



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:35 PM UTC

PDB ID : 4XIF / pdb_00004xif
Title : Human OGT in complex with UDP-5S-GlcNAc and substrate peptide (keratin-7)
Authors : Schimpl, M.; van Aalten, D.M.F.
Deposited on : 2015-01-06
Resolution : 3.20 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

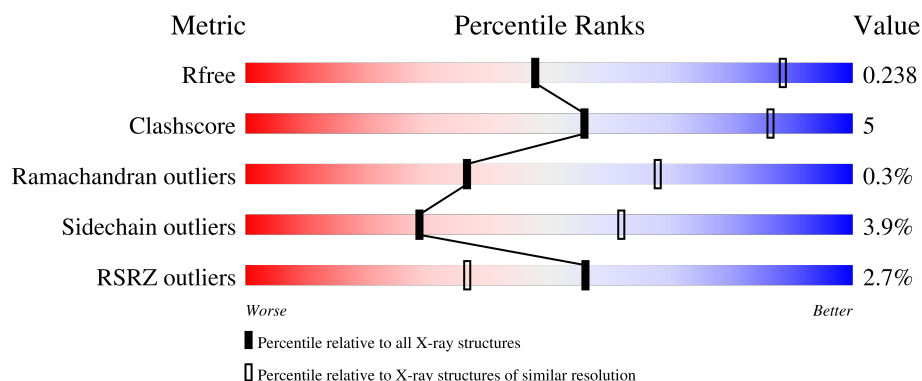
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



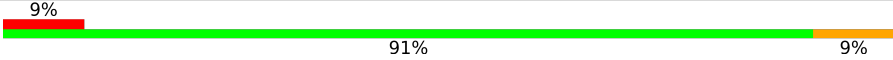
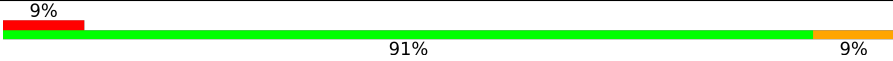
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 3% 83% 13% ..
1	B	723	 2% 85% 11% ..
1	C	723	 % 82% 13% ..
1	D	723	 4% 84% 12% ..
2	E	11	 36% 82% 9% 9%

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Mol	Chain	Length	Quality of chain
2	F	11	
2	G	11	
2	H	11	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22608 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	702	Total	C	N	O	S	0	0	0
			5535	3511	968	1017	39			
1	B	702	Total	C	N	O	S	0	0	0
			5535	3511	968	1017	39			
1	C	702	Total	C	N	O	S	0	0	0
			5535	3511	968	1017	39			
1	D	702	Total	C	N	O	S	0	0	0
			5535	3511	968	1017	39			

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

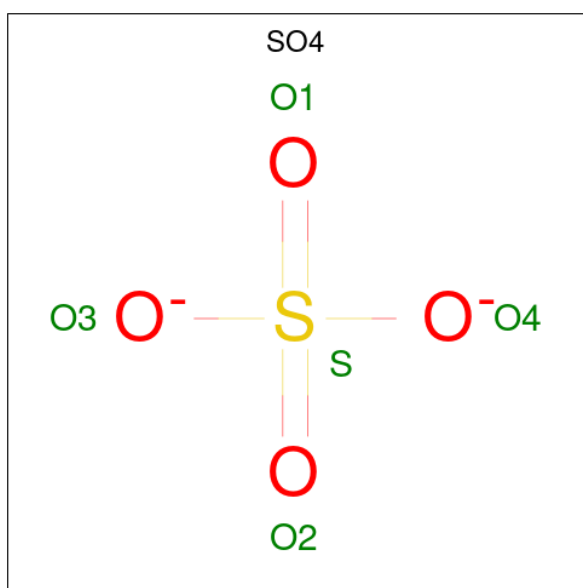
- Molecule 2 is a protein called Keratin, type II cytoskeletal 7.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	0	0	0
			73	45	14	14			
2	F	11	Total	C	N	O	0	0	0
			73	45	14	14			
2	G	11	Total	C	N	O	0	0	0
			73	45	14	14			
2	H	11	Total	C	N	O	0	0	0
			73	45	14	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	2007	GLY	-	expression tag	UNP P08729
E	2017	GLY	-	expression tag	UNP P08729
F	2007	GLY	-	expression tag	UNP P08729
F	2017	GLY	-	expression tag	UNP P08729
G	2007	GLY	-	expression tag	UNP P08729
G	2017	GLY	-	expression tag	UNP P08729
H	2007	GLY	-	expression tag	UNP P08729
H	2017	GLY	-	expression tag	UNP P08729

