Full wwPDB X-ray Structure Validation Report (i)

Jun 21, 2021 – 02:46 PM BST

PDB ID	:	6ZFH
Title	:	Structure of human galactokinase in complex with galactose and 2'-(benzo[d]oxazol-2-ylamino)-7',8'-dihydro-1'H-spiro[cyclopentane-1,4'-quinazolin]-5'(6'H)-one
Authors	:	Bezerra, G.A.; Mackinnon, S.; Zhang, M.; Foster, W.; Bailey, H.; Arrowsmith, C.; Edwards, A.; Bountra, C.; Lai, K.; Yue, W.W.; Structural Genomics Consortium (SGC)
Deposited on	:	2020-06-17
Resolution	:	2.44 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 following versions of software and data (see references (i)) were used in the production of this report:

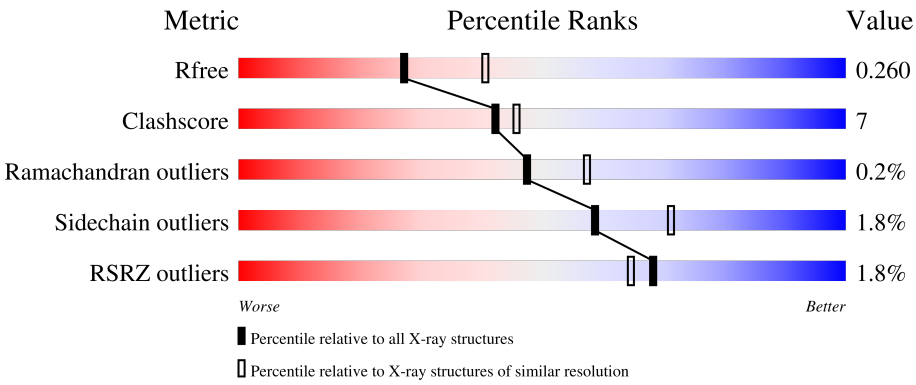
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	399	% 82% 15% •
1	B	399	% 83% 13% •
1	C	399	84% 13% •
1	D	399	% 80% 16% •
1	E	399	% 82% 14% • •

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Mol	Chain	Length	Quality of chain
1	F	399	5% 78% 18%
1	G	399	2% 81% 14%
1	H	399	4% 74% 19% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22813 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 Galactokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	386	2854	1786	512	540	16	0	0	0
1	B	386	2810	1765	498	531	16	0	0	0
1	C	388	2857	1790	514	537	16	0	0	0
1	D	385	2806	1759	499	532	16	0	0	0
1	E	386	2814	1764	503	531	16	0	0	0
1	F	384	2767	1741	486	524	16	0	0	0
1	G	383	2699	1701	478	504	16	0	0	0
1	H	376	2603	1639	462	489	13	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P51570
A	-5	ALA	-	expression tag	UNP P51570
A	-4	HIS	-	expression tag	UNP P51570
A	-3	HIS	-	expression tag	UNP P51570
A	-2	HIS	-	expression tag	UNP P51570
A	-1	HIS	-	expression tag	UNP P51570
A	0	HIS	-	expression tag	UNP P51570
A	1	HIS	-	expression tag	UNP P51570
A	252	ALA	LYS	conflict	UNP P51570
A	253	ALA	GLU	conflict	UNP P51570
B	-6	MET	-	initiating methionine	UNP P51570
B	-5	ALA	-	expression tag	UNP P51570
B	-4	HIS	-	expression tag	UNP P51570

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP P51570
B	-2	HIS	-	expression tag	UNP P51570
B	-1	HIS	-	expression tag	UNP P51570
B	0	HIS	-	expression tag	UNP P51570
B	1	HIS	-	expression tag	UNP P51570
B	252	ALA	LYS	conflict	UNP P51570
B	253	ALA	GLU	conflict	UNP P51570
C	-6	MET	-	initiating methionine	UNP P51570
C	-5	ALA	-	expression tag	UNP P51570
C	-4	HIS	-	expression tag	UNP P51570
C	-3	HIS	-	expression tag	UNP P51570
C	-2	HIS	-	expression tag	UNP P51570
C	-1	HIS	-	expression tag	UNP P51570
C	0	HIS	-	expression tag	UNP P51570
C	1	HIS	-	expression tag	UNP P51570
C	252	ALA	LYS	conflict	UNP P51570
C	253	ALA	GLU	conflict	UNP P51570
D	-6	MET	-	initiating methionine	UNP P51570
D	-5	ALA	-	expression tag	UNP P51570
D	-4	HIS	-	expression tag	UNP P51570
D	-3	HIS	-	expression tag	UNP P51570
D	-2	HIS	-	expression tag	UNP P51570
D	-1	HIS	-	expression tag	UNP P51570
D	0	HIS	-	expression tag	UNP P51570
D	1	HIS	-	expression tag	UNP P51570
D	252	ALA	LYS	conflict	UNP P51570
D	253	ALA	GLU	conflict	UNP P51570
E	-6	MET	-	initiating methionine	UNP P51570
E	-5	ALA	-	expression tag	UNP P51570
E	-4	HIS	-	expression tag	UNP P51570
E	-3	HIS	-	expression tag	UNP P51570
E	-2	HIS	-	expression tag	UNP P51570
E	-1	HIS	-	expression tag	UNP P51570
E	0	HIS	-	expression tag	UNP P51570
E	1	HIS	-	expression tag	UNP P51570
E	252	ALA	LYS	conflict	UNP P51570
E	253	ALA	GLU	conflict	UNP P51570
F	-6	MET	-	initiating methionine	UNP P51570
F	-5	ALA	-	expression tag	UNP P51570
F	-4	HIS	-	expression tag	UNP P51570
F	-3	HIS	-	expression tag	UNP P51570
F	-2	HIS	-	expression tag	UNP P51570

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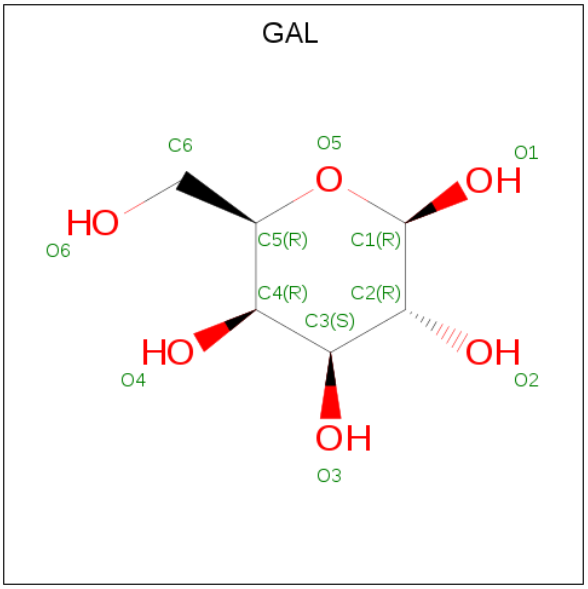
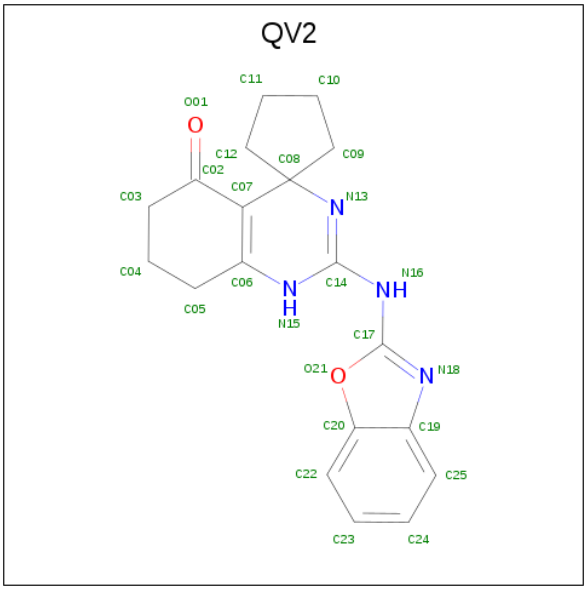
Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	HIS	-	expression tag	UNP P51570
F	0	HIS	-	expression tag	UNP P51570
F	1	HIS	-	expression tag	UNP P51570
F	252	ALA	LYS	conflict	UNP P51570
F	253	ALA	GLU	conflict	UNP P51570
G	-6	MET	-	initiating methionine	UNP P51570
G	-5	ALA	-	expression tag	UNP P51570
G	-4	HIS	-	expression tag	UNP P51570
G	-3	HIS	-	expression tag	UNP P51570
G	-2	HIS	-	expression tag	UNP P51570
G	-1	HIS	-	expression tag	UNP P51570
G	0	HIS	-	expression tag	UNP P51570
G	1	HIS	-	expression tag	UNP P51570
G	252	ALA	LYS	conflict	UNP P51570
G	253	ALA	GLU	conflict	UNP P51570
H	-6	MET	-	initiating methionine	UNP P51570
H	-5	ALA	-	expression tag	UNP P51570
H	-4	HIS	-	expression tag	UNP P51570
H	-3	HIS	-	expression tag	UNP P51570
H	-2	HIS	-	expression tag	UNP P51570
H	-1	HIS	-	expression tag	UNP P51570
H	0	HIS	-	expression tag	UNP P51570
H	1	HIS	-	expression tag	UNP P51570
H	252	ALA	LYS	conflict	UNP P51570
H	253	ALA	GLU	conflict	UNP P51570

- Molecule 2 is beta-D-galactopyranose (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
2	A	1	12	6	6		0	0
2	B	1	12	6	6		0	0
2	C	1	12	6	6		0	0
2	D	1	12	6	6		0	0
2	E	1	12	6	6		0	0
2	F	1	12	6	6		0	0
2	G	1	12	6	6		0	0
2	H	1	12	6	6		0	0

- Molecule 3 is 2-(1,3-benzoxazol-2-ylamino)spiro[1,6,7,8-tetrahydroquinazoline-4,1'-cyclopentane]-5-one (three-letter code: QV2) (formula: $C_{19}H_{20}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	25	19	4	2	0	0
3	B	1	25	19	4	2	0	0
3	C	1	25	19	4	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	D	1	25	19	4	2	0	0
			Total	C	N	O		
3	E	1	25	19	4	2	0	0
			Total	C	N	O		
3	F	1	25	19	4	2	0	0
			Total	C	N	O		
3	G	1	25	19	4	2	0	0

- Molecule 4 is water.

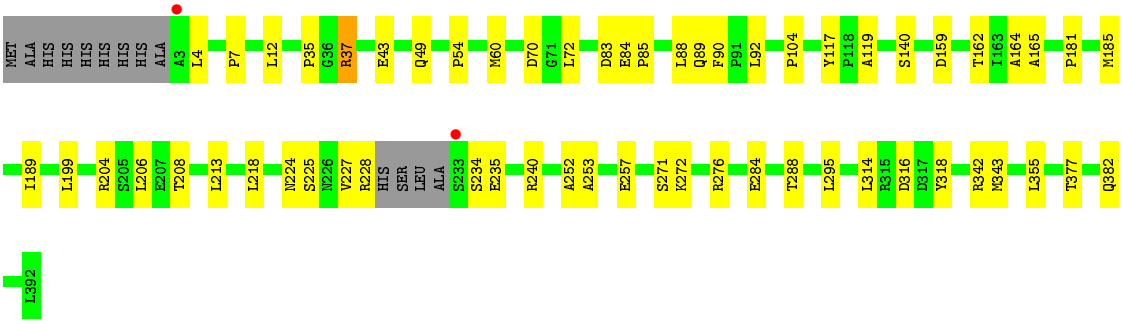
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	56	56	56	0	0
			Total	O		
4	B	49	49	49	0	0
			Total	O		
4	C	60	60	60	0	0
			Total	O		
4	D	56	56	56	0	0
			Total	O		
4	E	35	35	35	0	0
			Total	O		
4	F	36	36	36	0	0
			Total	O		
4	G	22	22	22	0	0
			Total	O		
4	H	18	18	18	0	0

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.

