Full wwPDB X-ray Structure Validation Report

Mar 21, 2016 – 06:03 PM EDT

PDB ID	:	5HG1
Title	:	Crystal Structure of Human Hexokinase 2 with cmpd 1, a C-2-substituted glucosamine
Authors	:	Campobasso, N.; Zhao, B.; Smallwood, A.
Deposited on	:	2016-01-07
Resolution	:	2.76 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

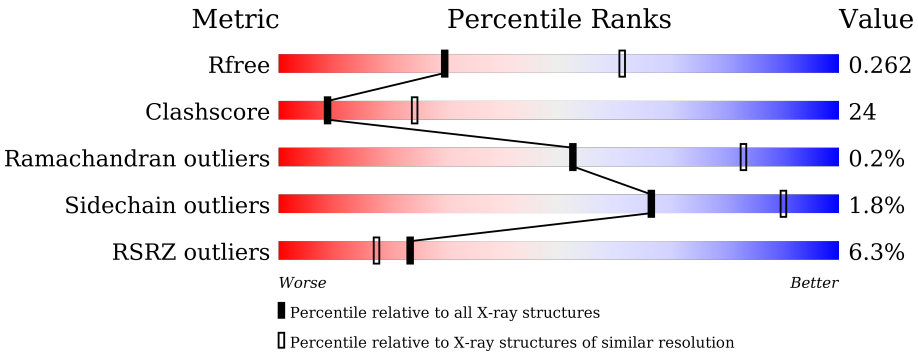
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

1 Overall quality at a glance

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

The reported resolution of this entry is 2.76 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	922	6% 63% 30% · 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	62C	A	1002	-	-	-	X
3	BG6	A	1003	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6652 atoms, of which 39 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.

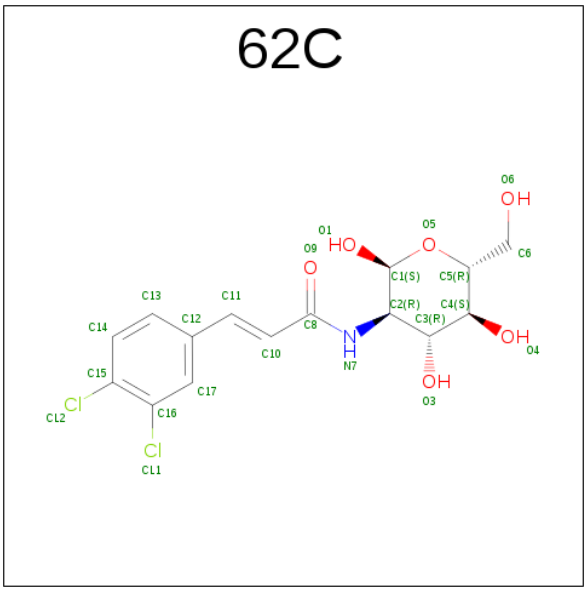
- Molecule 1 is a protein called Hexokinase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	867	Total	C	N	O	S	0	0	0
			6528	4084	1152	1233	59			

There are 22 discrepancies between the modelled and reference sequences:

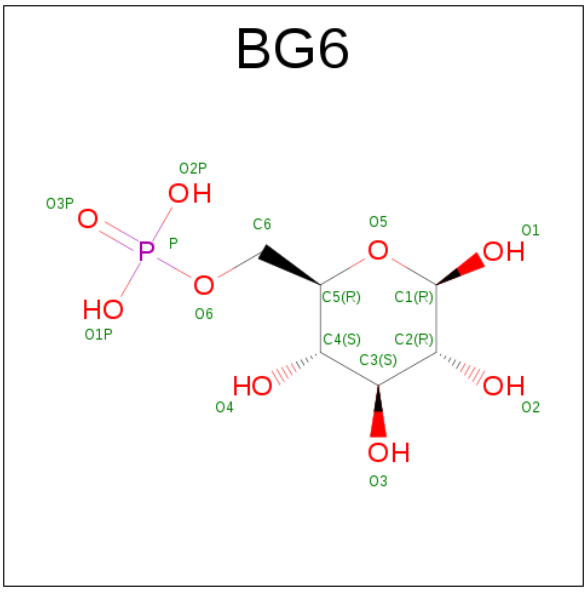
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP P52789
A	-4	GLY	-	expression tag	UNP P52789
A	-3	SER	-	expression tag	UNP P52789
A	-2	SER	-	expression tag	UNP P52789
A	-1	HIS	-	expression tag	UNP P52789
A	0	HIS	-	expression tag	UNP P52789
A	1	HIS	-	expression tag	UNP P52789
A	2	HIS	-	expression tag	UNP P52789
A	3	HIS	-	expression tag	UNP P52789
A	4	HIS	-	expression tag	UNP P52789
A	5	SER	-	expression tag	UNP P52789
A	6	SER	-	expression tag	UNP P52789
A	7	GLY	-	expression tag	UNP P52789
A	8	LEU	-	expression tag	UNP P52789
A	9	GLU	-	expression tag	UNP P52789
A	10	ASN	-	expression tag	UNP P52789
A	11	LEU	-	expression tag	UNP P52789
A	12	TYR	-	expression tag	UNP P52789
A	13	PHE	-	expression tag	UNP P52789
A	14	GLN	-	expression tag	UNP P52789
A	15	GLY	-	expression tag	UNP P52789
A	16	SER	-	expression tag	UNP P52789

- Molecule 2 is 2-deoxy-2-{[(2E)-3-(3,4-dichlorophenyl)prop-2-enoyl]amino}-alpha-D-glucopyranose (three-letter code: 62C) (formula: $C_{15}H_{17}Cl_2NO_6$).



