Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:01 am BST

PDB ID	:	4AY6
Title	:	Human O-GlcNAc transferase (OGT) in complex with UDP-5SGlcNAc and substrate peptide
Authors	:	Schimpl, M.; Zheng, X.; Blair, D.E.; Schuettelkopf, A.W.; Navratilova, I.; Aristotelous, T.; Ferenbach, A.T.; Macnaughtan, M.A.; Borodkin, V.S.; van Aalten, D.M.F.
Deposited on	:	2012-06-18
Resolution	:	3.30 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 ⓘ symbol.

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

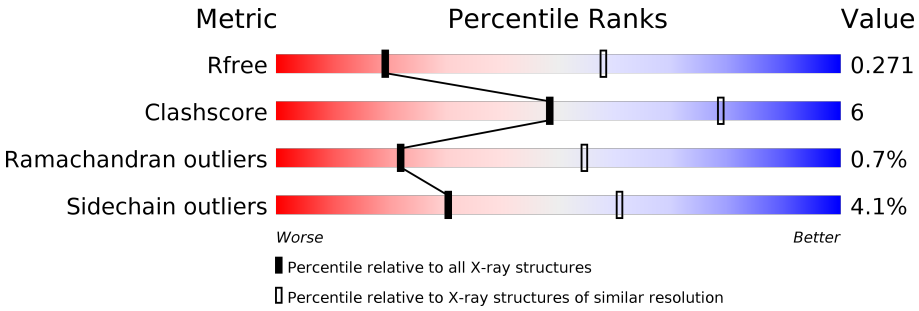
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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%

Mol	Chain	Length	Quality of chain
1	A	723	80% 15% • •
1	B	723	81% 14% • •
1	C	723	83% 12% • •
1	D	723	81% 14% • •
2	E	13	46% 31% 8% 15%
2	F	13	46% 31% 8% 15%
2	G	13	46% 31% 8% 15%

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Mol	Chain	Length	Quality of chain
2	H	13	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22544 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 UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYL GLUCOSAMINYLTRANS FERASE 110 KDA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	698	Total	C	N	O	S	0	0	0
			5514	3499	964	1013	38			
1	B	698	Total	C	N	O	S	0	0	0
			5514	3499	964	1013	38			
1	C	698	Total	C	N	O	S	0	0	0
			5514	3499	964	1013	38			
1	D	698	Total	C	N	O	S	0	0	0
			5514	3499	964	1013	38			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	GLY	-	expression tag	UNP O15294
A	310	PRO	-	expression tag	UNP O15294
A	311	GLY	-	expression tag	UNP O15294
A	312	SER	-	expression tag	UNP O15294
B	309	GLY	-	expression tag	UNP O15294
B	310	PRO	-	expression tag	UNP O15294
B	311	GLY	-	expression tag	UNP O15294
B	312	SER	-	expression tag	UNP O15294
C	309	GLY	-	expression tag	UNP O15294
C	310	PRO	-	expression tag	UNP O15294
C	311	GLY	-	expression tag	UNP O15294
C	312	SER	-	expression tag	UNP O15294
D	309	GLY	-	expression tag	UNP O15294
D	310	PRO	-	expression tag	UNP O15294
D	311	GLY	-	expression tag	UNP O15294
D	312	SER	-	expression tag	UNP O15294

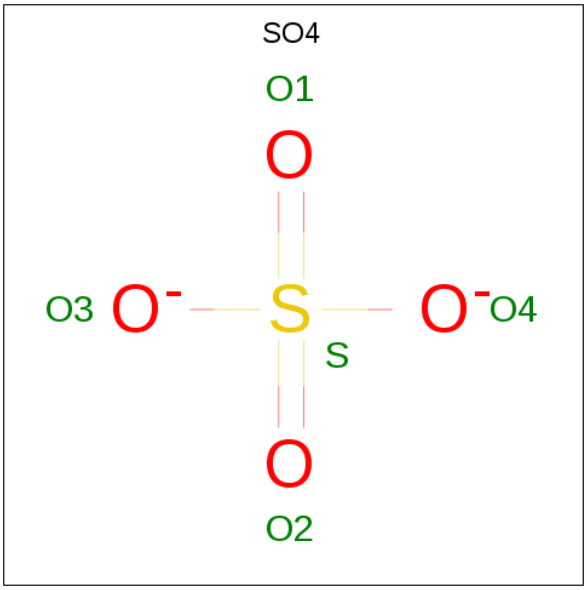
- Molecule 2 is a protein called TGF-BETA-ACTIVATED KINASE 1 AND MAP3K7-BINDING PROTEIN 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	0	0	0
			78	49	13	16			
2	F	11	Total	C	N	O	0	0	0
			78	49	13	16			
2	G	11	Total	C	N	O	0	0	0
			78	49	13	16			
2	H	11	Total	C	N	O	0	0	0
			78	49	13	16			

There are 4 discrepancies between the modelled and reference sequences:

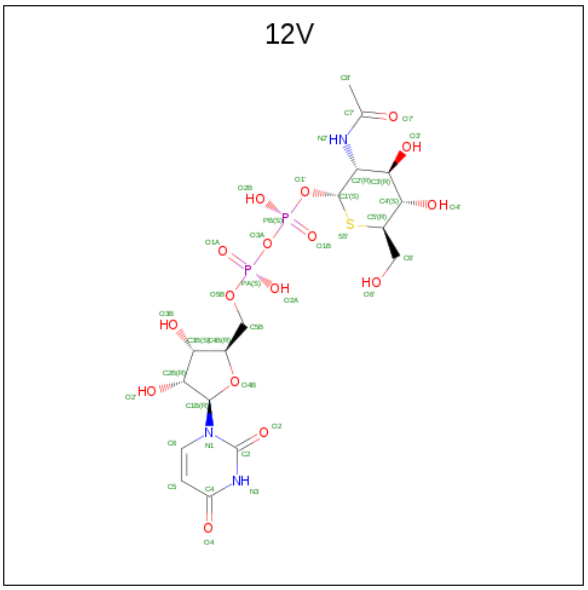
Chain	Residue	Modelled	Actual	Comment	Reference
E	1395	DNP	SER	SEE REMARK 999	UNP Q15750
F	1395	DNP	SER	SEE REMARK 999	UNP Q15750
G	1395	DNP	SER	SEE REMARK 999	UNP Q15750
H	1395	DNP	SER	SEE REMARK 999	UNP Q15750

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is (2S,3R,4R,5S,6R)-3-(acetylamino)-4,5-dihydroxy-6-(hydroxymethyl)tetrahydro-2H-thiopyran-2-yl [(2R,3S,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl dihydrogen diphosphate (three-letter code: 12V) (formula: $C_{17}H_{27}N_3O_{16}P_2S$).



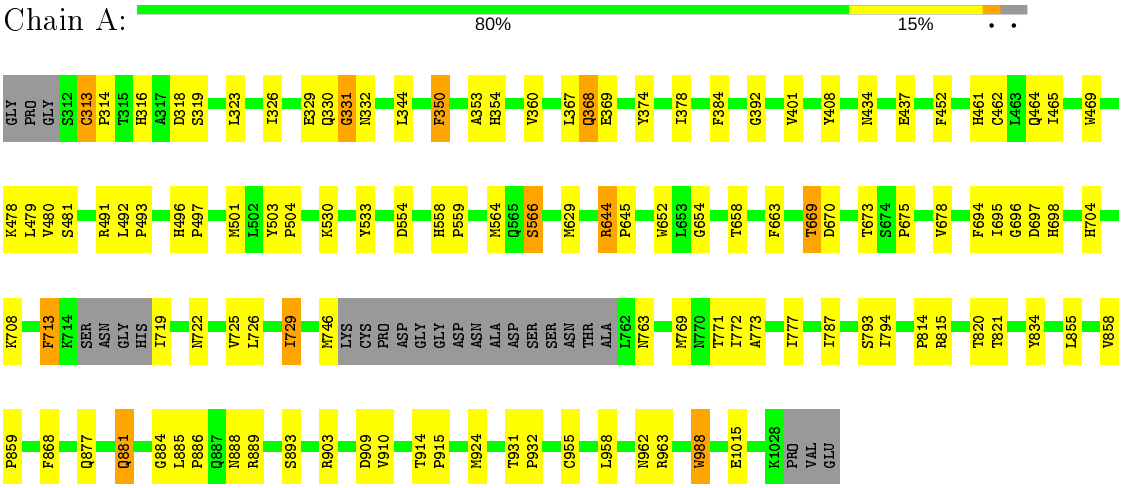
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
4	B	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
4	C	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
4	D	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

