



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 07:08 AM EDT

PDB ID : 4XI9  
Title : Human OGT in complex with UDP-5S-GlcNAc and substrate peptide (RBL2)  
Authors : Schimpl, M.; van Aalten, D.M.F.  
Deposited on : 2015-01-06  
Resolution : 3.10 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.37.1  
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) : 2.37.1

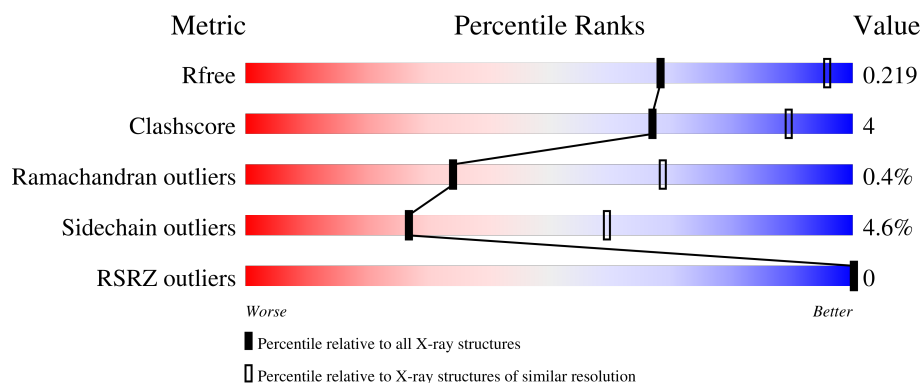
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	723	 86% 9% . .
1	B	723	 85% 10% . .
1	C	723	 86% 9% . .
1	D	723	 85% 11% . .
2	E	8	 62% 25% 12%

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Mol	Chain	Length	Quality of chain
2	F	8	 75% 12% 12%
2	G	8	 88% 12%
2	H	8	 75% 12% 12%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22400 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-acetylglucosaminyltransferase 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

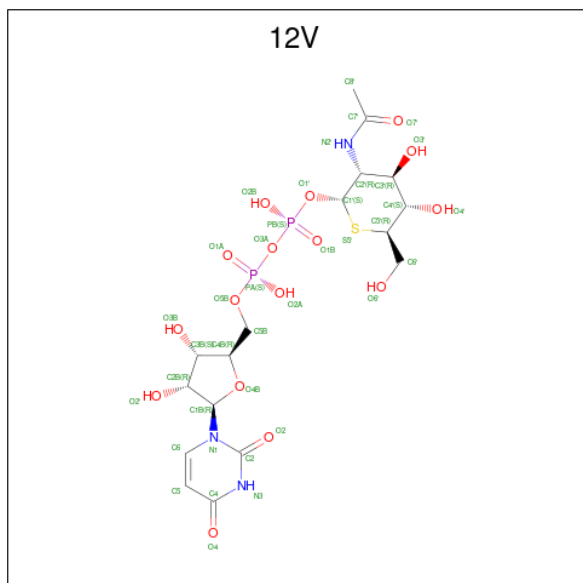
- Molecule 2 is a protein called Retinoblastoma-like protein 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	0	0	1
			47	29	8	10			
2	F	8	Total	C	N	O	0	0	1
			47	29	8	10			
2	G	8	Total	C	N	O	0	0	1
			47	29	8	10			
2	H	8	Total	C	N	O	0	0	1
			47	29	8	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1423	ALA	-	expression tag	UNP Q08999
F	1423	ALA	-	expression tag	UNP Q08999
G	1423	ALA	-	expression tag	UNP Q08999
H	1423	ALA	-	expression tag	UNP Q08999

- Molecule 3 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<sub>17</sub>H<sub>27</sub>N<sub>3</sub>O<sub>16</sub>P<sub>2</sub>S).



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

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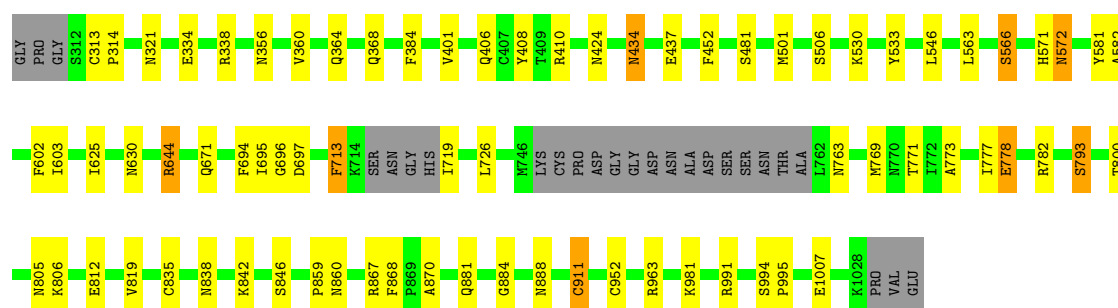
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
3	D	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		

### 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.

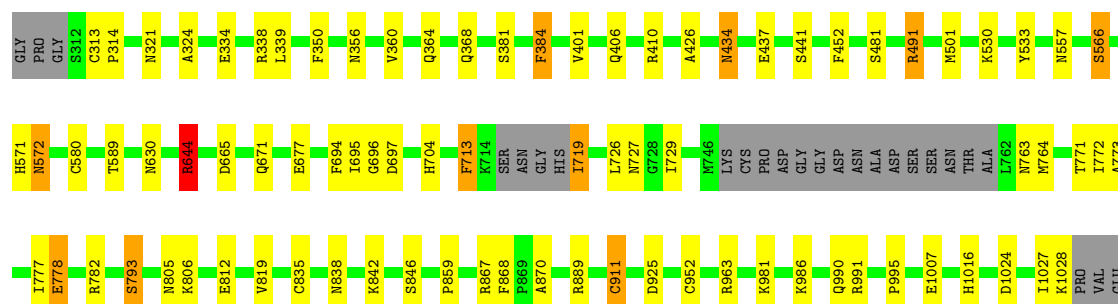
- Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit

Chain A: 




- Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit

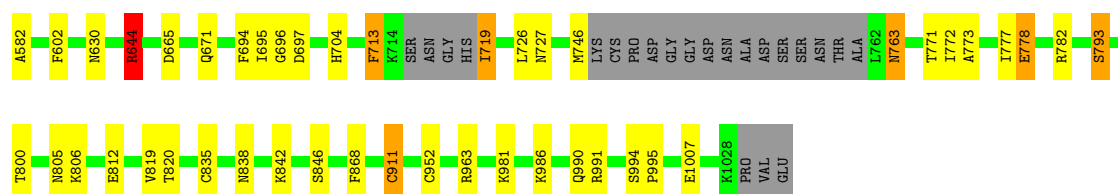
Chain B: 



- Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit

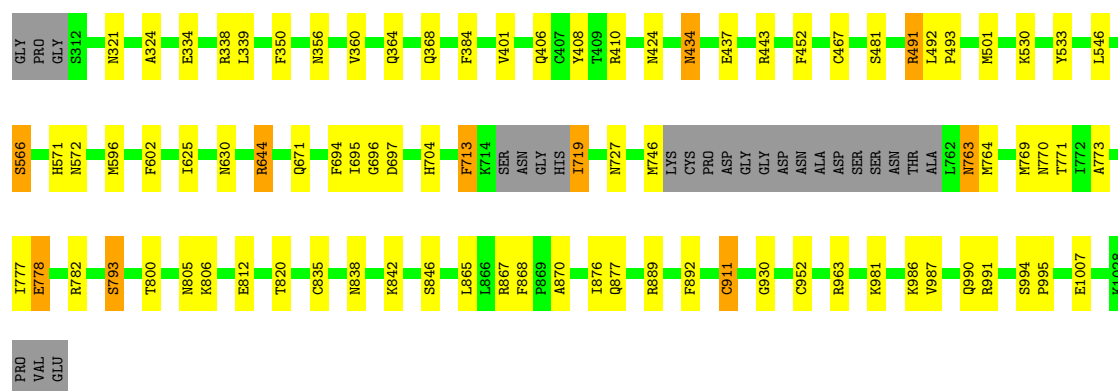
Chain C: 





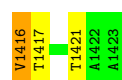
- Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit

Chain D: 85% 11% ..



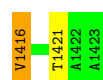
- Molecule 2: Retinoblastoma-like protein 2

Chain E: 62% 25% 12%



- Molecule 2: Retinoblastoma-like protein 2

Chain F: 75% 12% 12%



- Molecule 2: Retinoblastoma-like protein 2

Chain G: 88% 12%



- Molecule 2: Retinoblastoma-like protein 2

Chain H: 75% 12% 12%



Y1416	
T1421	
A1422	
A1423	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	273.91Å 273.91Å 142.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 3.10 25.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (25.00-3.10) 99.1 (25.00-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.203 , 0.223 0.199 , 0.219	Depositor DCC
$R_{free}$ test set	2196 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 11.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	22400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: 12V

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	0.65	2/5641 (0.0%)	0.66	0/7650
1	B	0.63	2/5641 (0.0%)	0.67	2/7650 (0.0%)
1	C	0.61	0/5641	0.67	1/7650 (0.0%)
1	D	0.62	1/5641 (0.0%)	0.65	0/7650
2	E	1.43	1/47 (2.1%)	1.19	0/66
2	F	1.55	2/47 (4.3%)	1.02	0/66
2	G	1.36	0/47	0.99	0/66
2	H	1.34	1/47 (2.1%)	0.97	0/66
All	All	0.64	9/22752 (0.0%)	0.67	3/30864 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	888	ASN	CB-CG	6.88	1.66	1.51
2	E	1416	VAL	CA-CB	5.94	1.67	1.54
1	D	368	GLN	CB-CG	5.78	1.68	1.52
2	H	1416	VAL	CA-CB	5.58	1.66	1.54
1	A	368	GLN	CB-CG	5.41	1.67	1.52
2	F	1416	VAL	CB-CG1	5.25	1.63	1.52
1	B	368	GLN	CB-CG	5.18	1.66	1.52
2	F	1416	VAL	CB-CG2	5.11	1.63	1.52
1	B	580	CYS	CB-SG	-5.01	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	644	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	B	644	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B	925	ASP	CB-CG-OD1	5.21	122.99	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	43	0
1	B	5514	0	5489	49	0
1	C	5514	0	5489	38	0
1	D	5514	0	5489	47	0
2	E	47	0	48	1	0
2	F	47	0	48	0	0
2	G	47	0	48	0	0
2	H	47	0	48	0	0
3	A	39	0	25	1	0
3	B	39	0	25	1	0
3	C	39	0	25	0	0
3	D	39	0	25	1	0
All	All	22400	0	22248	172	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 4.

