Full wwPDB X-ray Structure Validation Report (i)

Jan 16, 2024 – 03:11 am GMT

PDB ID	:	6Q91
Title	:	Structure of human galactokinase 1 bound with 5-Chloro-N-isobutyl-2-methoxybenzamide
Authors	:	Mackinnon, S.R.; Bezerra, G.A.; Zhang, M.; Foster, W.; Krojer, T.; Brandao-Neto, J.; Douangamath, A.; Arrowsmith, C.; Edwards, A.; Bountra, C.; Brennan, P.; Lai, K.; Yue, W.W.
Deposited on	:	2018-12-17
Resolution	:	2.40 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 (1)) were used in the production of this report:

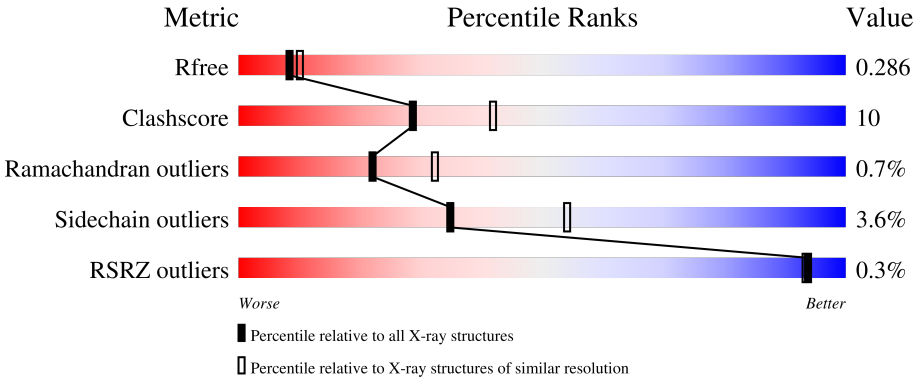
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	392	86% 12% •
1	B	392	86% 13% •
1	C	392	74% 24% •
1	D	392	% 73% 17% • 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11516 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.

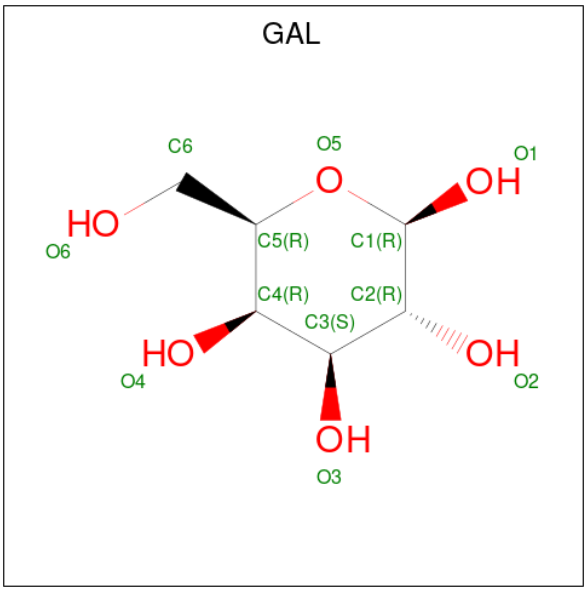
- Molecule 1 is a protein called Galactokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	5	1	0
			2879	1804	508	550	17			
1	B	392	Total	C	N	O	S	2	1	0
			2851	1780	505	551	15			
1	C	392	Total	C	N	O	S	0	0	0
			2791	1749	494	532	16			
1	D	360	Total	C	N	O	S	0	0	0
			2492	1558	441	480	13			

There are 12 discrepancies between the modelled and reference sequences:

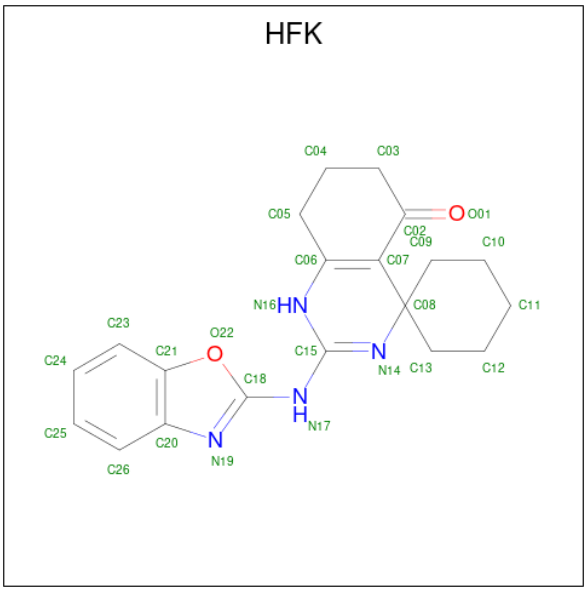
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP P51570
A	252	ALA	LYS	engineered mutation	UNP P51570
A	253	ALA	GLU	engineered mutation	UNP P51570
B	1	HIS	-	expression tag	UNP P51570
B	252	ALA	LYS	engineered mutation	UNP P51570
B	253	ALA	GLU	engineered mutation	UNP P51570
C	1	HIS	-	expression tag	UNP P51570
C	252	ALA	LYS	engineered mutation	UNP P51570
C	253	ALA	GLU	engineered mutation	UNP P51570
D	1	HIS	-	expression tag	UNP P51570
D	252	ALA	LYS	engineered mutation	UNP P51570
D	253	ALA	GLU	engineered mutation	UNP P51570

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



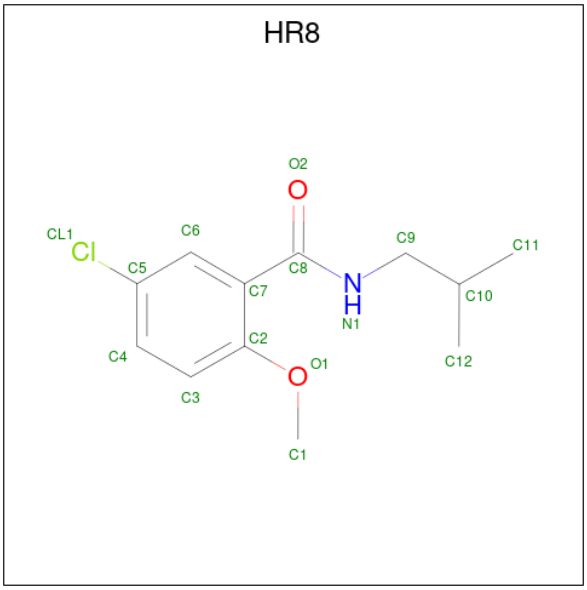
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0

- Molecule 3 is 2-(1,3-benzoxazol-2-ylamino)spiro[1,6,7,8-tetrahydroquinazoline-4,1'-cyclohexane]-5-one (three-letter code: HFK) (formula: $C_{20}H_{22}N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 26 20 4 2	0	0
3	B	1	Total C N O 26 20 4 2	0	0
3	C	1	Total C N O 26 20 4 2	0	0

- Molecule 4 is 5-chloranyl-2-methoxy- {N}-(2-methylpropyl)benzamide (three-letter code: HR8) (formula: $C_{12}H_{16}ClNO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Cl N O 16 12 1 1 2	0	0
4	B	1	Total C Cl N O 16 12 1 1 2	0	0
4	C	1	Total C Cl N O 16 12 1 1 2	0	0
4	D	1	Total C Cl N O 16 12 1 1 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	115	Total O 115 115	0	0
5	B	87	Total O 87 87	0	0

