	LEU	2.4
1	A	1012	LEU	2.4
2	E	812	VAL	2.4
2	B	856	LEU	2.4
3	I	102	LEU	2.4
1	D	61	ILE	2.4
1	D	377	THR	2.4
1	G	291	MET	2.4
2	B	731	GLY	2.4
3	F	257	LEU	2.4
1	G	237	ILE	2.4
1	D	230	ILE	2.4
1	D	253	ILE	2.4
1	D	76	LEU	2.4
3	C	193	LEU	2.4
3	C	199	LEU	2.4
1	G	62	ALA	2.4
3	I	58	PHE	2.4
2	B	743	LYS	2.4
1	G	121	ILE	2.4
1	A	41	ILE	2.4
3	I	178	ILE	2.4
2	B	926	LEU	2.4
2	H	863	SER	2.4
2	E	865	ILE	2.4
1	A	246	LEU	2.4
2	H	753	VAL	2.4
2	H	955	PRO	2.4
1	G	965	PHE	2.4
2	B	878	PHE	2.4
1	D	369	ARG	2.4
3	I	66	LEU	2.4
2	B	986	PHE	2.4
1	A	216	ALA	2.4
1	A	240	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	818	HIS	2.4
1	A	121	ILE	2.4
2	H	989	ILE	2.4
1	D	791	LEU	2.4
1	D	957	VAL	2.4
1	D	1004	VAL	2.4
3	I	148	LEU	2.4
1	D	1114	TYR	2.4
1	A	882	ALA	2.4
1	A	79	ILE	2.4
3	F	222	ILE	2.4
1	G	76	LEU	2.4
1	A	1004	VAL	2.4
1	D	202	PHE	2.4
2	B	988	PHE	2.4
1	D	178	ILE	2.4
2	E	737	THR	2.4
2	E	836	ILE	2.4
1	G	31	LEU	2.4
1	G	272	LEU	2.4
1	D	32	LEU	2.4
2	E	945	LEU	2.4
1	G	113	GLY	2.4
3	I	106	VAL	2.4
2	E	791	GLU	2.4
1	D	390	ILE	2.4
2	B	860	ILE	2.4
1	G	814	LEU	2.4
1	A	197	LEU	2.4
2	H	994	LEU	2.4
2	E	1020	LEU	2.4
3	C	100	LEU	2.4
1	D	281	PHE	2.3
3	C	238	PHE	2.3
2	H	811	LEU	2.3
1	D	1028	VAL	2.3
2	E	753	VAL	2.3
1	A	130	MET	2.3
1	A	881	LEU	2.3
2	H	997	LEU	2.3
1	D	735	VAL	2.3
1	A	67	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	809	PHE	2.3
3	I	94	VAL	2.3
2	H	755	LEU	2.3
1	A	113	GLY	2.3
1	G	197	LEU	2.3
3	I	71	LEU	2.3
3	I	147	LEU	2.3
3	F	161	TYR	2.3
1	G	219	VAL	2.3
2	E	1034	PRO	2.3
1	G	285	LEU	2.3
1	G	1089	ILE	2.3
1	D	314	LEU	2.3
2	H	733	ILE	2.3
3	F	38	LEU	2.3
1	D	888	VAL	2.3
1	G	362	MET	2.3
1	A	117	GLU	2.3
1	G	221	ALA	2.3
3	C	116	ILE	2.3
1	D	949	PHE	2.3
1	D	709	LYS	2.3
1	D	945	ILE	2.3
1	A	303	GLU	2.3
1	G	152	LEU	2.3
2	B	812	VAL	2.3
2	B	936	PHE	2.3
3	C	78	PHE	2.3
3	I	211	MET	2.3
1	G	1051	LEU	2.3
2	B	952	CYS	2.3
1	D	381	ALA	2.3
1	A	33	ILE	2.3
3	I	168	ALA	2.3
1	G	112	ILE	2.3
1	D	1140	HIS	2.3
3	I	97	ALA	2.3
2	B	844	MET	2.2
2	B	1001	LEU	2.2
1	A	100	ILE	2.2
1	G	977	CYS	2.2
1	D	997	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	1000	MET	2.2
2	B	1025	LEU	2.2
1	G	178	ILE	2.2
1	A	830	ILE	2.2
1	A	1020	THR	2.2
2	E	775	ILE	2.2
3	I	116	ILE	2.2
1	G	170	LEU	2.2
1	A	979	LYS	2.2
2	E	883	LEU	2.2
2	E	982	LEU	2.2
3	I	199	LEU	2.2
1	D	794	ILE	2.2
1	A	16	ASN	2.2
2	H	836	ILE	2.2
1	A	1132	VAL	2.2
1	D	928	ARG	2.2
1	G	816	LEU	2.2
2	H	752	LEU	2.2
3	F	78	PHE	2.2
1	D	1033	VAL	2.2
1	A	84	TYR	2.2
2	H	952	CYS	2.2
1	G	974	LEU	2.2
3	C	234	TRP	2.2
1	A	998	PHE	2.2
1	A	928	ARG	2.2
2	H	777	ILE	2.2
2	E	802	PHE	2.2
3	I	26	TRP	2.2
2	H	896	VAL	2.2
3	C	206	ILE	2.2
1	D	58	TYR	2.2
1	G	736	LEU	2.2
1	D	814	LEU	2.2
2	E	847	LEU	2.2