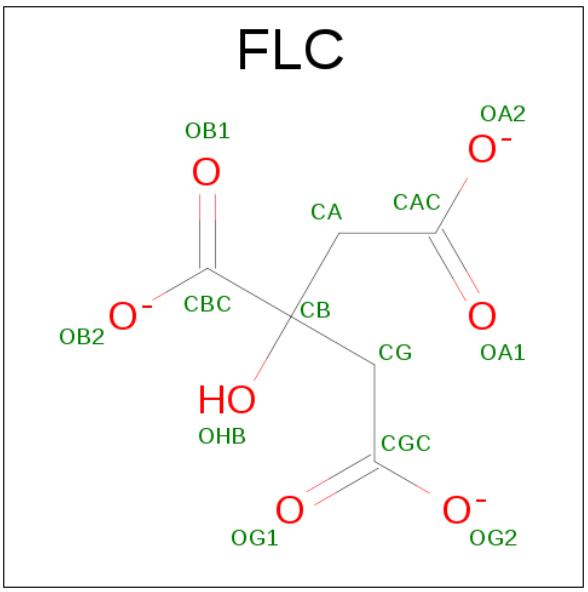
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	H	N	O	0	0
			41	15	2	17	1	6		
2	A	1	Total	C	Cl	H	N	O	0	0
			41	15	2	17	1	6		

- Molecule 3 is BETA-D-GLUCOSE-6-PHOSPHATE (three-letter code: BG6) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 18 6 5 7	0	0

- Molecule 5 is water.

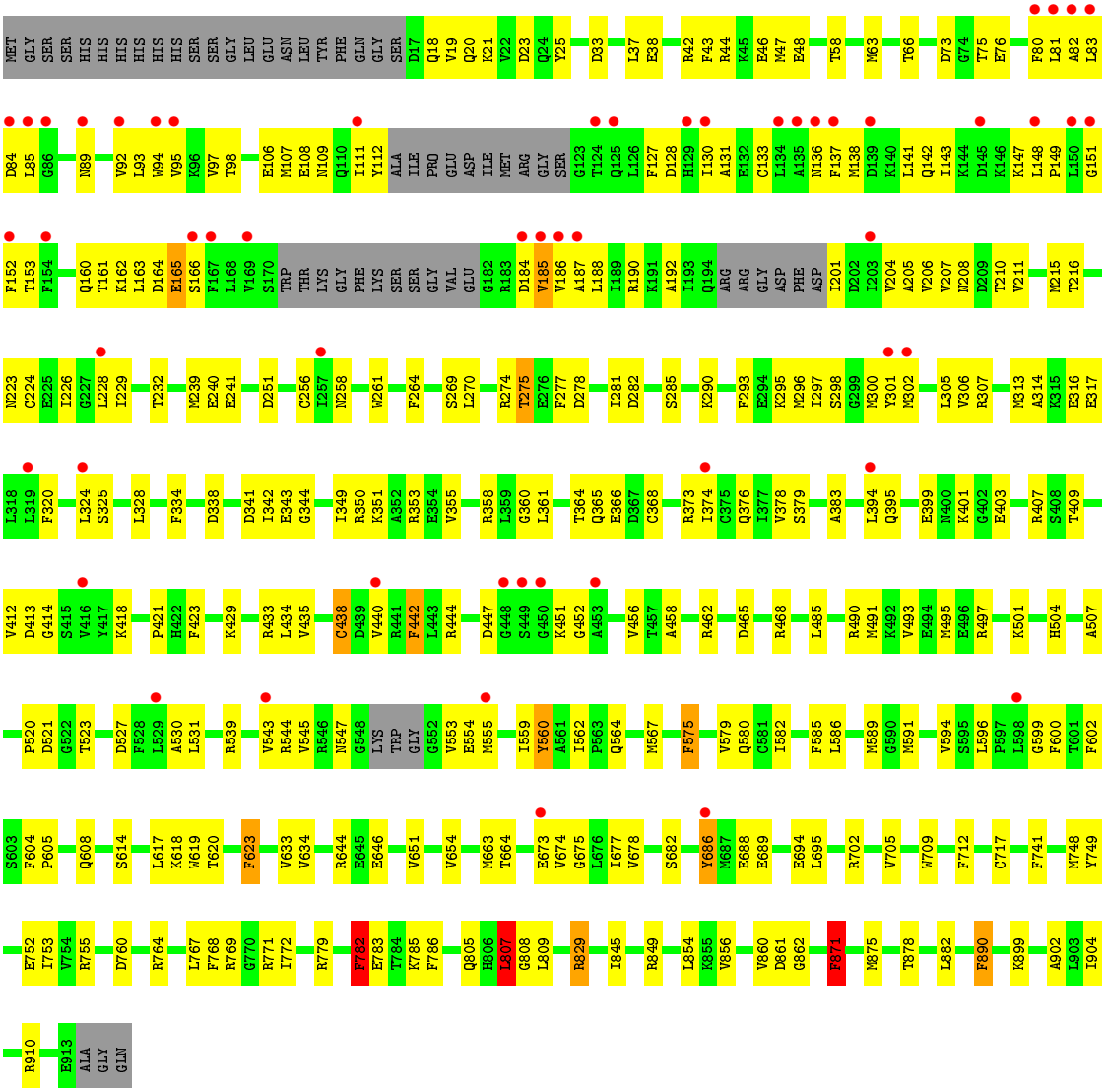
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	8	Total O 8 8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Hexokinase-2

