Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2020 – 09:51 AM BST

PDB ID	:	5HFU
Title	:	Crystal Structure of Human Hexokinase 2 with cmpd 27, a 2-amido-6-benzen esulfonamide glucosamine
Authors	:	Campobasso, N.; Zhao, B.; Smallwood, A.
Deposited on	:	2016-01-07
Resolution	:	2.92 Å(reported)

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

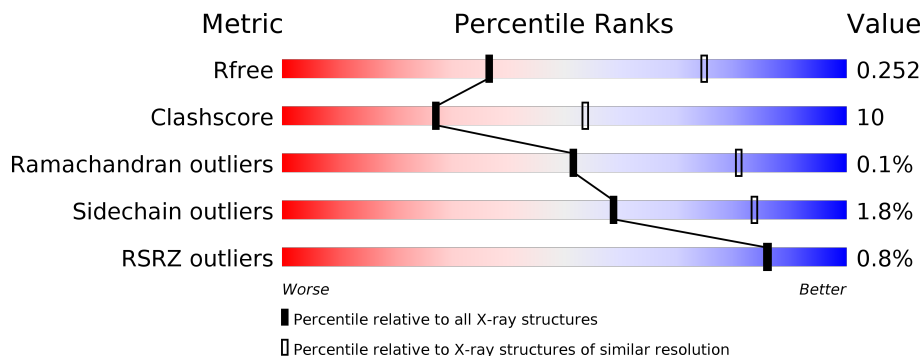|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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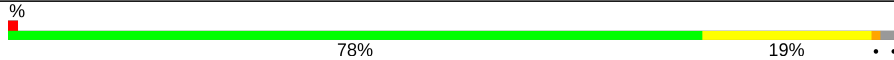*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.92 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 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	923	
1	B	923	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13964 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 Hexokinase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	895	Total 6872	C 4310	N 1207	O 1293	S 62	0	1	0
1	B	897	Total 6887	C 4321	N 1202	O 1302	S 62	0	0	0

There are 44 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
B	-5	MET	-	initiating methionine	UNP P52789
B	-4	GLY	-	expression tag	UNP P52789
B	-3	SER	-	expression tag	UNP P52789

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

- Molecule 2 is $\{N\}$-[(2 $\{S\}$,3 $\{R\}$,4 $\{R\}$,5 $\{S\}$,6 $\{R\}$)-6-[[(4-cyanophenyl)sulfonylamino]methyl]-2,4,5-tris(oxidanyl)oxan-3-yl]-3-phenyl-benzamide (three-letter code: 603) (formula: $C_{26}H_{25}N_3O_7S$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	37	26	3	7	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total C N O S	26	3	7	1	0	0
			37						
2	B	1	Total C N O S	26	3	7	1	0	0
			37						
2	B	1	Total C N O S	26	3	7	1	0	0
			37						

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total O	19	0	0
			19			
3	B	38	Total O	38	0	0
			38			

3 Residue-property plots ⓘ

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: Hexokinase-2

Chain A:

- Molecule 1: Hexokinase-2

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.88Å 154.99Å 114.20Å 90.00° 95.70° 90.00°	Depositor
Resolution (Å)	113.64 – 2.92 113.64 – 2.92	Depositor EDS
% Data completeness (in resolution range)	99.7 (113.64-2.92) 94.4 (113.64-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.86 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.182 , 0.252 0.183 , 0.252	Depositor DCC
R_{free} test set	2399 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	41.4	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.0	EDS
L-test for twinning[2]	$<|L|>=0.47$, $<L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13964	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 603