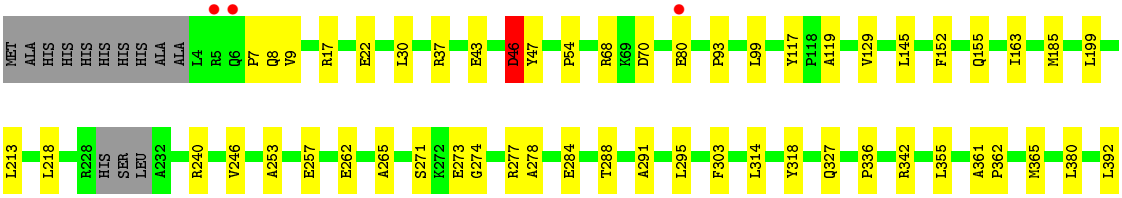
- Molecule 1: Galactokinase

Chain A:



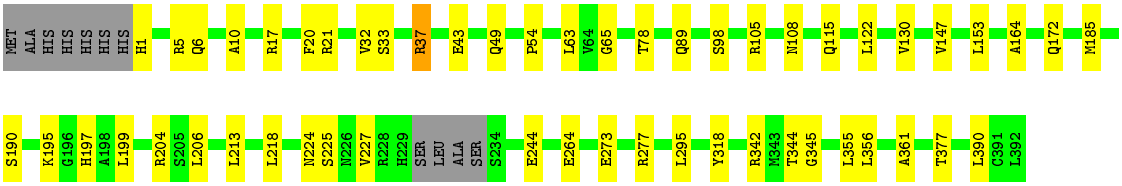
- Molecule 1: Galactokinase

Chain B:



- Molecule 1: Galactokinase

Chain C:

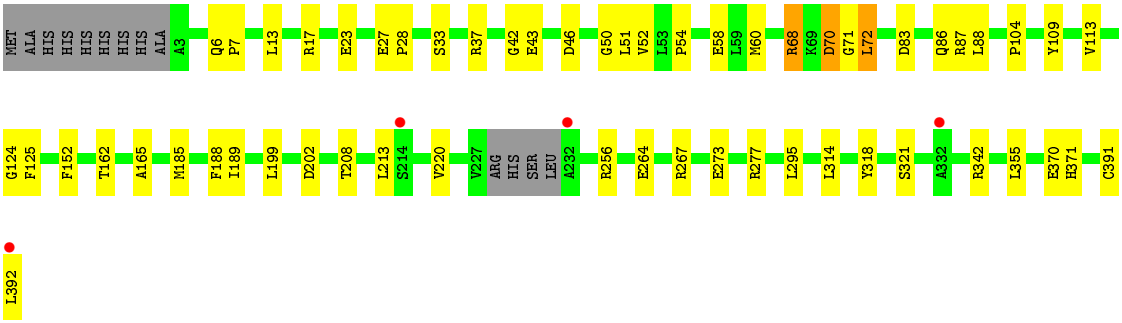


- Molecule 1: Galactokinase

Chain D:

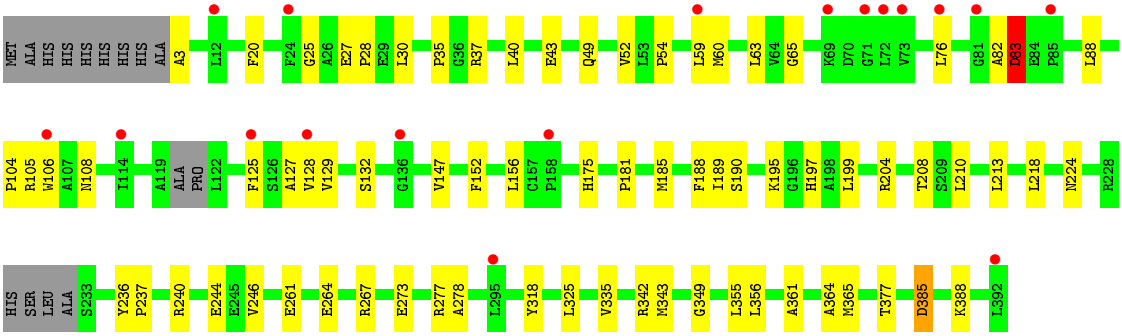
- Molecule 1: Galactokinase

Chain E:



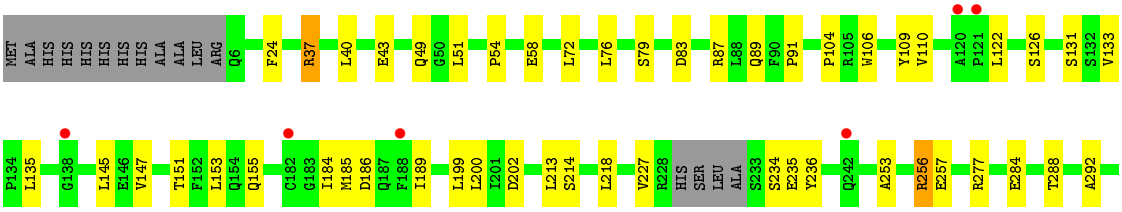
- Molecule 1: Galactokinase

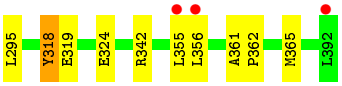
Chain F:



- Molecule 1: Galactokinase

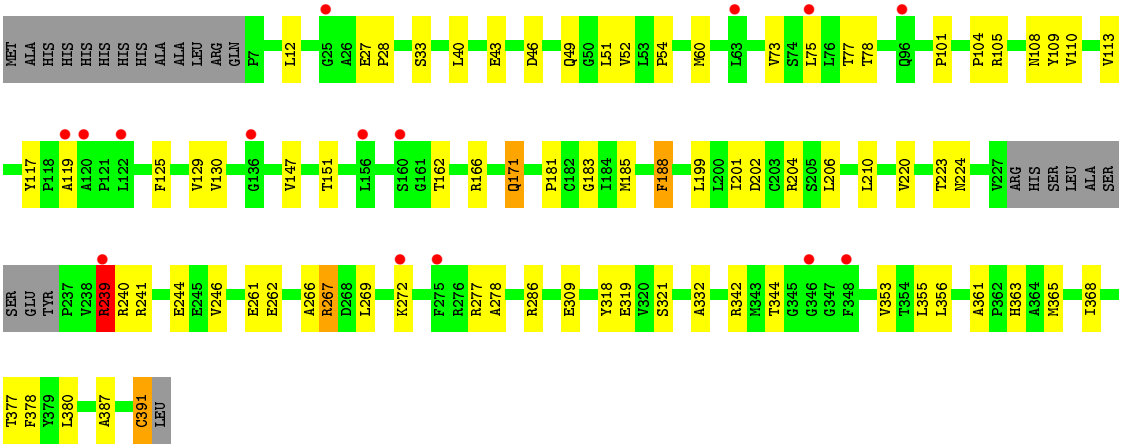
Chain G:





- Molecule 1: Galactokinase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	119.87Å 97.20Å 144.81Å 90.00° 98.51° 90.00°	Depositor
Resolution (Å)	98.79 – 2.44 98.79 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.1 (98.79-2.44) 99.3 (98.79-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.210 , 0.262 0.208 , 0.260	Depositor DCC
R_{free} test set	5996 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.803	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22813	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.05% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: QV2, GAL

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	0.28	0/2906	0.49	0/3949
1	B	0.27	0/2862	0.51	2/3896 (0.1%)
1	C	0.29	1/2911 (0.0%)	0.52	1/3959 (0.0%)
1	D	0.27	0/2858	0.48	0/3891
1	E	0.30	0/2866	0.54	5/3900 (0.1%)
1	F	0.29	0/2817	0.53	3/3836 (0.1%)
1	G	0.27	0/2749	0.47	0/3752
1	H	0.36	1/2652 (0.0%)	0.65	4/3627 (0.1%)
All	All	0.29	2/22621 (0.0%)	0.52	15/30810 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	244	GLU	CD-OE2	-6.08	1.19	1.25
1	H	309	GLU	CG-CD	-5.84	1.43	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	239	ARG	NE-CZ-NH1	-18.96	110.82	120.30
1	H	239	ARG	NE-CZ-NH2	13.54	127.07	120.30
1	C	172	GLN	CA-CB-CG	-8.13	95.51	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	86	GLN	CA-CB-CG	7.26	129.38	113.40
1	F	83	ASP	CB-CG-OD1	-6.45	112.50	118.30
1	F	83	ASP	CB-CG-OD2	6.16	123.84	118.30
1	B	46	ASP	CB-CG-OD1	-6.15	112.76	118.30
1	E	68	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	B	46	ASP	CB-CG-OD2	5.95	123.66	118.30
1	F	210	LEU	CA-CB-CG	5.88	128.82	115.30
1	H	309	GLU	CA-CB-CG	-5.79	100.66	113.40
1	E	68	ARG	CG-CD-NE	-5.46	100.34	111.80
1	H	239	ARG	CB-CG-CD	-5.38	97.60	111.60
1	E	72	LEU	CA-CB-CG	5.13	127.09	115.30
1	E	370	GLU	CA-CB-CG	-5.11	102.15	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	82	ALA	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2854	0	2808	42	0
1	B	2810	0	2739	38	0
1	C	2857	0	2793	30	0
1	D	2806	0	2719	38	0
1	E	2814	0	2744	31	1
1	F	2767	0	2675	41	0
1	G	2699	0	2579	39	0
1	H	2603	0	2439	55	1
2	A	12	0	12	0	0
2	B	12	0	12	0	0
2	C	12	0	12	0	0
2	D	12	0	12	0	0
2	E	12	0	12	0	0
2	F	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	12	0	12	1	0
2	H	12	0	12	1	0
3	A	25	0	0	0	0
3	B	25	0	0	0	0
3	C	25	0	0	1	0
3	D	25	0	0	0	0
3	E	25	0	0	0	0
3	F	25	0	0	0	0
3	G	25	0	0	0	0
4	A	56	0	0	1	0
4	B	49	0	0	3	0
4	C	60	0	0	2	0
4	D	56	0	0	3	0
4	E	35	0	0	1	0
4	F	36	0	0	3	0
4	G	22	0	0	1	0
4	H	18	0	0	1	0
All	All	22813	0	21592	305	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 7.