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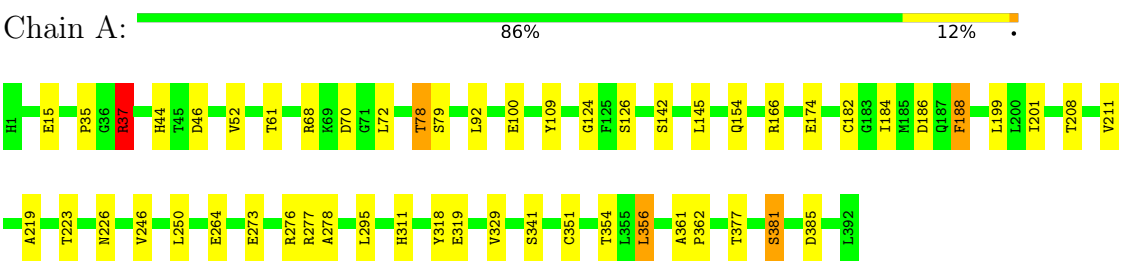
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	71	Total O 71 71	0	0
5	D	52	Total O 52 52	0	0

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.

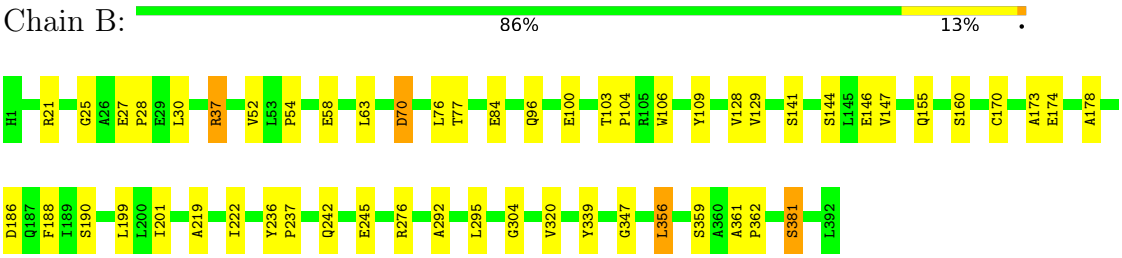
• Molecule 1: Galactokinase

Chain A:



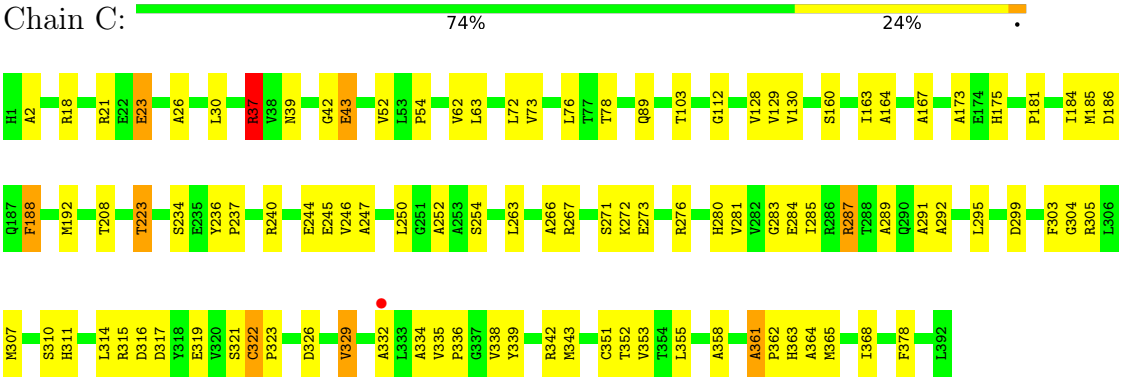
• Molecule 1: Galactokinase

Chain B:



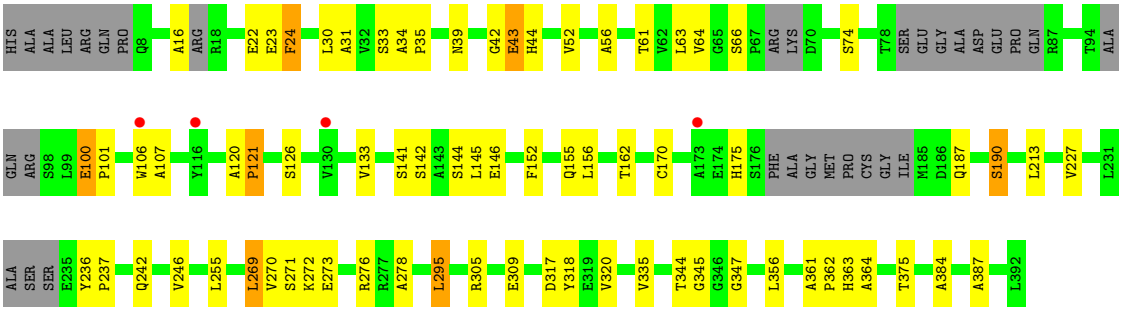
• Molecule 1: Galactokinase

Chain C:



• Molecule 1: Galactokinase

Chain D:


HIS ALA ALA LEU ARG GLN PRO Q8 A16 ARG R18 E22 E23 F24 L30 A31 V32 S33 A34 P35 N39 G42 E43 H44 V52 A56 T61 V62 L63 V64 G65 S66 P67 ARG LYS D70 S74 T78 SER GLU GLY ALA ASP GLU PRO GLN R87 T94 ALA
GLN ARG S98 L99 E100 P101 W106 A107 Y116 A120 P121 S126 V130 V133 S141 S142 A143 S144 L145 E146 F152 Q155 L156 T162 C170 A173 E174 H175 S176 PHE ALA GLY MET PRO CYS GLY ILE M185 D186 Q187 S190 L213 V227 L231
ALA SER SER E235 Y236 P237 Q242 V246 L255 L269 V270 S271 K272 E273 R276 R277 A278 L295 R305 E309 D317 Y318 E319 V320 V335 T344 G345 G346 G347 L356 A361 P362 H363 A364 T375 A384 A387 L392

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.32Å 114.96Å 120.92Å 90.00° 100.79° 90.00°	Depositor
Resolution (Å)	82.74 – 2.40 82.61 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.5 (82.74-2.40) 99.5 (82.61-2.27)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.216 , 0.285 0.220 , 0.286	Depositor DCC
R_{free} test set	4496 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 36.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11516	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: GAL, HR8, HFK