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	0.49	4/6984 (0.1%)	0.75	9/9410 (0.1%)
1	B	0.47	0/6996	0.67	2/9427 (0.0%)
All	All	0.48	4/13980 (0.0%)	0.71	11/18837 (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
1	B	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	502	GLU	CD-OE1	-7.15	1.17	1.25
1	A	494	GLU	CD-OE1	-6.09	1.19	1.25
1	A	494	GLU	CD-OE2	-5.83	1.19	1.25
1	A	502	GLU	CD-OE2	-5.13	1.20	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ARG	CG-CD-NE	6.65	125.77	111.80
1	A	142	GLN	CA-CB-CG	6.65	128.02	113.40
1	A	423	PHE	CB-CG-CD1	6.62	125.44	120.80
1	B	407	ARG	CG-CD-NE	-6.09	99.01	111.80
1	A	669	ASP	CB-CG-OD2	6.01	123.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	443	LEU	CA-CB-CG	5.88	128.81	115.30
1	A	163	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	750	LEU	CA-CB-CG	-5.40	102.89	115.30
1	A	307	ARG	CB-CG-CD	5.36	125.54	111.60
1	A	423	PHE	CB-CG-CD2	-5.25	117.13	120.80
1	A	451	LYS	CA-CB-CG	5.23	124.92	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	GLN	Peptide
1	A	150	LEU	Peptide
1	A	679	GLY	Peptide
1	B	154	PHE	Peptide
1	B	646	GLU	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	6872	0	6788	168	0
1	B	6887	0	6793	109	0
2	A	74	0	0	5	0
2	B	74	0	0	3	0
3	A	19	0	0	0	0
3	B	38	0	0	3	0
All	All	13964	0	13581	278	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 (278) 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:497:ARG:NH1	1:A:507:ALA:HA	1.67	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ARG:NH2	1:A:509:VAL:H	1.55	1.04
1:A:497:ARG:HH12	1:A:508:PRO:HD2	1.26	0.98
1:A:144:LYS:HZ1	1:A:198:ASP:HB2	1.31	0.92
1:A:497:ARG:HH12	1:A:508:PRO:CD	1.83	0.90
1:A:497:ARG:HH22	1:A:509:VAL:H	1.10	0.90
1:A:497:ARG:NH1	1:A:507:ALA:CA	2.40	0.85
1:A:686:TYR:HD2	1:A:841:VAL:HG13	1.46	0.81
1:B:673:GLU:OE1	1:B:849:ARG:NH2	2.14	0.77
1:A:683:ASN:HA	1:A:709:TRP:CD1	2.20	0.77
1:A:497:ARG:CZ	1:A:507:ALA:HB1	2.13	0.77
1:B:155:SER:HB3	2:B:1001:603:C7	2.16	0.76
1:A:793:ASP:O	1:A:820:LYS:NZ	2.17	0.75
1:B:688:GLU:OE2	1:B:848:ASN:ND2	2.23	0.71
1:A:307:ARG:NH1	1:A:331:THR:HA	2.06	0.70
1:B:663:MET:HG3	1:B:904:ILE:HG12	1.73	0.70
1:A:632:ASP:OD2	1:A:635:THR:HG23	1.91	0.70
1:B:524:GLU:OE2	1:B:910:ARG:NH1	2.24	0.70
1:A:96:LYS:HB3	1:A:106:GLU:HB3	1.71	0.70
1:A:497:ARG:NH1	1:A:508:PRO:HD2	2.03	0.69
1:A:686:TYR:CE1	1:A:688:GLU:HB2	2.27	0.69
1:A:141:LEU:O	1:A:142:GLN:HB3	1.92	0.69
1:A:83:LEU:HG	1:A:150:LEU:HD11	1.74	0.69
1:A:140:LYS:HG3	1:A:141:LEU:HD12	1.73	0.69
1:A:144:LYS:NZ	1:A:198:ASP:HB2	2.07	0.68
1:A:238:TYR:CD2	1:A:239:MET:O	2.47	0.68
1:A:327:GLU:OE1	1:A:333:ARG:NH2	2.27	0.68
1:A:238:TYR:CE2	1:A:240:GLU:HB2	2.30	0.68
1:A:686:TYR:HE1	1:A:688:GLU:HB2	1.58	0.68
1:A:238:TYR:HD2	1:A:239:MET:O	1.77	0.66
1:A:667:PHE:CZ	1:A:903:LEU:HD12	2.31	0.66
1:B:274:ARG:NH1	3:B:1102:HOH:O	2.28	0.65
1:A:687:MET:SD	1:A:704:CYS:HB2	2.37	0.65
1:A:497:ARG:HH12	1:A:507:ALA:HA	1.61	0.65
1:B:486:GLU:OE2	1:B:489:ARG:NH1	2.30	0.65
1:B:117:ASP:OD1	1:B:117:ASP:N	2.30	0.64
1:A:373:ARG:HH11	1:A:376:GLN:NE2	1.95	0.64
1:A:497:ARG:HH22	1:A:509:VAL:N	1.91	0.64
1:A:150:LEU:O	1:A:204:VAL:HA	1.98	0.63
1:B:431:VAL:HG11	1:B:442:PHE:HZ	1.64	0.63
1:A:180:VAL:O	1:A:183:ARG:HB3	2.00	0.62
1:A:515:TYR:CD1	1:A:703:MET:HE1	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:HG	1:B:138:MET:HE3	1.81	0.61
1:A:94:TRP:CH2	1:A:96:LYS:HB2	2.35	0.61
1:B:531:LEU:HB2	1:B:600:PHE:HB3	1.82	0.60
1:A:527:ASP:OD2	1:A:544:ARG:NH1	2.34	0.59
1:A:281:ILE:HD12	1:A:305:LEU:HD13	1.85	0.59
1:A:676:LEU:HD22	1:A:838:MET:HE3	1.84	0.59
1:B:663:MET:HE1	1:B:907:VAL:HG21	1.84	0.59
1:A:543:VAL:HG11	1:A:903:LEU:HD21	1.85	0.59
1:A:489:ARG:HA	1:A:492:LYS:HE2	1.84	0.58
1:B:658:THR:HG22	1:B:677:ILE:HD12	1.85	0.58
1:A:708:GLU:OE2	2:A:1002:603:N28	2.36	0.58
1:B:866:LYS:NZ	1:B:892:GLN:HB3	2.18	0.58
1:A:217:CYS:SG	1:A:445:SER:OG	2.48	0.58
1:A:115:PRO:HB2	1:A:117:ASP:OD1	2.04	0.58
1:A:82:ALA:HA	1:A:151:GLY:O	2.04	0.58
1:A:81:LEU:O	1:A:151:GLY:HA3	2.03	0.58
1:A:541:LEU:HD23	1:A:557:ASN:HB3	1.85	0.58
1:A:116:GLU:HA	1:A:119:MET:HB2	1.86	0.57
1:A:87:GLY:HA2	1:A:175:PHE:HZ	1.68	0.57
1:B:341:ASP:HB3	1:B:351:LYS:HD3	1.87	0.57
1:A:87:GLY:HA2	1:A:175:PHE:CZ	2.39	0.57
1:A:632:ASP:OD2	1:A:634:VAL:HG22	2.05	0.57
1:B:866:LYS:NZ	1:B:892:GLN:NE2	2.53	0.56
1:A:140:LYS:HD2	1:A:140:LYS:O	2.05	0.56
1:A:612:ASP:O	1:A:634:VAL:HG21	2.06	0.56
1:A:428:HIS:O	1:A:432:ARG:HG3	2.05	0.56
1:A:497:ARG:HH12	1:A:508:PRO:N	2.02	0.56
1:B:667:PHE:CE2	1:B:903:LEU:HD22	2.40	0.56
1:B:162:LYS:HB2	1:B:165:GLU:HB3	1.88	0.56
1:B:772:ILE:HG23	1:B:776:LEU:HD23	1.87	0.55