All (172) 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:644:ARG:HH11	1:A:644:ARG:HG2	1.49	0.76
1:A:859:PRO:O	1:B:1024:ASP:OD2	2.07	0.73
1:B:644:ARG:HH11	1:B:644:ARG:HG2	1.56	0.70
1:D:644:ARG:HG2	1:D:644:ARG:HH11	1.57	0.69
1:A:719:ILE:HG22	1:A:719:ILE:O	1.95	0.67
1:A:644:ARG:HH11	1:A:644:ARG:CG	2.08	0.65
1:D:835:CYS:SG	1:D:911:CYS:HB2	2.37	0.65
1:A:884:GLY:O	1:B:1027:ILE:HD12	1.97	0.65
1:C:719:ILE:O	1:C:719:ILE:HG22	1.96	0.64
1:D:719:ILE:HG22	1:D:719:ILE:O	1.98	0.64
1:C:713:PHE:H	1:C:713:PHE:HD1	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:ASN:OD1	1:B:1024:ASP:HB2	1.98	0.63
1:D:644:ARG:HH11	1:D:644:ARG:CG	2.13	0.62
1:A:713:PHE:H	1:A:713:PHE:HD1	1.47	0.61
1:B:644:ARG:HH11	1:B:644:ARG:CG	2.13	0.61
1:C:434:ASN:HB2	1:C:437:GLU:HG2	1.83	0.61
1:C:644:ARG:HG2	1:C:644:ARG:HH11	1.66	0.60
1:B:719:ILE:HG22	1:B:719:ILE:O	2.02	0.60
3:A:1200:12V:H1'	3:A:1200:12V:O1A	2.01	0.59
1:D:713:PHE:HD1	1:D:713:PHE:H	1.51	0.59
1:B:713:PHE:H	1:B:713:PHE:HD1	1.50	0.58
1:A:806:LYS:HB3	1:A:812:GLU:HG3	1.85	0.58
1:C:835:CYS:SG	1:C:911:CYS:HB2	2.45	0.57
1:A:434:ASN:HB2	1:A:437:GLU:HG2	1.87	0.57
1:A:952:CYS:SG	1:A:995:PRO:HG2	2.46	0.56
1:A:572:ASN:OD1	1:D:793:SER:HB3	2.06	0.56
1:D:566:SER:HB2	1:D:697:ASP:OD1	2.06	0.55
1:C:986:LYS:O	1:C:990:GLN:HG2	2.06	0.55
1:D:360:VAL:O	1:D:364:GLN:HG3	2.07	0.55
1:B:321:ASN:HD21	1:B:356:ASN:HD22	1.55	0.54
1:B:835:CYS:SG	1:B:911:CYS:HB2	2.48	0.54
1:B:644:ARG:NH2	1:B:665:ASP:OD1	2.41	0.54
1:B:726:LEU:HD22	1:B:819:VAL:HG22	1.89	0.54
1:D:805:ASN:ND2	1:D:805:ASN:H	2.05	0.54
1:A:571:HIS:HA	1:A:1007:GLU:OE2	2.07	0.54
1:C:952:CYS:SG	1:C:995:PRO:HG2	2.47	0.54
1:D:434:ASN:HB2	1:D:437:GLU:HG2	1.89	0.54
1:C:360:VAL:O	1:C:364:GLN:HG3	2.07	0.53
1:B:838:ASN:HB3	1:B:842:LYS:HD2	1.90	0.53
1:D:952:CYS:SG	1:D:995:PRO:HG2	2.49	0.53
1:A:881:GLN:OE1	1:B:677:GLU:HA	2.08	0.53
1:A:644:ARG:CG	1:A:644:ARG:NH1	2.71	0.53
1:A:566:SER:HB2	1:A:697:ASP:OD1	2.09	0.53
1:A:838:ASN:HB3	1:A:842:LYS:HD2	1.90	0.53
1:C:644:ARG:HH11	1:C:644:ARG:CG	2.21	0.52
1:C:806:LYS:HB3	1:C:812:GLU:HG3	1.90	0.52
1:D:805:ASN:H	1:D:805:ASN:HD22	1.56	0.52
1:C:805:ASN:H	1:C:805:ASN:HD22	1.57	0.52
1:B:805:ASN:HD22	1:B:805:ASN:H	1.58	0.51
1:C:434:ASN:HB2	1:C:437:GLU:CG	2.39	0.51
1:C:719:ILE:O	1:C:719:ILE:CG2	2.58	0.51
1:A:994:SER:HB2	1:A:995:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:HIS:HA	1:B:1007:GLU:OE2	2.11	0.51
1:A:719:ILE:O	1:A:719:ILE:CG2	2.58	0.51
1:C:530:LYS:HE2	1:C:533:TYR:OH	2.12	0.50
1:D:867:ARG:HB3	1:D:870:ALA:HA	1.94	0.49
1:A:773:ALA:O	1:A:777:ILE:HG22	2.13	0.49
1:B:1028:LYS:O	1:B:1028:LYS:HG3	2.12	0.49
1:C:838:ASN:HB3	1:C:842:LYS:HD2	1.93	0.49
1:D:838:ASN:HB3	1:D:842:LYS:HD2	1.92	0.49
1:B:406:GLN:O	1:B:410:ARG:HB2	2.12	0.49
1:C:571:HIS:HA	1:C:1007:GLU:OE2	2.13	0.49
1:D:571:HIS:HA	1:D:1007:GLU:OE2	2.12	0.49
1:A:835:CYS:SG	1:A:911:CYS:HB2	2.53	0.49
1:B:644:ARG:CG	1:B:644:ARG:NH1	2.76	0.49
1:A:406:GLN:O	1:A:410:ARG:HB2	2.13	0.49
1:A:434:ASN:HB2	1:A:437:GLU:CG	2.43	0.48
1:A:408:TYR:CE1	1:A:424:ASN:HB3	2.48	0.48
1:C:778:GLU:OE2	1:C:782:ARG:HD3	2.13	0.48
1:D:746:MET:HG3	1:D:763:ASN:HA	1.95	0.48
1:B:324:ALA:HB2	1:B:339:LEU:HB2	1.96	0.48
1:B:360:VAL:O	1:B:364:GLN:HG3	2.14	0.48
1:D:986:LYS:O	1:D:990:GLN:HG2	2.13	0.48
1:A:805:ASN:HD22	1:A:805:ASN:H	1.62	0.48
1:B:867:ARG:HB3	1:B:870:ALA:HA	1.95	0.47
1:D:719:ILE:O	1:D:719:ILE:CG2	2.61	0.47
1:A:778:GLU:OE2	1:A:782:ARG:HD3	2.14	0.47
1:A:793:SER:HB3	1:D:572:ASN:OD1	2.14	0.47
1:A:360:VAL:O	1:A:364:GLN:HG3	2.14	0.47
1:B:778:GLU:OE2	1:B:782:ARG:HD3	2.14	0.47
1:B:952:CYS:SG	1:B:995:PRO:HG2	2.55	0.47
1:D:434:ASN:HB2	1:D:437:GLU:CG	2.45	0.47
1:B:434:ASN:HB2	1:B:437:GLU:CG	2.45	0.47
1:C:805:ASN:H	1:C:805:ASN:ND2	2.12	0.47
1:B:434:ASN:HB2	1:B:437:GLU:HG2	1.96	0.46
1:B:572:ASN:OD1	1:C:793:SER:HB3	2.15	0.46
1:C:566:SER:HB2	1:C:697:ASP:OD1	2.15	0.46
1:A:859:PRO:HG2	1:B:1016:HIS:ND1	2.30	0.46
1:B:806:LYS:HB3	1:B:812:GLU:HG3	1.97	0.46
1:B:773:ALA:O	1:B:777:ILE:HG22	2.14	0.46
1:A:546:LEU:HD21	1:A:625:ILE:HD12	1.98	0.46
1:B:704:HIS:O	1:B:727:ASN:HB3	2.16	0.46
1:B:963:ARG:HG3	1:B:963:ARG:HH11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:PHE:CD1	1:C:713:PHE:N	2.83	0.46
1:B:719:ILE:O	1:B:719:ILE:CG2	2.64	0.46
1:B:566:SER:HB2	1:B:697:ASP:OD1	2.16	0.46
1:D:764:MET:O	1:D:764:MET:HG2	2.16	0.46
1:B:313:CYS:HA	1:B:314:PRO:HD2	1.88	0.45
1:C:963:ARG:HH11	1:C:963:ARG:HG3	1.81	0.45
1:A:805:ASN:H	1:A:805:ASN:ND2	2.15	0.45
1:D:530:LYS:HE2	1:D:533:TYR:OH	2.16	0.45
1:D:644:ARG:CG	1:D:644:ARG:NH1	2.74	0.45
1:D:778:GLU:OE2	1:D:782:ARG:HD3	2.17	0.45
1:C:695:ILE:HG13	1:C:696:GLY:N	2.31	0.45
1:B:793:SER:HB3	1:C:572:ASN:OD1	2.16	0.45
1:C:321:ASN:HD21	1:C:356:ASN:HD22	1.64	0.45
1:D:695:ILE:HG13	1:D:696:GLY:N	2.32	0.45
1:D:806:LYS:HB3	1:D:812:GLU:HG3	1.99	0.45
1:C:443:ARG:HG2	1:C:443:ARG:HH11	1.82	0.45
1:D:408:TYR:CZ	1:D:424:ASN:HB3	2.52	0.45
3:B:1200:12V:H1'	3:B:1200:12V:O1A	2.17	0.44
1:A:695:ILE:HG13	1:A:696:GLY:N	2.32	0.44
1:B:986:LYS:O	1:B:990:GLN:HG2	2.18	0.44
1:C:582:ALA:HB2	1:C:602:PHE:CZ	2.53	0.44
1:D:324:ALA:HB2	1:D:339:LEU:HB2	2.00	0.44
1:D:406:GLN:O	1:D:410:ARG:HB2	2.17	0.44
1:B:644:ARG:HH22	1:B:665:ASP:CG	2.21	0.44
1:A:726:LEU:HD22	1:A:819:VAL:HG22	1.99	0.44
1:B:491:ARG:HD2	1:B:491:ARG:HA	1.90	0.44
1:C:426:ALA:HB2	1:C:441:SER:CB	2.47	0.44
1:C:726:LEU:HD22	1:C:819:VAL:HG22	1.99	0.44
1:D:877:GLN:HA	1:D:877:GLN:OE1	2.17	0.44
1:B:805:ASN:H	1:B:805:ASN:ND2	2.16	0.43
1:A:582:ALA:HB2	1:A:602:PHE:CZ	2.53	0.43
1:B:324:ALA:HB2	1:B:339:LEU:CB	2.48	0.43
1:B:889:ARG:HH11	1:B:889:ARG:HG3	1.82	0.43
1:D:443:ARG:HH11	1:D:443:ARG:HG2	1.84	0.43
1:D:994:SER:HB2	1:D:995:PRO:HD2	2.00	0.43
1:A:963:ARG:HH11	1:A:963:ARG:HG3	1.84	0.43
1:D:491:ARG:HD2	1:D:491:ARG:HA	1.92	0.43
1:C:994:SER:HB2	1:C:995:PRO:HD2	2.01	0.43
1:D:704:HIS:O	1:D:727:ASN:HB3	2.19	0.43
1:D:930:GLY:HA2	1:D:987:VAL:HG12	2.00	0.43
1:B:729:ILE:HD13	1:B:729:ILE:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:CYS:HA	1:A:314:PRO:HD2	1.81	0.42
3:D:1200:12V:H1'	3:D:1200:12V:O1A	2.18	0.42
1:B:695:ILE:HG13	1:B:696:GLY:N	2.33	0.42
1:B:764:MET:O	1:B:764:MET:HG2	2.18	0.42
1:D:773:ALA:O	1:D:777:ILE:HG22	2.18	0.42
1:B:530:LYS:HE2	1:B:533:TYR:OH	2.20	0.42
1:A:408:TYR:CZ	1:A:424:ASN:HB3	2.54	0.42
1:D:408:TYR:CE1	1:D:424:ASN:HB3	2.55	0.42
1:A:713:PHE:CD1	1:A:713:PHE:N	2.83	0.42
1:C:509:PHE:O	1:C:513:ILE:HG13	2.20	0.42
1:C:746:MET:HG3	1:C:763:ASN:HA	2.02	0.41
1:A:321:ASN:HD21	1:A:356:ASN:HD22	1.66	0.41
1:C:644:ARG:HH22	1:C:665:ASP:CG	2.22	0.41
1:A:867:ARG:HB3	1:A:870:ALA:HA	2.03	0.41
1:C:381:SER:O	1:C:384:PHE:HB2	2.20	0.41
1:D:963:ARG:HH11	1:D:963:ARG:HG3	1.85	0.41
1:A:530:LYS:HE2	1:A:533:TYR:OH	2.20	0.41
1:A:581:TYR:CE1	1:A:603:ILE:HD13	2.56	0.41
1:B:713:PHE:CD1	1:B:713:PHE:N	2.86	0.41
1:C:644:ARG:NH2	1:C:665:ASP:OD1	2.49	0.41
1:D:596:MET:HG2	1:D:602:PHE:CD1	2.55	0.41
1:B:557:ASN:HB2	1:B:589:THR:HG21	2.03	0.41
1:D:321:ASN:HD21	1:D:356:ASN:HD22	1.67	0.41
1:A:563:LEU:HA	1:A:696:GLY:HA2	2.03	0.41
1:A:713:PHE:HD1	1:A:713:PHE:N	2.17	0.41
1:B:426:ALA:HB2	1:B:441:SER:CB	2.51	0.41
1:C:704:HIS:O	1:C:727:ASN:HB3	2.21	0.41
1:D:889:ARG:HH11	1:D:889:ARG:HG3	1.85	0.41
1:C:406:GLN:O	1:C:410:ARG:HB2	2.20	0.40
1:D:467:CYS:SG	1:D:876:ILE:HD11	2.60	0.40
1:D:492:LEU:HA	1:D:493:PRO:HD3	1.99	0.40
1:B:381:SER:O	1:B:384:PHE:HB2	2.22	0.40
2:E:1417:THR:O	2:E:1417:THR:OG1	2.39	0.40
1:D:546:LEU:HD21	1:D:625:ILE:HD12	2.03	0.40
1:D:770:ASN:H	1:D:773:ALA:HB3	1.86	0.40
1:C:773:ALA:O	1:C:777:ILE:HG22	2.22	0.40
1:D:713:PHE:CD1	1:D:713:PHE:N	2.85	0.40
1:D:865:LEU:O	1:D:892:PHE:HA	2.22	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	667 (96%)	22 (3%)	3 (0%)	34	69
1	B	692/723 (96%)	667 (96%)	23 (3%)	2 (0%)	41	73
1	C	692/723 (96%)	667 (96%)	23 (3%)	2 (0%)	41	73
1	D	692/723 (96%)	667 (96%)	22 (3%)	3 (0%)	34	69
2	E	6/8 (75%)	6 (100%)	0	0	100	100
2	F	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	G	6/8 (75%)	6 (100%)	0	0	100	100
2	H	6/8 (75%)	6 (100%)	0	0	100	100
All	All	2792/2924 (96%)	2691 (96%)	91 (3%)	10 (0%)	34	69