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	0.75	0/2937	0.92	1/3997 (0.0%)
1	B	0.75	0/2908	0.91	0/3962
1	C	0.79	0/2842	0.95	2/3875 (0.1%)
1	D	0.75	0/2530	0.93	0/3450
All	All	0.76	0/11217	0.93	3/15284 (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	A	0	2
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	37	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	C	37	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	C	23	GLU	CB-CA-C	-5.42	99.56	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	ARG	Peptide
1	A	381	SER	Peptide
1	C	363	HIS	Peptide
1	D	269	LEU	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	2879	0	2795	37	0
1	B	2851	0	2735	37	0
1	C	2791	0	2668	93	0
1	D	2492	0	2308	44	0
2	A	12	0	11	0	0
2	B	12	0	12	0	0
2	C	12	0	12	1	0
3	A	26	0	0	0	0
3	B	26	0	0	0	0
3	C	26	0	0	0	0
4	A	16	0	0	0	0
4	B	16	0	0	0	0
4	C	16	0	0	1	0
4	D	16	0	0	0	0
5	A	115	0	0	1	0
5	B	87	0	0	4	0
5	C	71	0	0	9	0
5	D	52	0	0	5	0
All	All	11516	0	10541	211	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (211) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:GLU:CB	5:C:569:HOH:O	1.83	1.25
1:B:96:GLN:CB	5:B:572:HOH:O	1.86	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:MET:SD	5:C:537:HOH:O	2.12	1.04
1:C:361:ALA:HB1	1:C:362:PRO:HD3	1.40	0.98
1:A:37:ARG:HG2	1:A:37:ARG:HH11	1.28	0.95
1:D:43:GLU:OE2	1:D:345:GLY:N	2.01	0.93
1:D:39:ASN:HB2	5:D:545:HOH:O	1.71	0.91
1:B:58:GLU:OE1	1:B:381:SER:OG	1.95	0.85
1:C:314:LEU:HB3	1:C:343:MET:HE1	1.59	0.83
1:C:63:LEU:HD11	1:C:129:VAL:HG22	1.61	0.82
1:B:37:ARG:HG2	1:B:37:ARG:HH21	1.43	0.80
1:C:78:THR:HG22	1:C:130:VAL:HG12	1.64	0.80
1:A:276:ARG:NH2	1:A:319:GLU:OE1	2.18	0.75
1:C:307:MET:CE	5:C:537:HOH:O	2.31	0.75
1:C:361:ALA:CB	1:C:362:PRO:CD	2.67	0.73
1:C:304:GLY:HA3	1:C:339:TYR:O	1.88	0.73
1:D:30:LEU:HD21	1:D:155:GLN:HB3	1.71	0.73
1:C:223:THR:O	1:C:351:CYS:HA	1.90	0.72
1:C:54:PRO:HB3	1:C:185:MET:CE	2.20	0.72
1:C:361:ALA:HB1	1:C:362:PRO:CD	2.16	0.71
1:C:361:ALA:CB	1:C:362:PRO:HD3	2.17	0.71
1:B:37:ARG:HG2	1:B:37:ARG:NH2	2.04	0.71
1:B:219:ALA:HB3	1:B:356:LEU:CD1	2.21	0.71
1:D:30:LEU:HD21	1:D:155:GLN:CB	2.22	0.70
1:C:54:PRO:HB3	1:C:185:MET:HE2	1.73	0.69
1:C:335:VAL:HG12	1:C:336:PRO:HD2	1.74	0.69
1:C:311:HIS:CE1	1:C:329:VAL:HG21	2.29	0.67
1:D:335:VAL:HG21	1:D:364:ALA:HA	1.77	0.67
1:D:74:SER:O	1:D:126:SER:HA	1.95	0.66
1:C:78:THR:CG2	1:C:130:VAL:HG12	2.27	0.64
1:C:314:LEU:O	1:C:319:GLU:N	2.31	0.63
1:D:43:GLU:OE2	1:D:344:THR:HA	1.98	0.63
1:C:283:GLY:C	1:C:287:ARG:HE	2.00	0.63
1:C:332:ALA:HA	1:C:335:VAL:HG21	1.81	0.63
1:C:355:LEU:CB	5:C:537:HOH:O	2.46	0.63
1:D:61:THR:HG21	1:D:145:LEU:HA	1.80	0.63
1:C:332:ALA:HB2	1:C:368:ILE:HD12	1.79	0.62
1:C:314:LEU:CB	1:C:343:MET:HE1	2.28	0.62
1:D:43:GLU:HB3	1:D:44:HIS:ND1	2.15	0.62
1:C:355:LEU:HB2	5:C:537:HOH:O	2.00	0.61
1:C:72:LEU:C	1:C:72:LEU:HD12	2.21	0.61
1:B:30:LEU:HD21	1:B:155:GLN:HB3	1.83	0.61
1:C:358:ALA:O	1:C:361:ALA:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ALA:HB3	1:D:144:SER:O	2.00	0.60
1:C:263:LEU:O	1:C:266:ALA:N	2.35	0.59
1:D:242:GLN:O	1:D:246:VAL:HG13	2.02	0.59
1:D:146:GLU:OE1	1:D:170:CYS:O	2.21	0.58
1:C:240:ARG:O	1:C:244:GLU:HG3	2.04	0.58
1:D:269:LEU:HD12	5:D:505:HOH:O	2.02	0.58
1:C:311:HIS:ND1	1:C:329:VAL:HG21	2.19	0.57
1:D:242:GLN:NE2	1:D:273:GLU:OE2	2.35	0.57
1:A:109:TYR:HB2	1:A:145:LEU:HD23	1.87	0.56
1:C:37:ARG:NE	1:C:186:ASP:OD1	2.38	0.56
1:C:291:ALA:HB1	1:C:303:PHE:CE1	2.39	0.56
1:B:30:LEU:HD21	1:B:155:GLN:CB	2.35	0.56
1:C:326:ASP:OD1	1:C:326:ASP:N	2.39	0.56
1:B:84:GLU:O	5:B:501:HOH:O	2.18	0.55
1:C:175:HIS:CD2	1:C:181:PRO:HA	2.41	0.55
1:B:63:LEU:HD11	1:B:129:VAL:HG22	1.88	0.55
1:C:37:ARG:HH21	1:C:37:ARG:HG2	1.70	0.55
1:A:15:GLU:OE2	1:A:78:THR:HG21	2.07	0.55
1:C:284:GLU:OE1	1:C:284:GLU:HA	2.07	0.55
1:C:223:THR:OG1	1:C:352:THR:OG1	2.23	0.55
1:C:283:GLY:O	1:C:287:ARG:HG3	2.06	0.55
1:B:37:ARG:HH21	1:B:37:ARG:CG	2.16	0.54
1:B:236:TYR:HB3	1:B:237:PRO:HD3	1.89	0.54
1:D:276:ARG:O	1:D:317:ASP:HB3	2.07	0.54
1:C:335:VAL:HG12	1:C:336:PRO:CD	2.38	0.54
1:C:164:ALA:HA	1:C:188:PHE:HE1	1.73	0.54
1:C:39:ASN:HB2	1:C:185:MET:HE1	1.88	0.53
1:D:246:VAL:CG2	1:D:255:LEU:HD21	2.37	0.53
1:B:219:ALA:HB3	1:B:356:LEU:HD11	1.89	0.53
1:A:100:GLU:HB3	5:A:543:HOH:O	2.07	0.53
1:A:361:ALA:HB3	1:A:362:PRO:HD3	1.91	0.53
1:C:63:LEU:CD1	1:C:129:VAL:HG22	2.37	0.53
1:C:332:ALA:O	1:C:338:VAL:HG11	2.08	0.53
1:A:311:HIS:CE1	1:A:329:VAL:HG21	2.44	0.52
1:C:271:SER:OG	1:C:272:LYS:N	2.41	0.52
1:C:236:TYR:HB3	1:C:237:PRO:HD3	1.91	0.52
1:D:42:GLY:O	1:D:52:VAL:HG12	2.10	0.52
1:C:364:ALA:O	1:C:368:ILE:HG22	2.10	0.52
1:A:92:LEU:HD11	1:A:124:GLY:N	2.25	0.51
1:A:72:LEU:C	1:A:72:LEU:HD12	2.30	0.51
1:C:335:VAL:CG1	1:C:336:PRO:HD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ASP:HB3	5:B:554:HOH:O	2.10	0.51
1:C:73:VAL:O	1:C:89:GLN:HA	2.10	0.51
1:D:31:ALA:HB2	1:D:64:VAL:HG12	1.93	0.51
1:C:280:HIS:O	1:C:284:GLU:HB2	2.12	0.50
1:B:52:VAL:HG22	1:B:201:ILE:HB	1.94	0.50
1:A:46:ASP:HB3	1:A:52:VAL:HG11	1.94	0.50
1:B:219:ALA:HB3	1:B:356:LEU:HD12	1.92	0.50
1:C:283:GLY:O	1:C:287:ARG:CG	2.60	0.49
1:A:37:ARG:HG2	1:A:37:ARG:NH1	2.07	0.49
1:D:320:VAL:O	1:D:347:GLY:HA3	2.11	0.49
1:C:247:ALA:HB1	1:C:252:ALA:O	2.11	0.49
1:B:141:SER:O	1:B:144:SER:OG	2.26	0.49