1:B:497:ARG:HG2	1:B:507:ALA:HB2	1.88	0.55
1:A:470:ARG:HB2	1:A:761:PHE:CZ	2.41	0.55
1:B:412:VAL:HG11	1:B:417:TYR:CD2	2.42	0.55
1:A:33:ASP:OD2	1:A:433:ARG:HD2	2.07	0.55
1:A:405:ARG:NH1	1:A:436:PRO:O	2.37	0.55
1:A:488:LYS:NZ	1:A:882:LEU:O	2.40	0.55
1:A:497:ARG:NH2	1:A:509:VAL:N	2.39	0.55
1:B:100:ASN:OD1	1:B:101:GLY:N	2.40	0.54
1:B:528:PHE:HD1	1:B:597:PRO:HG2	1.72	0.54
1:B:534:GLY:HA3	1:B:603:SER:HB2	1.89	0.54
1:A:307:ARG:HD2	1:A:328:LEU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASP:HB2	1:A:451:LYS:HE3	1.90	0.54
1:A:688:GLU:N	1:A:703:MET:O	2.39	0.54
1:B:83:LEU:HG	1:B:150:LEU:HD11	1.90	0.54
1:A:497:ARG:CZ	1:A:507:ALA:CB	2.84	0.54
1:A:271:ASN:ND2	1:A:274:ARG:HH11	2.05	0.53
1:A:619:TRP:CZ3	1:A:623:PHE:HD2	2.26	0.53
1:A:861:ASP:HB2	1:A:893:SER:OG	2.09	0.53
1:B:712:PHE:O	1:B:741:PHE:HB2	2.08	0.53
1:B:89:ASN:OD1	3:B:1101:HOH:O	2.19	0.53
1:A:610:SER:HB3	1:A:613:GLU:HB2	1.89	0.53
1:A:688:GLU:HG3	1:A:689:GLU:N	2.24	0.53
1:B:280:GLU:HB3	1:B:308:LEU:HD13	1.90	0.53
1:B:44:ARG:HA	1:B:47:MET:CE	2.39	0.53
1:A:294:GLU:OE2	2:A:1001:603:O36	2.25	0.53
1:A:218:GLY:HA2	1:A:221:ASP:O	2.10	0.52
1:B:530:ALA:HB2	1:B:902:ALA:HB2	1.92	0.52
1:A:62:LYS:HE3	2:A:1001:603:C8	2.39	0.52
1:A:673:GLU:OE2	1:A:849:ARG:NH2	2.42	0.52
1:A:423:PHE:CD1	1:A:423:PHE:C	2.83	0.52
1:B:601:THR:HG21	1:B:897:SER:HA	1.91	0.52
1:B:844:ARG:HH11	1:B:848:ASN:HD21	1.57	0.52
1:A:198:ASP:N	1:A:198:ASP:OD1	2.40	0.52
1:A:93:LEU:HD22	1:A:450:GLY:HA3	1.92	0.52
1:B:580:GLN:HG2	1:B:644:ARG:HH12	1.75	0.52
1:A:295:LYS:HA	1:A:301:TYR:CD2	2.45	0.51
1:A:25:TYR:OH	1:A:312:LYS:NZ	2.43	0.51
1:A:895:ASP:O	1:A:899:LYS:HB3	2.11	0.51
1:B:115:PRO:HG2	1:B:118:ILE:HD12	1.93	0.51
1:B:670:PRO:HG2	1:B:671:HIS:ND1	2.25	0.51
1:B:83:LEU:HD12	1:B:152:PHE:CE1	2.46	0.51
1:A:324:LEU:HD13	1:A:329:LEU:HD11	1.93	0.51
1:A:499:LEU:HD21	1:A:688:GLU:OE2	2.10	0.51
1:B:786:PHE:CE2	1:B:807:LEU:HD21	2.46	0.50
1:A:494:GLU:OE2	1:A:715:ASN:ND2	2.44	0.50
1:A:530:ALA:HB3	1:A:541:LEU:HB2	1.93	0.50
1:A:712:PHE:O	1:A:741:PHE:HB2	2.11	0.50
1:B:657:ASP:OD2	2:B:1002:603:O31	2.30	0.50
1:B:318:LEU:O	1:B:319:LEU:HD23	2.11	0.50
1:A:224:CYS:HA	1:A:409:THR:O	2.12	0.50
1:A:84:ASP:HA	1:A:153:THR:O	2.11	0.50
1:A:162:LYS:HB2	1:A:165:GLU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:HIS:CG	1:A:421:PRO:HD2	2.47	0.50
1:B:539:ARG:NH2	1:B:895:ASP:OD1	2.43	0.50
1:A:569:GLY:O	1:A:625:ALA:HA	2.12	0.49
1:A:497:ARG:HH11	1:A:507:ALA:HA	1.68	0.49
1:A:412:VAL:HG11	1:A:417:TYR:CD2	2.47	0.49
1:B:531:LEU:HB2	1:B:600:PHE:CB	2.42	0.49
1:B:664:THR:HG22	1:B:903:LEU:HD12	1.93	0.49
1:B:724:GLU:CD	1:B:724:GLU:H	2.14	0.49
1:B:295:LYS:HA	1:B:301:TYR:CD2	2.48	0.49
1:A:186:VAL:HA	1:A:189:ILE:HG22	1.94	0.49
1:B:695:LEU:HD12	3:B:1110:HOH:O	2.12	0.49
1:A:299:GLY:O	1:A:336:THR:OG1	2.28	0.48
1:A:678:VAL:CG1	1:A:865:TYR:HB2	2.44	0.48
1:B:682:SER:H	1:B:742:GLU:HG2	1.77	0.48
1:B:240:GLU:HG3	1:B:241:GLU:N	2.29	0.48
1:B:669:ASP:OD1	1:B:670:PRO:HD2	2.13	0.48
1:B:866:LYS:HZ1	1:B:892:GLN:NE2	2.11	0.48
1:A:520:PRO:HD3	1:A:663:MET:SD	2.53	0.48
1:B:144:LYS:HE2	1:B:198:ASP:OD1	2.13	0.48
1:A:90:PHE:CE2	1:A:130:ILE:HG12	2.48	0.48
1:A:63:MET:SD	1:A:259:MET:HG2	2.54	0.48
1:A:271:ASN:HD22	1:A:274:ARG:HD3	1.78	0.48
1:A:620:THR:HG22	1:A:621:LYS:N	2.29	0.48
1:B:763:LYS:HG3	1:B:772:ILE:HD11	1.95	0.48
1:B:191:LYS:HA	1:B:194:GLN:HG2	1.95	0.47
1:B:373:ARG:O	1:B:377:ILE:HG12	2.14	0.47
1:A:528:PHE:CD2	1:A:597:PRO:HG2	2.48	0.47
1:A:530:ALA:HB2	1:A:902:ALA:HB2	1.96	0.47
1:A:264:PHE:CD2	1:A:270:LEU:HD11	2.49	0.47
1:A:112:TYR:OH	1:A:137:PHE:HB2	2.14	0.47
1:B:243:ARG:HA	1:B:251:ASP:OD1	2.15	0.47
1:A:154:PHE:CE2	1:A:185:VAL:HG11	2.50	0.47
1:B:323:LYS:NZ	1:B:361:LEU:HA	2.29	0.47
1:B:570:THR:HA	1:B:626:SER:HB2	1.96	0.47
1:A:323:LYS:HA	1:A:323:LYS:HD3	1.58	0.47
1:A:497:ARG:HH21	1:A:509:VAL:HB	1.79	0.47
1:B:270:LEU:HD23	1:B:270:LEU:HA	1.72	0.47
1:B:483:GLN:O	1:B:487:VAL:HG23	2.15	0.46
1:B:532:ASP:O	1:B:538:PHE:HB2	2.15	0.46
1:B:691:ARG:HB3	1:B:699:GLU:HB3	1.96	0.46
1:A:417:TYR:C	1:A:417:TYR:CD1	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:VAL:O	1:A:638:LYS:HG2	2.15	0.46
1:A:390:LEU:HD12	1:A:427:LEU:HD21	1.97	0.46
1:B:854:LEU:HD12	1:B:855:LYS:H	1.78	0.46
1:A:447:ASP:OD2	1:A:451:LYS:HE3	2.15	0.46
1:B:470:ARG:HG2	1:B:761:PHE:CE2	2.51	0.46
1:A:524:GLU:O	1:A:547:ASN:HB3	2.16	0.46
1:B:44:ARG:HA	1:B:47:MET:HE3	1.97	0.46
1:B:528:PHE:CD1	1:B:597:PRO:HG2	2.51	0.46
1:B:678:VAL:HG12	1:B:864:LEU:HD23	1.97	0.46
2:B:1001:603:C13	2:B:1001:603:C26	2.94	0.46
1:B:441:ARG:NH1	1:B:443:LEU:HD13	2.31	0.46
1:B:480:SER:OG	1:B:483:GLN:HG3	2.15	0.46