All (305) 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:46:ASP:OD1	1:B:47:TYR:N	1.87	1.08
1:A:88:LEU:HD12	1:A:104:PRO:HD2	1.49	0.94
1:H:241:ARG:HA	1:H:244:GLU:OE1	1.68	0.91
1:F:59:LEU:HD22	1:F:132:SER:O	1.70	0.91
1:D:43:GLU:HG2	1:D:342:ARG:HH22	1.37	0.90
1:H:43:GLU:HG2	1:H:342:ARG:HH22	1.36	0.89
1:A:272:LYS:H	1:H:241:ARG:NH2	1.80	0.79
1:H:54:PRO:HB3	1:H:185:MET:HE2	1.64	0.79
1:D:76:LEU:HB3	1:D:128:VAL:HG12	1.66	0.78
1:F:59:LEU:HD23	1:F:132:SER:HB2	1.68	0.76
1:E:17:ARG:HD2	1:E:392:LEU:HD22	1.67	0.75
1:H:239:ARG:NH2	1:H:277:ARG:HH21	1.83	0.75
1:H:33:SER:OG	1:H:60:MET:SD	2.45	0.74
1:B:271:SER:HB2	1:B:274:GLY:H	1.54	0.73
1:D:49:GLN:HB3	1:D:204:ARG:HB2	1.69	0.72
1:F:76:LEU:HB3	1:F:128:VAL:HG12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:LYS:HB2	1:F:385:ASP:OD2	1.89	0.71
1:B:213:LEU:HD11	1:B:295:LEU:HD21	1.74	0.69
1:F:88:LEU:HD13	1:F:104:PRO:HD2	1.76	0.68
1:A:276:ARG:NH2	1:A:316:ASP:O	2.27	0.68
1:B:17:ARG:HE	1:B:392:LEU:HD22	1.58	0.67
1:E:70:ASP:OD2	1:E:72:LEU:HB2	1.93	0.67
1:G:83:ASP:HB3	1:G:104:PRO:HB2	1.76	0.67
1:B:327:GLN:NE2	4:B:501:HOH:O	2.28	0.67
1:E:162:THR:HG23	1:E:165:ALA:H	1.59	0.67
1:F:27:GLU:HG3	1:F:28:PRO:HD2	1.77	0.66
1:D:286:ARG:NH1	4:D:501:HOH:O	2.25	0.66
1:A:181:PRO:O	1:A:240:ARG:NH1	2.29	0.66
1:A:253:ALA:HB3	1:A:257:GLU:OE2	1.96	0.65
1:A:43:GLU:HB2	1:A:342:ARG:HH21	1.62	0.65
1:D:93:PRO:HB3	1:D:99:LEU:HD12	1.77	0.65
1:H:27:GLU:HG3	1:H:28:PRO:HD2	1.78	0.65
1:A:84:GLU:HG2	1:A:85:PRO:HA	1.78	0.65
1:F:3:ALA:N	4:F:502:HOH:O	2.31	0.64
1:D:94:THR:HG23	1:D:97:ARG:H	1.63	0.63
1:E:68:ARG:HB2	1:E:124:GLY:C	2.18	0.63
1:A:272:LYS:H	1:H:241:ARG:HH21	1.46	0.63
1:B:265:ALA:O	1:E:264:GLU:HG2	1.99	0.62
1:E:70:ASP:CG	1:E:72:LEU:H	2.02	0.62
1:H:239:ARG:HH21	1:H:277:ARG:NH2	1.95	0.62
1:C:213:LEU:HD11	1:C:295:LEU:HD21	1.81	0.62
1:H:49:GLN:HB3	1:H:204:ARG:HB2	1.82	0.61
1:G:155:GLN:NE2	4:G:504:HOH:O	2.33	0.61
1:E:70:ASP:OD1	1:E:71:GLY:N	2.33	0.61
1:A:253:ALA:N	1:A:257:GLU:OE1	2.34	0.60
1:F:125:PHE:HB3	1:F:156:LEU:HD11	1.83	0.60
1:H:266:ALA:HA	1:H:269:LEU:HD13	1.82	0.60
1:G:76:LEU:HD13	1:G:87:ARG:HG3	1.83	0.60
1:H:239:ARG:NH2	1:H:277:ARG:NH2	2.48	0.60
1:F:63:LEU:HG	1:F:129:VAL:HG12	1.83	0.60
1:H:188:PHE:CE2	1:H:206:LEU:HD12	2.37	0.59
1:A:162:THR:HG23	1:A:165:ALA:H	1.68	0.59
1:D:122:LEU:HD12	1:D:157:CYS:HB3	1.84	0.58
1:D:122:LEU:HD21	1:D:153:LEU:HD22	1.83	0.58
1:E:213:LEU:HD11	1:E:295:LEU:HD21	1.85	0.58
1:B:22:GLU:O	1:B:22:GLU:HG2	2.04	0.57
1:H:54:PRO:HD2	1:H:199:LEU:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLU:O	1:A:288:THR:HG23	2.05	0.57
1:D:99:LEU:HD23	1:D:111:LYS:HD2	1.87	0.57
1:A:70:ASP:OD1	1:A:72:LEU:HG	2.04	0.56
1:G:79:SER:HB3	1:G:135:LEU:HD11	1.88	0.56
1:D:273:GLU:O	1:D:277:ARG:HG2	2.05	0.56
1:C:164:ALA:HB1	1:C:206:LEU:HD13	1.88	0.56
1:C:122:LEU:HD11	1:C:153:LEU:HD22	1.88	0.55
1:D:224:ASN:HB3	1:D:377:THR:HB	1.88	0.55
1:E:27:GLU:HG3	1:E:28:PRO:HD2	1.89	0.55
1:H:223:THR:HG23	1:H:378:PHE:HE1	1.72	0.55
1:H:171:GLN:HE21	1:H:183:GLY:C	2.09	0.55
1:H:54:PRO:CB	1:H:185:MET:HE2	2.37	0.54
1:B:68:ARG:NH2	1:B:70:ASP:OD2	2.24	0.54
1:F:52:VAL:HG21	1:F:185:MET:HG3	1.88	0.54
1:F:59:LEU:CD2	1:F:132:SER:O	2.50	0.54
1:E:46:ASP:OD2	1:E:185:MET:HB3	2.07	0.54
1:D:27:GLU:HG3	1:D:28:PRO:HD2	1.90	0.54
1:G:213:LEU:HG	1:G:295:LEU:HD21	1.89	0.54
1:D:68:ARG:NH1	1:D:126:SER:OG	2.37	0.54
1:B:336:PRO:HG3	1:C:10:ALA:HB1	1.90	0.54
1:C:49:GLN:HB3	1:C:204:ARG:HB2	1.88	0.54
1:C:105:ARG:NH1	3:C:402:QV2:O01	2.40	0.54
1:G:122:LEU:HD21	1:G:153:LEU:HD22	1.90	0.54
1:B:218:LEU:HD11	1:B:355:LEU:CD2	2.38	0.54
1:G:200:LEU:HD12	1:G:292:ALA:CB	2.39	0.53
1:D:93:PRO:HD3	1:D:99:LEU:HD11	1.90	0.53
1:A:85:PRO:HD2	1:A:104:PRO:HD3	1.91	0.53
1:H:365:MET:HA	1:H:378:PHE:CE2	2.43	0.53
1:C:54:PRO:HD2	1:C:199:LEU:O	2.09	0.53
1:H:344:THR:HB	1:H:353:VAL:HG23	1.89	0.53
1:A:218:LEU:HD11	1:A:355:LEU:HD21	1.90	0.53
1:E:50:GLY:HA2	1:E:256:ARG:HD3	1.91	0.53
1:E:54:PRO:HD2	1:E:199:LEU:O	2.09	0.53
1:D:54:PRO:HD2	1:D:199:LEU:O	2.09	0.53
1:H:286:ARG:NH1	4:H:501:HOH:O	2.30	0.53
1:F:35:PRO:HA	1:F:60:MET:HA	1.91	0.52
1:H:75:LEU:CD1	1:H:110:VAL:HG21	2.39	0.52
1:H:54:PRO:HB3	1:H:185:MET:CE	2.36	0.52
1:A:89:GLN:HG2	1:G:89:GLN:HG2	1.91	0.52
1:D:276:ARG:NH2	1:D:319:GLU:OE1	2.38	0.52
1:B:43:GLU:HB2	1:B:342:ARG:HH12	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:LEU:HD23	1:G:202:ASP:HA	1.90	0.52
1:G:109:TYR:HB2	1:G:145:LEU:HD22	1.90	0.52
1:H:181:PRO:O	1:H:240:ARG:NH1	2.43	0.52
1:G:362:PRO:HA	1:G:365:MET:HE2	1.92	0.52
1:H:12:LEU:HD12	1:H:130:VAL:HG13	1.92	0.52
1:C:264:GLU:OE2	4:C:501:HOH:O	2.18	0.51
1:D:286:ARG:O	1:D:290:GLN:HG2	2.09	0.51
1:F:240:ARG:O	1:F:244:GLU:HG2	2.10	0.51
1:F:356:LEU:HD11	1:F:361:ALA:HA	1.92	0.51
1:A:252:ALA:HB1	1:A:257:GLU:OE1	2.10	0.51
1:B:253:ALA:N	1:B:257:GLU:OE2	2.42	0.51
1:G:37:ARG:NE	1:G:186:ASP:OD1	2.42	0.51
1:G:131:SER:OG	1:G:133:VAL:HG22	2.10	0.51
1:G:185:MET:O	1:G:189:ILE:HG22	2.11	0.51
1:C:273:GLU:O	1:C:277:ARG:HG2	2.10	0.51
1:H:151:THR:HG21	1:H:387:ALA:HB1	1.91	0.51
1:H:220:VAL:HG12	1:H:355:LEU:HD12	1.92	0.51
1:B:43:GLU:HB3	1:B:314:LEU:HD21	1.93	0.51
1:G:277:ARG:NH2	1:G:319:GLU:OE1	2.44	0.51
1:B:273:GLU:O	1:B:277:ARG:HG2	2.11	0.50
1:D:17:ARG:O	1:D:21:ARG:HG3	2.12	0.50
1:E:13:LEU:O	1:E:17:ARG:HG3	2.11	0.50
1:C:1:HIS:N	4:C:507:HOH:O	2.45	0.50
1:F:54:PRO:HD2	1:F:199:LEU:O	2.10	0.50
1:G:43:GLU:HB2	1:G:342:ARG:NH2	2.26	0.50
1:A:227:VAL:HG23	1:A:228:ARG:H	1.75	0.50
1:H:147:VAL:O	1:H:151:THR:HG23	2.12	0.50
1:F:49:GLN:HB3	1:F:204:ARG:HB2	1.93	0.50
1:E:33:SER:HB2	1:E:60:MET:HE2	1.93	0.50
1:H:239:ARG:HG2	1:H:277:ARG:HG3	1.93	0.50
1:H:356:LEU:HD11	1:H:361:ALA:HA	1.93	0.50
1:E:88:LEU:HD22	1:E:104:PRO:HD2	1.94	0.49
1:G:356:LEU:HD11	1:G:361:ALA:HA	1.94	0.49
1:A:382:GLN:NE2	4:A:505:HOH:O	2.45	0.49
1:G:49:GLN:O	1:G:256:ARG:HD3	2.12	0.49
1:F:218:LEU:HD11	1:F:355:LEU:HG	1.95	0.49
1:E:70:ASP:HB2	1:E:72:LEU:HD13	1.93	0.49
1:F:63:LEU:HD21	1:F:127:ALA:HB1	1.95	0.49
1:A:72:LEU:HD13	1:G:72:LEU:HD22	1.94	0.49
1:H:52:VAL:HG23	1:H:201:ILE:HB	1.93	0.49
1:E:43:GLU:HB3	1:E:314:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:PHE:CE2	1:F:65:GLY:HA2	2.48	0.48
1:D:312:ARG:NH1	4:D:509:HOH:O	2.45	0.48
1:A:224:ASN:HB3	1:A:377:THR:OG1	2.13	0.48
1:C:43:GLU:HB2	1:C:342:ARG:NH2	2.29	0.48
1:G:110:VAL:HG23	1:G:145:LEU:HD21	1.95	0.48
1:H:332:ALA:HB2	1:H:368:ILE:HD11	1.96	0.48
1:H:105:ARG:HA	1:H:108:ASN:ND2	2.28	0.48
1:B:54:PRO:HD2	1:B:199:LEU:O	2.12	0.48
1:G:234:SER:OG	1:G:235:GLU:N	2.47	0.48
1:D:94:THR:OG1	1:D:95:ALA:N	2.47	0.48
1:F:188:PHE:HE2	1:F:208:THR:HG21	1.79	0.48
1:C:32:VAL:HG22	1:C:63:LEU:HB2	1.95	0.48
1:D:15:GLU:HG2	1:D:130:VAL:HG11	1.95	0.48
1:F:147:VAL:HG21	1:F:190:SER:HB3	1.96	0.48
1:B:46:ASP:CG	1:B:47:TYR:N	2.64	0.48
1:B:284:GLU:O	1:B:288:THR:HG22	2.14	0.48
1:F:83:ASP:OD2	1:F:106:TRP:N	2.30	0.48
1:D:264:GLU:OE1	1:D:267:ARG:NH2	2.48	0.47
1:C:33:SER:HB3	1:C:390:LEU:HD11	1.96	0.47
1:D:68:ARG:NE	1:D:70:ASP:OD2	2.23	0.47
1:E:23:GLU:OE1	1:E:87:ARG:HD3	2.15	0.47
1:H:361:ALA:HB1	1:H:380:LEU:HD11	1.95	0.47
1:C:17:ARG:O	1:C:21:ARG:HG3	2.16	0.46
1:F:3:ALA:HB2	1:F:365:MET:SD	2.56	0.46
1:D:135:LEU:HD12	4:D:549:HOH:O	2.14	0.46
1:H:77:THR:HB	1:H:129:VAL:HG13	1.96	0.46
1:A:213:LEU:HD21	1:A:295:LEU:HD21	1.96	0.46
1:C:195:LYS:O	1:C:197:HIS:ND1	2.36	0.46
1:D:43:GLU:HG2	1:D:342:ARG:NH2	2.18	0.46
1:E:109:TYR:O	1:E:113:VAL:HG23	2.16	0.46
1:F:105:ARG:HA	1:F:108:ASN:ND2	2.30	0.46
1:H:267:ARG:NH1	1:H:272:LYS:HE2	2.30	0.46
1:D:70:ASP:OD1	1:D:72:LEU:N	2.47	0.46
1:G:147:VAL:O	1:G:151:THR:HG22	2.15	0.46
1:H:365:MET:HA	1:H:378:PHE:HE2	1.81	0.46
1:H:109:TYR:O	1:H:113:VAL:HG23	2.16	0.46
1:G:40:LEU:HD11	1:G:213:LEU:HD11	1.98	0.46
1:E:43:GLU:HB2	1:E:342:ARG:NH2	2.31	0.46
1:G:110:VAL:CG2	1:G:145:LEU:HD21	2.46	0.46
1:H:224:ASN:HB3	1:H:377:THR:HB	1.98	0.46
1:A:37:ARG:HG3	1:A:140:SER:OG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:SER:OG	1:A:227:VAL:HG22	2.16	0.46
1:B:218:LEU:HD21	1:B:355:LEU:HD21	1.97	0.46
1:A:54:PRO:HD2	1:A:199:LEU:O	2.15	0.46
1:B:218:LEU:HD11	1:B:355:LEU:HD21	1.97	0.45
1:F:25:GLY:O	4:F:501:HOH:O	2.21	0.45
1:H:78:THR:OG1	1:H:130:VAL:HG23	2.16	0.45
1:H:261:GLU:OE2	1:H:262:GLU:HG2	2.17	0.45
1:A:70:ASP:OD2	1:G:91:PRO:HD3	2.17	0.45
1:F:224:ASN:HB3	1:F:377:THR:OG1	2.17	0.45
1:G:51:LEU:HD22	1:G:200:LEU:HD21	1.99	0.45
1:D:194:GLN:HG3	1:D:210:LEU:HD13	1.98	0.45
1:G:184:ILE:O	1:G:184:ILE:HG13	2.16	0.45
1:G:284:GLU:O	1:G:288:THR:HG22	2.17	0.45
1:A:117:TYR:CE2	1:A:119:ALA:HB3	2.52	0.45
1:A:7:PRO:HB2	1:A:12:LEU:CD1	2.47	0.44
1:H:246:VAL:HG11	1:H:278:ALA:HB2	1.99	0.44
1:C:43:GLU:HB2	1:C:342:ARG:HH22	1.83	0.44
1:F:125:PHE:CD2	1:F:152:PHE:HE2	2.34	0.44
1:H:277:ARG:NH2	1:H:319:GLU:OE1	2.50	0.44
1:A:88:LEU:HD23	1:A:89:GLN:N	2.33	0.44
1:E:220:VAL:HG12	1:E:355:LEU:HD12	1.99	0.44
1:H:277:ARG:HD3	1:H:277:ARG:N	2.32	0.44
1:F:175:HIS:CD2	1:F:181:PRO:HA	2.52	0.44
1:B:246:VAL:HG11	1:B:278:ALA:HB2	1.99	0.44
1:G:236:TYR:HH	2:G:401:GAL:HO4	1.53	0.44
1:A:199:LEU:HD23	1:A:208:THR:HG21	2.00	0.44
1:B:93:PRO:HB3	1:B:99:LEU:HD13	1.99	0.44
1:C:218:LEU:HD11	1:C:355:LEU:HD12	1.99	0.44
1:B:30:LEU:HB2	1:B:152:PHE:HE1	1.82	0.44
1:B:117:TYR:CE2	1:B:119:ALA:HB3	2.53	0.44
1:H:101:PRO:HA	1:H:108:ASN:OD1	2.17	0.44
1:G:109:TYR:HB2	1:G:145:LEU:CD2	2.48	0.44
1:E:188:PHE:HE2	1:E:208:THR:HG21	1.83	0.43
1:F:30:LEU:HB2	1:F:152:PHE:HE1	1.83	0.43
1:D:55:MET:HE3	1:D:220:VAL:HG11	2.00	0.43
1:E:58:GLU:N	4:E:504:HOH:O	2.40	0.43
1:A:7:PRO:HB2	1:A:12:LEU:HD13	2.00	0.43
1:B:30:LEU:HD13	1:B:155:GLN:HB2	1.99	0.43
1:C:98:SER:HB2	1:C:115:GLN:HE22	1.83	0.43
1:F:40:LEU:HD11	1:F:213:LEU:HD11	2.00	0.43
1:H:40:LEU:O	1:H:342:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:PRO:HA	1:A:60:MET:HA	2.01	0.43
1:D:117:TYR:CE2	1:D:119:ALA:HB3	2.53	0.43
1:G:54:PRO:HD2	1:G:199:LEU:O	2.19	0.43
1:D:40:LEU:HD11	1:D:213:LEU:HD11	2.00	0.43
1:E:83:ASP:OD1	1:E:83:ASP:N	2.51	0.43
1:E:273:GLU:O	1:E:277:ARG:HG2	2.18	0.43
1:G:24:PHE:CE1	1:G:126:SER:HB2	2.54	0.43
1:B:46:ASP:OD1	1:B:47:TYR:CD2	2.71	0.43
1:F:264:GLU:O	1:F:267:ARG:HG2	2.19	0.43
1:H:51:LEU:HD23	1:H:202:ASP:HA	2.00	0.43
1:E:51:LEU:HD23	1:E:202:ASP:HA	2.00	0.43
1:G:277:ARG:NH1	1:G:318:TYR:O	2.52	0.43
1:A:185:MET:O	1:A:189:ILE:HG22	2.19	0.43
1:B:54:PRO:HB3	1:B:185:MET:HE3	2.01	0.43
1:B:362:PRO:HA	1:B:365:MET:HE2	2.00	0.43
1:C:37:ARG:HD3	1:C:185:MET:HE2	2.01	0.43
1:C:356:LEU:HD11	1:C:361:ALA:HA	2.01	0.43
1:F:43:GLU:HB2	1:F:342:ARG:HH12	1.84	0.43
1:G:83:ASP:HB3	1:G:106:TRP:HD1	1.84	0.43
1:H:183:GLY:N	2:H:401:GAL:O3	2.48	0.43
1:B:163:ILE:H	1:B:163:ILE:HG13	1.67	0.42
1:G:218:LEU:HD11	1:G:355:LEU:HD22	2.02	0.42
1:H:46:ASP:CG	1:H:183:GLY:HA3	2.40	0.42
1:H:117:TYR:CE2	1:H:119:ALA:HB3	2.54	0.42
1:H:162:THR:O	1:H:166:ARG:HG3	2.20	0.42
1:A:164:ALA:HB1	1:A:206:LEU:HD13	2.02	0.42
1:A:213:LEU:HD11	1:A:295:LEU:HD21	2.01	0.42
1:B:129:VAL:HG11	1:B:145:LEU:HD13	2.01	0.42
1:B:291:ALA:HB1	1:B:303:PHE:CE2	2.55	0.42
1:E:42:GLY:O	1:E:52:VAL:HG12	2.19	0.42
1:A:70:ASP:CG	1:G:91:PRO:HD3	2.40	0.42
1:C:54:PRO:HB3	1:C:185:MET:HE3	2.01	0.42
1:E:43:GLU:HB2	1:E:342:ARG:HH22	1.85	0.42
1:A:342:ARG:HG2	1:A:343:MET:O	2.20	0.42
1:B:218:LEU:HD11	1:B:355:LEU:HD23	2.00	0.42
1:C:105:ARG:HA	1:C:108:ASN:ND2	2.35	0.42
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.75	0.42
1:C:224:ASN:HB3	1:C:377:THR:HB	2.02	0.42
1:G:253:ALA:HB3	1:G:257:GLU:OE1	2.19	0.42
1:B:80:GLU:N	4:B:502:HOH:O	2.52	0.42
1:A:88:LEU:CD2	1:A:90:PHE:HD1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:MET:O	1:E:189:ILE:HG22	2.20	0.42
1:H:171:GLN:NE2	1:H:183:GLY:C	2.73	0.41
1:D:162:THR:O	1:D:166:ARG:HG3	2.20	0.41
1:B:262:GLU:OE1	1:E:267:ARG:NH2	2.51	0.41
1:C:147:VAL:HG21	1:C:190:SER:HB3	2.02	0.41
1:C:225:SER:OG	1:C:227:VAL:HG22	2.20	0.41
1:D:198:ALA:HB2	1:D:213:LEU:HD12	2.01	0.41
1:F:273:GLU:O	1:F:277:ARG:HG2	2.20	0.41
1:F:335:VAL:HG21	1:F:364:ALA:HA	2.02	0.41
1:H:104:PRO:O	1:H:108:ASN:ND2	2.53	0.41
1:H:363:HIS:O	1:H:363:HIS:ND1	2.53	0.41
1:C:20:PHE:CE2	1:C:65:GLY:HA2	2.56	0.41
1:C:78:THR:OG1	1:C:130:VAL:HG12	2.20	0.41
1:B:361:ALA:HB1	1:B:380:LEU:HD11	2.02	0.41
1:C:32:VAL:CG2	1:C:63:LEU:HB2	2.51	0.41
1:G:227:VAL:HG21	1:G:324:GLU:HG2	2.01	0.41
1:A:43:GLU:HB3	1:A:314:LEU:HD21	2.03	0.41
1:B:46:ASP:HB3	4:B:518:HOH:O	2.21	0.41
1:B:47:TYR:CD1	1:B:240:ARG:HG2	2.55	0.41
1:B:218:LEU:HA	1:B:218:LEU:HD12	1.85	0.41
1:C:89:GLN:HE21	1:C:89:GLN:HB2	1.73	0.41
1:D:63:LEU:HD22	1:D:152:PHE:CG	2.56	0.41
1:D:123:PRO:HD2	1:D:156:LEU:HB3	2.02	0.41
1:F:195:LYS:O	1:F:197:HIS:ND1	2.41	0.41
1:F:261:GLU:HB2	4:F:506:HOH:O	2.21	0.41
1:G:58:GLU:H	1:G:58:GLU:HG3	1.70	0.41
1:H:199:LEU:HD13	1:H:210:LEU:HD13	2.01	0.41
1:A:206:LEU:HD23	1:A:206:LEU:HA	1.92	0.41
1:A:227:VAL:HG23	1:A:228:ARG:N	2.36	0.41
1:B:8:GLN:HG3	1:B:9:VAL:H	1.85	0.41
1:D:202:ASP:O	1:D:206:LEU:N	2.54	0.40
1:F:236:TYR:N	1:F:237:PRO:HD2	2.36	0.40
1:C:344:THR:CG2	1:C:345:GLY:N	2.84	0.40
1:D:109:TYR:O	1:D:113:VAL:HG23	2.20	0.40
1:D:163:ILE:HG21	1:D:192:MET:SD	2.61	0.40
1:F:342:ARG:HG2	1:F:343:MET:O	2.21	0.40
1:A:49:GLN:HB3	1:A:204:ARG:HB2	2.02	0.40
1:D:149:THR:O	1:D:153:LEU:HG	2.21	0.40
1:F:325:LEU:HD11	1:F:349:GLY:O	2.21	0.40
1:E:125:PHE:CD2	1:E:152:PHE:HE2	2.39	0.40
1:F:185:MET:O	1:F:189:ILE:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:246:VAL:HG11	1:F:278:ALA:HB2	2.04	0.40
1:H:73:VAL:HA	1:H:125:PHE:O	2.22	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:E:391:CYS:SG	1:H:391:CYS:CB[2_544]	1.65	0.55