1:B:276:ARG:HD2	5:B:514:HOH:O	2.12	0.49
1:D:305:ARG:O	1:D:309:GLU:HG3	2.12	0.49
1:A:219:ALA:HB3	1:A:356:LEU:CD1	2.42	0.49
1:B:76:LEU:O	1:B:128:VAL:HA	2.13	0.49
1:C:332:ALA:HB2	1:C:368:ILE:CD1	2.43	0.49
1:A:174:GLU:HG2	1:A:182:CYS:SG	2.53	0.49
1:D:236:TYR:N	1:D:237:PRO:CD	2.76	0.49
1:B:37:ARG:HE	1:B:186:ASP:CG	2.16	0.48
1:C:62:VAL:O	1:C:63:LEU:HD12	2.13	0.48
1:D:272:LYS:O	5:D:501:HOH:O	2.19	0.48
1:D:187:GLN:CB	5:D:541:HOH:O	2.61	0.48
1:A:109:TYR:CE1	1:A:142:SER:HB2	2.47	0.48
1:C:43:GLU:OE2	2:C:401:GAL:O6	2.27	0.48
1:A:211:VAL:HG11	1:A:295:LEU:HD23	1.95	0.48
1:C:188:PHE:HE2	1:C:208:THR:HG21	1.79	0.47
1:D:213:LEU:HD12	1:D:295:LEU:HD11	1.95	0.47
1:C:43:GLU:HB2	1:C:342:ARG:NH2	2.28	0.47
1:D:361:ALA:N	1:D:362:PRO:HD2	2.30	0.47
1:D:142:SER:O	1:D:146:GLU:HG3	2.14	0.47
1:B:242:GLN:O	1:B:245:GLU:HB2	2.14	0.47
1:A:44:HIS:CG	1:A:318:TYR:CE2	3.03	0.47
1:A:52:VAL:CG2	1:A:201:ILE:HB	2.44	0.47
1:A:356:LEU:HD12	1:A:356:LEU:O	2.15	0.47
1:A:246:VAL:HG11	1:A:278:ALA:HB2	1.97	0.46
1:C:52:VAL:HG21	1:C:185:MET:HG3	1.97	0.46
1:A:37:ARG:NE	1:A:186:ASP:OD1	2.48	0.46
1:A:68:ARG:CZ	1:A:72:LEU:HD11	2.45	0.46
1:C:314:LEU:HD13	1:C:343:MET:HE3	1.97	0.46
1:D:31:ALA:CB	1:D:64:VAL:HG12	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:VAL:CG1	1:C:336:PRO:CD	2.94	0.46
1:B:54:PRO:HD2	1:B:199:LEU:O	2.15	0.46
1:B:37:ARG:NE	1:B:186:ASP:OD1	2.42	0.46
1:A:199:LEU:HD11	1:A:208:THR:HB	1.98	0.46
1:D:16:ALA:HB1	1:D:64:VAL:HG22	1.98	0.46
1:D:133:VAL:HG11	1:D:141:SER:HA	1.98	0.46
1:C:39:ASN:CB	1:C:185:MET:HE1	2.46	0.46
1:C:112:GLY:HA3	1:C:173:ALA:HB1	1.98	0.46
1:C:295:LEU:HD13	4:C:403:HR8:C4	2.46	0.46
1:D:33:SER:HA	1:D:61:THR:O	2.16	0.45
1:D:100:GLU:N	1:D:101:PRO:CD	2.80	0.45
1:C:321:SER:OG	1:C:326:ASP:OD1	2.26	0.45
1:C:192:MET:HE2	1:C:192:MET:HB3	1.71	0.45
1:C:299:ASP:CB	5:C:502:HOH:O	2.64	0.45
1:C:280:HIS:CE1	1:C:314:LEU:HG	2.52	0.45
1:A:246:VAL:O	1:A:250:LEU:HD13	2.17	0.44
1:A:273:GLU:O	1:A:277:ARG:HG2	2.17	0.44
1:C:315:ARG:NE	1:C:316:ASP:OD1	2.50	0.44
1:D:35:PRO:O	1:D:190:SER:OG	2.36	0.44
1:D:213:LEU:HD13	1:D:295:LEU:HD21	1.99	0.44
1:D:56:ALA:HB3	1:D:384:ALA:O	2.17	0.44
1:B:146:GLU:OE2	1:B:174:GLU:OE1	2.35	0.44
1:B:292:ALA:O	1:B:295:LEU:HB3	2.18	0.44
1:A:37:ARG:HH11	1:A:37:ARG:CG	2.15	0.44
1:C:245:GLU:CB	5:C:529:HOH:O	2.66	0.44
1:A:184:ILE:HG13	1:A:188:PHE:HD2	1.82	0.44
1:C:355:LEU:HB3	5:C:537:HOH:O	2.16	0.44
1:D:152:PHE:CE1	1:D:156:LEU:HD11	2.53	0.44
1:C:281:VAL:O	1:C:284:GLU:N	2.51	0.44
1:C:21:ARG:HA	1:C:26:ALA:O	2.18	0.43
1:A:341:SER:HG	1:A:354:THR:HG1	1.66	0.43
1:C:289:ALA:O	1:C:292:ALA:HB3	2.19	0.43
1:C:167:ALA:HB1	1:C:184:ILE:HD11	1.99	0.43
1:B:109:TYR:CE1	1:B:178:ALA:HB2	2.53	0.43
1:D:162:THR:OG1	5:D:502:HOH:O	2.21	0.43
1:D:213:LEU:CD1	1:D:295:LEU:HD21	2.49	0.43
1:C:276:ARG:C	1:C:317:ASP:OD1	2.57	0.43
1:B:77:THR:HA	1:B:129:VAL:O	2.19	0.43
1:C:43:GLU:OE2	1:C:43:GLU:HA	2.18	0.43
1:C:332:ALA:HA	1:C:335:VAL:CG2	2.47	0.43
1:D:33:SER:O	1:D:387:ALA:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:MET:O	1:C:310:SER:N	2.51	0.43
1:C:23:GLU:CG	1:C:76:LEU:HD22	2.48	0.43
1:A:52:VAL:HG22	1:A:201:ILE:HB	2.00	0.42
1:A:184:ILE:O	1:A:188:PHE:HB2	2.19	0.42
1:A:226:ASN:OD1	1:A:377:THR:OG1	2.37	0.42
1:C:42:GLY:O	1:C:52:VAL:HG12	2.19	0.42
1:C:280:HIS:CD2	1:C:280:HIS:C	2.87	0.42
1:C:163:ILE:HG21	1:C:192:MET:CG	2.48	0.42
1:A:61:THR:HG21	1:A:145:LEU:HA	2.00	0.42
1:C:362:PRO:HA	1:C:365:MET:HB2	2.00	0.42
1:C:353:VAL:O	1:C:353:VAL:HG13	2.19	0.42
1:B:104:PRO:HB2	1:B:106:TRP:CD1	2.55	0.42
1:A:154:GLN:HE22	1:A:166:ARG:CZ	2.32	0.42
1:A:68:ARG:HD2	1:A:126:SER:OG	2.20	0.42
1:B:27:GLU:OE1	1:B:28:PRO:HD2	2.20	0.42
1:B:320:VAL:O	1:B:347:GLY:HA3	2.20	0.42
1:D:246:VAL:HG21	1:D:278:ALA:CB	2.50	0.42
1:A:109:TYR:CB	1:A:145:LEU:HD23	2.48	0.41
1:B:63:LEU:CD1	1:B:129:VAL:HG22	2.50	0.41
1:C:246:VAL:O	1:C:250:LEU:HD13	2.19	0.41
1:C:322:CYS:O	1:C:323:PRO:C	2.57	0.41
1:C:365:MET:HA	1:C:378:PHE:CZ	2.54	0.41
1:D:106:TRP:CE3	1:D:107:ALA:N	2.88	0.41
1:D:23:GLU:O	1:D:24:PHE:CB	2.68	0.41
1:D:120:ALA:HA	1:D:121:PRO:HA	1.86	0.41
1:B:304:GLY:HA3	1:B:339:TYR:O	2.19	0.41
1:A:70:ASP:OD1	1:A:72:LEU:HG	2.20	0.41
1:A:223:THR:O	1:A:351:CYS:HA	2.20	0.41
1:A:35:PRO:HG3	1:A:385:ASP:O	2.21	0.41
1:B:21:ARG:O	1:B:25:GLY:N	2.40	0.41
1:B:361:ALA:N	1:B:362:PRO:CD	2.84	0.41
1:C:184:ILE:HA	1:C:184:ILE:HD12	1.78	0.41
1:B:147:VAL:HG21	1:B:190:SER:HB3	2.02	0.41
1:B:170:CYS:O	1:B:173:ALA:HB3	2.21	0.41
1:B:222:ILE:HD12	1:B:222:ILE:N	2.36	0.40
1:C:163:ILE:HG21	1:C:192:MET:HG3	2.02	0.40
1:C:284:GLU:OE2	1:C:310:SER:OG	2.30	0.40
1:D:43:GLU:HB3	1:D:44:HIS:CE1	2.56	0.40
1:C:18:ARG:HD2	5:C:506:HOH:O	2.21	0.40
1:C:304:GLY:O	1:C:305:ARG:C	2.60	0.40
1:C:314:LEU:CB	1:C:343:MET:CE	2.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ARG:HG2	1:C:37:ARG:NH2	2.35	0.40
1:C:76:LEU:O	1:C:128:VAL:HA	2.21	0.40
1:B:359:SER:O	1:B:362:PRO:HD2	2.21	0.40
1:D:246:VAL:HG21	1:D:278:ALA:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	391/392 (100%)	379 (97%)	12 (3%)	0	100	100
1	B	391/392 (100%)	376 (96%)	15 (4%)	0	100	100
1	C	390/392 (100%)	336 (86%)	48 (12%)	6 (2%)	10	14
1	D	346/392 (88%)	316 (91%)	25 (7%)	5 (1%)	11	15
All	All	1518/1568 (97%)	1407 (93%)	100 (7%)	11 (1%)	22	32