1:A:495:MET:CE	1:A:686:TYR:HE2	2.29	0.45
1:A:687:MET:HA	1:A:704:CYS:HA	1.97	0.45
1:B:115:PRO:HB2	1:B:117:ASP:OD1	2.16	0.45
1:B:406:LEU:HB3	1:B:438:CYS:SG	2.56	0.45
1:A:497:ARG:O	1:A:503:THR:OG1	2.25	0.45
1:B:293:PHE:O	1:B:297:ILE:HG12	2.17	0.45
1:A:644:ARG:HG2	1:A:647:PHE:HB2	1.98	0.45
1:A:667:PHE:CE2	1:A:903:LEU:HD12	2.52	0.45
1:A:720:ASP:N	1:A:720:ASP:OD1	2.46	0.45
1:B:264:PHE:O	1:B:293:PHE:HB2	2.17	0.45
1:B:327:GLU:HB2	1:B:359:LEU:O	2.17	0.45
1:A:447:ASP:HB2	1:A:451:LYS:CE	2.46	0.45
1:A:750:LEU:HD23	1:A:753:ILE:HD12	1.99	0.44
1:B:323:LYS:C	1:B:323:LYS:HD3	2.37	0.44
1:B:534:GLY:O	1:B:621:LYS:HE3	2.17	0.44
1:A:349:ILE:HG21	1:A:369:VAL:HG12	1.97	0.44
1:A:541:LEU:CD2	1:A:557:ASN:HB3	2.47	0.44
1:B:84:ASP:HA	1:B:153:THR:HG23	2.00	0.44
1:A:497:ARG:NH1	1:A:507:ALA:CB	2.80	0.44
1:A:90:PHE:HE2	1:A:130:ILE:HG12	1.83	0.44
1:A:527:ASP:OD1	1:A:544:ARG:HG3	2.17	0.44
1:A:708:GLU:OE2	2:A:1002:603:C22	2.66	0.44
1:A:490:ARG:NH1	1:A:717:CYS:O	2.48	0.44
1:B:156:PHE:HZ	1:B:175:PHE:CE1	2.36	0.44
1:B:167:PHE:HA	1:B:183:ARG:O	2.17	0.44
1:B:785:LYS:O	1:B:789:GLN:HG3	2.17	0.44
1:A:750:LEU:HD23	1:A:750:LEU:HA	1.60	0.43
1:B:366:GLU:H	1:B:366:GLU:CD	2.21	0.43
1:B:663:MET:HE1	1:B:907:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:VAL:HB	1:A:858:VAL:HG22	1.99	0.43
1:B:866:LYS:HZ1	1:B:892:GLN:HB3	1.82	0.43
1:B:854:LEU:HD12	1:B:855:LYS:N	2.34	0.43
1:A:117:ASP:OD1	1:A:118:ILE:HD12	2.18	0.43
1:A:495:MET:HE1	1:A:686:TYR:HE2	1.83	0.43
1:A:373:ARG:HH11	1:A:376:GLN:HE21	1.67	0.43
1:A:485:LEU:HA	1:A:485:LEU:HD23	1.88	0.43
1:A:846:ARG:HE	1:A:852:ASP:HA	1.83	0.43
1:A:849:ARG:HB3	1:A:851:LEU:HD13	2.01	0.43
1:B:278:ASP:OD1	1:B:296:MET:HG2	2.18	0.43
1:B:600:PHE:N	1:B:600:PHE:CD1	2.87	0.43
1:A:519:THR:OG1	1:A:520:PRO:HD2	2.18	0.42
1:A:423:PHE:C	1:A:423:PHE:HD1	2.21	0.42
1:B:678:VAL:O	1:B:862:GLY:HA3	2.19	0.42
1:A:115:PRO:HD2	1:A:118:ILE:CD1	2.49	0.42
1:A:305:LEU:HD21	1:A:381:ARG:NH2	2.35	0.42
1:B:80:PHE:CE2	1:B:458:ALA:HA	2.53	0.42
1:A:680:THR:HG23	2:A:1002:603:O32	2.18	0.42
1:A:641:ILE:HG23	1:A:647:PHE:HD2	1.84	0.42
1:B:652:VAL:HG23	1:B:653:ALA:N	2.35	0.42
1:B:793:ASP:O	1:B:820:LYS:HE3	2.20	0.42
1:A:680:THR:HA	1:A:747:GLY:HA2	2.02	0.42
1:B:612:ASP:HB3	1:B:652:VAL:O	2.19	0.42
1:A:153:THR:HG23	1:A:153:THR:O	2.19	0.42
1:A:121:GLY:O	1:A:177:SER:HA	2.20	0.42
1:A:669:ASP:OD1	1:A:857:THR:OG1	2.31	0.42
1:B:243:ARG:HB3	1:B:796:ALA:HB2	2.01	0.42
1:A:44:ARG:HA	1:A:47:MET:CE	2.49	0.42
1:A:274:ARG:HG2	1:A:296:MET:SD	2.60	0.41
1:A:903:LEU:HD13	1:A:903:LEU:HA	1.81	0.41
1:A:728:ALA:O	1:A:732:LEU:HD12	2.21	0.41
1:A:873:LYS:O	1:A:876:HIS:N	2.53	0.41
1:B:136:ASN:OD1	1:B:140:LYS:HE3	2.20	0.41
1:B:338:ASP:OD1	1:B:358:ARG:NH1	2.52	0.41
1:B:804:LEU:HD23	1:B:804:LEU:HA	1.88	0.41
1:A:226:ILE:HB	1:A:410:ILE:HG12	2.02	0.41
1:B:18:GLN:O	1:B:22:VAL:HG13	2.20	0.41
1:A:276:GLU:OE2	1:A:312:LYS:HE3	2.20	0.41
1:B:634:VAL:O	1:B:638:LYS:HG3	2.21	0.41
1:A:56:HIS:N	1:A:57:PRO:HD2	2.35	0.41
1:A:87:GLY:C	1:A:89:ASN:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ASP:OD1	1:A:118:ILE:N	2.47	0.41
1:A:683:ASN:HA	1:A:709:TRP:NE1	2.35	0.41
1:A:112:TYR:N	1:A:112:TYR:CD1	2.88	0.41
1:A:312:LYS:O	1:A:316:GLU:HG3	2.20	0.41
1:B:786:PHE:O	1:B:790:ILE:HG13	2.20	0.41
1:B:96:LYS:HB3	1:B:106:GLU:HB2	2.03	0.41
1:A:137:PHE:O	1:A:141:LEU:HB2	2.20	0.41
1:B:390:LEU:HD12	1:B:427:LEU:HD11	2.02	0.41
1:B:597:PRO:HA	1:B:650:ASP:O	2.21	0.41
1:B:688:GLU:HG3	1:B:689:GLU:N	2.36	0.41
1:B:32:SER:O	1:B:36:LEU:HG	2.21	0.41
1:B:228:LEU:HB3	1:B:412:VAL:HG22	2.03	0.41
1:B:838:MET:O	1:B:842:VAL:HG22	2.21	0.41
1:A:570:THR:HG22	1:A:573:GLU:CD	2.40	0.41
1:A:572:ASP:N	1:A:572:ASP:OD2	2.54	0.41
1:B:95:VAL:HG13	1:B:105:VAL:HG13	2.03	0.41
1:B:339:ILE:HG23	1:B:375:CYS:HB3	2.02	0.41
1:B:207:VAL:HG11	1:B:456:VAL:HG21	2.02	0.40
1:A:211:VAL:O	1:A:215:MET:HG2	2.21	0.40
1:A:33:ASP:OD1	1:A:433:ARG:NH1	2.55	0.40
1:B:92:VAL:HG12	1:B:137:PHE:CD2	2.57	0.40
1:B:497:ARG:HD3	1:B:507:ALA:HA	2.03	0.40
1:A:108:GLU:HB3	1:A:141:LEU:HD21	2.02	0.40
1:A:168:LEU:HB3	1:A:181:GLU:HA	2.02	0.40
1:A:572:ASP:HB3	1:A:643:ARG:HH12	1.85	0.40
1:A:874:VAL:HA	1:A:877:GLU:OE2	2.21	0.40
1:B:530:ALA:HA	1:B:599:GLY:O	2.21	0.40
1:A:678:VAL:O	1:A:678:VAL:HG13	2.21	0.40
1:A:772:ILE:HG23	1:A:776:LEU:HD23	2.02	0.40
1:A:207:VAL:HG21	1:A:456:VAL:HG21	2.04	0.40
1:A:510:LYS:HB2	1:A:512:LEU:HG	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	894/923 (97%)	875 (98%)	18 (2%)	1 (0%)	51	81
1	B	895/923 (97%)	881 (98%)	14 (2%)	0	100	100
All	All	1789/1846 (97%)	1756 (98%)	32 (2%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	897	SER