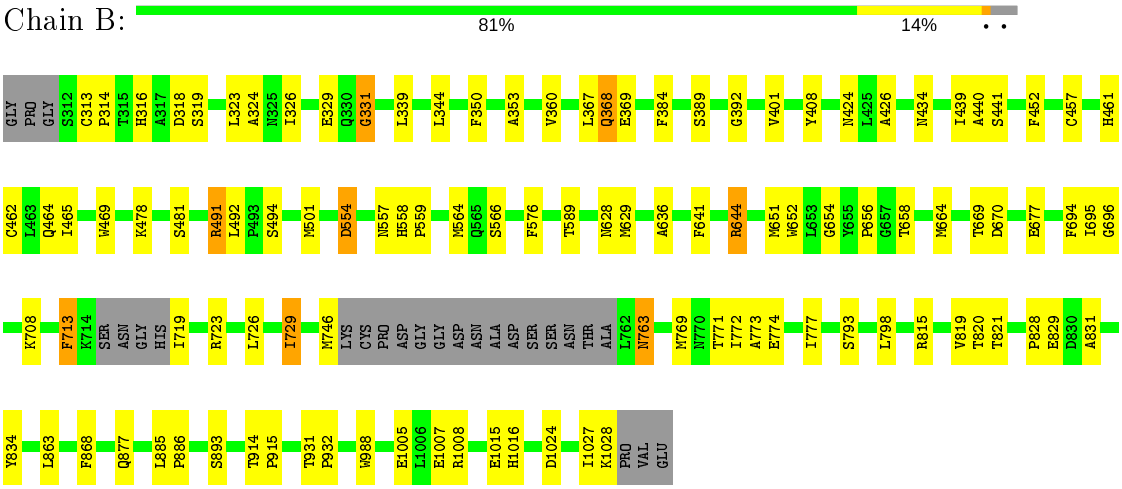
• Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYLTRANS FERASE 110 KDA SUBUNIT

Chain A:



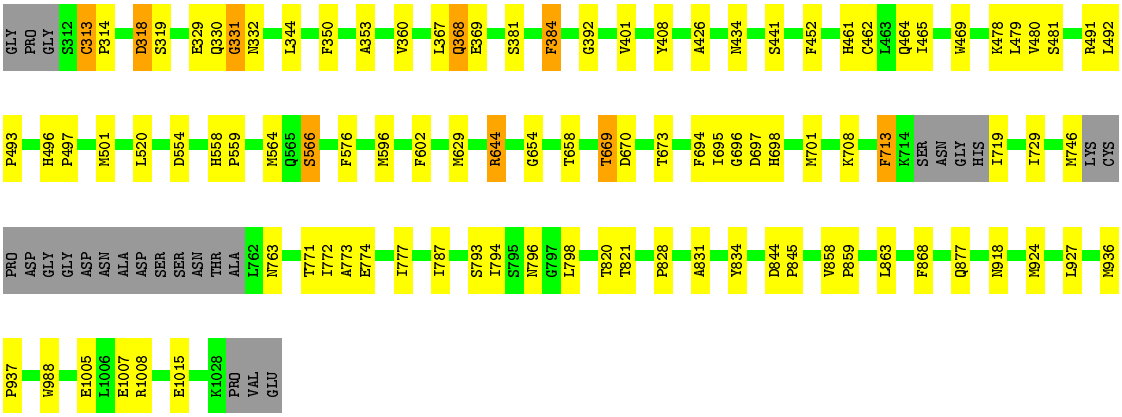
• Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYLTRANS FERASE 110 KDA SUBUNIT

Chain B:



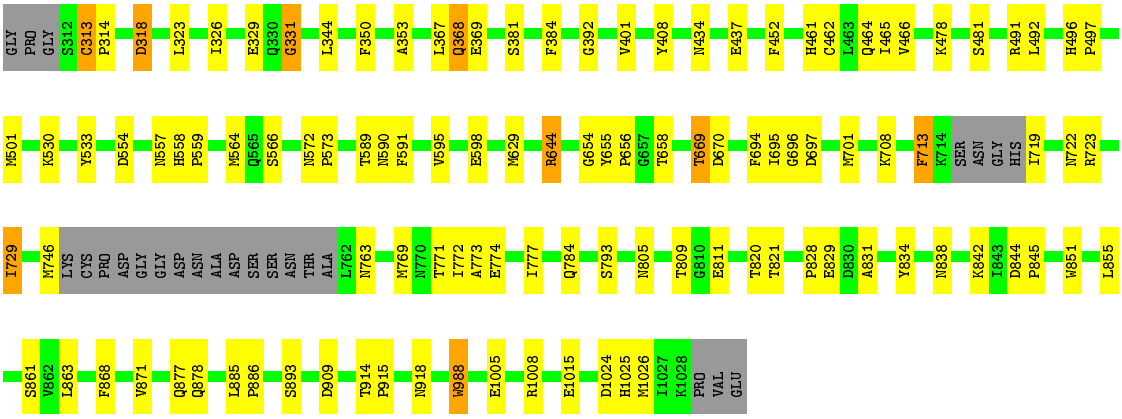
• Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYLTRANS FERASE 110 KDA SUBUNIT

Chain C:



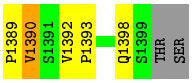
• Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYLTRANS FERASE 110 KDA SUBUNIT

Chain D:



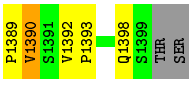
• Molecule 2: TGF-BETA-ACTIVATED KINASE 1 AND MAP3K7-BINDING PROTEIN 1

Chain E:



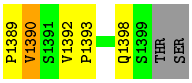
• Molecule 2: TGF-BETA-ACTIVATED KINASE 1 AND MAP3K7-BINDING PROTEIN 1

Chain F:



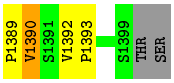
• Molecule 2: TGF-BETA-ACTIVATED KINASE 1 AND MAP3K7-BINDING PROTEIN 1

Chain G:



• Molecule 2: TGF-BETA-ACTIVATED KINASE 1 AND MAP3K7-BINDING PROTEIN 1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	275.44Å 275.44Å 142.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.30 25.01 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (40.00-3.30) 98.5 (25.01-3.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 3.30Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.227 , 0.272 0.226 , 0.271	Depositor DCC
R_{free} test set	435 reflections (0.48%)	wwPDB-VP
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , -2.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.237 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	22544	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 12V, DNP

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	0.62	3/5641 (0.1%)	0.66	1/7650 (0.0%)
1	B	0.61	2/5641 (0.0%)	0.67	0/7650
1	C	0.60	1/5641 (0.0%)	0.67	0/7650
1	D	0.57	2/5641 (0.0%)	0.63	0/7650
2	E	0.53	0/73	0.76	0/98
2	F	0.61	0/73	0.72	0/98
2	G	0.52	0/73	0.71	0/98
2	H	0.52	0/73	0.71	0/98
All	All	0.60	8/22856 (0.0%)	0.66	1/30992 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	988	TRP	CD2-CE2	5.75	1.48	1.41
1	D	988	TRP	CD2-CE2	5.70	1.48	1.41
1	B	469	TRP	CD2-CE2	5.33	1.47	1.41
1	C	469	TRP	CD2-CE2	5.29	1.47	1.41
1	A	469	TRP	CD2-CE2	5.17	1.47	1.41
1	D	851	TRP	CD2-CE2	5.14	1.47	1.41
1	A	652	TRP	CD2-CE2	5.10	1.47	1.41
1	B	652	TRP	CD2-CE2	5.09	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	903	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

There are no planarity outliers.

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	5514	0	5489	71	0
1	B	5514	0	5489	68	0
1	C	5514	0	5489	58	0
1	D	5514	0	5489	60	0
2	E	78	0	76	4	0
2	F	78	0	76	6	0
2	G	78	0	76	5	0
2	H	78	0	76	3	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
4	A	39	0	25	1	0
4	B	39	0	25	2	0
4	C	39	0	25	2	0
4	D	39	0	25	1	0
All	All	22544	0	22360	267	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 6.