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



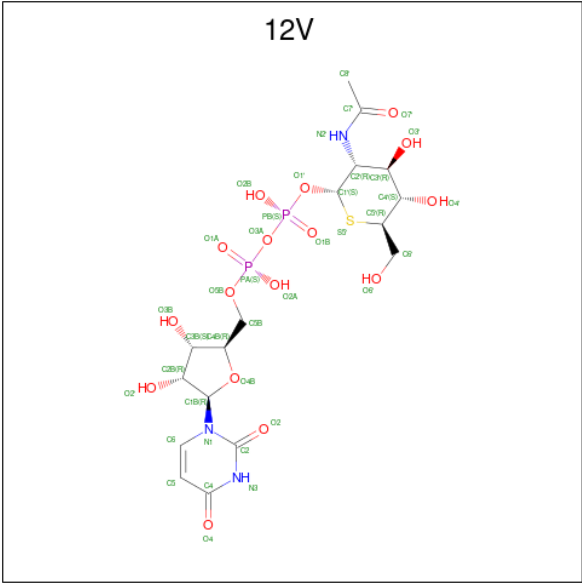
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	H	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 (CCD ID: 12V) (formula: C₁₇H₂₇N₃O₁₆P₂S).

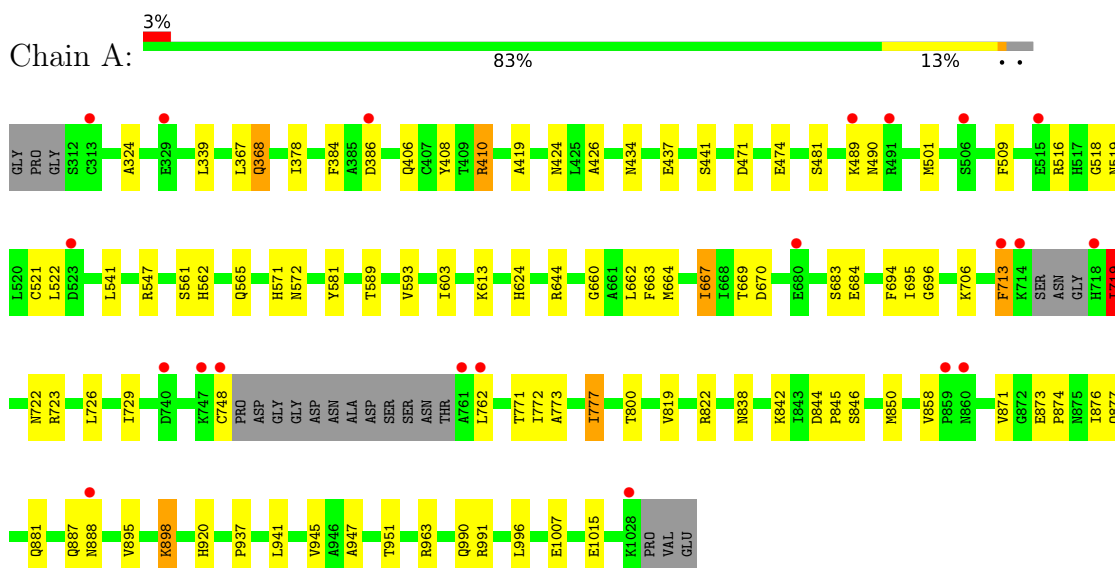


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
4	B	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
4	C	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
4	D	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		