Chain A: 



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	165.12Å 165.12Å 126.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	71.50 – 2.76 94.74 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (71.50-2.76) 94.0 (94.74-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.218 , 0.266 0.213 , 0.262	Depositor DCC
R_{free} test set	2315 reflections (4.79%)	DCC
Wilson B-factor (Å^2)	60.1	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 37.2	EDS
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 51671 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6652	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 62C, FLC, BG6

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	0.43	0/6622	0.71	7/8930 (0.1%)

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	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	251	ASP	N-CA-C	6.85	129.50	111.00
1	A	871	PHE	CB-CG-CD2	-6.01	116.59	120.80
1	A	871	PHE	CB-CG-CD1	5.96	124.97	120.80
1	A	782	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	A	829	ARG	CB-CG-CD	5.75	126.56	111.60
1	A	829	ARG	CG-CD-NE	5.39	123.12	111.80
1	A	807	LEU	C-N-CA	-5.16	111.46	122.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	438	CYS	Peptide
1	A	782	PHE	Sidechain
1	A	807	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	6528	0	6343	305	0
2	A	48	34	0	2	0
3	A	16	0	10	0	0
4	A	13	5	5	2	0
5	A	8	0	0	0	0
All	All	6613	39	6358	306	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 24.

All (306) 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:A:47:MET:HA	1:A:63:MET:HE3	1.29	1.06
1:A:47:MET:HA	1:A:63:MET:CE	1.92	0.99
1:A:185:VAL:HG23	1:A:186:VAL:H	1.29	0.97
1:A:608:GLN:HG2	1:A:614:SER:HB3	1.48	0.95
1:A:341:ASP:HB3	1:A:351:LYS:HD3	1.47	0.94
1:A:208:ASN:HD22	1:A:210:THR:HG22	1.30	0.94
1:A:89:ASN:HA	1:A:111:ILE:HD11	1.54	0.88
1:A:277:PHE:O	1:A:281:ILE:HD12	1.73	0.88
1:A:295:LYS:HA	1:A:301:TYR:CD2	2.08	0.87
1:A:275:THR:HG23	1:A:277:PHE:H	1.44	0.82
1:A:300:MET:HE3	1:A:301:TYR:CZ	2.16	0.81
1:A:343:GLU:OE2	1:A:376:GLN:HA	1.81	0.80
1:A:44:ARG:NH1	1:A:48:GLU:OE2	2.15	0.80
1:A:295:LYS:HG2	1:A:301:TYR:CE2	2.17	0.80
1:A:33:ASP:OD2	1:A:433:ARG:NH1	2.14	0.79
1:A:185:VAL:O	1:A:188:LEU:N	2.14	0.79
1:A:275:THR:HG22	1:A:278:ASP:H	1.46	0.79
1:A:341:ASP:HB3	1:A:351:LYS:CD	2.13	0.78
1:A:544:ARG:HB3	1:A:554:GLU:HB3	1.65	0.78
1:A:232:THR:O	1:A:298:SER:OG	2.00	0.78
1:A:208:ASN:ND2	1:A:210:THR:HG22	2.00	0.76
1:A:688:GLU:HG3	1:A:689:GLU:N	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:O	1:A:85:LEU:HD23	1.85	0.76
1:A:161:THR:O	1:A:162:LYS:HG3	1.87	0.75
1:A:133:CYS:HA	1:A:136:ASN:CB	2.16	0.74
1:A:43:PHE:O	1:A:47:MET:HG3	1.87	0.74
1:A:418:LYS:HE2	1:A:444:ARG:HG3	1.68	0.74
1:A:216:THR:HG23	1:A:452:GLY:HA2	1.71	0.73
1:A:215:MET:HG3	1:A:456:VAL:HG22	1.70	0.73
1:A:165:GLU:HA	1:A:186:VAL:HG11	1.71	0.73
1:A:84:ASP:HA	1:A:153:THR:CG2	2.19	0.72
1:A:184:ASP:O	1:A:185:VAL:HG22	1.90	0.72
1:A:306:VAL:HG23	1:A:374:ILE:HG22	1.71	0.72