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2	ALA
1	C	334	ALA
1	C	361	ALA
1	D	24	PHE
1	D	100	GLU
1	D	175	HIS
1	D	22	GLU
1	C	329	VAL
1	C	267	ARG
1	C	285	ILE
1	D	121	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	289/309 (94%)	282 (98%)	7 (2%)	49	68
1	B	283/309 (92%)	275 (97%)	8 (3%)	43	63
1	C	268/309 (87%)	257 (96%)	11 (4%)	30	48
1	D	230/309 (74%)	218 (95%)	12 (5%)	23	38
All	All	1070/1236 (87%)	1032 (96%)	38 (4%)	35	54

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	78	THR
1	A	79	SER
1	A	188	PHE
1	A	264	GLU
1	A	356	LEU
1	A	381	SER
1	B	37	ARG
1	B	70	ASP
1	B	100	GLU
1	B	103	THR
1	B	160	SER
1	B	188	PHE
1	B	356	LEU
1	B	381	SER
1	C	30	LEU
1	C	37	ARG
1	C	43	GLU
1	C	103	THR
1	C	160	SER
1	C	188	PHE
1	C	223	THR
1	C	234	SER
1	C	254	SER

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Mol	Chain	Res	Type
1	C	287	ARG
1	C	322	CYS
1	D	43	GLU
1	D	63	LEU
1	D	66	SER
1	D	190	SER
1	D	227	VAL
1	D	270	VAL
1	D	271	SER
1	D	295	LEU
1	D	318	TYR
1	D	356	LEU
1	D	363	HIS
1	D	375	THR

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

Mol	Chain	Res	Type
1	A	226	ASN
1	C	96	GLN
1	C	280	HIS
1	C	367	HIS
1	D	39	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

10 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	HR8	B	403	-	16,16,16	0.40	0	21,21,21	0.77	0
4	HR8	C	403	-	16,16,16	0.37	0	21,21,21	0.74	0
2	GAL	B	401	-	12,12,12	0.80	0	17,17,17	2.18	6 (35%)
3	HFK	B	402	-	26,30,30	4.15	8 (30%)	24,44,44	4.75	10 (41%)
3	HFK	A	402	-	26,30,30	4.10	9 (34%)	24,44,44	4.66	13 (54%)
2	GAL	C	401	-	12,12,12	0.58	0	17,17,17	2.18	6 (35%)
2	GAL	A	401	-	12,12,12	0.78	0	17,17,17	2.55	5 (29%)
3	HFK	C	402	-	26,30,30	4.02	8 (30%)	24,44,44	4.89	12 (50%)
4	HR8	D	401	-	16,16,16	0.35	0	21,21,21	0.61	0
4	HR8	A	403	-	16,16,16	0.37	0	21,21,21	0.57	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
4	HR8	B	403	-	-	4/11/11/11	0/1/1/1
4	HR8	C	403	-	-	0/11/11/11	0/1/1/1
2	GAL	B	401	-	-	1/2/22/22	0/1/1/1
3	HFK	B	402	-	-	2/2/43/43	0/5/5/5
3	HFK	A	402	-	-	2/2/43/43	0/5/5/5
2	GAL	C	401	-	-	2/2/22/22	0/1/1/1
2	GAL	A	401	-	-	2/2/22/22	0/1/1/1
3	HFK	C	402	-	-	2/2/43/43	0/5/5/5
4	HR8	D	401	-	-	2/11/11/11	0/1/1/1
4	HR8	A	403	-	-	2/11/11/11	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	HFK	C06-C07	15.05	1.56	1.37
3	A	402	HFK	C06-C07	14.20	1.55	1.37
3	C	402	HFK	C06-C07	13.56	1.54	1.37
3	A	402	HFK	C15-N16	7.55	1.48	1.36
3	B	402	HFK	C15-N14	7.55	1.49	1.30
3	C	402	HFK	C06-N16	7.49	1.49	1.37
3	C	402	HFK	C15-N16	7.48	1.48	1.36
3	A	402	HFK	C06-N16	7.39	1.49	1.37
3	C	402	HFK	C15-N14	7.33	1.49	1.30
3	B	402	HFK	C06-N16	7.11	1.49	1.37
3	B	402	HFK	C15-N16	7.05	1.48	1.36
3	A	402	HFK	C15-N14	6.59	1.47	1.30
3	A	402	HFK	C15-N17	5.48	1.46	1.36
3	B	402	HFK	C15-N17	5.41	1.46	1.36
3	C	402	HFK	C15-N17	4.70	1.45	1.36
3	C	402	HFK	C08-N14	4.62	1.51	1.46
3	A	402	HFK	C08-N14	3.72	1.50	1.46
3	B	402	HFK	C08-N14	3.43	1.49	1.46
3	A	402	HFK	C02-C07	2.59	1.54	1.46
3	B	402	HFK	C05-C06	2.53	1.54	1.49
3	A	402	HFK	C05-C06	2.50	1.53	1.49
3	C	402	HFK	C05-C06	2.43	1.53	1.49
3	A	402	HFK	C03-C02	2.37	1.53	1.50
3	C	402	HFK	C02-C07	2.26	1.53	1.46
3	B	402	HFK	C02-C07	2.20	1.53	1.46