All (267) 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:D:644:ARG:HH11	1:D:644:ARG:HG3	1.25	1.00
1:B:644:ARG:HG3	1:B:644:ARG:HH11	1.24	0.99
1:B:644:ARG:CG	1:B:644:ARG:HH11	1.77	0.98
1:D:644:ARG:HH11	1:D:644:ARG:CG	1.80	0.94
1:A:644:ARG:HH11	1:A:644:ARG:HG3	1.33	0.91
1:C:644:ARG:HH11	1:C:644:ARG:HG3	1.37	0.89
1:A:644:ARG:CG	1:A:644:ARG:HH11	1.91	0.84
1:B:644:ARG:NH1	1:B:644:ARG:HG3	1.93	0.82
1:C:644:ARG:HH11	1:C:644:ARG:CG	1.92	0.82
1:A:859:PRO:HB2	1:B:1016:HIS:CE1	2.16	0.81
1:B:629:MET:O	1:B:654:GLY:HA3	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:GLN:CG	1:A:369:GLU:H	1.95	0.79
1:D:644:ARG:NH1	1:D:644:ARG:HG3	1.93	0.76
1:B:368:GLN:CG	1:B:369:GLU:H	1.99	0.76
1:D:368:GLN:CG	1:D:369:GLU:H	1.99	0.75
1:C:629:MET:O	1:C:654:GLY:HA3	1.88	0.72
1:B:491:ARG:HH11	1:B:492:LEU:H	1.38	0.71
1:A:368:GLN:HG3	1:A:369:GLU:H	1.56	0.70
1:C:669:THR:OG1	1:C:670:ASP:N	2.25	0.70
1:A:881:GLN:HG2	1:B:677:GLU:HA	1.74	0.69
1:D:368:GLN:HG3	1:D:369:GLU:H	1.56	0.69
1:A:644:ARG:HG3	1:A:644:ARG:NH1	2.04	0.69
1:C:368:GLN:CG	1:C:369:GLU:H	2.05	0.68
1:B:368:GLN:HG3	1:B:369:GLU:H	1.57	0.68
1:A:491:ARG:HH11	1:A:492:LEU:H	1.41	0.67
1:C:491:ARG:HH11	1:C:492:LEU:H	1.42	0.65
1:C:392:GLY:HA3	1:C:408:TYR:CE1	2.32	0.65
1:D:491:ARG:HH11	1:D:492:LEU:H	1.43	0.65
1:D:629:MET:O	1:D:654:GLY:HA3	1.97	0.64
1:A:669:THR:OG1	1:A:670:ASP:N	2.30	0.64
1:A:462:CYS:HA	1:A:465:ILE:HD12	1.79	0.64
1:C:644:ARG:NH1	1:C:644:ARG:HG3	2.09	0.64
1:A:722:ASN:ND2	1:A:909:ASP:OD1	2.26	0.64
1:D:722:ASN:ND2	1:D:909:ASP:OD1	2.28	0.64
1:A:368:GLN:CG	1:A:369:GLU:N	2.61	0.62
1:B:392:GLY:HA3	1:B:408:TYR:CE1	2.35	0.61
1:D:559:PRO:HB2	4:D:1200:12V:H6'	1.83	0.61
1:D:368:GLN:CG	1:D:369:GLU:N	2.63	0.61
1:B:1028:LYS:O	1:B:1028:LYS:HG3	2.01	0.60
1:A:344:LEU:HD21	1:A:353:ALA:HB3	1.82	0.60
1:A:877:GLN:OE1	1:A:877:GLN:HA	2.01	0.60
1:B:368:GLN:CG	1:B:369:GLU:N	2.64	0.60
1:B:462:CYS:HA	1:B:465:ILE:HD12	1.83	0.59
1:B:576:PHE:CE1	1:B:1007:GLU:HG2	2.37	0.59
1:D:368:GLN:HG3	1:D:369:GLU:N	2.16	0.59
1:B:478:LYS:O	1:B:481:SER:HB3	2.02	0.59
1:B:491:ARG:NH1	1:B:492:LEU:H	2.02	0.58
1:C:877:GLN:HA	1:C:877:GLN:OE1	2.02	0.58
1:A:859:PRO:O	1:B:1024:ASP:OD2	2.22	0.58
1:C:368:GLN:CG	1:C:369:GLU:N	2.66	0.58
1:D:669:THR:OG1	1:D:670:ASP:N	2.37	0.58
1:C:461:HIS:O	1:C:465:ILE:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:462:CYS:HA	1:D:465:ILE:HD12	1.87	0.57
1:D:491:ARG:NH1	1:D:492:LEU:H	2.02	0.57
1:A:478:LYS:O	1:A:481:SER:HB3	2.05	0.57
1:C:491:ARG:NH1	1:C:492:LEU:H	2.03	0.57
2:F:1392:VAL:HG12	2:F:1393:PRO:HD2	1.88	0.56
1:B:368:GLN:HG3	1:B:369:GLU:N	2.20	0.56
1:A:368:GLN:HG3	1:A:369:GLU:N	2.19	0.56
1:D:877:GLN:OE1	1:D:877:GLN:HA	2.06	0.56
1:A:491:ARG:NH1	1:A:492:LEU:H	2.04	0.56
2:G:1389:PRO:O	2:G:1390:VAL:O	2.23	0.55
2:F:1389:PRO:O	2:F:1390:VAL:O	2.24	0.55
1:C:368:GLN:HG3	1:C:369:GLU:H	1.72	0.55
1:B:554:ASP:HB3	1:B:558:HIS:CG	2.41	0.55
1:B:877:GLN:OE1	1:B:877:GLN:HA	2.07	0.54
1:C:559:PRO:HB2	4:C:1200:12V:H6'	1.90	0.54
1:C:344:LEU:HD21	1:C:353:ALA:HB3	1.89	0.54
1:D:392:GLY:HA3	1:D:408:TYR:CE1	2.42	0.54
2:H:1389:PRO:O	2:H:1390:VAL:O	2.25	0.54
2:E:1392:VAL:HG12	2:E:1393:PRO:HD2	1.90	0.54
1:B:344:LEU:HD21	1:B:353:ALA:HB3	1.89	0.54
1:A:392:GLY:HA3	1:A:408:TYR:CE1	2.43	0.54
1:B:651:MET:HG2	1:B:664:MET:HE2	1.89	0.54
1:D:461:HIS:O	1:D:464:GLN:HB3	2.08	0.53
1:A:773:ALA:O	1:A:777:ILE:HG22	2.08	0.53
1:B:461:HIS:O	1:B:465:ILE:HG13	2.08	0.53
1:A:644:ARG:CG	1:A:644:ARG:NH1	2.61	0.53
1:A:629:MET:O	1:A:654:GLY:HA3	2.08	0.52
1:B:772:ILE:HG22	1:B:773:ALA:N	2.23	0.52
4:B:1200:12V:O2	2:F:1392:VAL:HG11	2.09	0.52
1:B:461:HIS:O	1:B:464:GLN:HB3	2.10	0.52
1:D:772:ILE:HG22	1:D:773:ALA:N	2.25	0.52
1:A:559:PRO:HB2	4:A:1200:12V:H6'	1.91	0.52
2:H:1392:VAL:HG12	2:H:1393:PRO:HD2	1.91	0.52
1:B:708:LYS:HG2	1:B:988:TRP:CH2	2.45	0.52
1:B:828:PRO:HG2	1:B:831:ALA:CB	2.39	0.51
1:A:881:GLN:CG	1:B:677:GLU:HA	2.40	0.51
1:C:1015:GLU:OE1	1:C:1015:GLU:HA	2.10	0.51
2:E:1389:PRO:O	2:E:1390:VAL:O	2.28	0.51
1:B:669:THR:OG1	1:B:670:ASP:N	2.43	0.51
1:C:368:GLN:HG3	1:C:369:GLU:N	2.26	0.51
2:F:1392:VAL:CG1	2:F:1393:PRO:HD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1392:VAL:CG1	2:H:1393:PRO:HD2	2.42	0.50
1:D:344:LEU:HD21	1:D:353:ALA:HB3	1.94	0.50
1:B:329:GLU:C	1:B:331:GLY:H	2.15	0.50
1:B:557:ASN:HB2	1:B:589:THR:HG21	1.93	0.50
1:D:695:ILE:HG13	1:D:696:GLY:N	2.27	0.49
1:C:478:LYS:O	1:C:481:SER:HB3	2.12	0.49
1:C:576:PHE:CE1	1:C:1007:GLU:HG2	2.47	0.49
1:A:461:HIS:O	1:A:465:ILE:HG13	2.12	0.49
1:D:530:LYS:HE2	1:D:533:TYR:OH	2.12	0.49
1:A:884:GLY:O	1:B:1027:ILE:HD12	2.12	0.49
1:B:367:LEU:O	1:B:368:GLN:C	2.51	0.49
1:A:719:ILE:HG22	1:A:719:ILE:O	2.13	0.49
1:D:708:LYS:HG2	1:D:988:TRP:CH2	2.47	0.49
1:B:457:CYS:SG	1:B:494:SER:HB2	2.53	0.49
1:D:723:ARG:NE	1:D:829:GLU:O	2.45	0.49
1:C:772:ILE:HG22	1:C:773:ALA:N	2.29	0.48
2:E:1392:VAL:CG1	2:E:1393:PRO:HD2	2.43	0.48
1:B:636:ALA:HB3	2:F:1398:GLN:NE2	2.29	0.48
1:D:466:VAL:HG12	1:D:871:VAL:HG23	1.95	0.48
1:D:496:HIS:CG	1:D:497:PRO:HD2	2.49	0.48
1:B:636:ALA:HB3	2:F:1398:GLN:HE22	1.78	0.48
1:A:329:GLU:C	1:A:331:GLY:H	2.17	0.48
1:D:367:LEU:O	1:D:368:GLN:C	2.52	0.48
1:D:557:ASN:HB2	1:D:589:THR:HG21	1.94	0.48
1:C:330:GLN:O	1:C:332:ASN:N	2.47	0.48
1:D:1015:GLU:OE1	1:D:1015:GLU:HA	2.13	0.48
1:D:478:LYS:O	1:D:481:SER:HB3	2.14	0.48
1:D:554:ASP:HB3	1:D:558:HIS:CG	2.49	0.48
2:G:1392:VAL:HG12	2:G:1393:PRO:HD2	1.94	0.48
1:C:368:GLN:HG2	1:C:369:GLU:H	1.77	0.48
1:C:461:HIS:O	1:C:464:GLN:HB3	2.14	0.47
1:C:462:CYS:HA	1:C:465:ILE:HD12	1.95	0.47
1:D:655:TYR:HA	1:D:656:PRO:HD3	1.77	0.47
1:D:855:LEU:HD23	1:D:861:SER:OG	2.15	0.47
4:C:1200:12V:O2	2:G:1392:VAL:HG11	2.14	0.47
1:A:368:GLN:HG2	1:A:369:GLU:H	1.76	0.47
1:C:698:HIS:CE1	1:C:924:MET:HB3	2.49	0.47
1:D:773:ALA:O	1:D:777:ILE:HG22	2.14	0.47
1:A:1015:GLU:OE1	1:A:1015:GLU:HA	2.14	0.47
1:C:697:ASP:HB3	1:C:701:MET:HG3	1.96	0.47
1:D:564:MET:SD	1:D:564:MET:C	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:708:LYS:HG2	1:C:988:TRP:CH2	2.50	0.47
1:C:719:ILE:HG22	1:C:719:ILE:O	2.15	0.47
1:C:844:ASP:HB2	1:C:845:PRO:HD2	1.96	0.47
1:D:774:GLU:HA	1:D:777:ILE:HG22	1.96	0.47