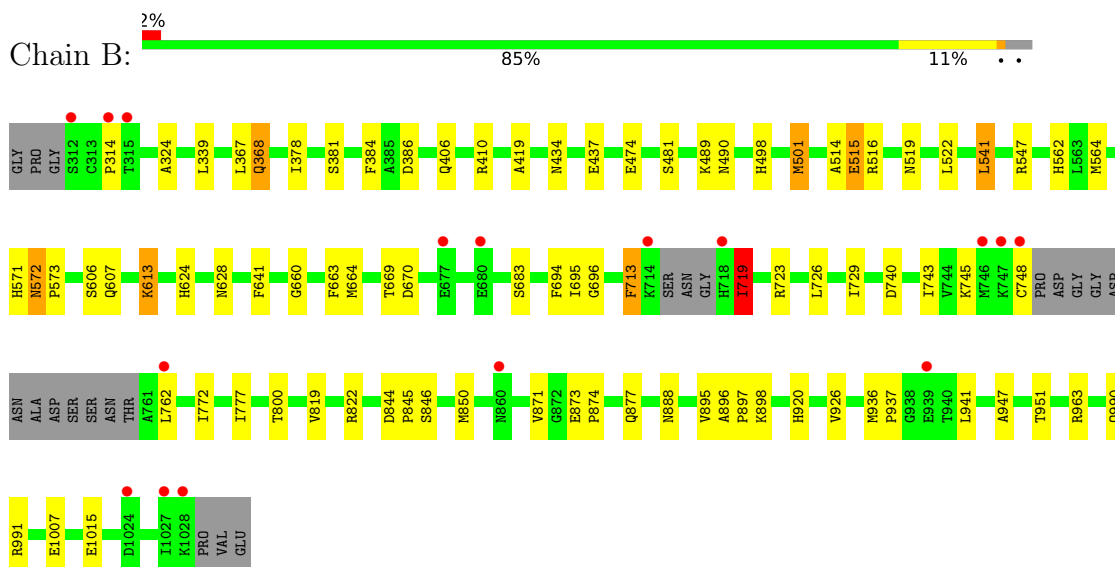
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

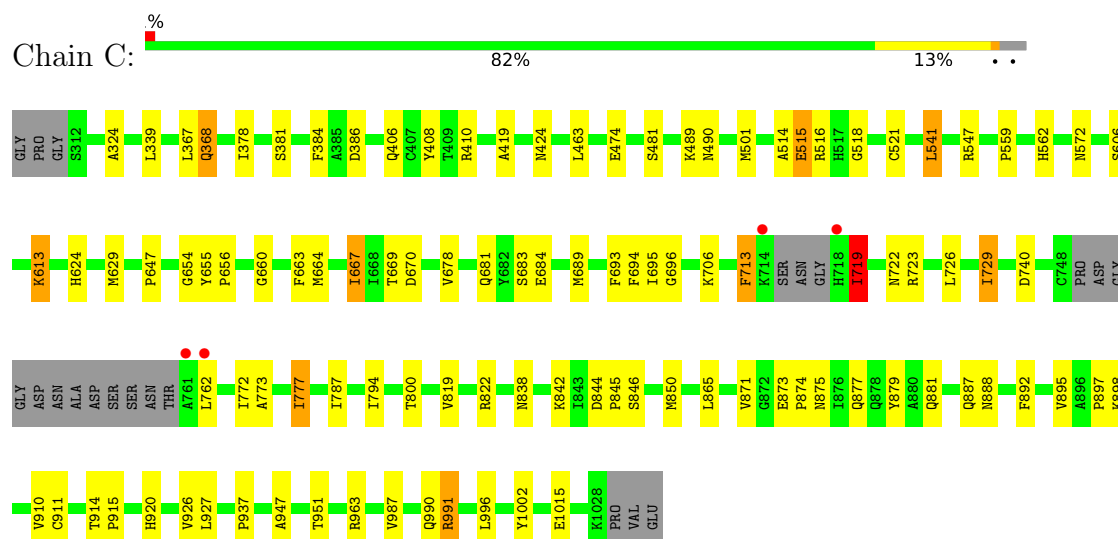
- Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit



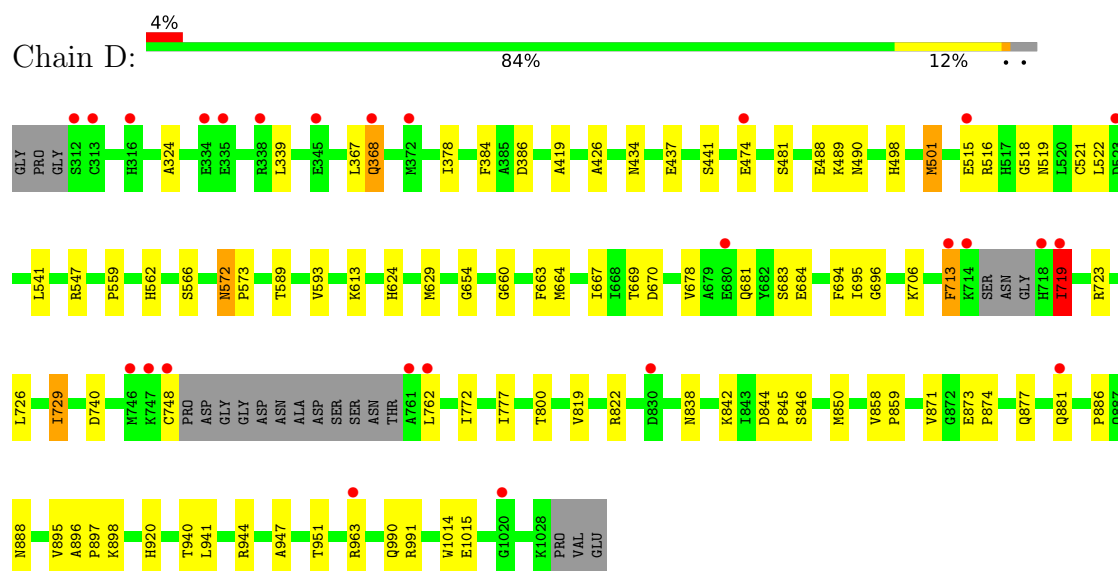
- Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit



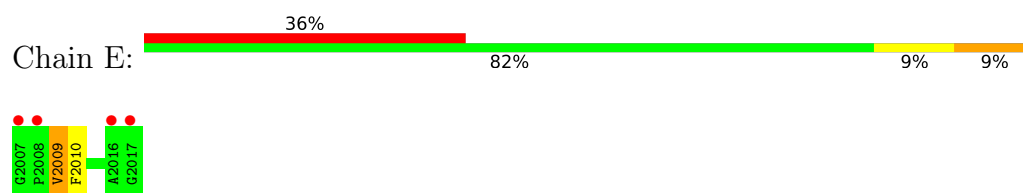
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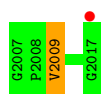


- Molecule 2: Keratin, type II cytoskeletal 7

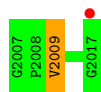
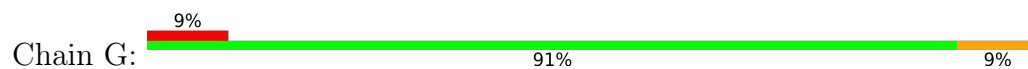


- Molecule 2: Keratin, type II cytoskeletal 7

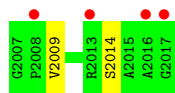
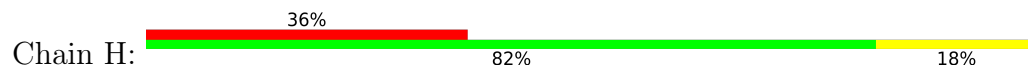




- Molecule 2: Keratin, type II cytoskeletal 7



- Molecule 2: Keratin, type II cytoskeletal 7



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	275.14Å 275.14Å 143.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 3.20 25.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (25.00-3.20) 98.8 (25.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 3.17Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.216 , 0.239 0.211 , 0.238	Depositor DCC
R_{free} test set	1015 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 4.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22608	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, SO4