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	HFK	C02-C07-C06	-14.02	105.85	119.17
3	B	402	HFK	C15-N16-C06	-13.37	104.67	120.67
3	B	402	HFK	C02-C07-C06	-10.89	108.83	119.17
3	A	402	HFK	C02-C07-C06	-10.53	109.17	119.17
3	C	402	HFK	C05-C06-C07	-10.51	109.11	122.97
3	A	402	HFK	C05-C06-C07	-10.29	109.40	122.97
3	A	402	HFK	C15-N16-C06	-9.72	109.04	120.67
3	B	402	HFK	N16-C15-N14	-9.61	107.80	123.88
3	C	402	HFK	N16-C15-N14	-8.90	108.99	123.88
3	C	402	HFK	C15-N16-C06	-8.75	110.20	120.67
3	A	402	HFK	N16-C15-N14	-8.24	110.10	123.88
3	B	402	HFK	C05-C06-C07	-8.05	112.36	122.97
3	A	402	HFK	C08-C07-C06	-7.42	113.37	121.75
2	A	401	GAL	C1-O5-C5	-6.72	100.98	113.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	HFK	C08-C07-C06	-5.75	115.26	121.75
3	C	402	HFK	C08-C07-C06	-5.73	115.29	121.75
2	B	401	GAL	C1-O5-C5	-5.64	103.03	113.66
3	C	402	HFK	N17-C15-N14	-4.73	109.95	117.81
2	A	401	GAL	C1-C2-C3	-4.50	100.97	110.31
2	C	401	GAL	O2-C2-C1	4.33	119.20	109.16
3	B	402	HFK	C05-C06-N16	-4.29	108.74	115.34
3	A	402	HFK	C09-C10-C11	4.21	117.89	111.37
2	C	401	GAL	C1-O5-C5	-3.79	106.52	113.66
2	C	401	GAL	O1-C1-C2	3.55	119.03	109.03
2	C	401	GAL	O5-C1-C2	-3.50	104.05	110.28
3	A	402	HFK	N17-C15-N14	-3.46	112.05	117.81
2	B	401	GAL	C1-C2-C3	-3.41	103.23	110.31
3	C	402	HFK	C03-C02-C07	3.35	123.61	117.36
2	A	401	GAL	O1-C1-C2	3.29	118.29	109.03
3	A	402	HFK	O01-C02-C03	-3.25	115.54	120.86
3	A	402	HFK	C13-C12-C11	3.04	116.07	111.37
2	A	401	GAL	O3-C3-C4	2.90	117.06	110.35
3	C	402	HFK	C13-C12-C11	2.77	115.65	111.37
3	C	402	HFK	C05-C06-N16	-2.69	111.21	115.34
2	C	401	GAL	C1-C2-C3	-2.68	104.75	110.31
3	A	402	HFK	C03-C02-C07	2.65	122.31	117.36
3	C	402	HFK	O01-C02-C03	-2.54	116.69	120.86
3	A	402	HFK	C05-C06-N16	-2.54	111.43	115.34
3	B	402	HFK	N17-C15-N14	-2.53	113.60	117.81
2	B	401	GAL	O5-C5-C6	2.44	112.50	106.44
3	B	402	HFK	C26-C20-N19	2.40	137.72	130.78
3	C	402	HFK	C26-C20-N19	2.37	137.66	130.78
2	B	401	GAL	O4-C4-C3	2.35	115.78	110.35
2	B	401	GAL	O5-C1-C2	-2.28	106.21	110.28
2	C	401	GAL	C3-C4-C5	2.27	114.29	110.24
2	A	401	GAL	O1-C1-O5	-2.26	103.59	110.38
3	A	402	HFK	C26-C20-N19	2.25	137.31	130.78
3	C	402	HFK	C26-C20-C21	-2.23	116.61	120.53
3	B	402	HFK	O01-C02-C07	2.18	124.54	121.54
2	B	401	GAL	O1-C1-C2	2.17	115.15	109.03
3	A	402	HFK	C21-C20-N19	-2.08	103.20	108.04
3	B	402	HFK	C04-C03-C02	-2.06	109.92	113.58

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	HFK	N14-C15-N17-C18
3	A	402	HFK	N16-C15-N17-C18
3	B	402	HFK	N14-C15-N17-C18
3	C	402	HFK	N14-C15-N17-C18
3	C	402	HFK	N16-C15-N17-C18
4	B	403	HR8	C7-C8-N1-C9
4	B	403	HR8	C12-C10-C9-N1
4	B	403	HR8	O2-C8-N1-C9
2	A	401	GAL	O5-C5-C6-O6
2	C	401	GAL	O5-C5-C6-O6
2	C	401	GAL	C4-C5-C6-O6
4	A	403	HR8	C11-C10-C9-N1
4	D	401	HR8	C11-C10-C9-N1
2	B	401	GAL	O5-C5-C6-O6
4	B	403	HR8	C11-C10-C9-N1
2	A	401	GAL	C4-C5-C6-O6
3	B	402	HFK	N16-C15-N17-C18
4	D	401	HR8	C12-C10-C9-N1
4	A	403	HR8	C12-C10-C9-N1

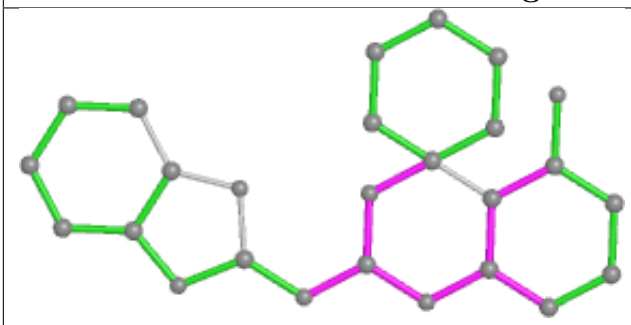
There are no ring outliers.