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	382/399 (96%)	371 (97%)	10 (3%)	1 (0%)	41	49
1	B	382/399 (96%)	371 (97%)	10 (3%)	1 (0%)	41	49
1	C	384/399 (96%)	368 (96%)	14 (4%)	2 (0%)	29	34
1	D	381/399 (96%)	371 (97%)	10 (3%)	0	100	100
1	E	382/399 (96%)	371 (97%)	10 (3%)	1 (0%)	41	49
1	F	378/399 (95%)	368 (97%)	9 (2%)	1 (0%)	41	49
1	G	379/399 (95%)	366 (97%)	13 (3%)	0	100	100
1	H	372/399 (93%)	363 (98%)	9 (2%)	0	100	100
All	All	3040/3192 (95%)	2949 (97%)	85 (3%)	6 (0%)	47	57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	83	ASP
1	C	5	ARG
1	A	4	LEU

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Mol	Chain	Res	Type
1	E	7	PRO
1	C	6	GLN
1	B	7	PRO

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	291/315 (92%)	284 (98%)	7 (2%)	49	61
1	B	281/315 (89%)	278 (99%)	3 (1%)	73	83
1	C	287/315 (91%)	285 (99%)	2 (1%)	84	90
1	D	280/315 (89%)	275 (98%)	5 (2%)	59	71
1	E	281/315 (89%)	275 (98%)	6 (2%)	53	66
1	F	273/315 (87%)	268 (98%)	5 (2%)	59	71
1	G	256/315 (81%)	252 (98%)	4 (2%)	62	74
1	H	238/315 (76%)	231 (97%)	7 (3%)	42	54
All	All	2187/2520 (87%)	2148 (98%)	39 (2%)	59	71

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	83	ASP
1	A	159	ASP
1	A	234	SER
1	A	235	GLU
1	A	271	SER
1	A	318	TYR
1	B	37	ARG
1	B	46	ASP
1	B	318	TYR
1	C	37	ARG
1	C	318	TYR

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Mol	Chain	Res	Type
1	D	18	ARG
1	D	37	ARG
1	D	99	LEU
1	D	180	MET
1	D	318	TYR
1	E	6	GLN
1	E	37	ARG
1	E	70	ASP
1	E	318	TYR
1	E	321	SER
1	E	371	HIS
1	F	37	ARG
1	F	83	ASP
1	F	318	TYR
1	F	385	ASP
1	F	388	LYS
1	G	37	ARG
1	G	214	SER
1	G	256	ARG
1	G	318	TYR
1	H	171	GLN
1	H	188	PHE
1	H	239	ARG
1	H	267	ARG
1	H	318	TYR
1	H	321	SER
1	H	391	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	363	HIS
1	D	86	GLN
1	E	6	GLN
1	H	39	ASN
1	H	171	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