1:C:834:TYR:O	1:C:863:LEU:HD12	2.15	0.47
1:B:1005:GLU:OE1	1:B:1005:GLU:HA	2.14	0.46
1:A:713:PHE:HD1	1:A:713:PHE:H	1.62	0.46
1:B:313:CYS:SG	1:B:316:HIS:HB2	2.55	0.46
1:B:559:PRO:HB2	4:B:1200:12V:H6'	1.97	0.46
1:B:723:ARG:NE	1:B:829:GLU:O	2.48	0.46
1:B:576:PHE:CZ	1:B:1007:GLU:HG2	2.50	0.46
1:D:461:HIS:O	1:D:465:ILE:HG13	2.15	0.46
1:B:644:ARG:HH11	1:B:644:ARG:HG2	1.73	0.46
1:C:554:ASP:HB3	1:C:558:HIS:CG	2.51	0.46
1:A:772:ILE:HG22	1:A:773:ALA:N	2.30	0.46
1:B:389:SER:OG	1:B:424:ASN:ND2	2.48	0.46
1:A:374:TYR:O	1:A:378:ILE:HG12	2.16	0.46
1:C:496:HIS:CG	1:C:497:PRO:HD2	2.51	0.46
1:C:367:LEU:O	1:C:368:GLN:C	2.54	0.45
1:A:704:HIS:NE2	1:A:814:PRO:HG2	2.30	0.45
1:C:695:ILE:HG13	1:C:696:GLY:N	2.32	0.45
1:D:914:THR:HA	1:D:915:PRO:HD3	1.83	0.45
1:A:725:VAL:HG12	1:A:726:LEU:N	2.30	0.45
1:B:729:ILE:HD13	1:B:729:ILE:HA	1.82	0.45
1:D:590:ASN:ND2	1:D:811:GLU:HB3	2.31	0.45
1:A:344:LEU:CD2	1:A:353:ALA:HB3	2.47	0.45
1:A:695:ILE:HG13	1:A:696:GLY:N	2.32	0.45
1:B:323:LEU:O	1:B:326:ILE:HB	2.17	0.45
1:A:491:ARG:HD2	1:A:491:ARG:HA	1.73	0.45
1:B:695:ILE:HG13	1:B:696:GLY:N	2.31	0.45
1:C:566:SER:HB2	1:C:697:ASP:OD1	2.17	0.45
1:D:591:PHE:O	1:D:595:VAL:HG23	2.18	0.45
1:A:313:CYS:HA	1:A:314:PRO:HD2	1.85	0.44
1:A:885:LEU:HA	1:A:886:PRO:HD2	1.84	0.44
1:C:461:HIS:CE1	1:C:465:ILE:HD11	2.52	0.44
1:B:324:ALA:HB2	1:B:339:LEU:HB2	1.99	0.44
1:B:885:LEU:HA	1:B:886:PRO:HD2	1.86	0.44
1:D:1024:ASP:CG	1:D:1025:HIS:H	2.21	0.44
1:C:774:GLU:HA	1:C:777:ILE:HG22	1.98	0.44
1:D:834:TYR:O	1:D:863:LEU:HD12	2.18	0.44
1:B:644:ARG:CG	1:B:644:ARG:NH1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:PRO:O	1:C:318:ASP:HB2	2.17	0.44
1:A:815:ARG:CZ	1:D:598:GLU:HG2	2.48	0.44
1:D:885:LEU:HA	1:D:886:PRO:HD2	1.85	0.44
1:C:329:GLU:C	1:C:331:GLY:H	2.21	0.43
1:D:844:ASP:HB2	1:D:845:PRO:HD2	2.00	0.43
1:A:855:LEU:O	1:A:889:ARG:NH2	2.46	0.43
1:D:314:PRO:O	1:D:318:ASP:HB2	2.18	0.43
1:D:746:MET:HG3	1:D:763:ASN:HA	2.00	0.43
1:A:492:LEU:HA	1:A:493:PRO:HD3	1.86	0.43
1:A:914:THR:HA	1:A:915:PRO:HD3	1.79	0.43
3:A:1100:SO4:O1	2:E:1398:GLN:HG3	2.17	0.43
1:C:713:PHE:HD1	1:C:713:PHE:H	1.65	0.43
1:A:496:HIS:CG	1:A:497:PRO:HD2	2.54	0.43
1:A:787:ILE:HG13	1:A:794:ILE:HB	1.99	0.43
1:B:713:PHE:H	1:B:713:PHE:HD1	1.65	0.43
1:D:1005:GLU:OE1	1:D:1008:ARG:HD3	2.18	0.43
3:C:1100:SO4:O1	2:G:1398:GLN:HG3	2.18	0.43
1:A:367:LEU:O	1:A:368:GLN:C	2.56	0.43
1:B:914:THR:HA	1:B:915:PRO:HD3	1.80	0.43
1:A:962:ASN:O	1:A:963:ARG:C	2.55	0.43
1:D:491:ARG:HD2	1:D:491:ARG:HA	1.72	0.43
1:D:784:GLN:HB2	1:D:784:GLN:HE21	1.64	0.43
1:A:644:ARG:N	1:A:645:PRO:HD3	2.33	0.43
1:B:439:ILE:O	1:B:440:ALA:C	2.55	0.43
1:B:457:CYS:SG	1:B:494:SER:CB	3.07	0.43
1:B:1005:GLU:OE1	1:B:1008:ARG:HD3	2.19	0.43
1:B:564:MET:SD	1:B:564:MET:C	2.97	0.43
1:A:330:GLN:O	1:A:332:ASN:N	2.51	0.43
1:A:313:CYS:SG	1:A:316:HIS:HB2	2.59	0.42
1:C:313:CYS:HA	1:C:314:PRO:HD2	1.82	0.42
1:B:815:ARG:NH1	1:B:815:ARG:HG3	2.34	0.42
1:D:918:ASN:HD22	1:D:918:ASN:N	2.16	0.42
1:B:726:LEU:CD2	1:B:819:VAL:HG22	2.49	0.42
1:D:713:PHE:HD1	1:D:713:PHE:H	1.68	0.42
1:D:329:GLU:C	1:D:331:GLY:H	2.21	0.42
1:A:746:MET:HG3	1:A:763:ASN:HA	2.01	0.42
1:B:368:GLN:HG2	1:B:369:GLU:H	1.82	0.42
1:B:628:ASN:HB2	1:B:641:PHE:CZ	2.55	0.42
1:A:461:HIS:O	1:A:464:GLN:HB3	2.20	0.42
1:B:726:LEU:HD22	1:B:819:VAL:HG22	2.02	0.42
1:B:774:GLU:HA	1:B:777:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:931:THR:HA	1:B:932:PRO:HD3	1.89	0.42
1:D:313:CYS:HA	1:D:314:PRO:HD2	1.86	0.42
1:D:323:LEU:O	1:D:326:ILE:HB	2.19	0.42
1:D:828:PRO:HG2	1:D:831:ALA:CB	2.50	0.42
1:A:955:CYS:HB3	1:A:958:LEU:HD12	2.02	0.42
2:G:1392:VAL:CG1	2:G:1393:PRO:HD2	2.50	0.42
1:A:530:LYS:HE2	1:A:533:TYR:OH	2.19	0.41
1:A:564:MET:SD	1:A:564:MET:C	2.98	0.41
1:A:858:VAL:HA	1:A:859:PRO:HD3	1.92	0.41
1:B:746:MET:HG3	1:B:763:ASN:HA	2.02	0.41
1:A:675:PRO:O	1:A:678:VAL:HG22	2.20	0.41
1:C:479:LEU:O	1:C:480:VAL:C	2.58	0.41
1:C:596:MET:HG2	1:C:602:PHE:CG	2.55	0.41
1:C:936:MET:HA	1:C:937:PRO:HD2	1.93	0.41
1:A:566:SER:HB2	1:A:697:ASP:OD1	2.20	0.41
1:D:838:ASN:HB3	1:D:842:LYS:HD2	2.01	0.41
1:A:931:THR:HA	1:A:932:PRO:HD3	1.93	0.41
1:C:844:ASP:HB2	1:C:845:PRO:CD	2.51	0.41
1:C:426:ALA:HB2	1:C:441:SER:CB	2.50	0.41
1:C:520:LEU:HD23	1:C:520:LEU:HA	1.93	0.41
1:C:858:VAL:HA	1:C:859:PRO:HD3	1.84	0.41
1:A:350:PHE:O	1:A:354:HIS:HD2	2.02	0.41
1:C:1005:GLU:OE1	1:C:1008:ARG:HD3	2.21	0.41
1:C:576:PHE:CZ	1:C:1007:GLU:HG2	2.56	0.41
1:A:503:TYR:HB3	1:A:504:PRO:HD2	2.03	0.41
1:A:323:LEU:O	1:A:326:ILE:HB	2.20	0.41
1:C:787:ILE:HG13	1:C:794:ILE:HB	2.02	0.41
1:C:828:PRO:HG2	1:C:831:ALA:CB	2.51	0.41
1:D:805:ASN:O	1:D:809:THR:HG23	2.21	0.41
1:B:1015:GLU:HA	1:B:1015:GLU:OE1	2.21	0.41
1:B:313:CYS:HA	1:B:314:PRO:HD2	1.91	0.41
1:D:697:ASP:HB3	1:D:701:MET:HG3	2.03	0.41
1:B:491:ARG:HD2	1:B:491:ARG:HA	1.68	0.41
1:B:834:TYR:O	1:B:863:LEU:HD12	2.21	0.41
1:C:564:MET:SD	1:C:564:MET:C	2.99	0.41
1:C:796:ASN:OD1	1:C:798:LEU:HB2	2.21	0.41
1:D:729:ILE:HD13	1:D:729:ILE:HA	1.80	0.41
1:A:644:ARG:HE	1:A:663:PHE:HA	1.86	0.41
1:B:426:ALA:HB2	1:B:441:SER:CB	2.51	0.41
1:C:927:LEU:HA	1:C:927:LEU:HD23	1.83	0.41
1:A:708:LYS:HG2	1:A:988:TRP:CH2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:LEU:HA	1:C:493:PRO:HD3	1.86	0.40
1:A:479:LEU:O	1:A:480:VAL:C	2.59	0.40
1:C:918:ASN:HD22	1:C:918:ASN:N	2.19	0.40
1:A:479:LEU:HD23	1:A:479:LEU:HA	1.90	0.40
1:A:554:ASP:HB3	1:A:558:HIS:CG	2.56	0.40
1:A:698:HIS:CE1	1:A:924:MET:HB3	2.56	0.40
1:C:746:MET:HG3	1:C:763:ASN:HA	2.04	0.40
1:D:572:ASN:HA	1:D:573:PRO:HD2	1.90	0.40
1:A:729:ILE:HA	1:A:729:ILE:HD13	1.83	0.40
1:A:834:TYR:HA	1:A:910:VAL:O	2.22	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	692/723 (96%)	648 (94%)	40 (6%)	4 (1%)	25	57
1	B	692/723 (96%)	641 (93%)	46 (7%)	5 (1%)	22	54
1	C	692/723 (96%)	643 (93%)	46 (7%)	3 (0%)	34	66
1	D	692/723 (96%)	643 (93%)	45 (6%)	4 (1%)	25	57
2	E	8/13 (62%)	6 (75%)	1 (12%)	1 (12%)	0	1
2	F	8/13 (62%)	6 (75%)	1 (12%)	1 (12%)	0	1
2	G	8/13 (62%)	6 (75%)	1 (12%)	1 (12%)	0	1
2	H	8/13 (62%)	6 (75%)	1 (12%)	1 (12%)	0	1
All	All	2800/2944 (95%)	2599 (93%)	181 (6%)	20 (1%)	22	54