5.3.2　Protein sidechains ⓘ

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	729/782 (93%)	715 (98%)	14 (2%)	57	83
1	B	732/782 (94%)	720 (98%)	12 (2%)	62	85
All	All	1461/1564 (93%)	1435 (98%)	26 (2%)	59	83

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	PHE
1	A	112	TYR
1	A	261	TRP
1	A	307	ARG
1	A	334	PHE
1	A	417	TYR
1	A	423	PHE
1	A	497	ARG
1	A	572	ASP
1	A	686	TYR
1	A	709	TRP
1	A	748	MET

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Mol	Chain	Res	Type
1	A	843	ASP
1	A	871	PHE
1	B	22	VAL
1	B	90	PHE
1	B	152	PHE
1	B	166	SER
1	B	220	ASP
1	B	261	TRP
1	B	334	PHE
1	B	408	SER
1	B	441	ARG
1	B	546	ARG
1	B	600	PHE
1	B	709	TRP

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	271	ASN
1	A	376	GLN
1	A	608	GLN
1	A	739	GLN
1	A	892	GLN
1	B	608	GLN
1	B	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 monosaccharides 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	603	A	1002	-	40,40,40	1.43	4 (10%)	57,57,57	1.53	9 (15%)
2	603	B	1002	-	40,40,40	1.33	1 (2%)	57,57,57	1.63	12 (21%)
2	603	A	1001	-	40,40,40	1.34	2 (5%)	57,57,57	1.42	10 (17%)
2	603	B	1001	-	40,40,40	1.45	2 (5%)	57,57,57	2.11	13 (22%)

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	603	A	1002	-	-	6/26/46/46	0/4/4/4
2	603	B	1002	-	-	7/26/46/46	0/4/4/4
2	603	A	1001	-	-	3/26/46/46	0/4/4/4
2	603	B	1001	-	-	7/26/46/46	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	603	S37-N29	7.06	1.72	1.61
2	A	1002	603	S37-N29	6.90	1.72	1.61
2	A	1001	603	S37-N29	6.56	1.71	1.61
2	B	1002	603	S37-N29	6.37	1.71	1.61
2	A	1002	603	O31-S37	2.14	1.46	1.43
2	A	1002	603	O32-S37	2.11	1.45	1.43
2	A	1002	603	C17-C16	-2.10	1.43	1.49
2	B	1001	603	C18-C20	-2.00	1.46	1.50
2	A	1001	603	C18-C20	-2.00	1.46	1.50