2 monomers are involved in 2 short contacts:

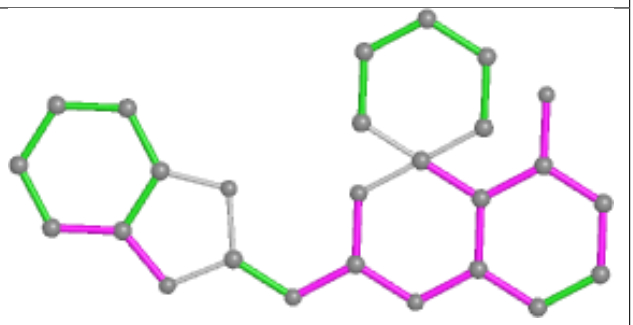
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403	HR8	1	0
2	C	401	GAL	1	0

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.

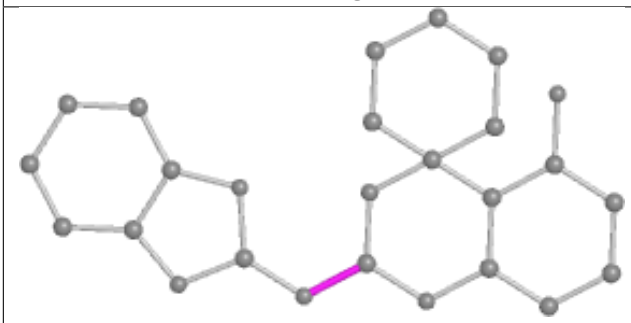
Ligand HFK B 402



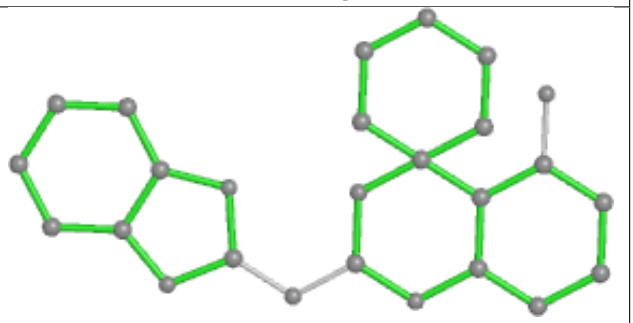
Bond lengths



Bond angles

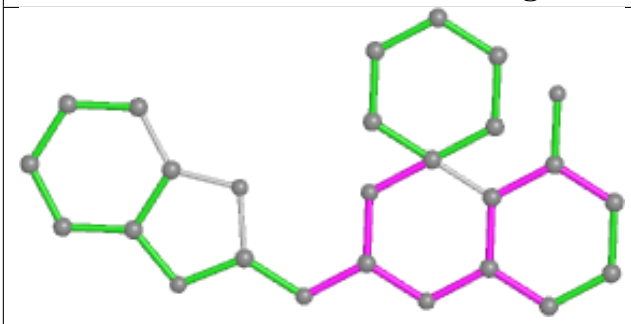


Torsions

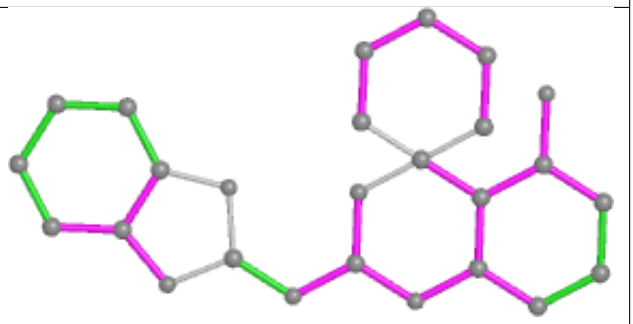


Rings

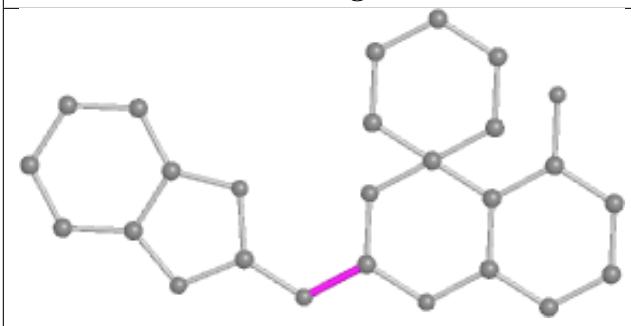
Ligand HFK A 402



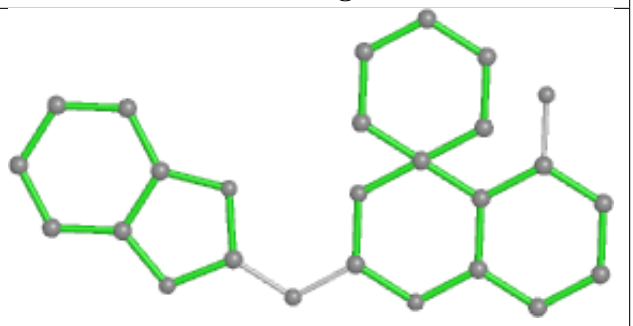
Bond lengths



Bond angles

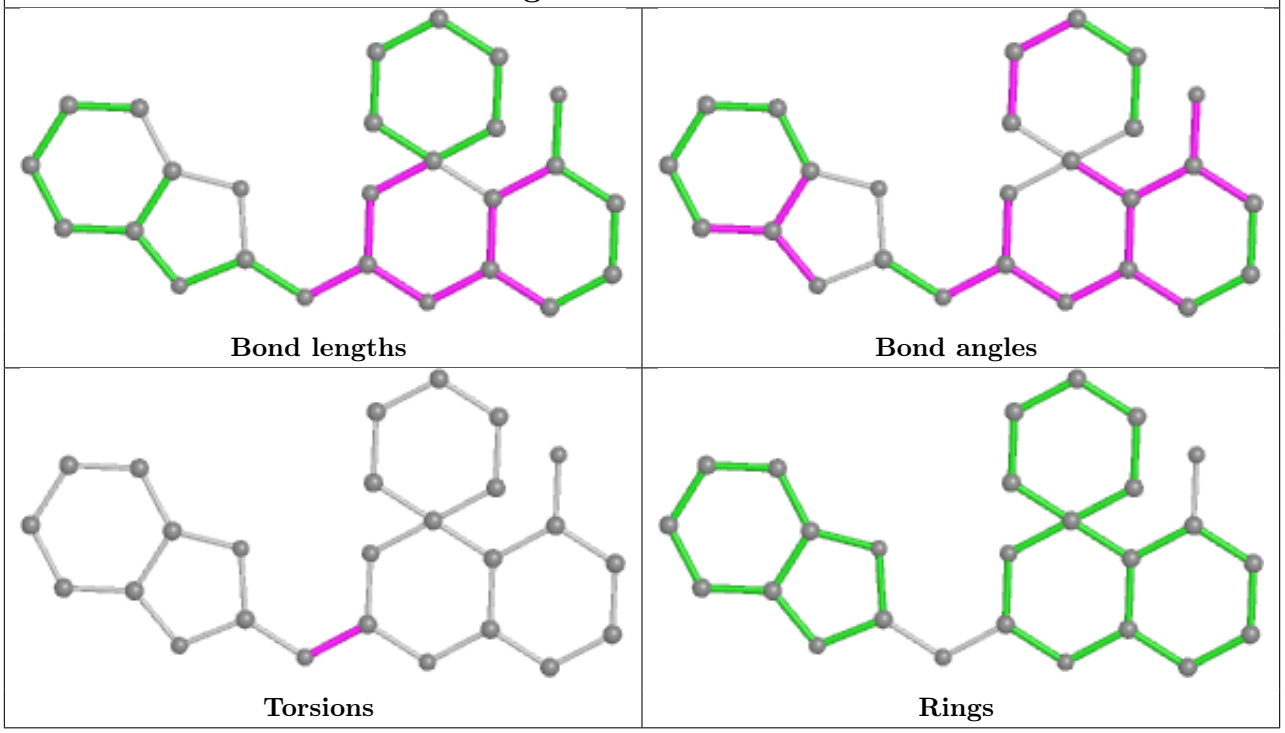


Torsions



Rings

Ligand HFK C 402



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	392/392 (100%)	-0.51	0	100	100	25, 40, 63, 97	0
1	B	392/392 (100%)	-0.43	0	100	100	27, 45, 77, 107	0
1	C	392/392 (100%)	-0.27	1 (0%)	94	93	25, 49, 88, 115	0
1	D	360/392 (91%)	-0.19	4 (1%)	80	79	26, 56, 99, 123	0
All	All	1536/1568 (97%)	-0.35	5 (0%)	94	93	25, 47, 88, 123	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	106	TRP	3.2
1	C	332	ALA	3.0
1	D	116	TYR	2.5
1	D	130	VAL	2.3
1	D	173	ALA	2.2

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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,