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	334	GLU
1	B	334	GLU
1	C	334	GLU
1	D	334	GLU
1	A	769	MET
1	D	763	ASN
1	A	763	ASN
1	C	763	ASN
1	B	763	ASN
1	D	769	MET

### 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	600/618 (97%)	576 (96%)	24 (4%)	31	65
1	B	600/618 (97%)	573 (96%)	27 (4%)	27	60
1	C	600/618 (97%)	573 (96%)	27 (4%)	27	60
1	D	600/618 (97%)	574 (96%)	26 (4%)	29	62
2	E	6/6 (100%)	4 (67%)	2 (33%)	0	0
2	F	6/6 (100%)	4 (67%)	2 (33%)	0	0
2	G	6/6 (100%)	5 (83%)	1 (17%)	2	9
2	H	6/6 (100%)	4 (67%)	2 (33%)	0	0
All	All	2424/2496 (97%)	2313 (95%)	111 (5%)	27	59

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	338	ARG
1	A	384	PHE
1	A	401	VAL
1	A	434	ASN
1	A	452	PHE
1	A	481	SER
1	A	501	MET
1	A	506	SER
1	A	566	SER
1	A	572	ASN
1	A	630	ASN
1	A	644	ARG
1	A	671	GLN
1	A	694	PHE
1	A	713	PHE
1	A	771	THR
1	A	778	GLU
1	A	793	SER
1	A	800	THR
1	A	846	SER
1	A	868	PHE
1	A	911	CYS
1	A	981	LYS
1	A	991	ARG