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1001	603	O33-C25-C21	7.68	117.23	109.52
2	B	1001	603	C26-C24-C23	-6.04	101.60	113.54
2	A	1002	603	C19-S37-N29	-4.76	100.95	107.55
2	A	1002	603	C26-C24-C23	-4.66	104.33	113.54
2	B	1001	603	O31-S37-N29	4.52	114.10	107.04
2	B	1002	603	C19-S37-N29	-4.51	101.29	107.55
2	A	1001	603	C19-S37-N29	-4.00	102.01	107.55
2	B	1002	603	C24-C26-N29	-3.59	105.30	112.51
2	B	1002	603	C25-O33-C24	-3.47	107.11	113.66
2	B	1002	603	O31-S37-C19	-3.45	103.71	107.97
2	B	1001	603	O34-C22-C23	-3.45	102.37	110.35
2	B	1002	603	O32-S37-C19	3.42	112.19	107.97
2	B	1001	603	O30-C20-N28	3.29	128.50	122.45
2	A	1001	603	C23-C22-C21	-3.22	105.63	110.34
2	B	1001	603	C14-C17-C16	-3.19	115.59	120.86
2	A	1001	603	O33-C25-C21	3.15	112.68	109.52
2	A	1001	603	C24-C26-N29	-3.13	106.23	112.51
2	B	1001	603	O31-S37-C19	-3.09	104.17	107.97
2	A	1002	603	O31-S37-C19	-3.03	104.24	107.97
2	A	1001	603	C26-C24-C23	-2.89	107.84	113.54
2	B	1002	603	C26-C24-C23	-2.80	108.01	113.54
2	B	1001	603	C2-C4-C9	-2.78	115.95	120.19
2	B	1001	603	C3-C8-C16	-2.76	117.09	120.56
2	B	1002	603	O30-C20-N28	2.74	127.50	122.45
2	A	1002	603	O31-S37-N29	2.65	111.18	107.04
2	A	1002	603	O34-C22-C23	-2.57	104.42	110.35
2	B	1002	603	O31-S37-N29	2.54	111.01	107.04
2	A	1002	603	O32-S37-O31	2.52	122.64	119.55
2	B	1001	603	C9-C16-C17	-2.51	117.01	121.36
2	A	1001	603	C21-N28-C20	-2.42	118.58	122.39
2	A	1001	603	C11-C18-C14	2.30	121.95	119.24
2	A	1002	603	C13-C19-S37	-2.26	117.31	119.77
2	B	1002	603	C13-C19-S37	-2.26	117.31	119.77
2	A	1002	603	O35-C23-C22	-2.23	105.19	110.35
2	B	1002	603	C14-C17-C16	-2.21	117.20	120.86
2	B	1002	603	C18-C20-N28	-2.18	112.88	117.06
2	A	1002	603	C6-C12-C19	-2.14	117.23	119.45
2	B	1001	603	C11-C18-C14	2.13	121.76	119.24
2	A	1001	603	O32-S37-O31	2.11	122.14	119.55
2	A	1001	603	C26-N29-S37	-2.11	115.85	120.02
2	B	1001	603	C10-C17-C16	2.09	124.98	121.36
2	A	1001	603	C5-C11-C18	-2.07	117.89	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	603	C18-C20-N28	-2.04	113.15	117.06
2	B	1002	603	C25-C21-N28	2.01	113.06	110.73

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1002	603	O33-C24-C26-N29
2	B	1002	603	C23-C24-C26-N29
2	B	1002	603	O33-C24-C26-N29
2	A	1001	603	C23-C24-C26-N29
2	A	1001	603	O33-C24-C26-N29
2	B	1002	603	C8-C16-C17-C10
2	B	1002	603	C8-C16-C17-C14
2	B	1002	603	C9-C16-C17-C14
2	B	1002	603	C9-C16-C17-C10
2	A	1002	603	C11-C18-C20-O30
2	A	1002	603	C11-C18-C20-N28
2	A	1002	603	C14-C18-C20-O30
2	A	1002	603	C14-C18-C20-N28
2	B	1001	603	C18-C20-N28-C21
2	A	1002	603	C23-C24-C26-N29
2	B	1001	603	O30-C20-N28-C21
2	A	1001	603	C22-C21-N28-C20
2	B	1002	603	C26-N29-S37-O31
2	B	1001	603	C26-N29-S37-O31
2	B	1001	603	C12-C19-S37-O31
2	B	1001	603	C11-C18-C20-O30
2	B	1001	603	C13-C19-S37-O31
2	B	1001	603	C14-C18-C20-O30

There are no ring outliers.
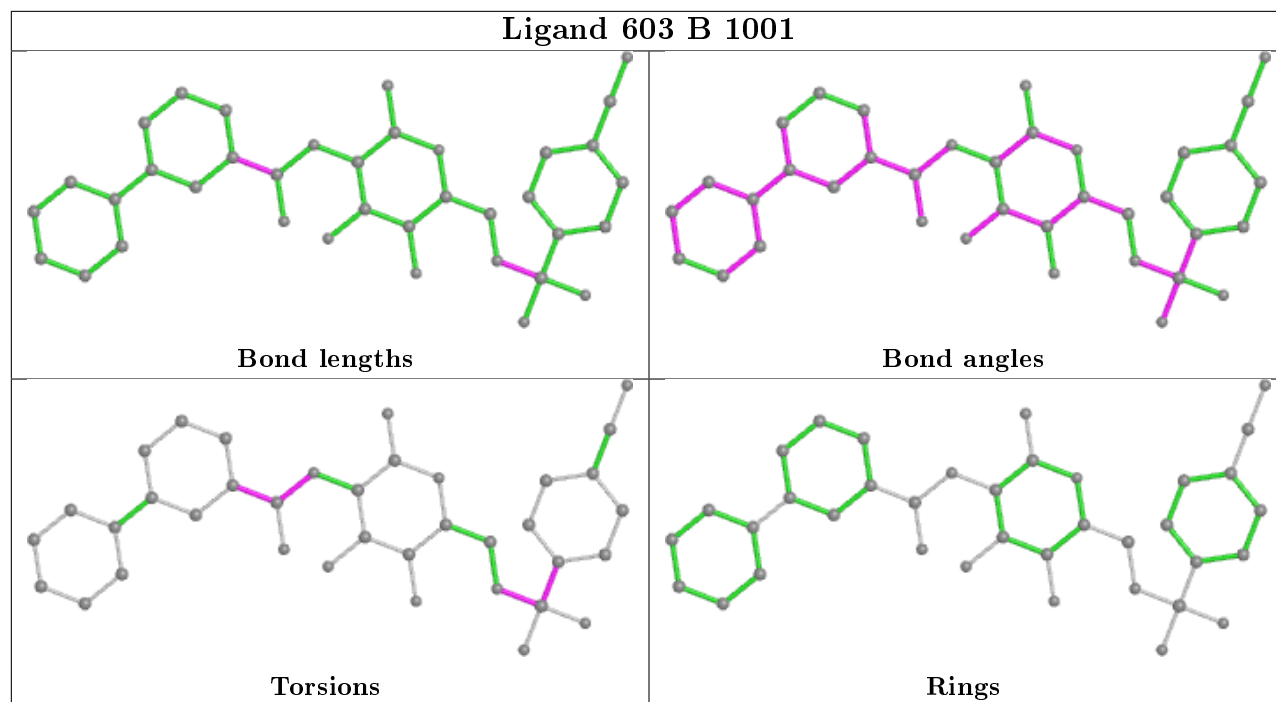
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	603	3	0
2	B	1002	603	1	0
2	A	1001	603	2	0
2	B	1001	603	2	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 603 A 1002