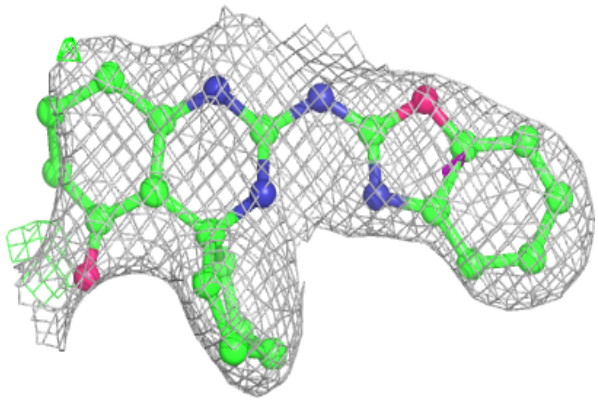
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

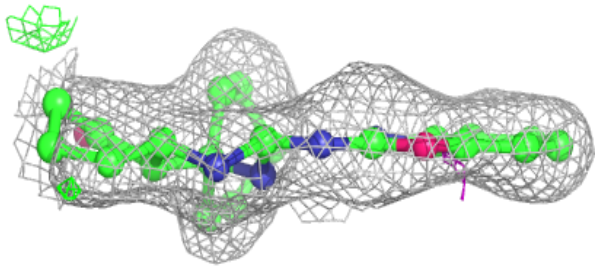
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HFK	B	402	26/26	0.81	0.22	60,79,97,106	0
4	HR8	D	401	16/16	0.86	0.22	55,64,80,81	0
3	HFK	C	402	26/26	0.88	0.20	47,70,80,83	0
4	HR8	C	403	16/16	0.89	0.20	51,70,79,82	0
4	HR8	A	403	16/16	0.90	0.19	56,63,68,73	0
3	HFK	A	402	26/26	0.93	0.13	39,48,55,61	0
4	HR8	B	403	16/16	0.93	0.14	44,47,53,59	0
2	GAL	C	401	12/12	0.95	0.11	37,42,49,51	0
2	GAL	B	401	12/12	0.96	0.12	32,40,47,54	0
2	GAL	A	401	12/12	0.98	0.10	23,28,33,38	0

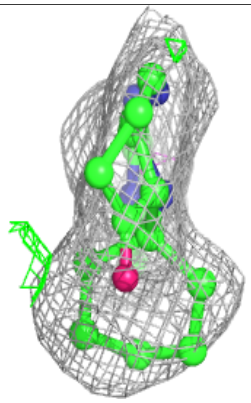
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HFK B 402:

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

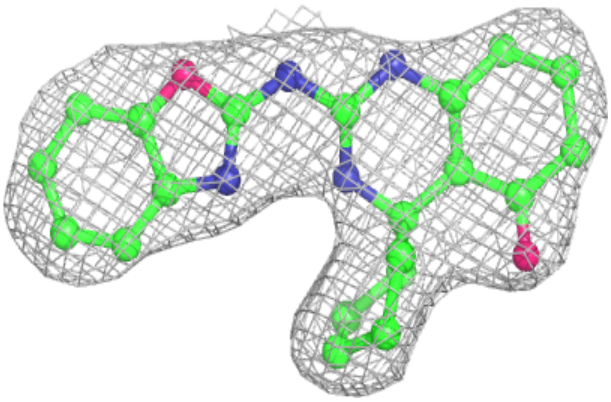


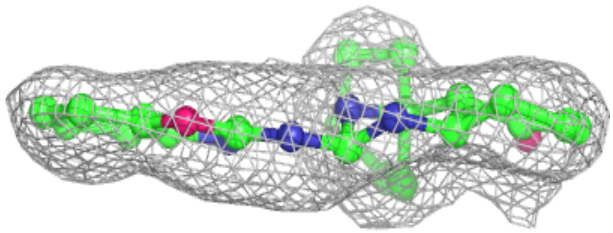


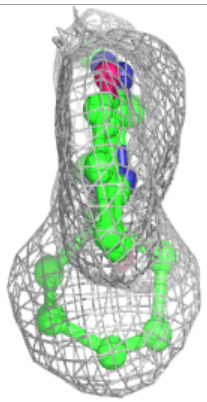


Electron density around HFK C 402:

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

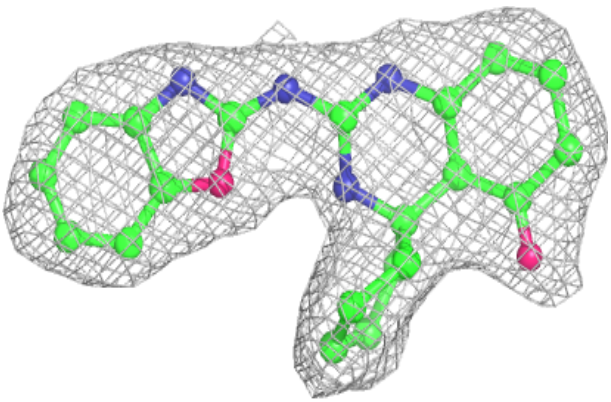


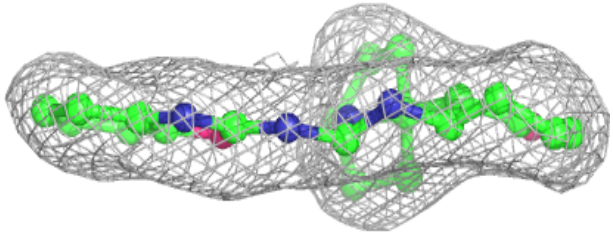


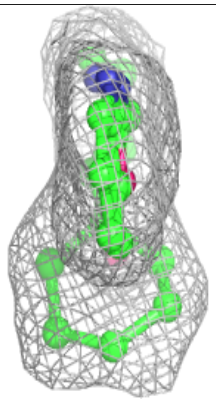


Electron density around HFK A 402:

$2mF_o$-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.