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Mol	Chain	Res	Type
1	B	338	ARG
1	B	350	PHE
1	B	384	PHE
1	B	401	VAL
1	B	434	ASN
1	B	452	PHE
1	B	481	SER
1	B	491	ARG
1	B	501	MET
1	B	566	SER
1	B	572	ASN
1	B	630	ASN
1	B	644	ARG
1	B	671	GLN
1	B	694	PHE
1	B	713	PHE
1	B	719	ILE
1	B	771	THR
1	B	772	ILE
1	B	778	GLU
1	B	793	SER
1	B	846	SER
1	B	859	PRO
1	B	868	PHE
1	B	911	CYS
1	B	981	LYS
1	B	991	ARG
1	C	338	ARG
1	C	350	PHE
1	C	384	PHE
1	C	401	VAL
1	C	434	ASN
1	C	452	PHE
1	C	481	SER
1	C	491	ARG
1	C	501	MET
1	C	566	SER
1	C	630	ASN
1	C	644	ARG
1	C	671	GLN
1	C	694	PHE
1	C	713	PHE

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Mol	Chain	Res	Type
1	C	719	ILE
1	C	771	THR
1	C	772	ILE
1	C	778	GLU
1	C	793	SER
1	C	800	THR
1	C	820	THR
1	C	846	SER
1	C	868	PHE
1	C	911	CYS
1	C	981	LYS
1	C	991	ARG
1	D	338	ARG
1	D	350	PHE
1	D	384	PHE
1	D	401	VAL
1	D	434	ASN
1	D	452	PHE
1	D	481	SER
1	D	491	ARG
1	D	501	MET
1	D	566	SER
1	D	630	ASN
1	D	644	ARG
1	D	671	GLN
1	D	694	PHE
1	D	713	PHE
1	D	719	ILE
1	D	771	THR
1	D	778	GLU
1	D	793	SER
1	D	800	THR
1	D	820	THR
1	D	846	SER
1	D	868	PHE
1	D	911	CYS
1	D	981	LYS
1	D	991	ARG
2	E	1416	VAL
2	E	1421	THR
2	F	1416	VAL
2	F	1421	THR

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Mol	Chain	Res	Type
2	G	1416	VAL
2	H	1416	VAL
2	H	1421	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	321	ASN
1	A	424	ASN
1	A	434	ASN
1	A	681	GLN
1	A	805	ASN
1	B	321	ASN
1	B	424	ASN
1	B	434	ASN
1	B	681	GLN
1	B	805	ASN
1	C	321	ASN
1	C	434	ASN
1	C	681	GLN
1	C	805	ASN
1	D	321	ASN
1	D	424	ASN
1	D	434	ASN
1	D	681	GLN
1	D	805	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

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
3	12V	D	1200	-	36,41,41	1.79	6 (16%)	50,62,62	1.98	11 (22%)
3	12V	B	1200	-	36,41,41	1.15	3 (8%)	50,62,62	1.84	6 (12%)
3	12V	C	1200	-	36,41,41	1.23	4 (11%)	50,62,62	1.80	10 (20%)
3	12V	A	1200	-	36,41,41	1.27	5 (13%)	50,62,62	2.03	10 (20%)

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
3	12V	D	1200	-	-	8/25/63/63	0/3/3/3
3	12V	B	1200	-	-	4/25/63/63	0/3/3/3
3	12V	C	1200	-	-	5/25/63/63	0/3/3/3
3	12V	A	1200	-	-	2/25/63/63	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1200	12V	C4'-C5'	-6.93	1.47	1.53
3	D	1200	12V	C5'-S5'	-3.93	1.76	1.82
3	D	1200	12V	PB-O1'	3.59	1.69	1.60
3	D	1200	12V	C2-N1	-3.53	1.32	1.38
3	B	1200	12V	C2-N1	-2.94	1.33	1.38
3	C	1200	12V	C5'-S5'	-2.62	1.78	1.82
3	C	1200	12V	O4B-C1B	2.57	1.48	1.42
3	A	1200	12V	O4B-C4B	-2.42	1.39	1.45
3	B	1200	12V	C6'-C5'	2.42	1.54	1.52
3	C	1200	12V	C6-C5	2.40	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1200	12V	C2-N1	-2.36	1.34	1.38
3	D	1200	12V	C6-C5	2.28	1.40	1.35
3	C	1200	12V	PB-O1'	2.22	1.66	1.60
3	A	1200	12V	PB-O1'	2.15	1.66	1.60
3	A	1200	12V	C5'-S5'	-2.09	1.78	1.82
3	A	1200	12V	C6-C5	2.09	1.39	1.35
3	B	1200	12V	PB-O1'	2.02	1.65	1.60
3	D	1200	12V	C2B-C1B	-2.02	1.47	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1200	12V	C4-N3-C2	-6.56	117.93	126.58
3	D	1200	12V	N3-C2-N1	6.22	123.14	114.89
3	D	1200	12V	C4-N3-C2	-6.01	118.65	126.58
3	A	1200	12V	O1'-C1'-C2'	5.96	116.48	107.47
3	B	1200	12V	O1'-C1'-C2'	5.57	115.90	107.47
3	A	1200	12V	N3-C2-N1	5.52	122.22	114.89
3	B	1200	12V	C4-N3-C2	-5.34	119.54	126.58
3	C	1200	12V	C4-N3-C2	-5.19	119.73	126.58
3	C	1200	12V	N3-C2-N1	5.14	121.71	114.89
3	B	1200	12V	N3-C2-N1	4.67	121.09	114.89
3	A	1200	12V	C5-C4-N3	4.18	121.09	114.84
3	D	1200	12V	O1'-C1'-C2'	3.98	113.48	107.47
3	C	1200	12V	O1'-C1'-C2'	3.90	113.36	107.47
3	D	1200	12V	O2-C2-N1	-3.88	117.64	122.79
3	D	1200	12V	PB-O3A-PA	-3.78	119.85	132.83
3	C	1200	12V	C1'-C2'-N2'	-3.70	104.28	111.17
3	B	1200	12V	C5-C4-N3	3.66	120.31	114.84
3	C	1200	12V	C5-C4-N3	3.33	119.81	114.84
3	A	1200	12V	C5-C6-N1	-3.04	116.71	121.81
3	D	1200	12V	O4B-C1B-N1	3.01	115.24	108.36
3	D	1200	12V	C5-C4-N3	2.98	119.29	114.84
3	A	1200	12V	O4B-C4B-C5B	-2.78	100.22	109.37
3	C	1200	12V	O2-C2-N3	-2.77	116.35	121.50
3	D	1200	12V	O4B-C4B-C5B	-2.72	100.41	109.37
3	C	1200	12V	PB-O3A-PA	-2.55	124.08	132.83
3	A	1200	12V	C3B-C2B-C1B	-2.50	96.67	101.43
3	B	1200	12V	O4B-C1B-C2B	-2.40	101.40	106.64
3	A	1200	12V	O2-C2-N1	-2.36	119.65	122.79
3	C	1200	12V	C2B-C1B-N1	2.36	119.89	113.22
3	D	1200	12V	C5-C6-N1	-2.33	117.91	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1200	12V	O4-C4-N3	-2.27	115.97	119.31
3	D	1200	12V	O4'-C4'-C5'	-2.20	104.03	108.82
3	A	1200	12V	C2B-C1B-N1	2.12	119.22	113.22
3	B	1200	12V	O4B-C1B-N1	-2.12	103.52	108.36
3	C	1200	12V	C3'-C2'-N2'	2.09	114.56	110.62
3	D	1200	12V	C1'-C2'-N2'	-2.06	107.34	111.17
3	C	1200	12V	O4-C4-N3	-2.04	116.31	119.31