1	G	722	ARG	2.2
1	A	851	PHE	2.2
1	A	874	VAL	2.2
1	A	1052	LEU	2.2
2	E	761	ASP	2.2
1	G	916	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	377	THR	2.2
3	C	84	PHE	2.2
1	D	830	ILE	2.2
1	G	890	LEU	2.2
1	G	914	LEU	2.2
1	G	7	VAL	2.2
1	D	252	ILE	2.2
2	H	840	MET	2.2
3	I	151	ILE	2.2
3	C	254	ILE	2.2
1	G	1136	LEU	2.2
2	B	755	LEU	2.2
1	G	100	ILE	2.2
1	G	735	VAL	2.2
1	G	1022	THR	2.2
2	E	840	MET	2.2
1	D	942	PHE	2.1
1	G	358	PRO	2.1
1	G	363	CYS	2.1
1	D	99	ASP	2.1
2	E	888	GLU	2.1
3	C	196	THR	2.1
3	C	247	LEU	2.1
1	G	34	ALA	2.1
1	G	65	GLU	2.1
2	E	743	LYS	2.1
2	E	915	PRO	2.1
1	G	1112	LEU	2.1
1	D	966	LEU	2.1
3	F	155	LEU	2.1
1	G	813	ALA	2.1
1	D	778	HIS	2.1
1	D	807	PHE	2.1
3	I	80	ARG	2.1
1	G	390	ILE	2.1
1	G	830	ILE	2.1
2	E	1031	PRO	2.1
2	E	997	LEU	2.1
2	B	767	PHE	2.1
1	G	87	CYS	2.1
1	G	921	ILE	2.1
1	A	1139	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	358	PRO	2.1
1	D	1052	LEU	2.1
2	B	908	LEU	2.1
2	H	1019	PHE	2.1
1	A	4	ASN	2.1
1	A	957	VAL	2.1
2	E	917	ILE	2.1
1	A	300	LEU	2.1
2	H	847	LEU	2.1
2	H	1001	LEU	2.1
2	E	755	LEU	2.1
1	D	65	GLU	2.1
1	G	389	ILE	2.1
1	D	181	VAL	2.1
2	H	743	LYS	2.1
2	B	997	LEU	2.1
3	C	64	LEU	2.1
3	F	56	PHE	2.1
1	A	232	ILE	2.1
1	A	347	VAL	2.1
2	H	925	ILE	2.1
2	H	1023	VAL	2.1
2	H	1020	LEU	2.1
2	B	720	GLY	2.1
2	B	760	LEU	2.1
1	A	949	PHE	2.1
2	H	826	SER	2.1
1	G	232	ILE	2.1
1	G	752	LEU	2.1
1	G	922	LEU	2.1
1	G	1088	PHE	2.1
1	G	302	VAL	2.1
1	G	786	VAL	2.1
2	H	758	VAL	2.1
1	G	710	LEU	2.1
1	G	858	LEU	2.1
1	A	997	LEU	2.1
2	B	761	ASP	2.1
1	D	1054	MET	2.1
2	H	1000	MET	2.1
1	G	975	PHE	2.1
3	F	84	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	738	TYR	2.1
1	G	6	VAL	2.1
1	G	884	ILE	2.1
1	G	246	LEU	2.1
1	G	333	LEU	2.1
1	A	1119	GLY	2.1
2	H	883	LEU	2.1
2	E	828	LEU	2.1
2	E	818	HIS	2.1
3	I	225	TRP	2.1
1	G	40	GLU	2.1
1	D	951	PRO	2.1
3	C	239	VAL	2.1
1	D	336	LEU	2.1
2	H	935	ILE	2.1
1	D	1036	MET	2.1
2	H	767	PHE	2.0
2	E	986	PHE	2.0
1	D	327	ARG	2.0
2	E	922	CYS	2.0
1	D	923	VAL	2.0
2	B	892	TYR	2.0
1	A	1005	ASN	2.0
3	F	106	VAL	2.0
1	D	736	LEU	2.0
1	D	1094	ILE	2.0
2	E	748	ASP	2.0
1	D	1006	VAL	2.0
3	C	165	LEU	2.0
3	I	144	GLU	2.0
3	I	149	GLN	2.0
2	E	913	TYR	2.0
2	H	932	LYS	2.0
3	F	164	LEU	2.0
2	B	810	TYR	2.0
1	D	165	ILE	2.0
2	B	843	LEU	2.0
3	C	75	ILE	2.0
2	H	934	PRO	2.0
1	G	372	GLN	2.0
1	D	717	LEU	2.0
2	H	730	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1079	GLU	2.0
2	B	757	LYS	2.0
1	G	957	VAL	2.0
1	A	960	LEU	2.0
1	A	1080	ARG	2.0
2	H	908	LEU	2.0
2	H	1003	LEU	2.0
2	E	1001	LEU	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	TPO	E	893	11/12	0.61	0.18	185,192,232,235	6
2	TPO	H	893	11/12	0.74	0.19	190,198,235,241	5
2	TPO	B	893	11/12	0.77	0.20	145,162,191,196	6