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	GLN
1	B	368	GLN
1	C	368	GLN
1	D	368	GLN
2	E	1390	VAL
2	F	1390	VAL
2	G	1390	VAL
2	H	1390	VAL
1	A	331	GLY
1	B	331	GLY
1	C	331	GLY
1	D	331	GLY
1	B	769	MET
1	D	769	MET
1	C	384	PHE
1	A	769	MET
1	A	888	ASN
1	B	763	ASN
1	D	878	GLN
1	B	656	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	600/618 (97%)	574 (96%)	26 (4%)	29	59
1	B	600/618 (97%)	575 (96%)	25 (4%)	30	60
1	C	600/618 (97%)	576 (96%)	24 (4%)	31	61
1	D	600/618 (97%)	575 (96%)	25 (4%)	30	60
2	E	9/11 (82%)	9 (100%)	0	100	100
2	F	9/11 (82%)	9 (100%)	0	100	100
2	G	9/11 (82%)	9 (100%)	0	100	100
2	H	9/11 (82%)	9 (100%)	0	100	100
All	All	2436/2516 (97%)	2336 (96%)	100 (4%)	30	61

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	313	CYS
1	A	318	ASP
1	A	319	SER
1	A	350	PHE
1	A	360	VAL
1	A	384	PHE
1	A	401	VAL
1	A	434	ASN
1	A	437	GLU
1	A	452	PHE
1	A	501	MET
1	A	566	SER
1	A	644	ARG
1	A	658	THR
1	A	669	THR
1	A	673	THR
1	A	694	PHE
1	A	713	PHE
1	A	729	ILE
1	A	771	THR
1	A	793	SER
1	A	820	THR
1	A	821	THR
1	A	868	PHE
1	A	881	GLN
1	A	893	SER
1	B	318	ASP
1	B	319	SER
1	B	350	PHE
1	B	360	VAL
1	B	384	PHE
1	B	401	VAL
1	B	434	ASN
1	B	452	PHE
1	B	491	ARG
1	B	501	MET
1	B	554	ASP
1	B	566	SER
1	B	644	ARG
1	B	658	THR
1	B	694	PHE
1	B	713	PHE

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Mol	Chain	Res	Type
1	B	719	ILE
1	B	729	ILE
1	B	771	THR
1	B	793	SER
1	B	798	LEU
1	B	820	THR
1	B	821	THR
1	B	868	PHE
1	B	893	SER
1	C	313	CYS
1	C	318	ASP
1	C	319	SER
1	C	350	PHE
1	C	360	VAL
1	C	381	SER
1	C	384	PHE
1	C	401	VAL
1	C	434	ASN
1	C	452	PHE
1	C	501	MET
1	C	566	SER
1	C	644	ARG
1	C	658	THR
1	C	669	THR
1	C	673	THR
1	C	694	PHE
1	C	713	PHE
1	C	729	ILE
1	C	771	THR
1	C	793	SER
1	C	820	THR
1	C	821	THR
1	C	868	PHE
1	D	313	CYS
1	D	318	ASP
1	D	350	PHE
1	D	381	SER
1	D	384	PHE
1	D	401	VAL
1	D	434	ASN
1	D	437	GLU
1	D	452	PHE

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Mol	Chain	Res	Type
1	D	501	MET
1	D	566	SER
1	D	644	ARG
1	D	658	THR
1	D	669	THR
1	D	694	PHE
1	D	713	PHE
1	D	719	ILE
1	D	729	ILE
1	D	771	THR
1	D	793	SER
1	D	820	THR
1	D	821	THR
1	D	868	PHE
1	D	893	SER
1	D	1026	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	321	ASN
1	A	356	ASN
1	A	363	GLN
1	A	402	GLN
1	A	406	GLN
1	A	424	ASN
1	A	434	ASN
1	A	784	GLN
1	A	824	GLN
1	A	1012	GLN
1	B	321	ASN
1	B	363	GLN
1	B	402	GLN
1	B	406	GLN
1	B	424	ASN
1	B	434	ASN
1	B	784	GLN
1	B	1012	GLN
1	C	321	ASN
1	C	363	GLN
1	C	406	GLN
1	C	424	ASN