15 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	$\#\|Z\| > 2$
2	GAL	C	401	-	12,12,12	0.36	0	17,17,17	0.76	0
2	GAL	D	401	-	12,12,12	0.46	0	17,17,17	0.83	0
2	GAL	H	401	-	12,12,12	0.54	0	17,17,17	0.85	0
2	GAL	G	401	-	12,12,12	0.49	0	17,17,17	0.85	1 (5%)
3	QV2	G	402	-	25,29,29	4.49	17 (68%)	25,43,43	1.15	4 (16%)
3	QV2	D	402	-	25,29,29	4.50	17 (68%)	25,43,43	1.23	5 (20%)
2	GAL	E	401	-	12,12,12	0.46	0	17,17,17	0.80	0
3	QV2	B	402	-	25,29,29	4.44	17 (68%)	25,43,43	1.23	4 (16%)
3	QV2	E	402	-	25,29,29	4.47	17 (68%)	25,43,43	1.34	4 (16%)
3	QV2	F	402	-	25,29,29	4.46	17 (68%)	25,43,43	1.20	4 (16%)
3	QV2	C	402	-	25,29,29	4.46	17 (68%)	25,43,43	1.23	5 (20%)
2	GAL	B	401	-	12,12,12	0.92	1 (8%)	17,17,17	1.06	1 (5%)
3	QV2	A	402	-	25,29,29	4.47	17 (68%)	25,43,43	1.25	4 (16%)
2	GAL	F	401	-	12,12,12	0.44	0	17,17,17	0.76	0
2	GAL	A	401	-	12,12,12	0.47	0	17,17,17	1.00	1 (5%)

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	GAL	C	401	-	-	1/2/22/22	0/1/1/1
2	GAL	D	401	-	-	2/2/22/22	0/1/1/1
2	GAL	H	401	-	-	1/2/22/22	0/1/1/1
2	GAL	G	401	-	-	2/2/22/22	0/1/1/1
3	QV2	G	402	-	-	2/2/42/42	0/5/5/5
3	QV2	D	402	-	-	2/2/42/42	0/5/5/5
2	GAL	E	401	-	-	1/2/22/22	0/1/1/1
3	QV2	B	402	-	-	2/2/42/42	0/5/5/5
3	QV2	E	402	-	-	2/2/42/42	0/5/5/5
3	QV2	F	402	-	-	2/2/42/42	0/5/5/5
3	QV2	C	402	-	-	2/2/42/42	0/5/5/5
2	GAL	B	401	-	-	2/2/22/22	0/1/1/1
3	QV2	A	402	-	-	2/2/42/42	0/5/5/5
2	GAL	F	401	-	-	1/2/22/22	0/1/1/1
2	GAL	A	401	-	-	2/2/22/22	0/1/1/1

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	QV2	C06-C07	11.25	1.51	1.37
3	D	402	QV2	C06-C07	11.23	1.51	1.37
3	A	402	QV2	C06-C07	11.21	1.51	1.37
3	E	402	QV2	C06-C07	11.07	1.51	1.37
3	F	402	QV2	C06-C07	10.97	1.51	1.37
3	G	402	QV2	C06-C07	10.96	1.51	1.37
3	B	402	QV2	C06-C07	10.95	1.51	1.37
3	D	402	QV2	C14-N16	8.14	1.51	1.36
3	G	402	QV2	C14-N16	8.13	1.51	1.36
3	E	402	QV2	C14-N16	8.08	1.51	1.36
3	C	402	QV2	C14-N16	8.04	1.51	1.36
3	A	402	QV2	C14-N16	8.03	1.51	1.36
3	F	402	QV2	C14-N16	8.02	1.51	1.36
3	G	402	QV2	C14-N15	7.99	1.49	1.36
3	B	402	QV2	C14-N16	7.96	1.51	1.36
3	D	402	QV2	C14-N15	7.93	1.49	1.36
3	E	402	QV2	C14-N15	7.92	1.49	1.36
3	F	402	QV2	C14-N15	7.88	1.49	1.36
3	C	402	QV2	C14-N15	7.86	1.49	1.36
3	B	402	QV2	C14-N15	7.85	1.49	1.36
3	A	402	QV2	C14-N15	7.79	1.49	1.36
3	B	402	QV2	C14-N13	7.10	1.48	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	402	QV2	C14-N13	7.09	1.48	1.30
3	A	402	QV2	C14-N13	7.05	1.48	1.30
3	D	402	QV2	C14-N13	7.03	1.48	1.30
3	F	402	QV2	C14-N13	7.01	1.48	1.30
3	E	402	QV2	C14-N13	7.00	1.48	1.30
3	C	402	QV2	C14-N13	7.00	1.48	1.30
3	G	402	QV2	C17-N16	5.40	1.46	1.36
3	E	402	QV2	C17-N16	5.37	1.46	1.36
3	D	402	QV2	C17-N16	5.31	1.46	1.36
3	A	402	QV2	C17-N16	5.24	1.45	1.36
3	F	402	QV2	C17-N16	5.24	1.45	1.36
3	C	402	QV2	C17-N16	5.23	1.45	1.36
3	E	402	QV2	C02-C07	5.14	1.61	1.46
3	F	402	QV2	C02-C07	5.10	1.61	1.46
3	D	402	QV2	C02-C07	5.09	1.61	1.46
3	B	402	QV2	C17-N16	5.08	1.45	1.36
3	A	402	QV2	C02-C07	5.04	1.61	1.46
3	B	402	QV2	C02-C07	5.04	1.61	1.46
3	G	402	QV2	C02-C07	5.04	1.61	1.46
3	C	402	QV2	C02-C07	4.99	1.61	1.46
3	F	402	QV2	C12-C11	-4.89	1.35	1.52
3	A	402	QV2	C05-C06	4.81	1.57	1.49
3	E	402	QV2	C12-C11	-4.80	1.36	1.52
3	D	402	QV2	C05-C06	4.79	1.57	1.49
3	A	402	QV2	C12-C11	-4.78	1.36	1.52
3	B	402	QV2	C12-C11	-4.77	1.36	1.52
3	C	402	QV2	C12-C11	-4.77	1.36	1.52
3	G	402	QV2	C12-C11	-4.76	1.36	1.52
3	D	402	QV2	C12-C11	-4.75	1.36	1.52
3	C	402	QV2	C05-C06	4.67	1.57	1.49
3	F	402	QV2	C05-C06	4.65	1.57	1.49
3	G	402	QV2	C05-C06	4.65	1.57	1.49
3	E	402	QV2	C05-C06	4.57	1.57	1.49
3	B	402	QV2	C05-C06	4.50	1.57	1.49
3	F	402	QV2	C09-C10	-4.35	1.37	1.52
3	B	402	QV2	C09-C10	-4.34	1.37	1.52
3	C	402	QV2	C09-C10	-4.34	1.37	1.52
3	G	402	QV2	C09-C10	-4.33	1.37	1.52
3	D	402	QV2	C09-C10	-4.32	1.37	1.52
3	A	402	QV2	C09-C10	-4.30	1.37	1.52
3	E	402	QV2	C09-C10	-4.28	1.37	1.52
3	G	402	QV2	C08-N13	4.03	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	QV2	C08-N13	3.96	1.50	1.46
3	G	402	QV2	C23-C22	3.93	1.45	1.36
3	E	402	QV2	C23-C22	3.91	1.45	1.36
3	F	402	QV2	C23-C22	3.90	1.45	1.36
3	D	402	QV2	C08-N13	3.89	1.50	1.46
3	D	402	QV2	C23-C22	3.89	1.45	1.36
3	B	402	QV2	C23-C22	3.87	1.45	1.36
3	A	402	QV2	C23-C22	3.86	1.45	1.36
3	C	402	QV2	C23-C22	3.83	1.45	1.36
3	F	402	QV2	C08-N13	3.71	1.50	1.46
3	A	402	QV2	C08-N13	3.69	1.50	1.46
3	G	402	QV2	C24-C25	3.65	1.45	1.36
3	D	402	QV2	C24-C25	3.60	1.44	1.36
3	E	402	QV2	C24-C25	3.59	1.44	1.36
3	F	402	QV2	C24-C25	3.59	1.44	1.36
3	A	402	QV2	C24-C25	3.55	1.44	1.36
3	E	402	QV2	C08-N13	3.52	1.50	1.46
3	B	402	QV2	C24-C25	3.47	1.44	1.36
3	C	402	QV2	C24-C25	3.47	1.44	1.36
3	C	402	QV2	C08-N13	3.26	1.49	1.46
3	B	402	QV2	C17-N18	-2.95	1.31	1.35
3	F	402	QV2	C17-N18	-2.93	1.31	1.35
3	A	402	QV2	C17-N18	-2.88	1.31	1.35
3	C	402	QV2	C17-N18	-2.87	1.31	1.35
3	E	402	QV2	C17-N18	-2.83	1.31	1.35
3	D	402	QV2	C17-N18	-2.76	1.31	1.35
3	G	402	QV2	C17-N18	-2.73	1.31	1.35
3	C	402	QV2	C06-N15	2.69	1.42	1.37
3	G	402	QV2	C06-N15	2.66	1.41	1.37
3	D	402	QV2	C06-N15	2.65	1.41	1.37
3	E	402	QV2	C06-N15	2.60	1.41	1.37
3	F	402	QV2	C06-N15	2.57	1.41	1.37
3	C	402	QV2	C11-C10	2.57	1.66	1.48
3	E	402	QV2	C11-C10	2.56	1.66	1.48
3	A	402	QV2	C11-C10	2.55	1.66	1.48
3	F	402	QV2	C11-C10	2.55	1.66	1.48
3	D	402	QV2	C11-C10	2.55	1.66	1.48
3	B	402	QV2	C11-C10	2.55	1.66	1.48
3	G	402	QV2	C11-C10	2.54	1.66	1.48
3	A	402	QV2	C06-N15	2.52	1.41	1.37
3	B	402	QV2	C06-N15	2.45	1.41	1.37
2	B	401	GAL	O4-C4	-2.29	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	QV2	C25-C19	2.26	1.45	1.41
3	G	402	QV2	C25-C19	2.25	1.45	1.41
3	D	402	QV2	C25-C19	2.23	1.45	1.41
3	E	402	QV2	C25-C19	2.22	1.45	1.41
3	F	402	QV2	C25-C19	2.19	1.45	1.41
3	C	402	QV2	C12-C08	2.19	1.61	1.54
3	A	402	QV2	C12-C08	2.18	1.61	1.54
3	B	402	QV2	C25-C19	2.17	1.45	1.41
3	G	402	QV2	C12-C08	2.16	1.61	1.54
3	B	402	QV2	C12-C08	2.15	1.61	1.54
3	D	402	QV2	C12-C08	2.15	1.61	1.54
3	C	402	QV2	C25-C19	2.13	1.45	1.41
3	E	402	QV2	C12-C08	2.04	1.60	1.54
3	F	402	QV2	C12-C08	2.02	1.60	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	402	QV2	C05-C06-N15	2.94	119.87	115.34
3	E	402	QV2	C05-C06-C07	-2.94	119.10	122.97
3	B	402	QV2	C05-C06-C07	-2.91	119.14	122.97
3	F	402	QV2	C05-C06-C07	-2.89	119.15	122.97
3	G	402	QV2	C05-C06-N15	2.88	119.77	115.34
3	A	402	QV2	C02-C07-C06	-2.85	116.46	119.17
3	B	402	QV2	C05-C06-N15	2.84	119.70	115.34
3	G	402	QV2	C05-C06-C07	-2.79	119.29	122.97
3	F	402	QV2	C05-C06-N15	2.73	119.55	115.34
3	A	402	QV2	C05-C06-C07	-2.72	119.38	122.97
3	D	402	QV2	C05-C06-C07	-2.70	119.41	122.97
3	E	402	QV2	C08-C07-C06	-2.68	118.72	121.75
3	D	402	QV2	C02-C07-C06	-2.55	116.74	119.17
3	C	402	QV2	C17-N16-C14	-2.50	120.94	126.49
3	C	402	QV2	C05-C06-C07	-2.46	119.73	122.97
2	B	401	GAL	O3-C3-C4	-2.43	104.74	110.35
2	A	401	GAL	O5-C5-C4	2.40	114.06	109.69
3	C	402	QV2	N15-C14-N13	-2.34	119.96	123.88
3	E	402	QV2	N15-C14-N13	-2.32	119.99	123.88
3	C	402	QV2	C05-C06-N15	2.29	118.87	115.34
3	D	402	QV2	N15-C14-N13	-2.27	120.08	123.88
3	F	402	QV2	N15-C14-N13	-2.22	120.17	123.88
3	G	402	QV2	N16-C14-N13	2.21	121.49	117.81
3	G	402	QV2	N15-C14-N13	-2.21	120.18	123.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	QV2	C08-C07-C06	-2.20	119.26	121.75
3	A	402	QV2	C08-C07-C06	-2.20	119.27	121.75
3	A	402	QV2	N15-C14-N13	-2.20	120.20	123.88
3	B	402	QV2	N16-C14-N13	2.13	121.35	117.81
3	D	402	QV2	C08-C07-C06	-2.10	119.38	121.75
3	B	402	QV2	N15-C14-N13	-2.08	120.41	123.88
3	F	402	QV2	C17-N16-C14	-2.06	121.92	126.49
2	G	401	GAL	O5-C5-C4	2.01	113.35	109.69
3	D	402	QV2	N16-C14-N13	2.01	121.14	117.81