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	0.88	1/5662 (0.0%)	0.97	7/7679 (0.1%)
1	B	0.90	1/5662 (0.0%)	0.98	7/7679 (0.1%)
1	C	0.80	1/5662 (0.0%)	0.97	7/7679 (0.1%)
1	D	0.91	1/5662 (0.0%)	0.99	7/7679 (0.1%)
2	E	1.37	0/74	1.17	0/99
2	F	1.31	0/74	1.17	0/99
2	G	1.46	0/74	1.11	0/99
2	H	1.31	0/74	1.20	0/99
All	All	0.88	4/22944 (0.0%)	0.98	28/31112 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	719	ILE	N-CA	5.62	1.53	1.46
1	D	719	ILE	N-CA	5.59	1.53	1.46
1	C	719	ILE	N-CA	5.53	1.53	1.46
1	A	719	ILE	N-CA	5.10	1.52	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	722	ASN	N-CA-C	7.01	118.68	110.41
1	A	858	VAL	CA-C-N	6.50	126.00	119.24
1	A	858	VAL	C-N-CA	6.50	126.00	119.24
1	C	762	LEU	N-CA-C	6.48	120.19	110.14
1	C	419	ALA	N-CA-C	6.26	117.77	111.07
1	D	762	LEU	N-CA-C	6.22	119.78	110.14
1	B	762	LEU	N-CA-C	6.00	119.49	109.95
1	D	419	ALA	N-CA-C	5.99	117.48	111.07
1	A	419	ALA	N-CA-C	5.98	118.29	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	996	LEU	N-CA-C	5.89	118.18	111.11
1	C	693	PHE	N-CA-C	-5.88	106.11	113.28
1	D	740	ASP	N-CA-C	5.79	117.47	109.54
1	A	762	LEU	N-CA-C	5.72	119.05	109.95
1	B	740	ASP	N-CA-C	5.69	117.33	109.54
1	D	858	VAL	CA-C-N	5.67	125.13	119.24
1	D	858	VAL	C-N-CA	5.67	125.13	119.24
1	A	722	ASN	N-CA-C	5.49	116.89	110.41
1	C	740	ASP	N-CA-C	5.44	117.00	109.54
1	A	996	LEU	N-CA-C	5.40	116.85	111.07
1	B	896	ALA	CA-C-N	5.32	125.26	119.78
1	B	896	ALA	C-N-CA	5.32	125.26	119.78
1	B	419	ALA	N-CA-C	5.29	117.45	111.11
1	B	606	SER	N-CA-C	-5.17	106.80	113.01
1	D	896	ALA	CA-C-N	5.16	125.15	119.89
1	D	896	ALA	C-N-CA	5.16	125.15	119.89
1	A	945	VAL	N-CA-C	5.13	115.35	110.53
1	B	743	ILE	N-CA-C	5.12	113.75	106.53
1	C	606	SER	N-CA-C	-5.06	106.94	113.01