1:A:401:LYS:HG2	1:A:403:GLU:HG2	1.72	0.72
1:A:608:GLN:HE21	1:A:654:VAL:HG23	1.56	0.71
1:A:164:ASP:O	1:A:165:GLU:HB2	1.91	0.70
1:A:215:MET:HG3	1:A:456:VAL:CG2	2.22	0.70
1:A:608:GLN:CG	1:A:614:SER:HB3	2.22	0.70
1:A:184:ASP:OD2	1:A:187:ALA:HB3	1.92	0.69
1:A:190:ARG:HH21	1:A:204:VAL:HG12	1.57	0.69
1:A:438:CYS:HB2	1:A:440:VAL:HG23	1.75	0.69
1:A:306:VAL:HG23	1:A:374:ILE:CG2	2.22	0.69
1:A:663:MET:HG3	1:A:904:ILE:CG1	2.23	0.69
1:A:281:ILE:HD13	1:A:305:LEU:HD13	1.74	0.69
1:A:805:GLN:O	1:A:808:GLY:HA2	1.93	0.68
1:A:634:VAL:HG13	1:A:651:VAL:HG11	1.74	0.68
1:A:688:GLU:HG3	1:A:689:GLU:H	1.57	0.68
1:A:807:LEU:O	1:A:809:LEU:HG	1.92	0.68
1:A:338:ASP:O	1:A:342:ILE:HD12	1.93	0.68
1:A:274:ARG:HE	1:A:296:MET:CE	2.06	0.67
1:A:93:LEU:HA	1:A:109:ASN:HB3	1.76	0.67
1:A:152:PHE:HD2	1:A:206:VAL:HG22	1.60	0.67
1:A:23:ASP:OD1	1:A:373:ARG:NE	2.16	0.67
1:A:580:GLN:HG3	1:A:644:ARG:HH22	1.59	0.67
1:A:600:PHE:CD2	1:A:654:VAL:HG12	2.29	0.67
1:A:152:PHE:CD2	1:A:206:VAL:HG22	2.31	0.66
1:A:185:VAL:HG23	1:A:186:VAL:N	2.08	0.66
1:A:644:ARG:HD2	1:A:646:GLU:CD	2.16	0.66
1:A:353:ARG:HB2	1:A:368:CYS:SG	2.37	0.65
1:A:95:VAL:HA	1:A:106:GLU:O	1.96	0.65
1:A:83:LEU:HD11	1:A:152:PHE:CE1	2.32	0.65
1:A:527:ASP:OD1	1:A:544:ARG:HG3	1.97	0.64
1:A:223:ASN:ND2	1:A:407:ARG:HG3	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASN:HA	1:A:137:PHE:CZ	2.32	0.64
1:A:165:GLU:HA	1:A:186:VAL:CG1	2.28	0.64
1:A:491:MET:O	1:A:495:MET:HG3	1.98	0.64
1:A:686:TYR:H	1:A:686:TYR:HD1	1.46	0.64
1:A:83:LEU:O	1:A:83:LEU:HD12	1.98	0.64
1:A:871:PHE:C	1:A:871:PHE:HD1	2.00	0.64
1:A:83:LEU:HD11	1:A:152:PHE:CD1	2.33	0.63
1:A:141:LEU:HB2	1:A:143:ILE:HG23	1.78	0.63
1:A:47:MET:HG2	1:A:63:MET:HE1	1.79	0.63
1:A:523:THR:OG1	1:A:547:ASN:ND2	2.31	0.63
1:A:530:ALA:HA	1:A:599:GLY:O	1.99	0.62
1:A:854:LEU:HG	1:A:856:VAL:HG22	1.82	0.62
1:A:223:ASN:HD21	1:A:407:ARG:HG3	1.65	0.62
1:A:582:ILE:O	1:A:586:LEU:HD13	1.99	0.62
1:A:465:ASP:HA	1:A:468:ARG:NH1	2.16	0.61
1:A:83:LEU:O	1:A:153:THR:HG22	2.01	0.61
1:A:108:GLU:O	1:A:137:PHE:HZ	1.83	0.61
1:A:47:MET:CB	1:A:63:MET:HE1	2.31	0.61
1:A:871:PHE:C	1:A:871:PHE:CD1	2.74	0.61
1:A:543:VAL:CG2	1:A:902:ALA:HB1	2.30	0.61
1:A:364:THR:HG22	1:A:365:GLN:N	2.15	0.60
1:A:302:MET:HE3	1:A:379:SER:HA	1.82	0.60
1:A:33:ASP:CG	1:A:433:ARG:HH12	2.04	0.60
1:A:138:MET:O	1:A:142:GLN:N	2.35	0.59
1:A:543:VAL:HG21	1:A:902:ALA:CB	2.32	0.59
1:A:344:GLY:HA2	1:A:421:PRO:HG3	1.84	0.59
1:A:295:LYS:HA	1:A:301:TYR:HD2	1.68	0.59
1:A:608:GLN:NE2	1:A:654:VAL:HG23	2.16	0.58
1:A:18:GLN:NE2	1:A:21:LYS:HE2	2.17	0.58
1:A:760:ASP:OD2	1:A:764:ARG:NH1	2.36	0.58
1:A:73:ASP:N	1:A:76:GLU:OE2	2.18	0.58
1:A:349:ILE:H	1:A:349:ILE:HD12	1.68	0.58
1:A:306:VAL:HG13	1:A:334:PHE:CD2	2.39	0.58
1:A:360:GLY:C	1:A:361:LEU:HD12	2.23	0.58
1:A:94:TRP:O	1:A:107:MET:HA	2.03	0.58
1:A:543:VAL:HG21	1:A:902:ALA:HB1	1.86	0.58
1:A:350:ARG:HG3	1:A:351:LYS:N	2.19	0.57
1:A:165:GLU:CA	1:A:186:VAL:HG11	2.35	0.57
1:A:854:LEU:HG	1:A:856:VAL:CG2	2.34	0.57