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1200	12V	O4B-C4B-C5B-O5B
3	C	1200	12V	C5B-O5B-PA-O1A
3	C	1200	12V	C5B-O5B-PA-O3A
3	C	1200	12V	C3B-C4B-C5B-O5B
3	C	1200	12V	O4B-C4B-C5B-O5B
3	D	1200	12V	C5B-O5B-PA-O3A
3	D	1200	12V	C3B-C4B-C5B-O5B
3	D	1200	12V	O4B-C4B-C5B-O5B
3	D	1200	12V	C4'-C5'-C6'-O6'
3	D	1200	12V	S5'-C5'-C6'-O6'
3	A	1200	12V	C3B-C4B-C5B-O5B
3	B	1200	12V	C3B-C4B-C5B-O5B
3	B	1200	12V	O4B-C4B-C5B-O5B
3	B	1200	12V	PA-O3A-PB-O2B
3	C	1200	12V	C5B-O5B-PA-O2A
3	D	1200	12V	C5B-O5B-PA-O1A
3	B	1200	12V	PA-O3A-PB-O1B
3	D	1200	12V	PA-O3A-PB-O2B
3	D	1200	12V	C5B-O5B-PA-O2A

There are no ring outliers.

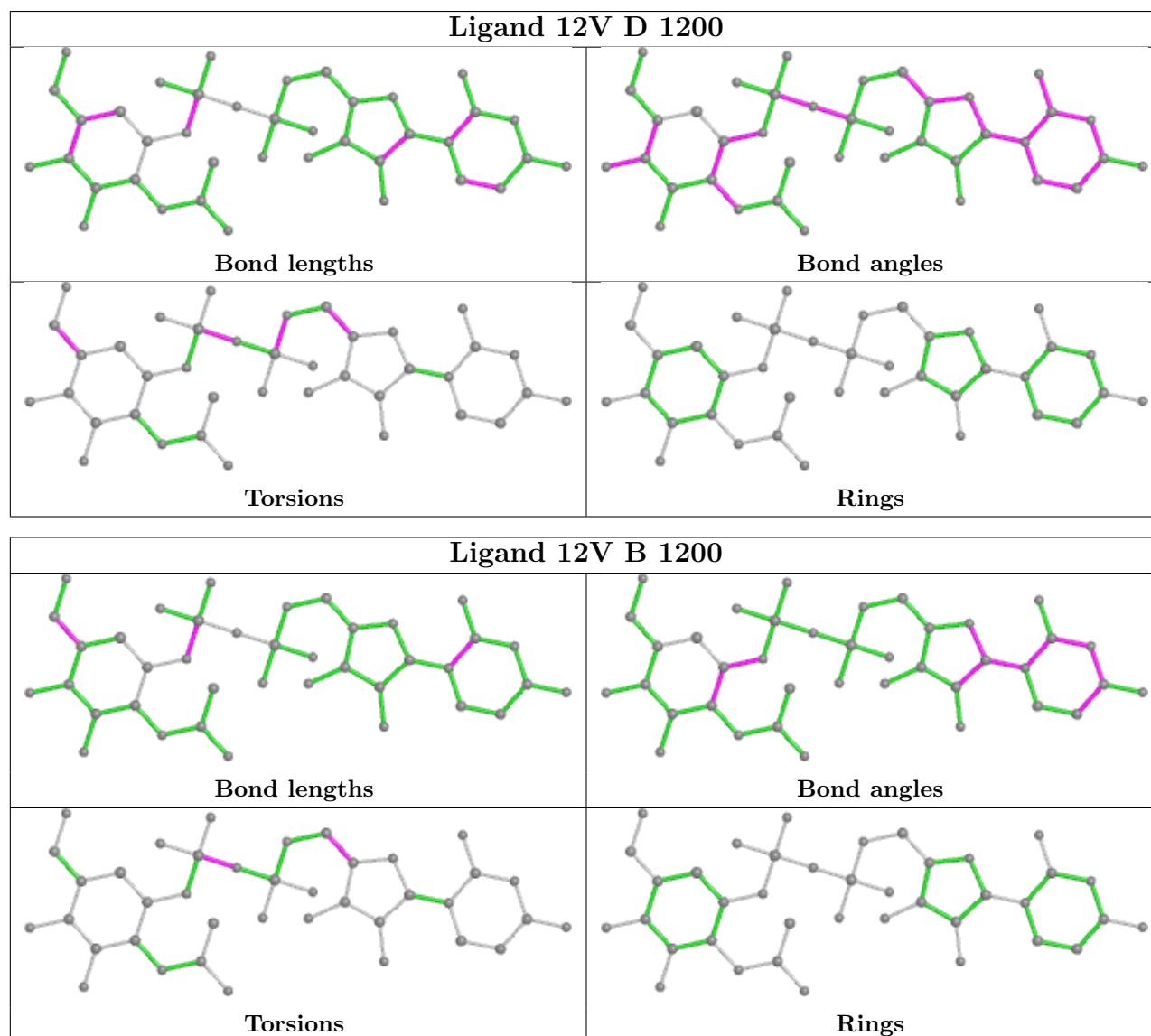
3 monomers are involved in 3 short contacts:

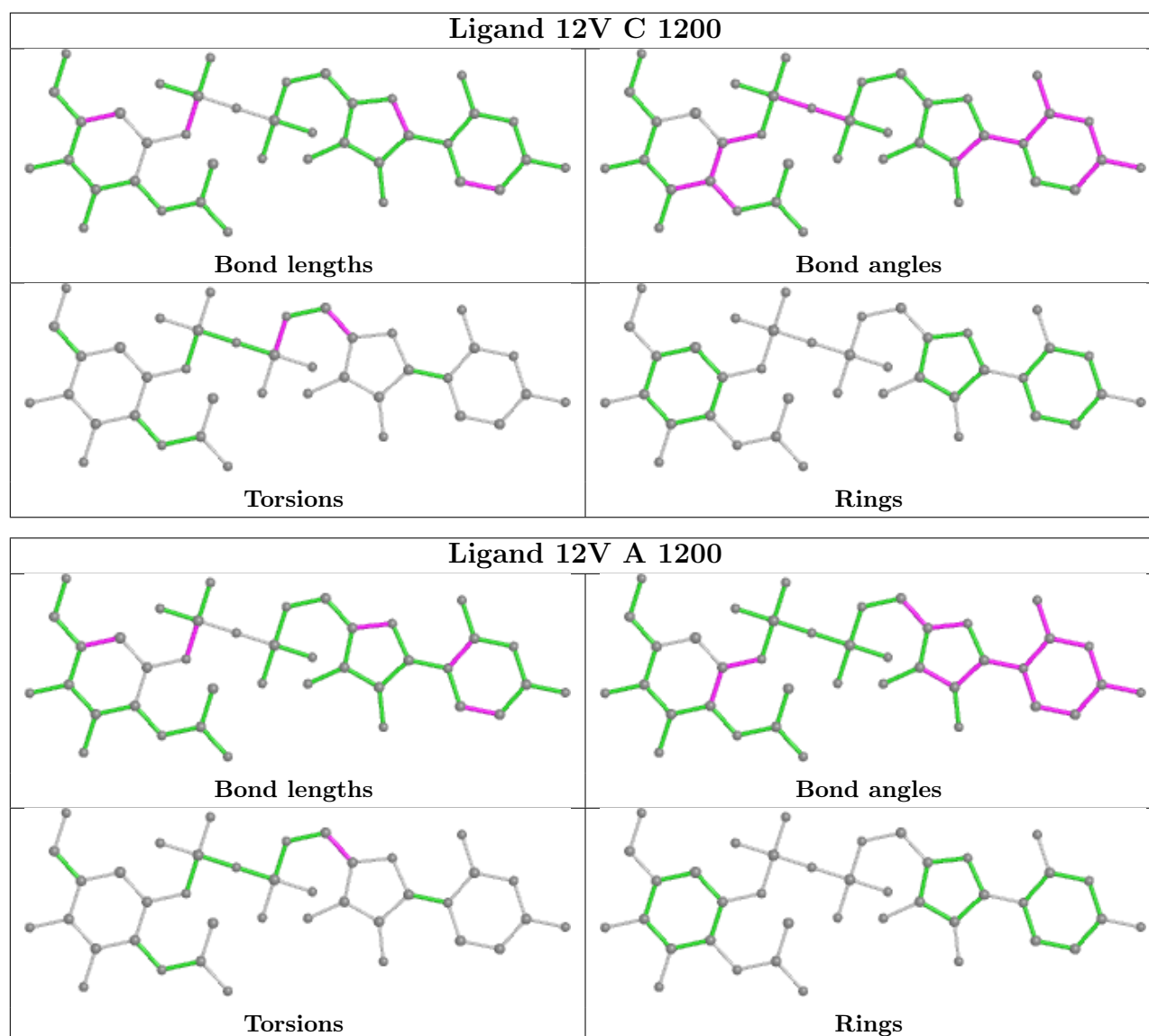
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1200	12V	1	0
3	B	1200	12V	1	0
3	A	1200	12V	1	0

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 than 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.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	698/723 (96%)	-0.56	0 100 100	18, 34, 59, 101	0
1	B	698/723 (96%)	-0.58	0 100 100	18, 34, 59, 101	0
1	C	698/723 (96%)	-0.56	0 100 100	18, 34, 59, 101	0
1	D	698/723 (96%)	-0.64	0 100 100	18, 34, 59, 101	0
2	E	8/8 (100%)	0.11	0 100 100	33, 36, 40, 40	0
2	F	8/8 (100%)	-0.03	0 100 100	37, 39, 40, 43	0
2	G	8/8 (100%)	0.07	0 100 100	34, 38, 40, 40	0
2	H	8/8 (100%)	-0.32	0 100 100	43, 45, 47, 48	0
All	All	2824/2924 (96%)	-0.58	0 100 100	18, 34, 59, 101	0

There are no RSRZ outliers to report.

### 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](#)

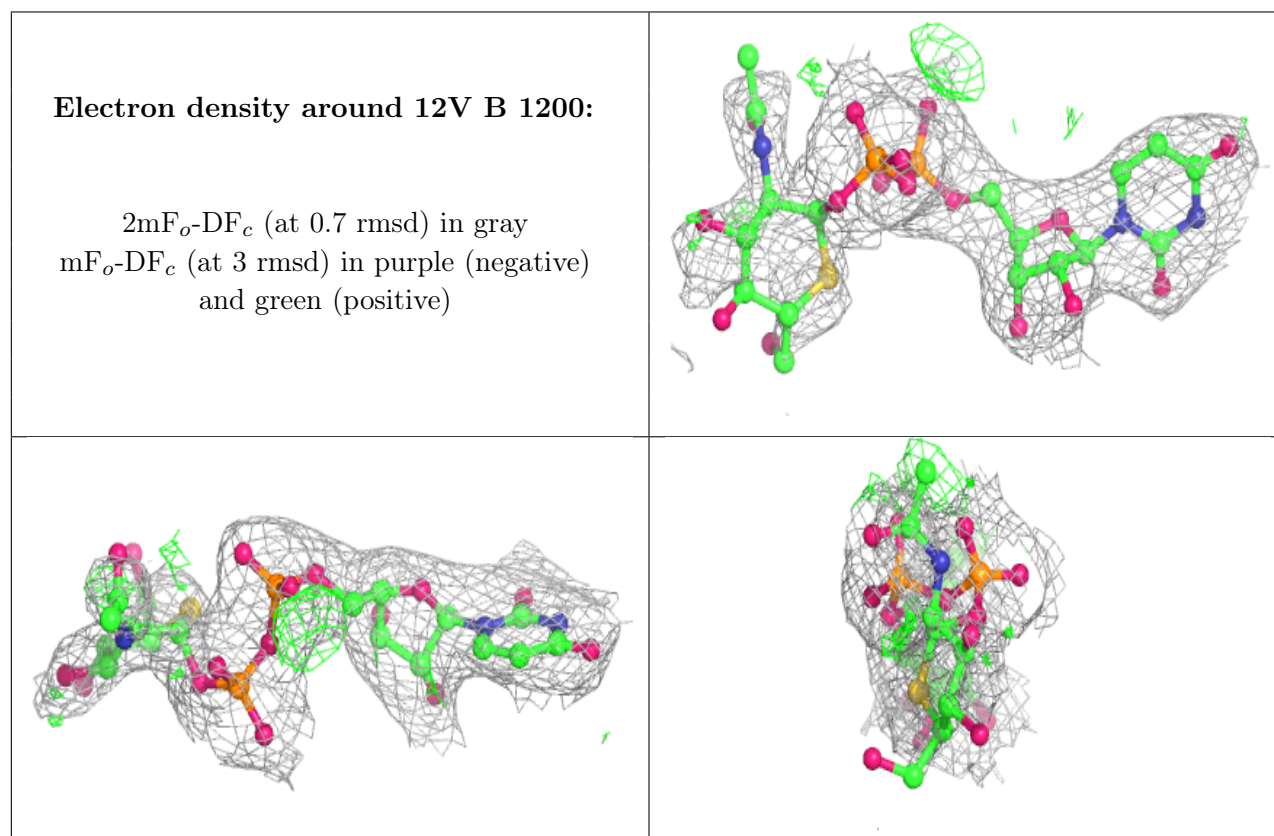
There are no monosaccharides in this entry.

### 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, 95<sup>th</sup> 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.