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
4	SO4	F	301	5/5	0.79	0.17	152,159,165,209	0
4	SO4	A	1201	5/5	0.81	0.19	164,165,175,222	0
4	SO4	G	1201	5/5	0.82	0.23	140,146,151,191	0
5	RQE	E	1101	32/32	0.90	0.41	91,128,155,157	22
5	RQE	H	1101	32/32	0.91	0.41	116,129,158,162	22
4	SO4	I	301	5/5	0.91	0.20	142,143,146,175	0
4	SO4	C	301	5/5	0.92	0.14	154,154,163,195	0

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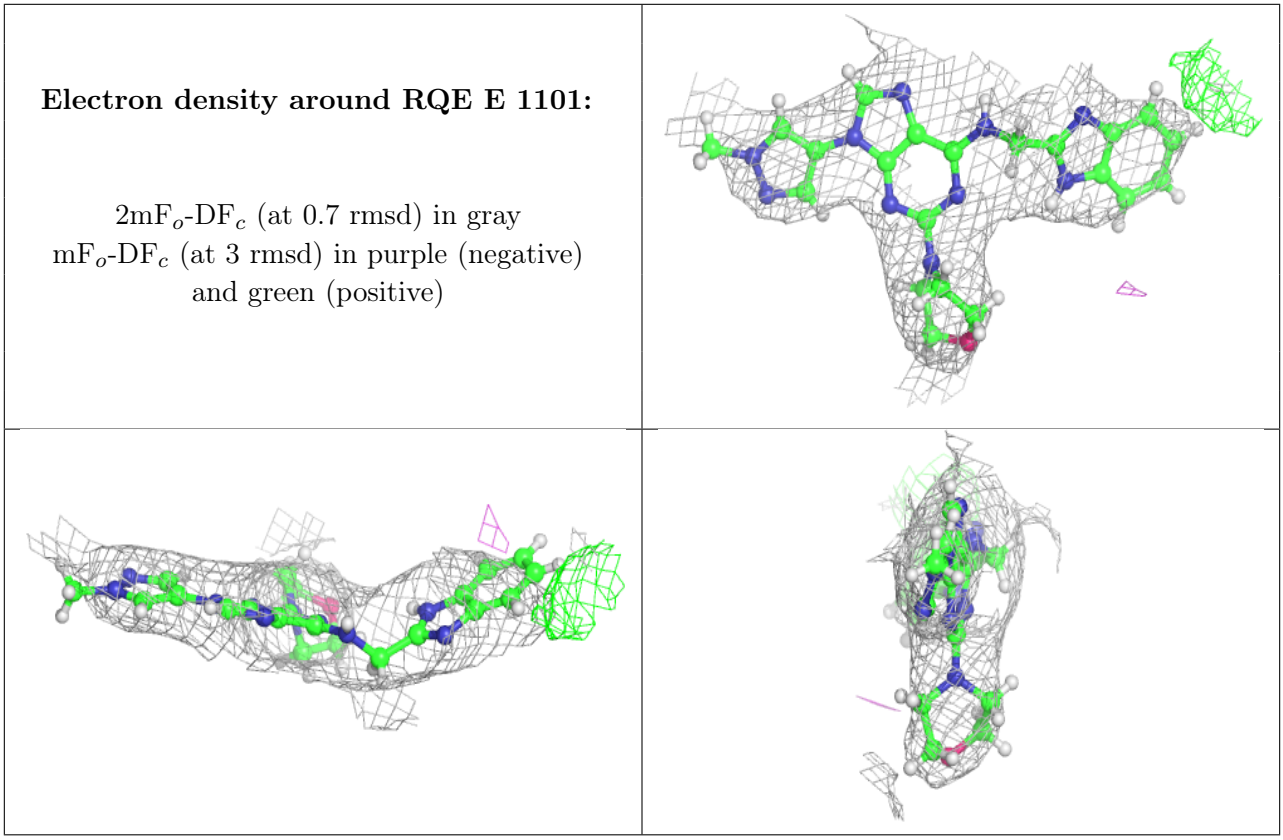
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	RQE	B	1101	32/32	0.92	0.38	104,116,141,145	22
4	SO4	F	302	5/5	0.97	0.19	133,135,138,156	0