1:A:130:ILE:HG22	1:A:130:ILE:O	2.04	0.57
1:A:497:ARG:HG2	1:A:507:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:LEU:CG	1:A:856:VAL:HG22	2.35	0.57
1:A:148:LEU:HG	1:A:149:PRO:HD2	1.87	0.56
1:A:47:MET:CA	1:A:63:MET:CE	2.77	0.56
1:A:580:GLN:HG3	1:A:644:ARG:NH2	2.20	0.56
1:A:47:MET:HG2	1:A:63:MET:CE	2.35	0.56
1:A:290:LYS:HG3	2:A:1002:62C:CL1	2.43	0.56
1:A:185:VAL:CG2	1:A:186:VAL:H	2.11	0.56
1:A:164:ASP:HB2	1:A:186:VAL:HG21	1.87	0.56
1:A:295:LYS:HG2	1:A:301:TYR:CZ	2.40	0.55
1:A:485:LEU:HD23	1:A:882:LEU:HD22	1.88	0.55
1:A:19:VAL:HG23	1:A:20:GLN:N	2.21	0.55
1:A:128:ASP:OD1	1:A:192:ALA:HB1	2.07	0.55
1:A:240:GLU:HG3	1:A:241:GLU:N	2.22	0.55
1:A:663:MET:HG3	1:A:904:ILE:HG13	1.88	0.55
1:A:25:TYR:CD2	1:A:313:MET:CE	2.91	0.54
1:A:47:MET:HA	1:A:63:MET:HE1	1.87	0.54
1:A:523:THR:HG23	1:A:523:THR:O	2.06	0.54
1:A:769:ARG:O	1:A:769:ARG:HG2	2.07	0.54
1:A:184:ASP:O	1:A:185:VAL:CG2	2.54	0.54
1:A:364:THR:HG22	1:A:366:GLU:H	1.73	0.54
1:A:207:VAL:CG2	1:A:211:VAL:HB	2.37	0.54
1:A:128:ASP:HA	1:A:131:ALA:HB3	1.90	0.54
1:A:300:MET:CE	1:A:301:TYR:CZ	2.88	0.54
1:A:343:GLU:OE2	1:A:376:GLN:CA	2.56	0.54
1:A:521:ASP:OD2	1:A:910:ARG:NH2	2.41	0.54
1:A:413:ASP:OD1	1:A:414:GLY:N	2.37	0.54
1:A:38:GLU:O	1:A:42:ARG:HG3	2.07	0.53
1:A:208:ASN:HD22	1:A:210:THR:CG2	2.13	0.53
1:A:94:TRP:HB2	1:A:137:PHE:HE2	1.73	0.53
1:A:325:SER:HB3	1:A:360:GLY:O	2.08	0.53
1:A:442:PHE:CD1	1:A:442:PHE:N	2.77	0.53
1:A:92:VAL:O	1:A:109:ASN:HB2	2.09	0.53
1:A:686:TYR:HB2	1:A:845:ILE:HD11	1.90	0.53
1:A:664:THR:HG23	1:A:899:LYS:HD3	1.90	0.53
1:A:302:MET:CE	1:A:378:VAL:HG12	2.39	0.53
1:A:127:PHE:O	1:A:131:ALA:HB2	2.09	0.52
1:A:748:MET:HG3	1:A:749:TYR:N	2.17	0.52
1:A:829:ARG:HH21	1:A:829:ARG:HG2	1.73	0.52
1:A:47:MET:CG	1:A:63:MET:HE1	2.38	0.52
1:A:779:ARG:NH2	4:A:1004:FLC:OA2	2.42	0.52
1:A:623:PHE:CD1	1:A:623:PHE:N	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:VAL:O	1:A:435:VAL:HG23	2.10	0.52
1:A:497:ARG:HD2	1:A:507:ALA:HA	1.92	0.52
1:A:270:LEU:O	1:A:274:ARG:HG3	2.10	0.52
1:A:320:PHE:CD1	1:A:361:LEU:HD23	2.45	0.52
1:A:644:ARG:HD2	1:A:646:GLU:OE2	2.10	0.52
1:A:127:PHE:HE2	1:A:188:LEU:CB	2.23	0.51
1:A:523:THR:CB	1:A:547:ASN:HD22	2.24	0.51
1:A:531:LEU:HB2	1:A:600:PHE:HD1	1.76	0.51
1:A:600:PHE:HD2	1:A:654:VAL:HG12	1.72	0.51
1:A:748:MET:HE1	1:A:752:GLU:HG3	1.93	0.51
1:A:829:ARG:HH21	1:A:829:ARG:CG	2.24	0.51
4:A:1004:FLC:OA2	4:A:1004:FLC:CBC	2.58	0.51
1:A:712:PHE:O	1:A:741:PHE:HB2	2.10	0.51
1:A:749:TYR:O	1:A:753:ILE:HG13	2.11	0.51
1:A:81:LEU:HB2	1:A:148:LEU:HD22	1.93	0.51
1:A:207:VAL:HG22	1:A:211:VAL:HB	1.93	0.51
1:A:109:ASN:HA	1:A:137:PHE:HZ	1.74	0.50
1:A:543:VAL:HG12	1:A:555:MET:SD	2.51	0.50
1:A:560:TYR:CD1	1:A:560:TYR:N	2.80	0.50
1:A:42:ARG:NH1	1:A:269:SER:O	2.44	0.50
1:A:760:ASP:O	1:A:764:ARG:HG3	2.10	0.50
1:A:560:TYR:OH	1:A:585:PHE:HB2	2.12	0.50
1:A:141:LEU:CB	1:A:143:ILE:HG23	2.42	0.50
1:A:860:VAL:HG12	1:A:861:ASP:N	2.27	0.50
1:A:619:TRP:HB3	1:A:623:PHE:O	2.12	0.50
1:A:293:PHE:CZ	1:A:297:ILE:HD11	2.47	0.50