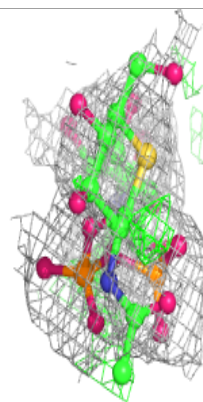
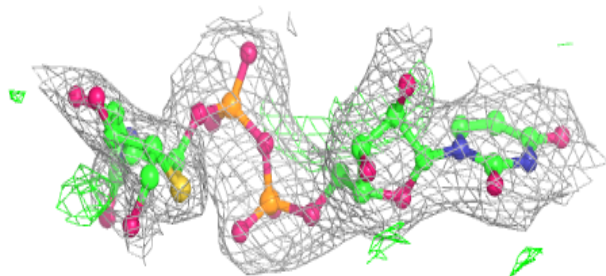
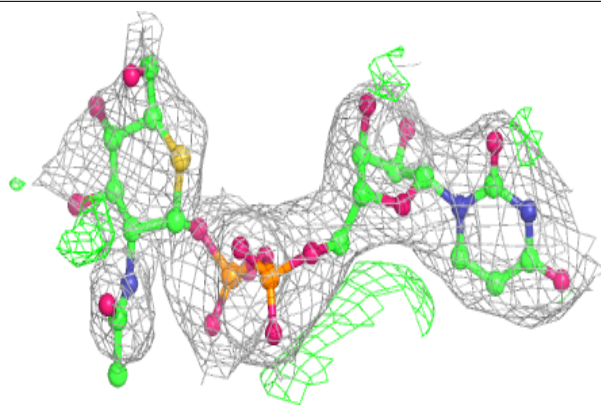
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	12V	B	1200	39/39	0.97	0.13	16,19,23,24	14
3	12V	C	1200	39/39	0.97	0.12	15,20,23,24	14
3	12V	D	1200	39/39	0.97	0.13	28,31,35,36	14
3	12V	A	1200	39/39	0.98	0.13	18,21,23,25	14

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.

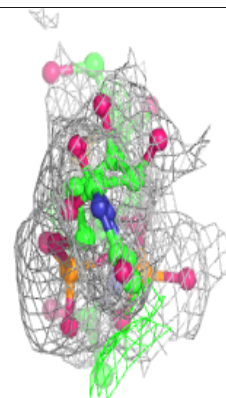
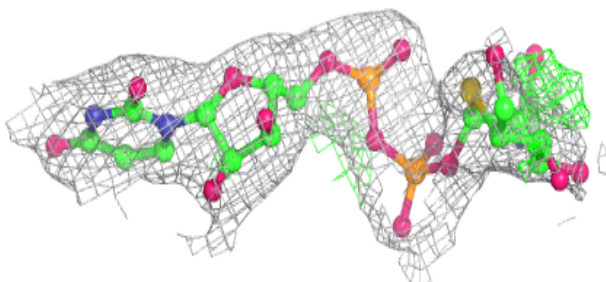
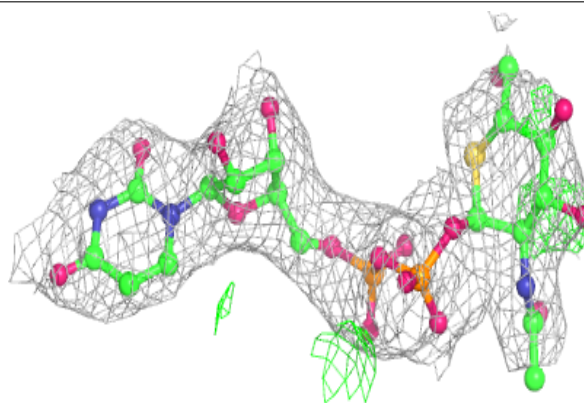


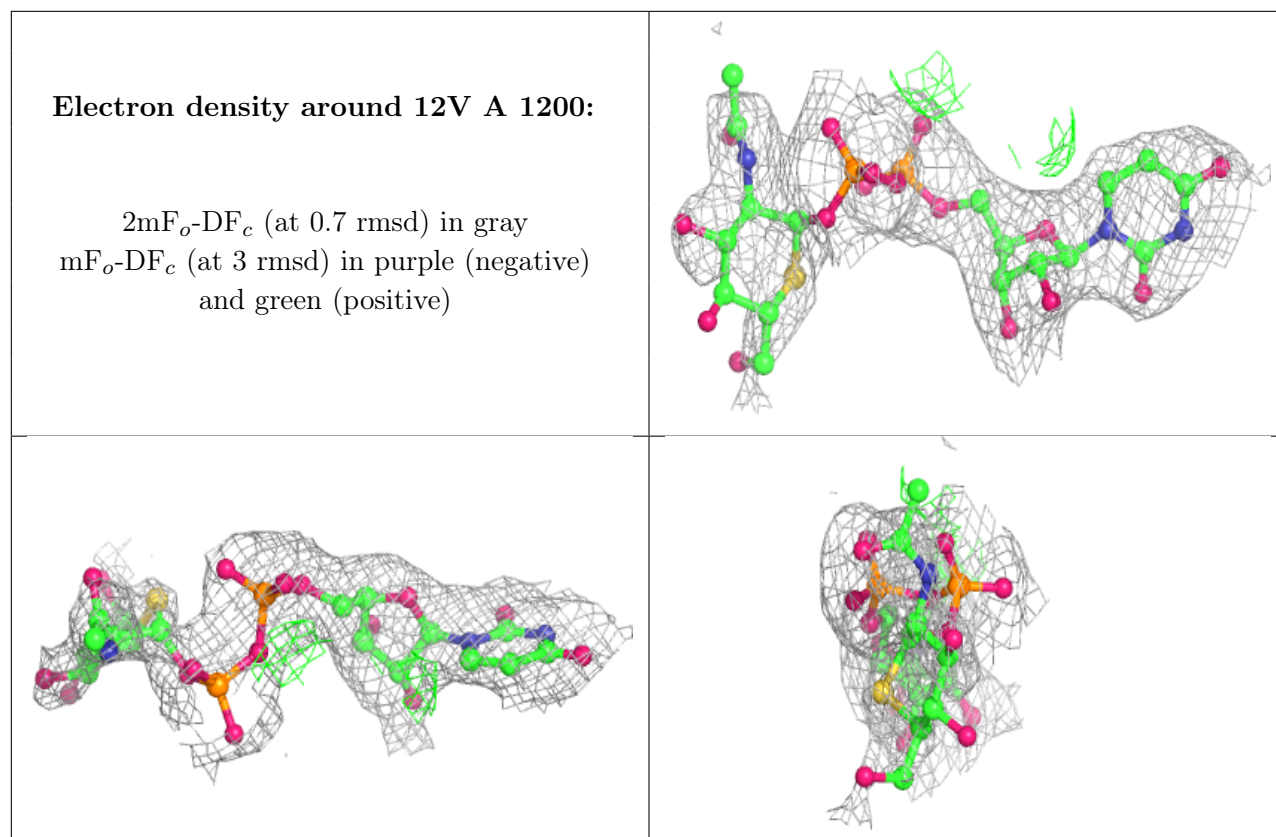
**Electron density around 12V C 1200:**

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

**Electron density around 12V 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.