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	5535	0	5503	54	0
1	B	5535	0	5503	50	0
1	C	5535	0	5503	60	0
1	D	5535	0	5503	52	0
2	E	73	0	70	3	0
2	F	73	0	70	2	0
2	G	73	0	70	2	0
2	H	73	0	70	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5	0	0	0	0
3	H	5	0	0	0	0
4	A	39	0	25	1	0
4	B	39	0	25	0	0
4	C	39	0	25	1	0
4	D	39	0	25	1	0
All	All	22608	0	22392	211	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:ARG:H	1:B:624:HIS:HD2	1.10	0.98
1:A:547:ARG:H	1:A:624:HIS:HD2	1.08	0.98
1:C:547:ARG:H	1:C:624:HIS:HD2	1.14	0.94
1:D:547:ARG:H	1:D:624:HIS:HD2	1.10	0.88
1:A:547:ARG:H	1:A:624:HIS:CD2	1.92	0.87
1:D:547:ARG:H	1:D:624:HIS:CD2	1.93	0.85
1:C:547:ARG:H	1:C:624:HIS:CD2	1.99	0.79
1:B:547:ARG:H	1:B:624:HIS:CD2	1.98	0.79
1:A:368:GLN:NE2	1:A:368:GLN:HA	1.98	0.78
1:D:368:GLN:NE2	1:D:368:GLN:HA	1.99	0.76
1:B:368:GLN:NE2	1:B:368:GLN:HA	2.06	0.70
1:A:368:GLN:HA	1:A:368:GLN:HE21	1.58	0.68
1:D:474:GLU:OE1	1:D:474:GLU:HA	1.92	0.67
1:C:368:GLN:NE2	1:C:368:GLN:HA	2.08	0.67
1:D:719:ILE:HG22	1:D:719:ILE:O	1.94	0.67
1:C:719:ILE:O	1:C:719:ILE:HG22	1.95	0.66
1:A:547:ARG:N	1:A:624:HIS:HD2	1.89	0.65
1:A:719:ILE:HG22	1:A:719:ILE:O	1.95	0.65
1:C:873:GLU:HB3	1:C:874:PRO:HD3	1.79	0.64
1:B:368:GLN:HA	1:B:368:GLN:HE21	1.64	0.62
1:A:410:ARG:NH2	1:B:410:ARG:NH2	2.48	0.61
1:D:547:ARG:N	1:D:624:HIS:HD2	1.91	0.61
1:A:695:ILE:HG13	1:A:696:GLY:N	2.14	0.61
1:D:368:GLN:HA	1:D:368:GLN:HE21	1.65	0.61
1:A:895:VAL:HG11	2:E:2009:VAL:HG21	1.83	0.60
1:D:559:PRO:HB2	4:D:1200:12V:H6'	1.83	0.60
1:D:895:VAL:HG11	2:H:2009:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:719:ILE:HG22	1:B:719:ILE:O	2.01	0.59
1:C:877:GLN:HA	1:C:877:GLN:OE1	2.01	0.59
1:C:474:GLU:HA	1:C:474:GLU:OE1	2.03	0.59
1:B:562:HIS:ND1	1:B:898:LYS:HE3	2.18	0.58
1:B:726:LEU:HD22	1:B:819:VAL:HG22	1.86	0.58
1:B:663:PHE:CD1	1:B:664:MET:HE2	2.39	0.58
1:C:895:VAL:HG11	2:G:2009:VAL:HG21	1.83	0.58
1:C:663:PHE:CD1	1:C:664:MET:HE2	2.39	0.57
1:D:562:HIS:ND1	1:D:898:LYS:HE3	2.19	0.57
1:A:562:HIS:ND1	1:A:898:LYS:HE3	2.18	0.57
1:D:895:VAL:HG11	2:H:2009:VAL:CG2	2.35	0.57
1:B:695:ILE:HG13	1:B:696:GLY:N	2.20	0.57
1:C:667:ILE:HG22	1:C:684:GLU:HB2	1.87	0.56
1:A:663:PHE:CD1	1:A:664:MET:HE2	2.42	0.55
1:B:474:GLU:HA	1:B:474:GLU:OE1	2.06	0.55
1:B:844:ASP:HB2	1:B:845:PRO:CD	2.37	0.54
1:B:895:VAL:HG11	2:F:2009:VAL:HG21	1.87	0.54
1:C:368:GLN:HA	1:C:368:GLN:HE21	1.72	0.54
1:A:1015:GLU:HA	1:A:1015:GLU:OE1	2.08	0.54
1:C:562:HIS:ND1	1:C:898:LYS:HE3	2.22	0.54
1:A:410:ARG:HH22	1:B:410:ARG:NH2	2.02	0.54
1:A:669:THR:OG1	1:A:670:ASP:N	2.41	0.54
1:A:713:PHE:CD2	1:A:713:PHE:N	2.75	0.54
1:B:947:ALA:O	1:B:951:THR:HG23	2.08	0.53
1:C:895:VAL:HG11	2:G:2009:VAL:CG2	2.37	0.53
1:A:406:GLN:O	1:A:410:ARG:HB2	2.09	0.53
1:B:723:ARG:HD2	1:B:822:ARG:HD2	1.91	0.53
1:A:947:ALA:O	1:A:951:THR:HG23	2.09	0.52
1:D:713:PHE:N	1:D:713:PHE:CD2	2.78	0.52
1:C:695:ILE:HG13	1:C:696:GLY:N	2.25	0.51
1:B:873:GLU:HB3	1:B:874:PRO:HD3	1.91	0.51