1:A:504:HIS:CD2	1:A:695:LEU:HD21	2.47	0.49
1:A:861:ASP:OD1	1:A:862:GLY:N	2.41	0.49
1:A:447:ASP:CB	1:A:451:LYS:CB	2.90	0.49
1:A:82:ALA:HA	1:A:151:GLY:O	2.12	0.49
1:A:274:ARG:HG2	1:A:296:MET:CE	2.43	0.49
1:A:42:ARG:O	1:A:46:GLU:HG2	2.12	0.49
1:A:111:ILE:HG12	1:A:112:TYR:N	2.28	0.49
1:A:19:VAL:HB	1:A:373:ARG:CD	2.43	0.49
1:A:25:TYR:CD2	1:A:313:MET:HE3	2.48	0.49
1:A:560:TYR:N	1:A:560:TYR:HD1	2.10	0.49
1:A:282:ASP:O	1:A:285:SER:OG	2.27	0.49
1:A:553:VAL:O	1:A:553:VAL:HG23	2.12	0.49
1:A:890:PHE:N	1:A:890:PHE:CD1	2.81	0.48
1:A:264:PHE:O	1:A:293:PHE:HB2	2.13	0.48
1:A:314:ALA:HB1	1:A:324:LEU:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLY:CA	1:A:421:PRO:HG3	2.43	0.48
1:A:293:PHE:CE2	1:A:297:ILE:CD1	2.96	0.48
1:A:520:PRO:HD3	1:A:663:MET:HE1	1.94	0.48
1:A:418:LYS:HE2	1:A:444:ARG:CG	2.42	0.48
1:A:591:MET:CE	1:A:594:VAL:HG21	2.43	0.48
1:A:591:MET:HE2	1:A:594:VAL:HG21	1.94	0.48
1:A:543:VAL:CG2	1:A:902:ALA:CB	2.91	0.48
1:A:109:ASN:HA	1:A:137:PHE:CE1	2.49	0.48
1:A:25:TYR:CD2	1:A:313:MET:HE2	2.49	0.48
1:A:293:PHE:CE2	1:A:297:ILE:HD12	2.49	0.48
1:A:302:MET:HE3	1:A:378:VAL:HG12	1.96	0.48
1:A:678:VAL:HG11	1:A:871:PHE:CZ	2.49	0.48
1:A:111:ILE:HG12	1:A:112:TYR:H	1.78	0.47
1:A:37:LEU:CD2	1:A:434:LEU:HD22	2.44	0.47
1:A:783:GLU:OE1	1:A:785:LYS:HE2	2.15	0.47
1:A:364:THR:HG22	1:A:365:GLN:H	1.79	0.47
1:A:395:GLN:O	1:A:399:GLU:HG3	2.14	0.47
1:A:160:GLN:HB3	1:A:166:SER:OG	2.15	0.47
1:A:591:MET:O	1:A:594:VAL:HG13	2.14	0.47
1:A:689:GLU:OE2	1:A:702:ARG:NH1	2.47	0.47
1:A:25:TYR:HD2	1:A:313:MET:CE	2.27	0.47
1:A:216:THR:CG2	1:A:452:GLY:HA2	2.42	0.47
1:A:782:PHE:CE1	1:A:786:PHE:HB2	2.50	0.47
1:A:89:ASN:CA	1:A:111:ILE:HD11	2.36	0.47
1:A:66:THR:OG1	1:A:256:CYS:O	2.20	0.47
1:A:412:VAL:HG12	1:A:413:ASP:N	2.29	0.46
1:A:674:VAL:HG12	1:A:675:GLY:N	2.30	0.46
1:A:47:MET:CA	1:A:63:MET:HE1	2.44	0.46
1:A:18:GLN:HE22	1:A:21:LYS:NZ	2.14	0.46
1:A:768:PHE:CZ	1:A:809:LEU:HD13	2.50	0.46
1:A:520:PRO:HD3	1:A:663:MET:CE	2.45	0.46
1:A:163:LEU:HD22	1:A:205:ALA:HB1	1.98	0.46
1:A:355:VAL:HG13	1:A:358:ARG:HH11	1.81	0.45
1:A:769:ARG:HH21	1:A:771:ARG:NH1	2.14	0.45
1:A:320:PHE:CE1	1:A:361:LEU:HD23	2.52	0.45
1:A:686:TYR:CD1	1:A:686:TYR:N	2.81	0.45
1:A:871:PHE:O	1:A:871:PHE:HD1	1.99	0.45
1:A:274:ARG:HG2	1:A:296:MET:HE1	1.99	0.45
1:A:275:THR:HG23	1:A:277:PHE:N	2.20	0.45
1:A:429:LYS:O	1:A:433:ARG:HG3	2.17	0.45
1:A:66:THR:HG23	1:A:256:CYS:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:VAL:O	1:A:543:VAL:HG23	2.17	0.44
1:A:575:PHE:O	1:A:579:VAL:HG22	2.18	0.44
1:A:564:GLN:HA	1:A:567:MET:CE	2.47	0.44
1:A:83:LEU:C	1:A:83:LEU:HD12	2.37	0.44
1:A:84:ASP:HA	1:A:153:THR:HG23	1.95	0.44
1:A:539:ARG:NH2	1:A:559:ILE:HD11	2.33	0.44
1:A:878:THR:HG22	1:A:882:LEU:HD12	1.98	0.44
1:A:97:VAL:HG12	1:A:98:THR:N	2.33	0.44
1:A:562:ILE:HG22	1:A:567:MET:HG3	2.00	0.44
1:A:490:ARG:NH1	1:A:717:CYS:O	2.47	0.44
1:A:435:VAL:HG23	1:A:438:CYS:HB3	1.99	0.44
1:A:748:MET:CG	1:A:749:TYR:N	2.79	0.44
1:A:686:TYR:CB	1:A:845:ILE:HD11	2.48	0.44