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	GAL	O5-C5-C6-O6
2	A	401	GAL	O5-C5-C6-O6
2	G	401	GAL	O5-C5-C6-O6
2	B	401	GAL	O5-C5-C6-O6
2	E	401	GAL	O5-C5-C6-O6
2	H	401	GAL	O5-C5-C6-O6
2	D	401	GAL	C4-C5-C6-O6
2	C	401	GAL	O5-C5-C6-O6
2	F	401	GAL	O5-C5-C6-O6
3	B	402	QV2	N15-C14-N16-C17
3	D	402	QV2	N15-C14-N16-C17
3	E	402	QV2	N15-C14-N16-C17
3	A	402	QV2	N13-C14-N16-C17
3	A	402	QV2	N15-C14-N16-C17
3	B	402	QV2	N13-C14-N16-C17
3	C	402	QV2	N13-C14-N16-C17
3	C	402	QV2	N15-C14-N16-C17
3	D	402	QV2	N13-C14-N16-C17
3	E	402	QV2	N13-C14-N16-C17
3	F	402	QV2	N13-C14-N16-C17
3	F	402	QV2	N15-C14-N16-C17
3	G	402	QV2	N13-C14-N16-C17
3	G	402	QV2	N15-C14-N16-C17
2	A	401	GAL	C4-C5-C6-O6
2	G	401	GAL	C4-C5-C6-O6
2	B	401	GAL	C4-C5-C6-O6

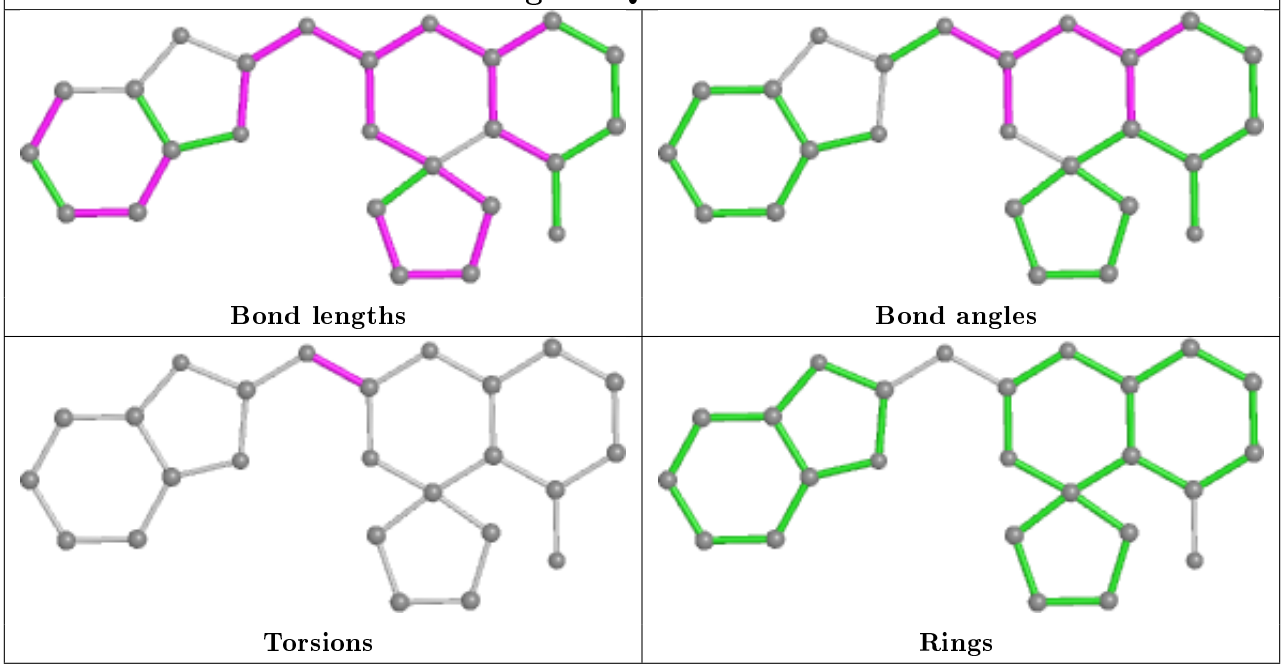
There are no ring outliers.

3 monomers are involved in 3 short contacts:

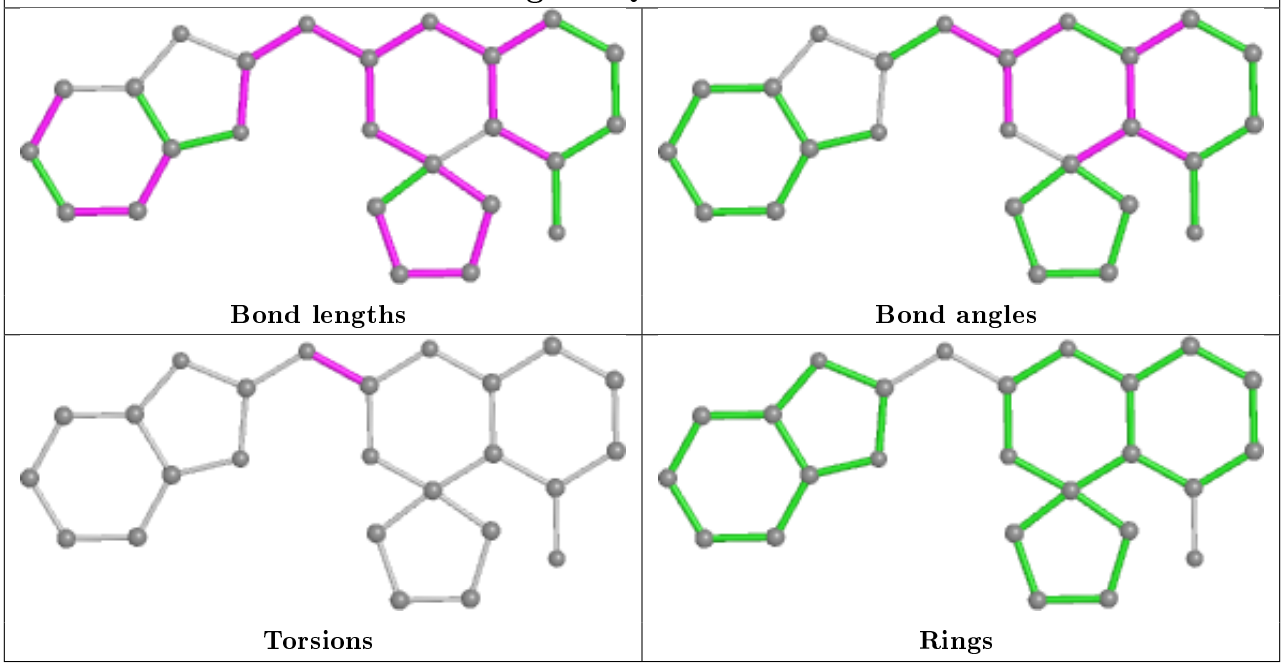
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	401	GAL	1	0
2	G	401	GAL	1	0
3	C	402	QV2	1	0

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.