Bond lengths

Bond angles

Torsions

Rings

Ligand 603 B 1002

Bond lengths

Bond angles

Torsions

Rings

Ligand 603 A 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand 603 B 1001

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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(Å²)	Q<0.9
1	A	895/923 (96%)	0.08	7 (0%)	86	86	23, 48, 75, 98	0
1	B	897/923 (97%)	-0.03	7 (0%)	86	86	21, 38, 68, 92	0
All	All	1792/1846 (97%)	0.02	14 (0%)	86	86	21, 43, 72, 98	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	GLY	3.6
1	B	87	GLY	3.2
1	A	172	THR	3.1
1	A	447	ASP	3.1
1	B	550	TRP	2.9
1	A	86	GLY	2.9
1	B	155	SER	2.6
1	A	171	TRP	2.6
1	B	627	GLY	2.5
1	A	854	LEU	2.4
1	B	549	LYS	2.4
1	A	90	PHE	2.3
1	B	172	THR	2.2
1	B	154	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.
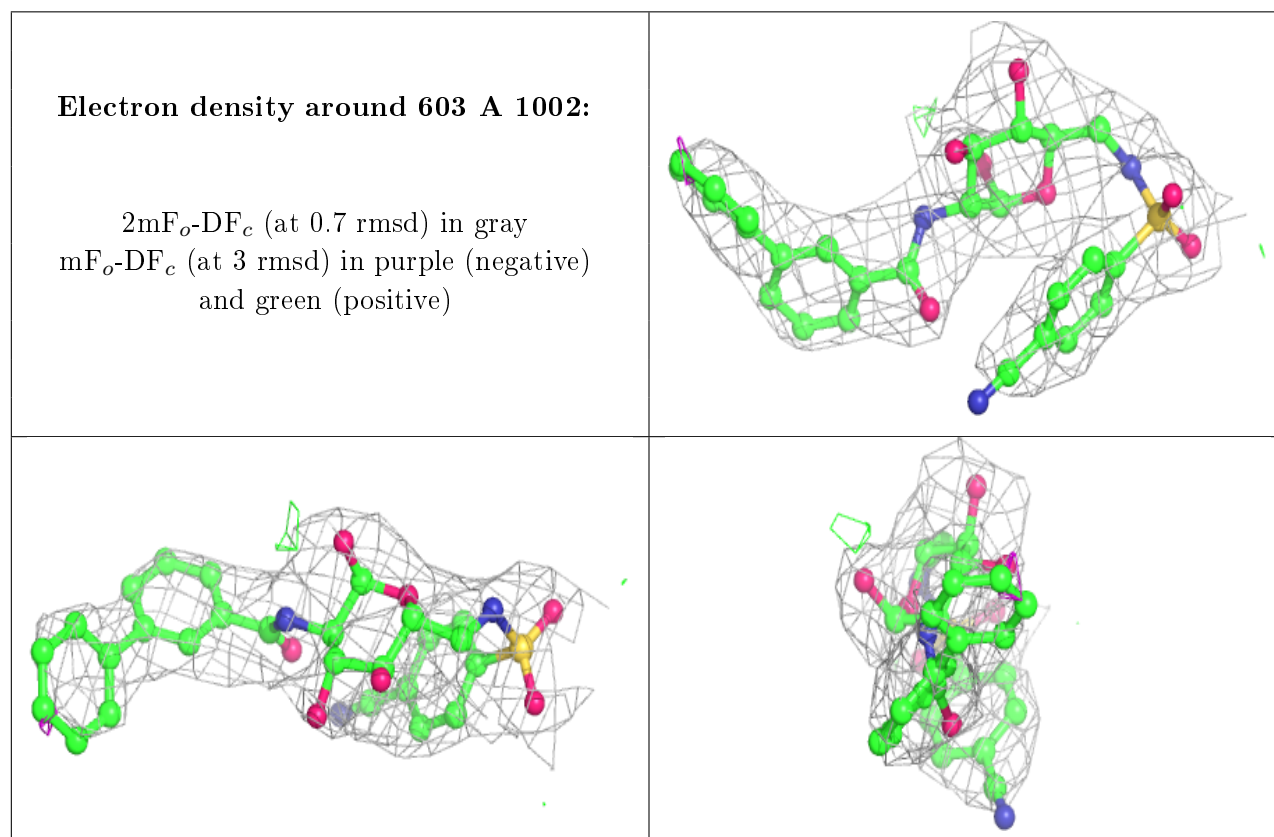
6.3 Carbohydrates (i)

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.
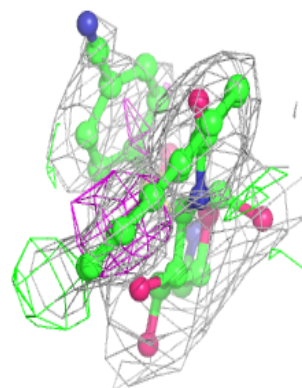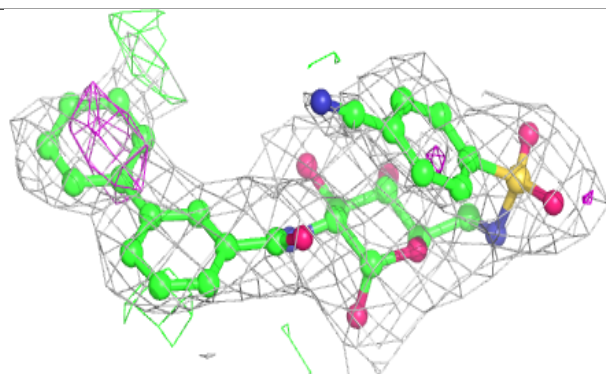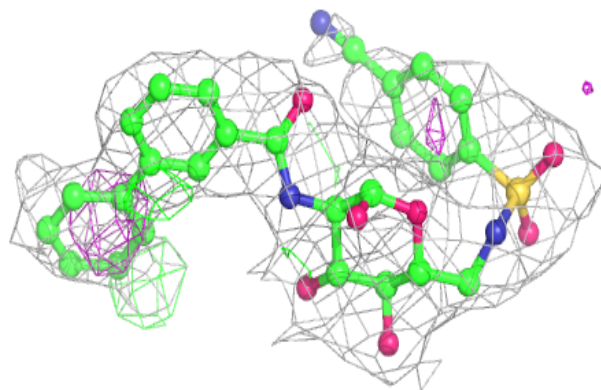
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	603	A	1002	37/37	0.93	0.23	46,54,70,76	0
2	603	A	1001	37/37	0.93	0.23	28,41,53,54	0
2	603	B	1001	37/37	0.94	0.21	32,42,57,60	0
2	603	B	1002	37/37	0.96	0.22	32,43,54,59	0