1:A:875:MET:CE	1:A:890:PHE:HE2	2.30	0.44
1:A:316:GLU:O	1:A:317:GLU:HB2	2.17	0.43
1:A:328:LEU:O	1:A:328:LEU:HG	2.18	0.43
1:A:224:CYS:HA	1:A:409:THR:O	2.18	0.43
1:A:306:VAL:HG11	1:A:334:PHE:CE2	2.53	0.43
1:A:705:VAL:O	1:A:705:VAL:HG23	2.18	0.43
1:A:361:LEU:HD12	1:A:361:LEU:N	2.34	0.43
1:A:58:THR:O	1:A:58:THR:CG2	2.65	0.43
1:A:66:THR:OG1	1:A:256:CYS:HB3	2.19	0.43
1:A:80:PHE:CZ	1:A:458:ALA:HA	2.53	0.43
1:A:688:GLU:CG	1:A:689:GLU:N	2.76	0.43
1:A:166:SER:O	1:A:184:ASP:O	2.36	0.43
1:A:274:ARG:HE	1:A:296:MET:HE1	1.80	0.43
1:A:73:ASP:HB2	1:A:462:ARG:CZ	2.47	0.43
1:A:383:ALA:HB2	1:A:423:PHE:CD1	2.53	0.43
1:A:442:PHE:HD1	1:A:442:PHE:N	2.17	0.43
1:A:216:THR:HG23	1:A:452:GLY:CA	2.46	0.43
1:A:226:ILE:HD11	1:A:394:LEU:HD23	2.00	0.43
1:A:623:PHE:HD1	1:A:623:PHE:N	2.15	0.43
1:A:147:LYS:HA	1:A:201:ILE:CB	2.49	0.43
1:A:130:ILE:CG2	1:A:130:ILE:O	2.66	0.43
1:A:293:PHE:CZ	1:A:297:ILE:CD1	3.01	0.43
1:A:138:MET:CB	1:A:142:GLN:HA	2.49	0.42
1:A:161:THR:C	1:A:162:LYS:HG3	2.38	0.42
1:A:338:ASP:O	1:A:342:ILE:CD1	2.66	0.42
1:A:589:MET:HB2	1:A:591:MET:HG2	2.00	0.42
1:A:239:MET:SD	1:A:256:CYS:HB2	2.58	0.42
1:A:677:ILE:O	1:A:682:SER:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:ARG:NH1	1:A:779:ARG:HA	2.34	0.42
1:A:589:MET:CB	1:A:591:MET:HG2	2.49	0.42
1:A:258:ASN:OD1	1:A:258:ASN:C	2.57	0.42
1:A:320:PHE:CE1	1:A:361:LEU:CD2	3.03	0.42
1:A:772:ILE:HG23	1:A:772:ILE:O	2.18	0.42
1:A:81:LEU:HB2	1:A:148:LEU:CD2	2.49	0.42
1:A:307:ARG:HB2	1:A:334:PHE:HB3	2.01	0.42
1:A:306:VAL:HG23	1:A:374:ILE:HG21	1.96	0.42
1:A:620:THR:HG21	2:A:1001:62C:C11	2.50	0.42
1:A:25:TYR:HD2	1:A:313:MET:HE2	1.85	0.42
1:A:295:LYS:HA	1:A:301:TYR:CE2	2.52	0.42
1:A:545:VAL:O	1:A:545:VAL:HG13	2.19	0.42
1:A:604:PHE:HB3	1:A:605:PRO:HD2	2.01	0.41
1:A:302:MET:HE3	1:A:379:SER:CA	2.49	0.41
1:A:663:MET:HG3	1:A:904:ILE:HD11	2.02	0.41
1:A:228:LEU:HD12	1:A:229:ILE:N	2.36	0.41
1:A:314:ALA:HB1	1:A:324:LEU:HD11	2.03	0.41
1:A:618:LYS:HG2	1:A:619:TRP:O	2.20	0.41
1:A:73:ASP:OD2	1:A:75:THR:OG1	2.26	0.41
1:A:767:LEU:HD23	1:A:768:PHE:CE2	2.55	0.41
1:A:18:GLN:HE22	1:A:21:LYS:HE2	1.86	0.41
1:A:605:PRO:O	1:A:617:LEU:HB2	2.20	0.41
1:A:591:MET:HE2	1:A:596:LEU:HD11	2.01	0.41
1:A:19:VAL:CG2	1:A:20:GLN:N	2.84	0.41
1:A:306:VAL:CG1	1:A:334:PHE:CE2	3.03	0.41
1:A:306:VAL:HG11	1:A:334:PHE:HE2	1.86	0.41
1:A:875:MET:HE1	1:A:890:PHE:HE2	1.85	0.41
1:A:295:LYS:CG	1:A:301:TYR:CE2	2.98	0.40
1:A:673:GLU:CD	1:A:849:ARG:HH12	2.24	0.40
1:A:111:ILE:CG1	1:A:112:TYR:H	2.35	0.40
1:A:686:TYR:HD2	1:A:845:ILE:HG13	1.85	0.40
1:A:686:TYR:HD2	1:A:845:ILE:CG1	2.33	0.40
1:A:300:MET:HE1	1:A:301:TYR:OH	2.21	0.40
1:A:302:MET:HE1	1:A:379:SER:HB3	2.03	0.40
1:A:435:VAL:O	1:A:438:CYS:SG	2.80	0.40
1:A:501:LYS:HG2	1:A:694:GLU:OE1	2.21	0.40
1:A:165:GLU:N	1:A:186:VAL:HG11	2.37	0.40
1:A:602:PHE:CE2	1:A:633:VAL:HG21	2.56	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	857/922 (93%)	822 (96%)	33 (4%)	2 (0%)	52 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	VAL
1	A	165	GLU