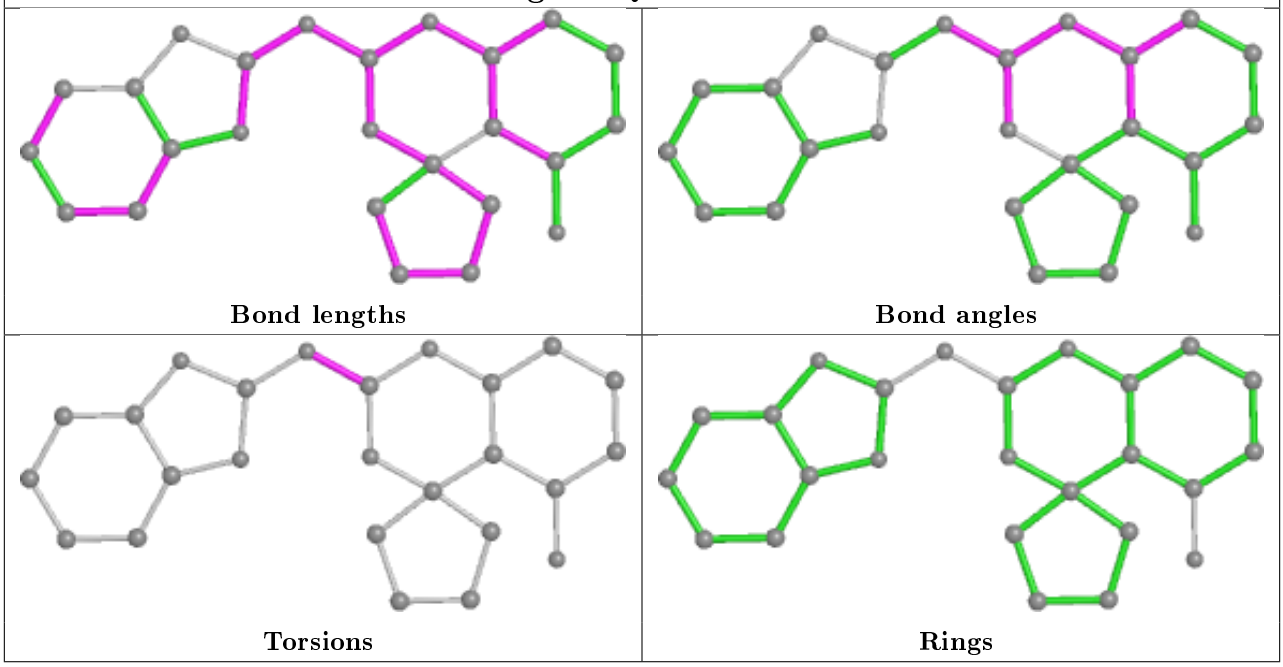
Ligand QV2 G 402



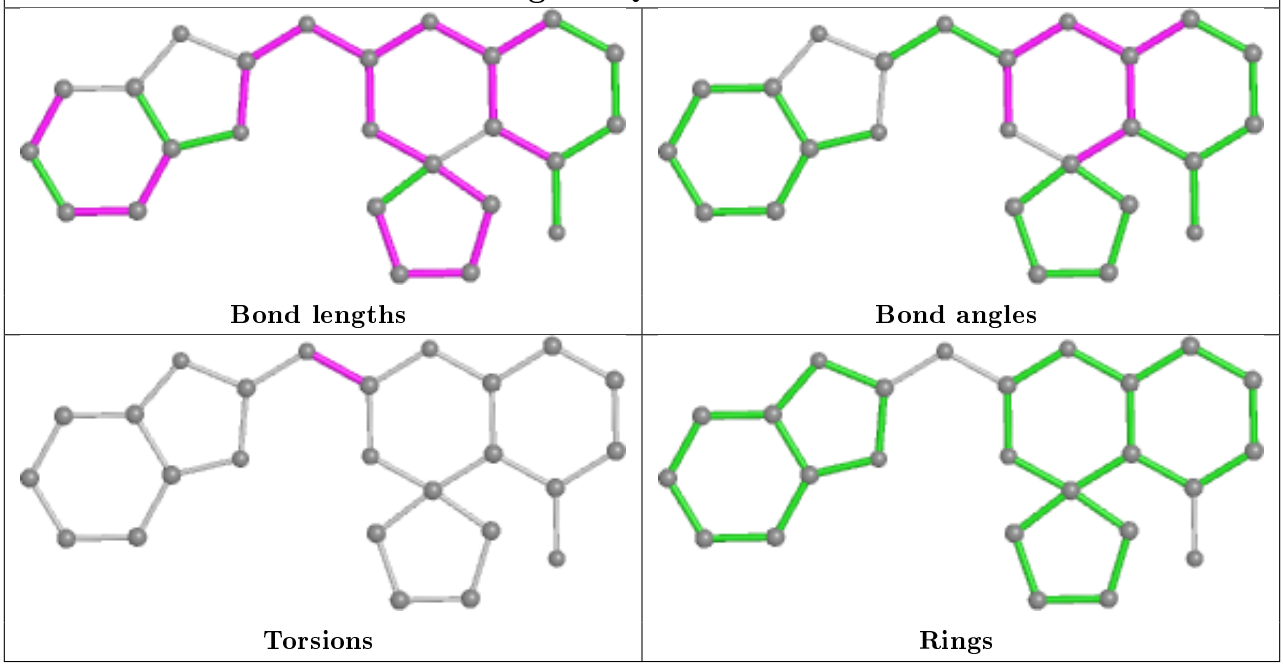
Ligand QV2 D 402



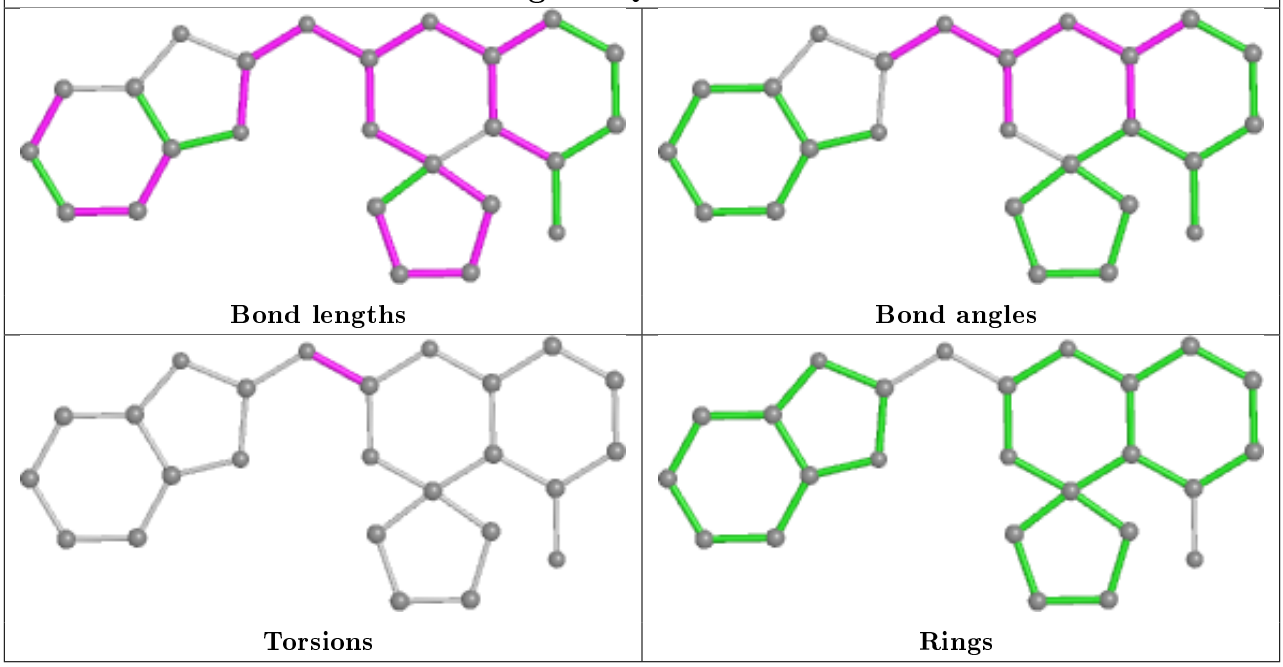
Ligand QV2 B 402



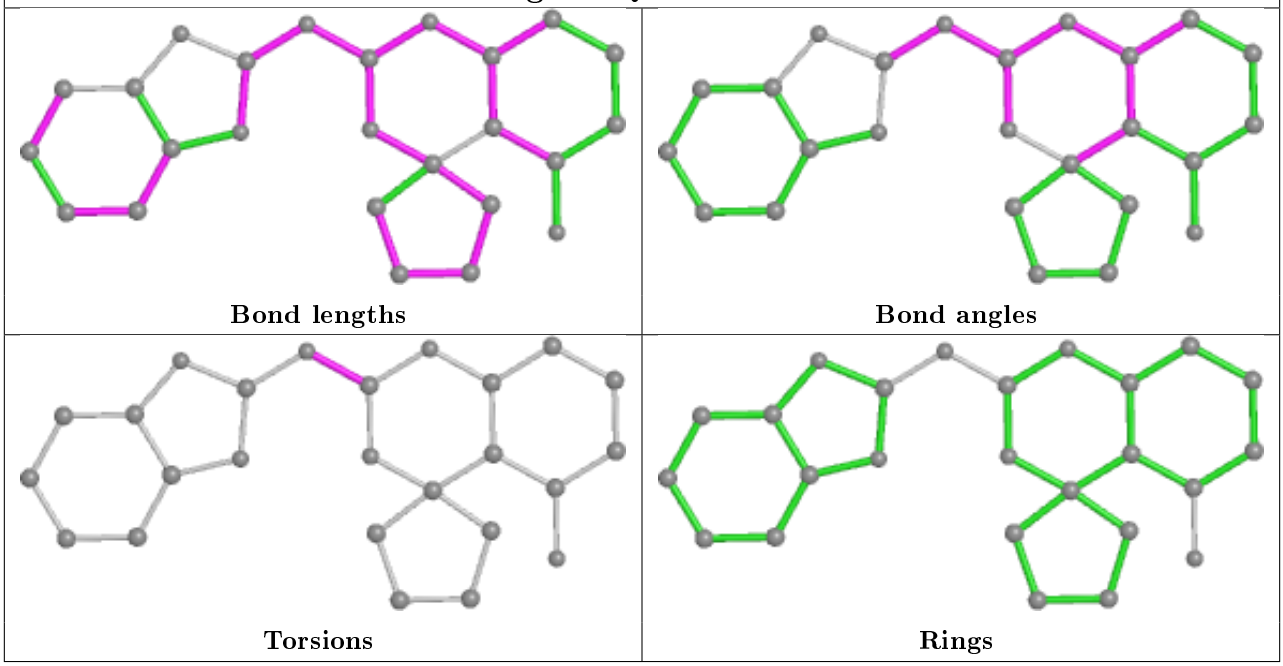
Ligand QV2 E 402



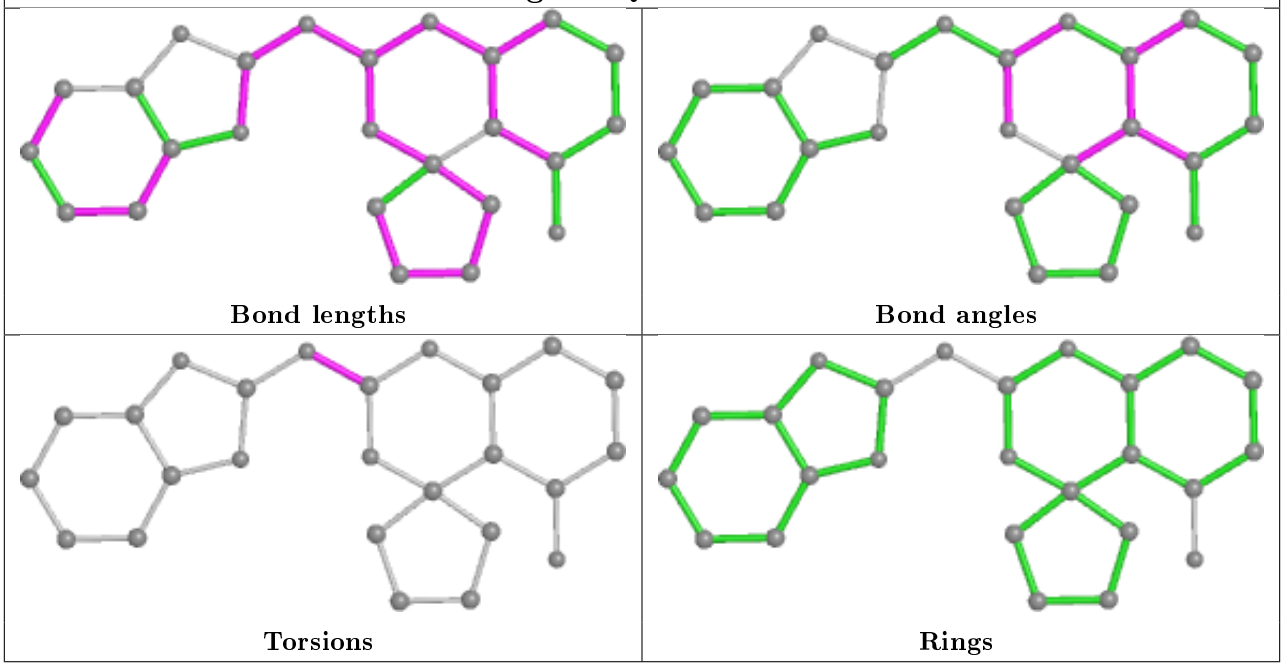
Ligand QV2 F 402



Ligand QV2 C 402



Ligand QV2 A 402



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	386/399 (96%)	-0.04	2 (0%)	91	91	26, 46, 76, 122	0
1	B	386/399 (96%)	-0.06	3 (0%)	86	85	27, 48, 78, 120	0
1	C	388/399 (97%)	-0.11	0	100	100	23, 43, 70, 102	0
1	D	385/399 (96%)	-0.00	3 (0%)	86	85	27, 52, 87, 119	0
1	E	386/399 (96%)	-0.05	4 (1%)	82	81	30, 51, 85, 121	0
1	F	384/399 (96%)	0.23	18 (4%)	31	29	32, 61, 103, 128	0
1	G	383/399 (95%)	0.25	9 (2%)	60	56	47, 67, 96, 121	0
1	H	376/399 (94%)	0.35	15 (3%)	38	35	41, 83, 117, 134	0
All	All	3074/3192 (96%)	0.07	54 (1%)	68	64	23, 56, 100, 134	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	392	LEU	6.0
1	E	392	LEU	5.6
1	H	122	LEU	4.9
1	F	71	GLY	4.2
1	H	25	GLY	4.0
1	H	119	ALA	3.8
1	D	392	LEU	3.6
1	F	24	PHE	3.5
1	F	158	PRO	3.4
1	H	120	ALA	3.4
1	F	72	LEU	3.3
1	D	95	ALA	3.3
1	B	80	GLU	3.3
1	B	5	ARG	3.1
1	E	332	ALA	3.1
1	F	136	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	85	PRO	3.0
1	D	122	LEU	2.9
1	F	295	LEU	2.9
1	H	348	PHE	2.9
1	F	106	TRP	2.7
1	H	136	GLY	2.7
1	H	239	ARG	2.6
1	H	96	GLN	2.6
1	F	128	VAL	2.6
1	H	63	LEU	2.6
1	G	242	GLN	2.6
1	F	81	GLY	2.5
1	F	12	LEU	2.5
1	G	121	PRO	2.4
1	H	272	LYS	2.4
1	F	59	LEU	2.4
1	G	355	LEU	2.4
1	F	69	LYS	2.3
1	G	392	LEU	2.3
1	A	3	ALA	2.3
1	E	214	SER	2.3
1	H	75	LEU	2.2
1	B	6	GLN	2.2
1	F	76	LEU	2.2
1	H	156	LEU	2.2
1	G	182	CYS	2.2
1	H	160	SER	2.2
1	A	233	SER	2.2
1	F	73	VAL	2.1
1	F	114	ILE	2.1
1	F	125	PHE	2.1
1	G	120	ALA	2.1
1	E	232	ALA	2.0
1	G	356	LEU	2.0
1	G	138	GLY	2.0
1	H	346	GLY	2.0
1	G	188	PHE	2.0
1	H	275	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