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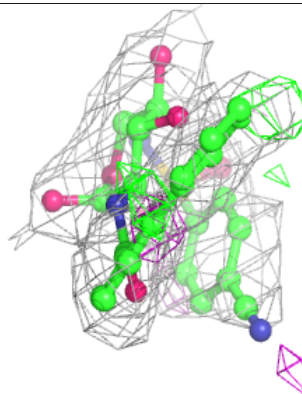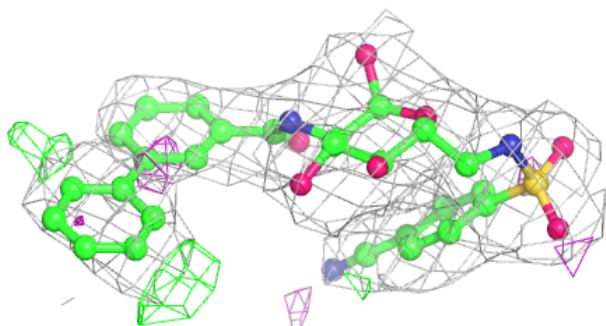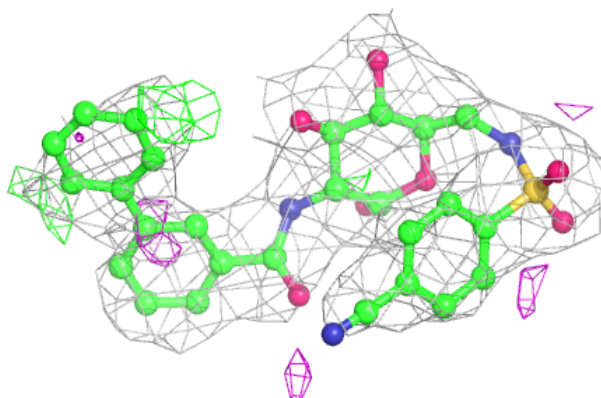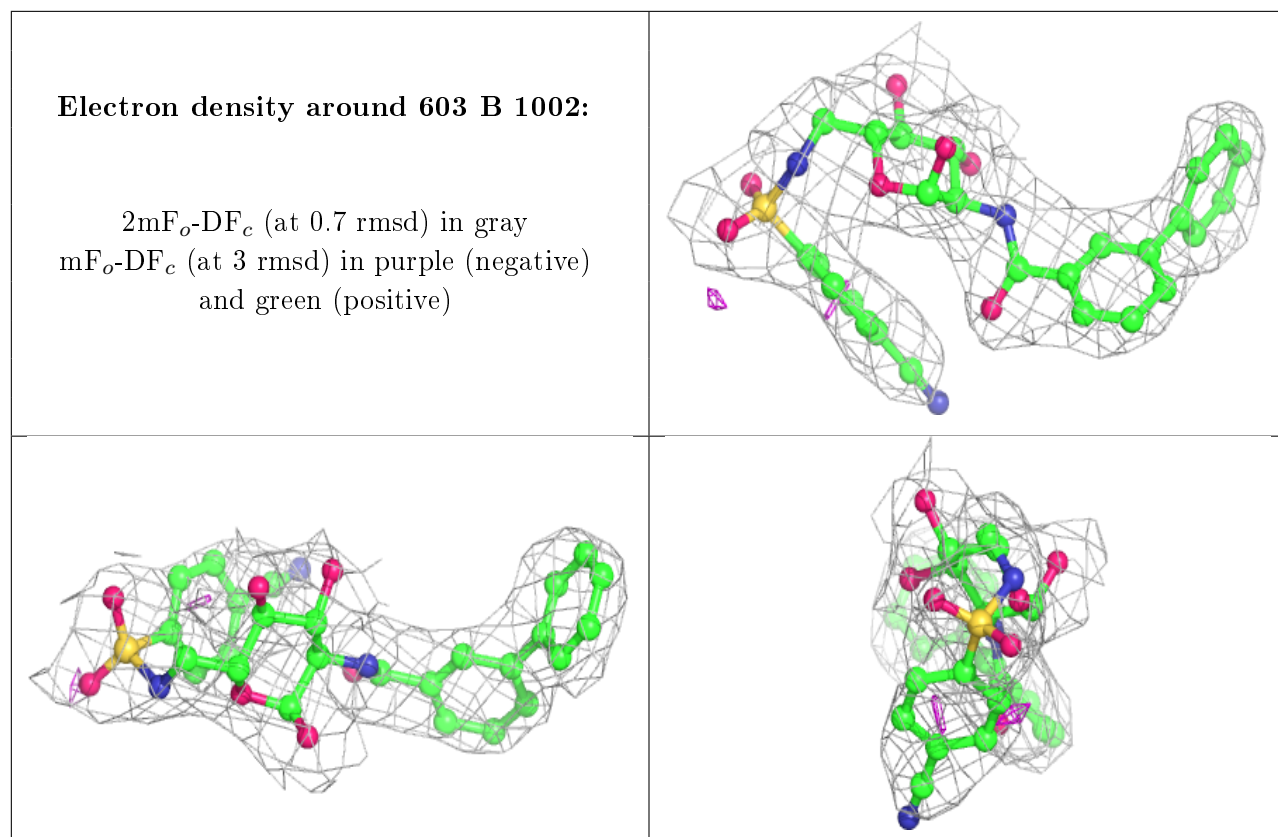

Electron density around 603 A 1002:

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

Electron density around 603 A 1001:

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 603 B 1001:

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 603 B 1002:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.