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.

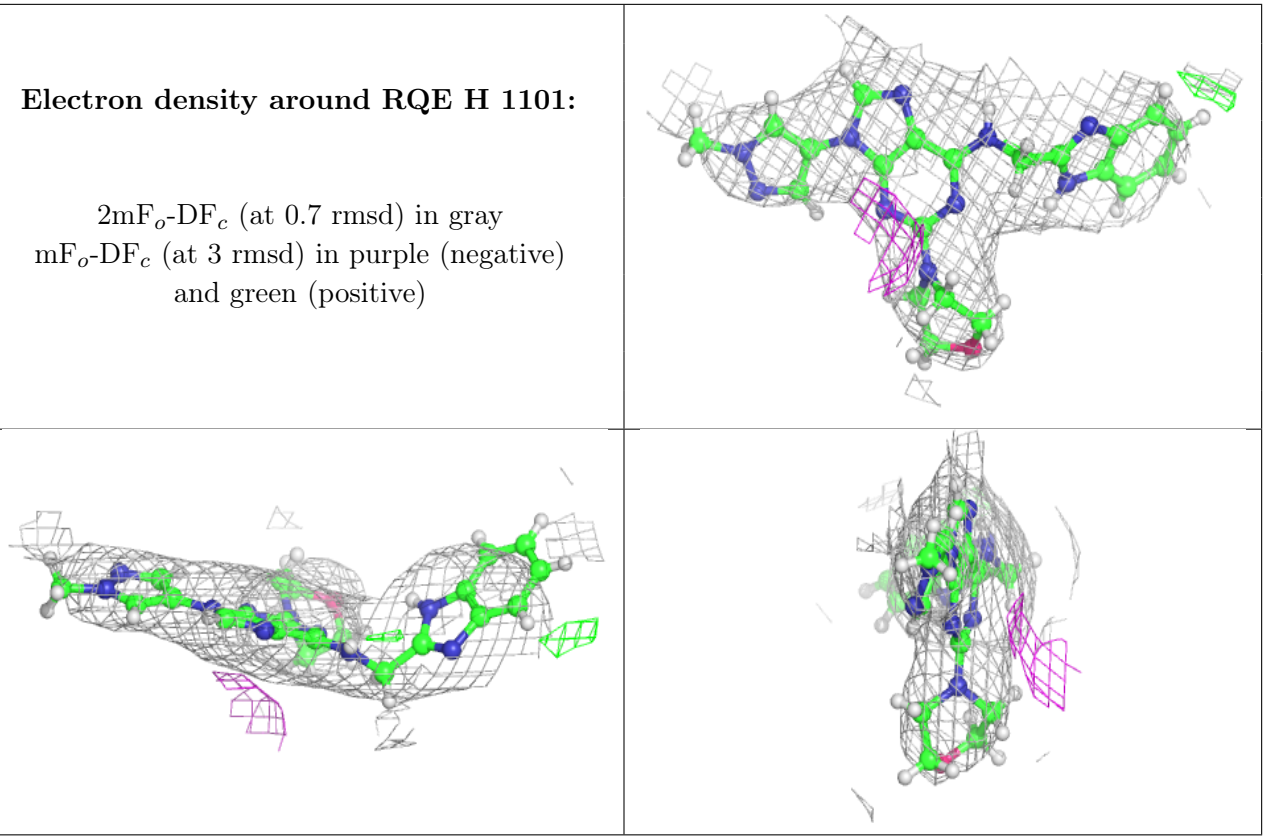
Electron density around RQE E 1101:

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



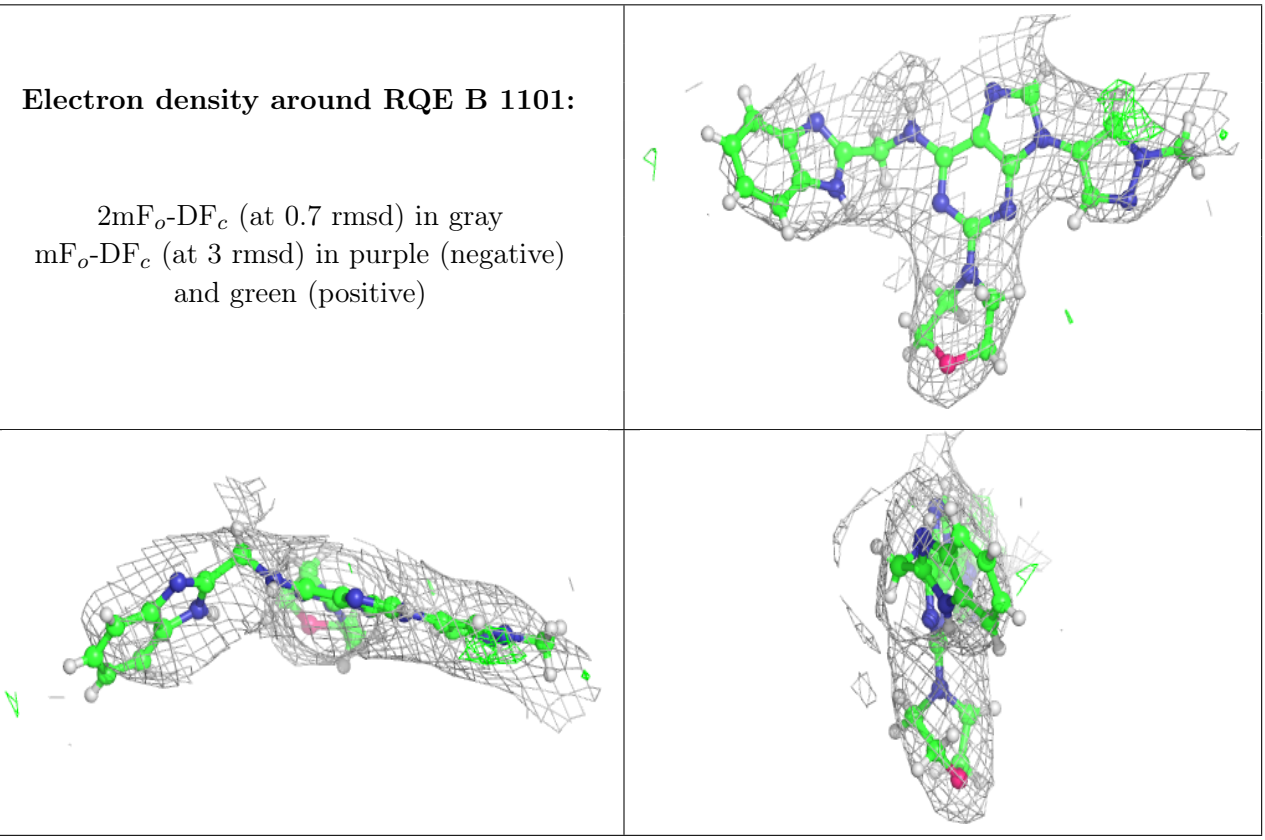
Electron density around RQE H 1101:

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



Electron density around RQE B 1101:

$2mF_o$-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 (i)

There are no such residues in this entry.