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Mol	Chain	Res	Type
1	C	434	ASN
1	C	784	GLN
1	C	1012	GLN
1	D	321	ASN
1	D	356	ASN
1	D	363	GLN
1	D	390	ASN
1	D	406	GLN
1	D	424	ASN
1	D	434	ASN
1	D	784	GLN
1	D	1012	GLN
2	F	1398	GLN
2	G	1398	GLN
2	H	1398	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DNP	G	1395	2	3,5,6	0.54	0	1,5,7	0.20	0
2	DNP	E	1395	2	3,5,6	1.08	0	1,5,7	0.01	0
2	DNP	H	1395	2	3,5,6	0.67	0	1,5,7	0.12	0
2	DNP	F	1395	2	3,5,6	0.71	0	1,5,7	0.32	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
2	DNP	G	1395	2	-	1/2/4/6	-
2	DNP	E	1395	2	-	1/2/4/6	-
2	DNP	H	1395	2	-	1/2/4/6	-
2	DNP	F	1395	2	-	1/2/4/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1395	DNP	N-CA-CB-NG
2	E	1395	DNP	N-CA-CB-NG
2	H	1395	DNP	N-CA-CB-NG
2	F	1395	DNP	N-CA-CB-NG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	12V	D	1200	-	32,41,41	1.42	5 (15%)	38,62,62	1.38	6 (15%)
3	SO4	A	1100	-	4,4,4	0.33	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	12V	B	1200	-	32,41,41	1.43	4 (12%)	38,62,62	1.55	8 (21%)
4	12V	C	1200	-	32,41,41	1.49	6 (18%)	38,62,62	1.34	5 (13%)
4	12V	A	1200	-	32,41,41	1.68	3 (9%)	38,62,62	1.49	4 (10%)
3	SO4	B	1100	-	4,4,4	0.26	0	6,6,6	0.26	0
3	SO4	C	1100	-	4,4,4	0.30	0	6,6,6	0.19	0
3	SO4	D	1100	-	4,4,4	0.17	0	6,6,6	0.27	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	12V	A	1200	-	-	6/23/63/63	0/3/3/3
4	12V	D	1200	-	-	5/23/63/63	0/3/3/3
4	12V	B	1200	-	-	7/23/63/63	0/3/3/3
4	12V	C	1200	-	-	6/23/63/63	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1200	12V	C6-N1	5.89	1.43	1.35
4	B	1200	12V	O4B-C1B	4.42	1.47	1.41
4	A	1200	12V	C4-N3	4.29	1.40	1.33
4	D	1200	12V	C6-N1	4.15	1.41	1.35
4	D	1200	12V	C5'-S5'	-3.80	1.76	1.82
4	A	1200	12V	C5'-S5'	-3.71	1.76	1.82
4	C	1200	12V	C6-N1	3.41	1.40	1.35
4	B	1200	12V	C6-N1	3.27	1.39	1.35
4	C	1200	12V	C2B-C1B	-3.13	1.49	1.53
4	C	1200	12V	O4B-C1B	3.12	1.45	1.41
4	D	1200	12V	C2B-C1B	-3.05	1.49	1.53
4	C	1200	12V	C5'-S5'	-3.03	1.77	1.82
4	B	1200	12V	C5'-S5'	-2.77	1.78	1.82
4	D	1200	12V	C4-N3	2.59	1.37	1.33
4	C	1200	12V	C4'-C5'	-2.57	1.51	1.53
4	B	1200	12V	C2B-C1B	-2.54	1.49	1.53
4	C	1200	12V	C4-N3	2.30	1.37	1.33
4	D	1200	12V	O4B-C1B	2.16	1.44	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1200	12V	O4B-C1B-C2B	-5.23	99.29	106.93
4	B	1200	12V	O1'-C1'-C2'	4.36	114.06	107.47
4	A	1200	12V	O1'-C1'-C2'	4.17	113.78	107.47
4	B	1200	12V	O4B-C1B-C2B	-3.77	101.42	106.93
4	D	1200	12V	PB-O3A-PA	-3.47	120.92	132.83
4	C	1200	12V	O4B-C1B-C2B	-3.45	101.88	106.93
4	D	1200	12V	O4B-C1B-C2B	-3.40	101.96	106.93
4	B	1200	12V	PB-O3A-PA	-3.33	121.39	132.83
4	C	1200	12V	PB-O3A-PA	-3.30	121.49	132.83
4	A	1200	12V	PB-O3A-PA	-2.97	122.62	132.83
4	C	1200	12V	C1'-C2'-N2'	-2.76	106.04	111.17
4	B	1200	12V	C1'-C2'-N2'	-2.72	106.11	111.17
4	C	1200	12V	O1'-C1'-C2'	2.71	111.56	107.47
4	D	1200	12V	O1'-C1'-C2'	2.68	111.52	107.47
4	D	1200	12V	C1'-C2'-N2'	-2.67	106.20	111.17
4	B	1200	12V	C3B-C2B-C1B	-2.50	97.21	100.98
4	A	1200	12V	C1'-C2'-N2'	-2.35	106.79	111.17
4	C	1200	12V	C3B-C2B-C1B	-2.34	97.46	100.98
4	B	1200	12V	O3B-C3B-C4B	-2.24	104.56	111.05
4	D	1200	12V	C3B-C2B-C1B	-2.23	97.63	100.98
4	B	1200	12V	O4'-C4'-C3'	-2.09	105.53	110.35
4	D	1200	12V	O4'-C4'-C3'	-2.06	105.58	110.35
4	B	1200	12V	C5-C4-N3	-2.02	118.86	123.31

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1200	12V	C2B-C1B-N1-C6
4	D	1200	12V	C3B-C4B-C5B-O5B
4	D	1200	12V	O4B-C4B-C5B-O5B
4	D	1200	12V	C4'-C5'-C6'-O6'
4	B	1200	12V	C2B-C1B-N1-C6
4	B	1200	12V	O4B-C1B-N1-C6
4	B	1200	12V	C3B-C4B-C5B-O5B
4	B	1200	12V	O4B-C4B-C5B-O5B
4	B	1200	12V	C4'-C5'-C6'-O6'
4	C	1200	12V	C2B-C1B-N1-C6
4	C	1200	12V	C3B-C4B-C5B-O5B
4	C	1200	12V	O4B-C4B-C5B-O5B
4	C	1200	12V	C4'-C5'-C6'-O6'
4	A	1200	12V	C2B-C1B-N1-C6
4	A	1200	12V	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
4	A	1200	12V	O4B-C4B-C5B-O5B
4	A	1200	12V	C4'-C5'-C6'-O6'
4	D	1200	12V	PA-O3A-PB-O2B
4	B	1200	12V	PA-O3A-PB-O2B
4	C	1200	12V	PA-O3A-PB-O2B
4	A	1200	12V	PA-O3A-PB-O2B
4	C	1200	12V	PA-O3A-PB-O1B
4	B	1200	12V	PA-O3A-PB-O1B
4	A	1200	12V	PA-O3A-PB-O1B

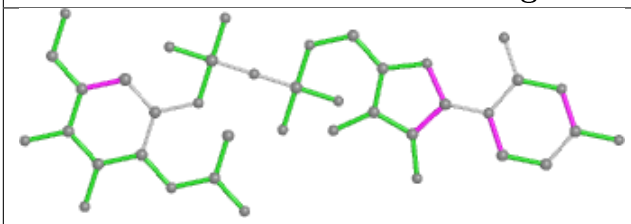
There are no ring outliers.