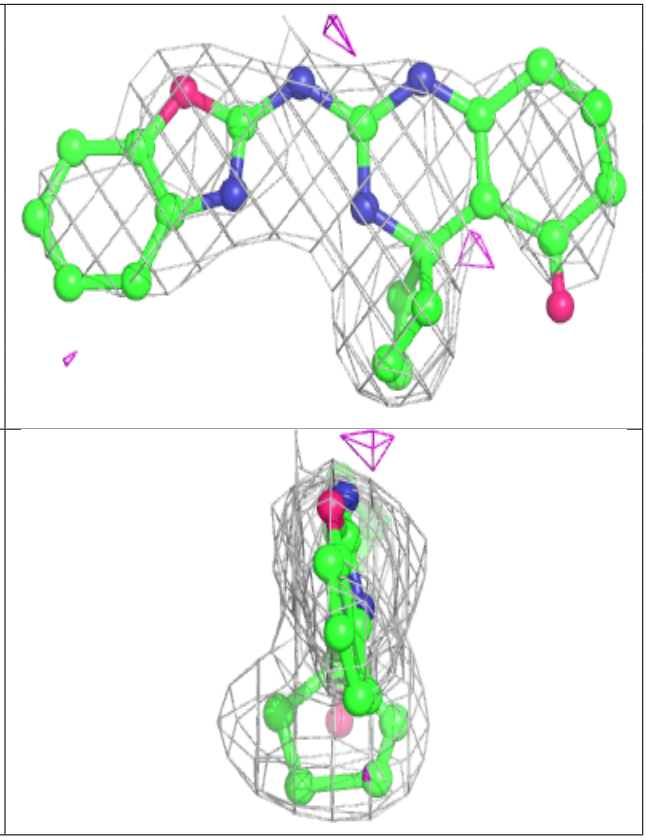
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	QV2	F	402	25/25	0.82	0.31	64,78,83,90	0
2	GAL	H	401	12/12	0.88	0.18	57,86,90,97	0
3	QV2	D	402	25/25	0.89	0.30	54,70,75,77	0
3	QV2	E	402	25/25	0.90	0.17	50,63,71,73	0
2	GAL	A	401	12/12	0.91	0.16	27,43,46,61	0
3	QV2	G	402	25/25	0.91	0.26	54,65,71,76	0
3	QV2	C	402	25/25	0.93	0.21	40,51,57,62	0
2	GAL	G	401	12/12	0.93	0.14	63,67,69,70	0
2	GAL	D	401	12/12	0.93	0.15	34,43,52,63	0
3	QV2	A	402	25/25	0.93	0.20	40,51,68,72	0
3	QV2	B	402	25/25	0.93	0.25	45,56,62,73	0
2	GAL	B	401	12/12	0.94	0.17	35,50,52,61	0
2	GAL	E	401	12/12	0.94	0.15	26,47,53,66	0
2	GAL	F	401	12/12	0.94	0.18	40,58,75,78	0
2	GAL	C	401	12/12	0.96	0.13	28,40,59,70	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.

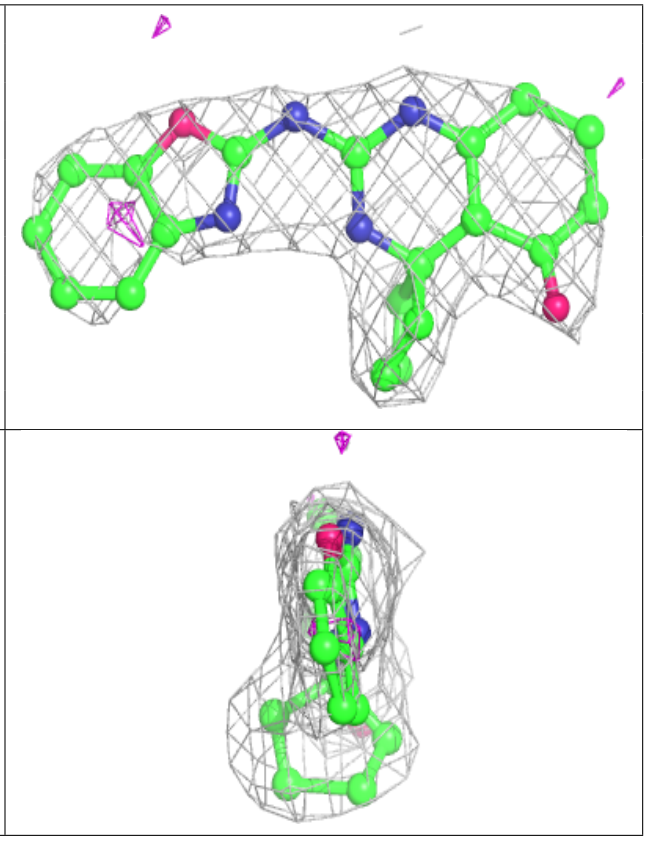
Electron density around QV2 F 402:

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



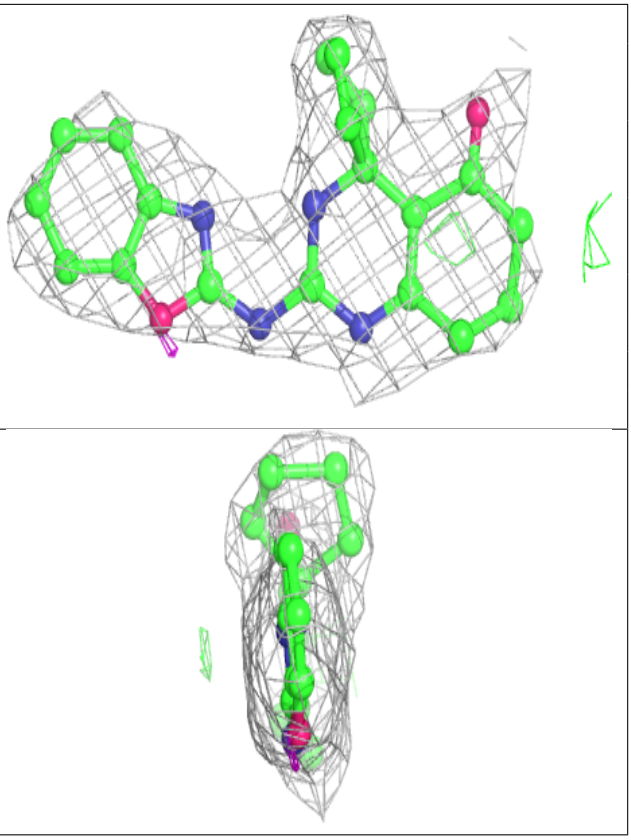
Electron density around QV2 D 402:

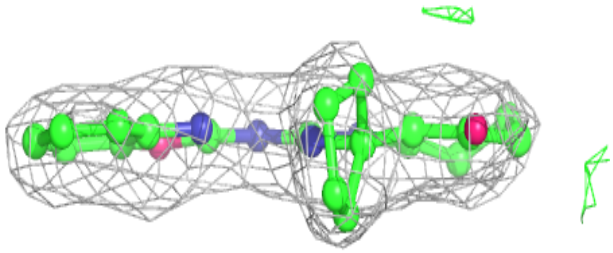
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around QV2 E 402:

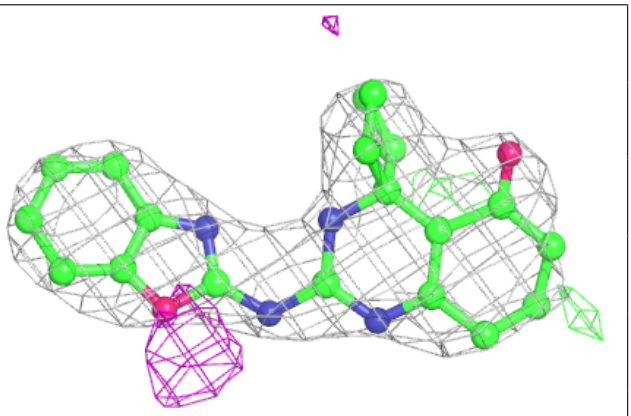
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

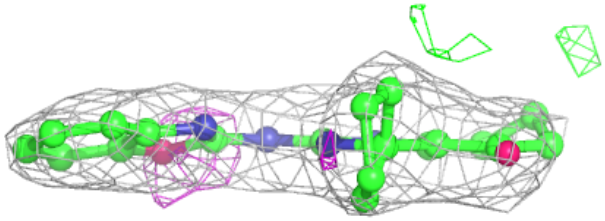


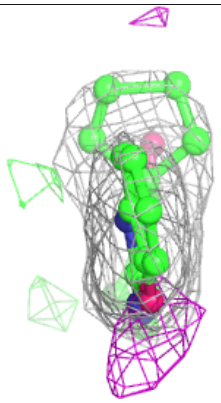


Electron density around QV2 G 402:

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







Electron density around QV2 C 402:

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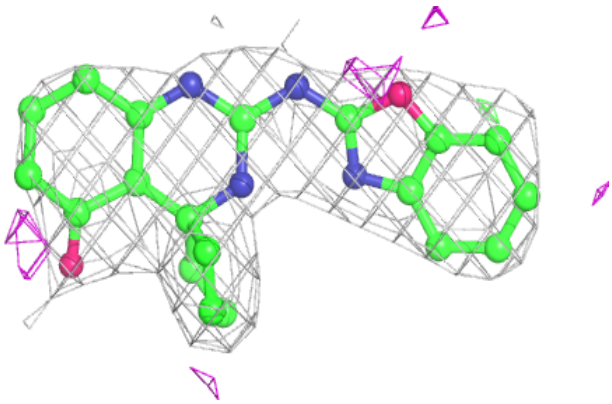
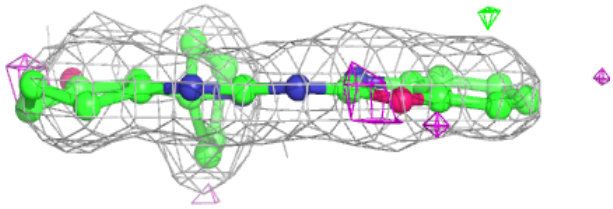
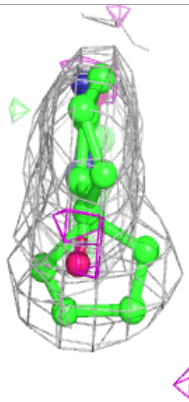
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around QV2 A 402:

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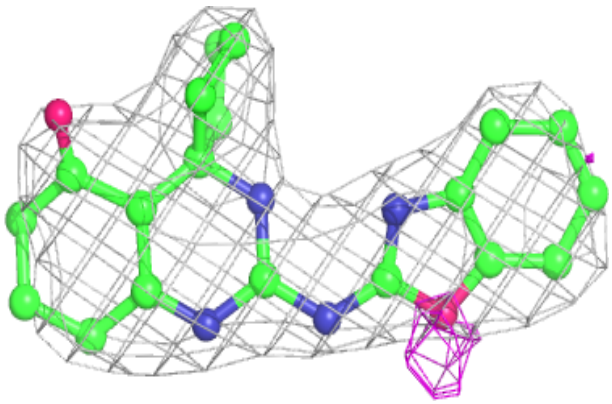
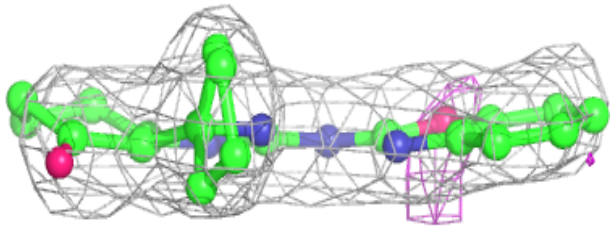
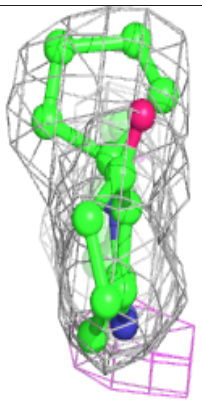
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around QV2 B 402:

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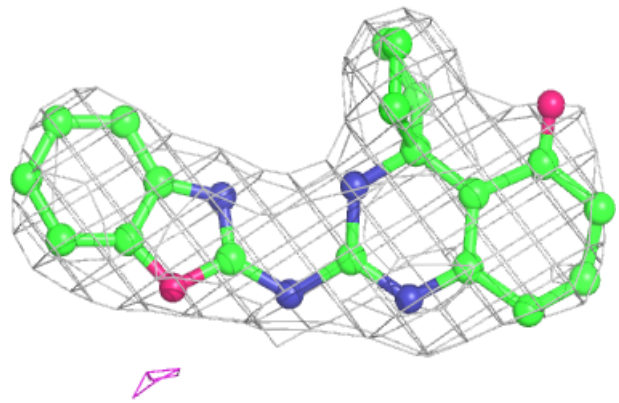
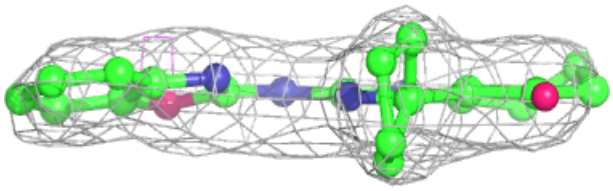
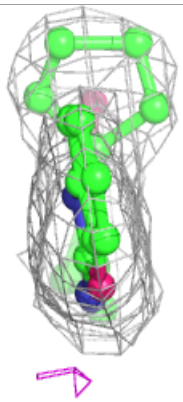
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.