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	673/781 (86%)	661 (98%)	12 (2%)	66 90

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	TRP
1	A	275	THR
1	A	442	PHE
1	A	493	VAL
1	A	560	TYR
1	A	575	PHE
1	A	623	PHE
1	A	686	TYR
1	A	709	TRP

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Mol	Chain	Res	Type
1	A	782	PHE
1	A	871	PHE
1	A	890	PHE

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

Mol	Chain	Res	Type
1	A	18	GLN
1	A	208	ASN
1	A	223	ASN
1	A	547	ASN
1	A	556	HIS
1	A	608	GLN
1	A	892	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	62C	A	1001	-	25,25,25	0.49	1 (4%)	31,35,35	0.59	1 (3%)
2	62C	A	1002	-	25,25,25	0.33	0	31,35,35	0.32	0
3	BG6	A	1003	-	16,16,16	0.35	0	23,24,24	0.57	0
4	FLC	A	1004	-	3,12,12	0.53	0	3,17,17	2.12	1 (33%)

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	62C	A	1001	-	-	0/11/31/31	0/2/2/2
2	62C	A	1002	-	-	0/11/31/31	0/2/2/2
3	BG6	A	1003	-	-	0/6/26/26	0/1/1/1
4	FLC	A	1004	-	-	0/6/16/16	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	62C	O5-C1	-2.02	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	62C	C2-N7-C8	-2.05	118.83	122.13
4	A	1004	FLC	CB-CA-CAC	3.45	120.34	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	62C	1	0
2	A	1002	62C	1	0
4	A	1004	FLC	2	0

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	867/922 (94%)	0.49	55 (6%)	23	17	43, 63, 132, 161	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	LEU	5.6
1	A	95	VAL	5.3
1	A	151	GLY	5.3
1	A	83	LEU	4.9
1	A	89	ASN	4.8
1	A	169	VAL	4.8
1	A	81	LEU	4.6
1	A	125	GLN	4.6
1	A	137	PHE	4.6
1	A	152	PHE	4.6
1	A	80	PHE	4.4
1	A	82	ALA	4.3
1	A	135	ALA	4.2
1	A	86	GLY	4.2
1	A	154	PHE	4.2
1	A	92	VAL	4.1
1	A	150	LEU	4.1
1	A	129	HIS	3.9
1	A	124	THR	3.8
1	A	94	TRP	3.6
1	A	145	ASP	3.5
1	A	529	LEU	3.3
1	A	85	LEU	3.2
1	A	184	ASP	3.1
1	A	167	PHE	3.1
1	A	302	MET	3.0
1	A	148	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	450	GLY	2.9
1	A	84	ASP	2.9
1	A	686	TYR	2.8
1	A	111	ILE	2.8
1	A	374	ILE	2.8
1	A	186	VAL	2.7
1	A	394	LEU	2.6
1	A	203	ILE	2.6
1	A	449	SER	2.6
1	A	453	ALA	2.5
1	A	166	SER	2.5
1	A	185	VAL	2.4
1	A	257	ILE	2.4
1	A	324	LEU	2.4
1	A	187	ALA	2.4
1	A	301	TYR	2.3
1	A	448	GLY	2.3
1	A	416	VAL	2.3
1	A	673	GLU	2.2
1	A	319	LEU	2.1
1	A	136	ASN	2.1
1	A	139	ASP	2.1
1	A	228	LEU	2.1
1	A	440	VAL	2.1
1	A	598	LEU	2.0
1	A	543	VAL	2.0
1	A	555	MET	2.0
1	A	130	ILE	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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	62C	A	1002	24/24	0.91	0.32	2.99	57,73,119,128	0
3	BG6	A	1003	16/16	0.93	0.27	2.39	66,76,86,90	0
2	62C	A	1001	24/24	0.95	0.21	0.52	41,56,77,101	0
4	FLC	A	1004	13/13	0.91	0.17	-1.18	60,78,87,95	0

6.5 Other polymers (i)

There are no such residues in this entry.