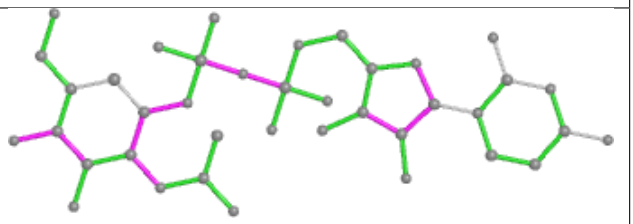
6 monomers are involved in 8 short contacts:

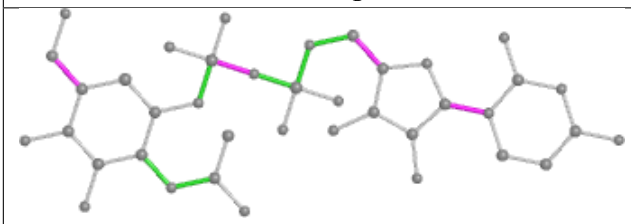
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1200	12V	1	0
3	A	1100	SO4	1	0
4	B	1200	12V	2	0
4	C	1200	12V	2	0
4	A	1200	12V	1	0
3	C	1100	SO4	1	0

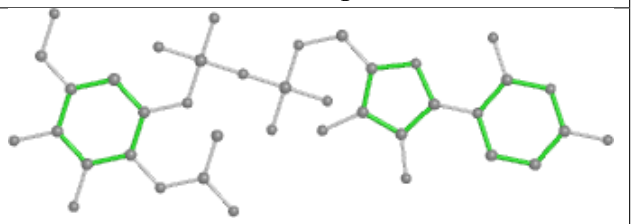
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 12V D 1200

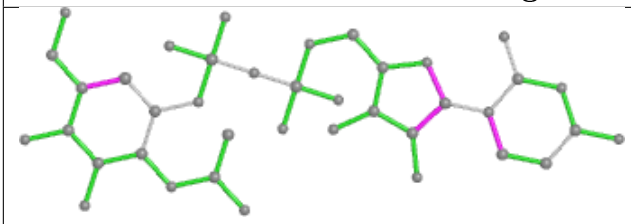

Bond lengths

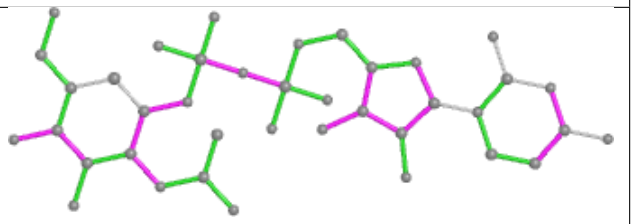

Bond angles

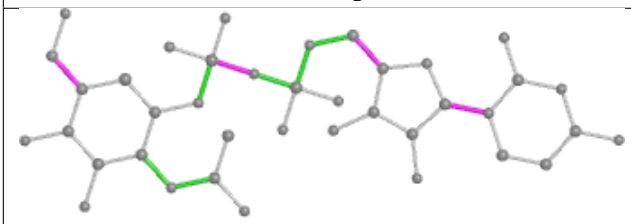

Torsions

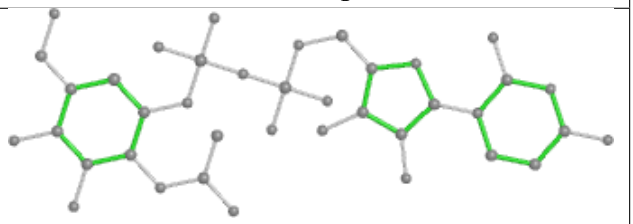

Rings

Ligand 12V B 1200

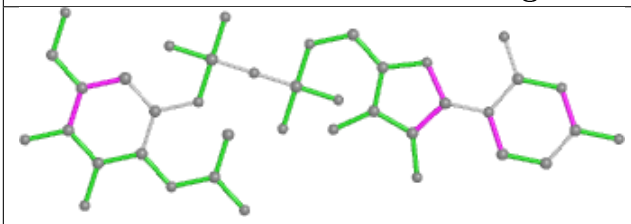

Bond lengths

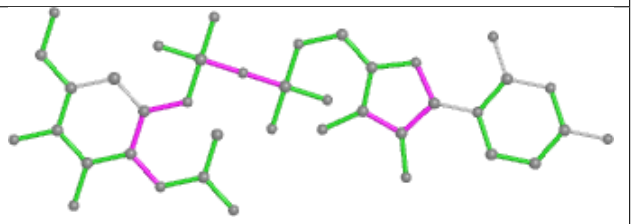

Bond angles

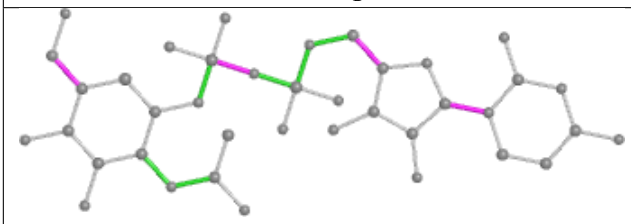

Torsions

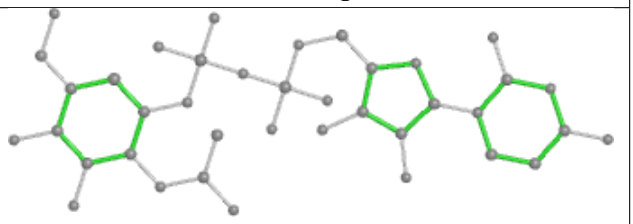

Rings

Ligand 12V C 1200

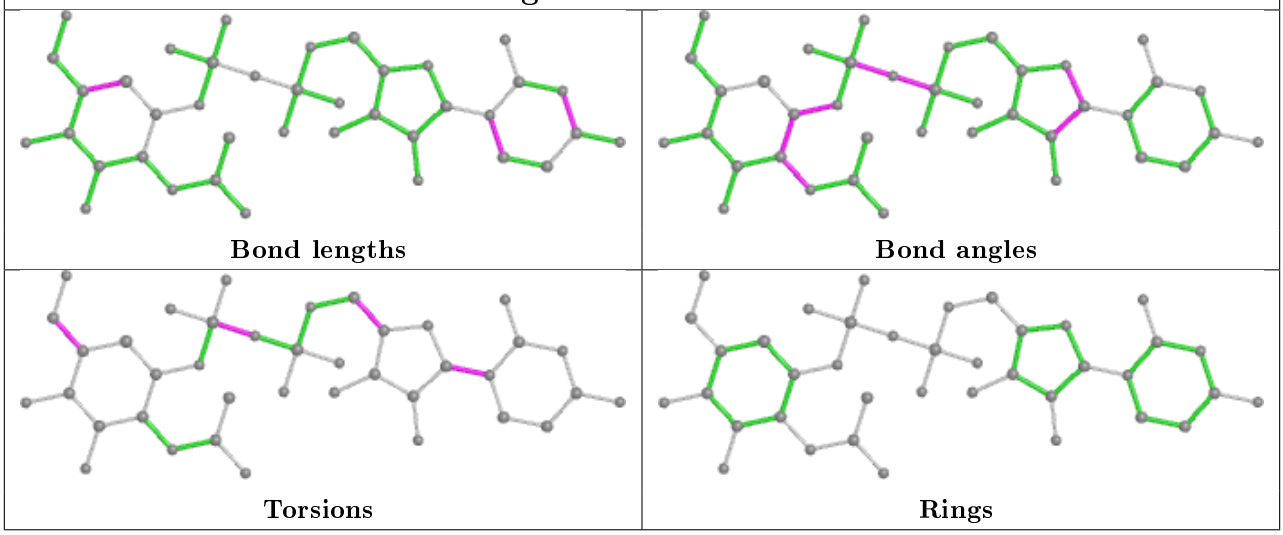

Bond lengths


Bond angles


Torsions


Rings

Ligand 12V A 1200



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

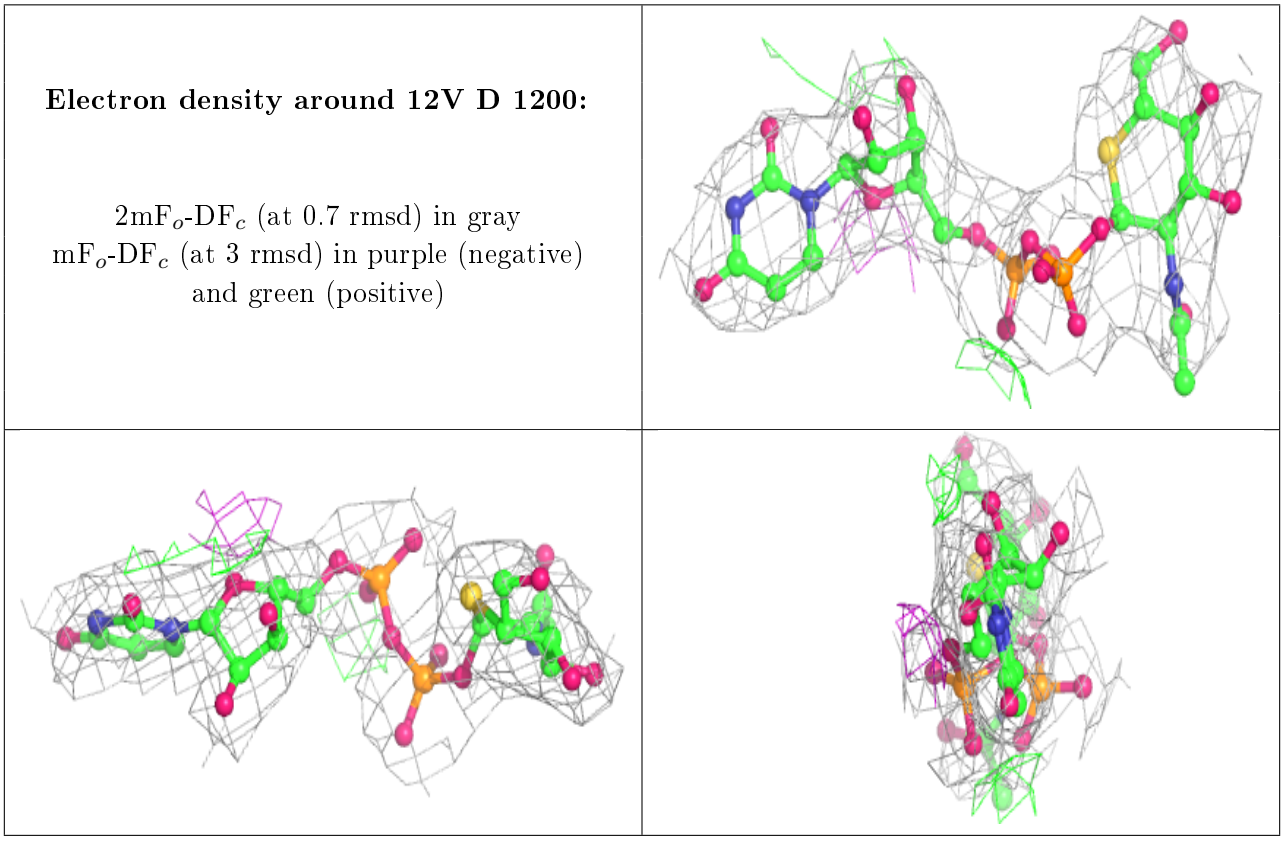
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

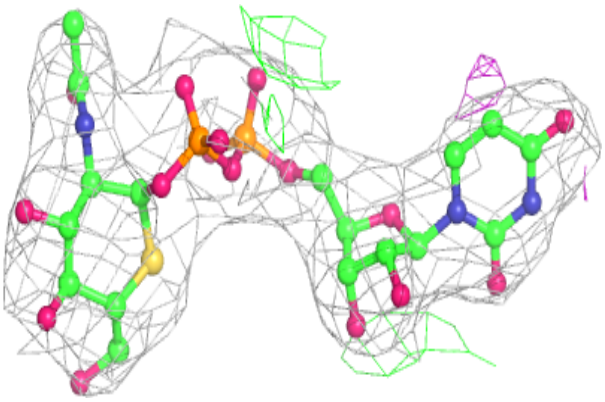
Electron density around 12V D 1200:

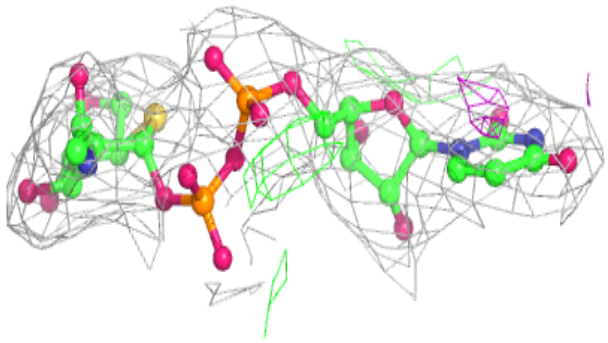
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

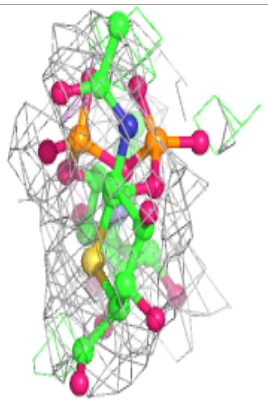


Electron density around 12V B 1200:

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

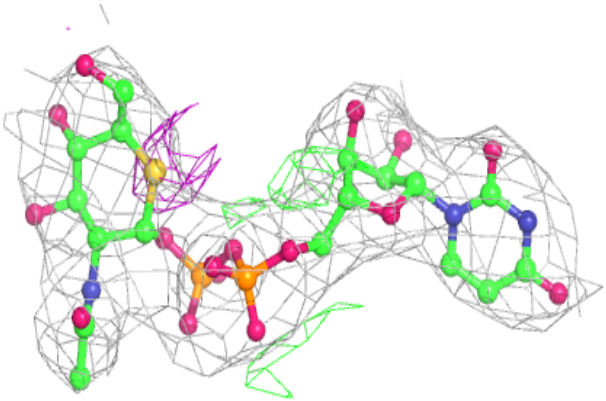


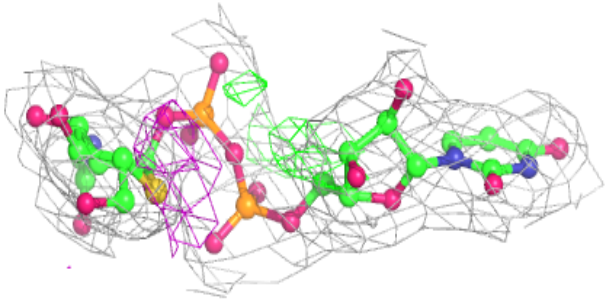


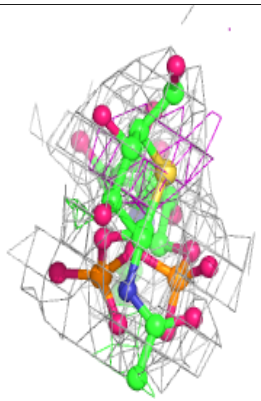


Electron density around 12V C 1200:

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

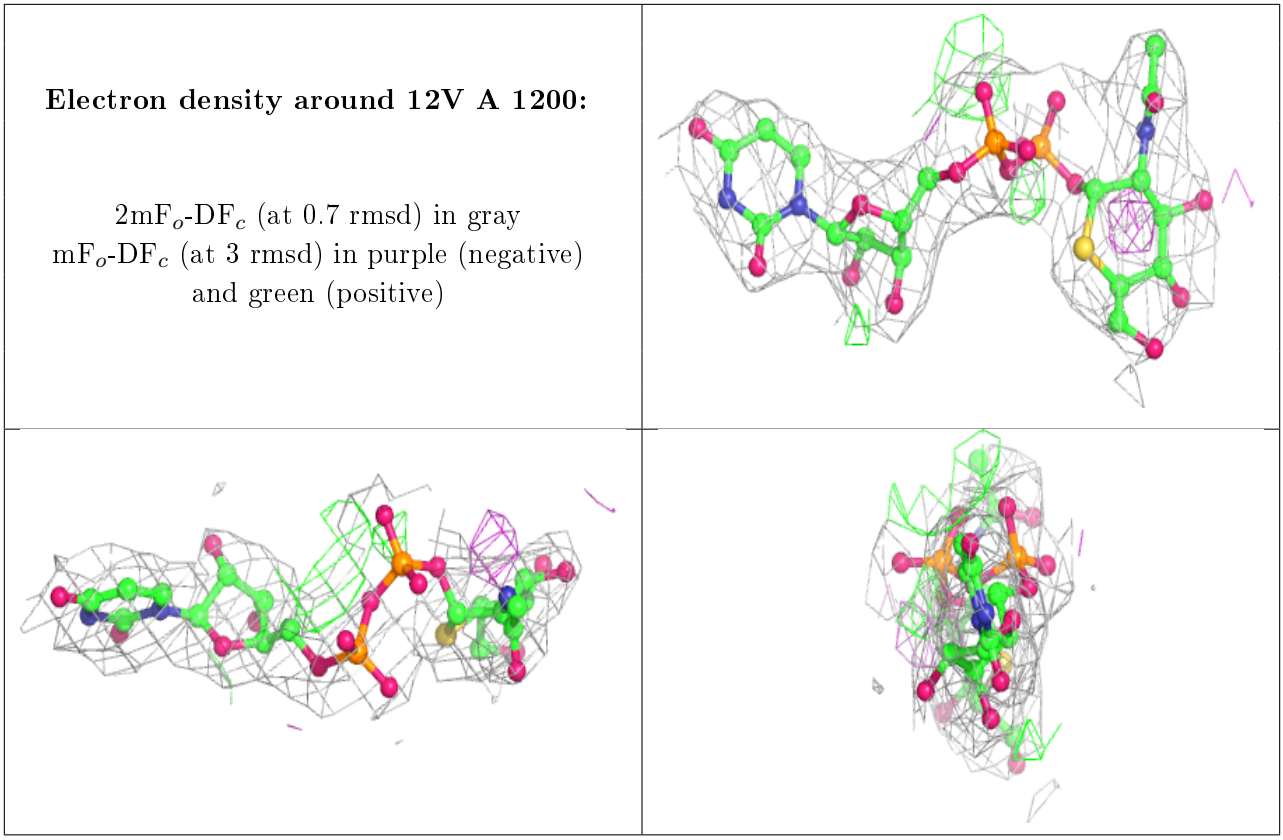






Electron density around 12V A 1200:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.