1:A:660:GLY:HA2	1:A:683:SER:HB3	1.92	0.51
1:A:895:VAL:HG11	2:E:2009:VAL:CG2	2.40	0.51
1:B:541:LEU:HD12	1:B:541:LEU:H	1.75	0.51
1:C:947:ALA:O	1:C:951:THR:HG23	2.10	0.51
1:D:947:ALA:O	1:D:951:THR:HG23	2.11	0.50
1:C:629:MET:O	1:C:654:GLY:HA3	2.11	0.50
1:A:474:GLU:HA	1:A:474:GLU:OE1	2.10	0.50
1:C:937:PRO:HG3	1:C:947:ALA:HB2	1.92	0.50
1:D:844:ASP:HB2	1:D:845:PRO:CD	2.41	0.50
1:A:662:LEU:HD21	1:D:886:PRO:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:723:ARG:HD2	1:C:822:ARG:HD2	1.94	0.50
1:D:519:ASN:HA	1:D:522:LEU:HD12	1.94	0.50
1:D:663:PHE:CD1	1:D:664:MET:HE2	2.47	0.49
1:A:490:ASN:HA	1:A:516:ARG:NH2	2.27	0.49
1:A:726:LEU:HD22	1:A:819:VAL:HG22	1.93	0.49
1:D:719:ILE:O	1:D:719:ILE:CG2	2.60	0.49
1:D:873:GLU:HB3	1:D:874:PRO:HD3	1.94	0.49
1:B:877:GLN:HA	1:B:877:GLN:OE1	2.13	0.49
1:D:726:LEU:HD22	1:D:819:VAL:HG22	1.93	0.49
1:D:695:ILE:HG13	1:D:696:GLY:N	2.27	0.49
1:A:873:GLU:HB3	1:A:874:PRO:HD3	1.95	0.49
1:A:937:PRO:HG3	1:A:947:ALA:HB2	1.94	0.49
1:A:368:GLN:NE2	1:A:368:GLN:CA	2.74	0.49
1:A:667:ILE:HG22	1:A:684:GLU:HB2	1.94	0.49
1:A:723:ARG:HD2	1:A:822:ARG:HD2	1.95	0.49
1:B:941:LEU:C	1:B:941:LEU:HD23	2.38	0.49
1:C:713:PHE:N	1:C:713:PHE:CD2	2.79	0.49
1:D:434:ASN:HB3	1:D:437:GLU:OE1	2.13	0.48
1:B:406:GLN:O	1:B:410:ARG:HB2	2.13	0.48
1:D:669:THR:OG1	1:D:670:ASP:N	2.44	0.48
1:A:773:ALA:O	1:A:777:ILE:HG12	2.14	0.48
1:B:713:PHE:CD2	1:B:713:PHE:N	2.82	0.48
1:B:547:ARG:N	1:B:624:HIS:HD2	1.93	0.48
1:B:850:MET:HE2	1:B:963:ARG:HG2	1.94	0.48
1:D:490:ASN:HA	1:D:516:ARG:NH2	2.28	0.48
1:B:324:ALA:HB2	1:B:339:LEU:HB2	1.95	0.48
1:C:408:TYR:CZ	1:C:424:ASN:HB3	2.49	0.48
1:C:660:GLY:HA2	1:C:683:SER:HB3	1.95	0.48
1:C:865:LEU:O	1:C:892:PHE:HA	2.14	0.48
1:A:368:GLN:HE21	1:A:368:GLN:CA	2.24	0.48
1:C:559:PRO:HB2	4:C:1102:12V:H6'	1.95	0.48
1:C:490:ASN:HA	1:C:516:ARG:NH2	2.28	0.47
1:D:723:ARG:HD2	1:D:822:ARG:HD2	1.96	0.47
1:D:877:GLN:O	1:D:881:GLN:OE1	2.32	0.47
1:A:898:LYS:HE2	4:A:1102:12V:O3B	2.14	0.47
1:B:434:ASN:HB3	1:B:437:GLU:OE1	2.15	0.47
1:C:406:GLN:O	1:C:410:ARG:HB2	2.14	0.47
1:C:844:ASP:HB2	1:C:845:PRO:CD	2.45	0.47
1:B:660:GLY:HA2	1:B:683:SER:HB3	1.97	0.46
1:B:519:ASN:HA	1:B:522:LEU:HD12	1.97	0.46
1:A:581:TYR:CE1	1:A:603:ILE:HD13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:ILE:O	1:A:719:ILE:CG2	2.62	0.46
1:A:877:GLN:HA	1:A:877:GLN:OE1	2.15	0.46
1:A:434:ASN:HB3	1:A:437:GLU:OE1	2.16	0.46
1:B:897:PRO:O	1:B:898:LYS:C	2.59	0.46
1:A:850:MET:HE2	1:A:963:ARG:HG2	1.98	0.46
1:B:628:ASN:HB2	1:B:641:PHE:CZ	2.51	0.46
1:D:368:GLN:HE21	1:D:368:GLN:CA	2.28	0.46
1:D:729:ILE:HD13	1:D:729:ILE:HA	1.88	0.46
1:A:384:PHE:CE2	1:A:386:ASP:HB3	2.51	0.45
1:D:572:ASN:HA	1:D:573:PRO:HD3	1.83	0.45
1:C:719:ILE:O	1:C:719:ILE:CG2	2.63	0.45
1:B:694:PHE:CZ	1:B:920:HIS:HB3	2.52	0.45
1:C:624:HIS:O	1:C:647:PRO:HG2	2.16	0.45
1:A:881:GLN:HE22	1:A:887:GLN:HG2	1.82	0.45
1:D:368:GLN:NE2	1:D:368:GLN:CA	2.75	0.45
1:D:660:GLY:HA2	1:D:683:SER:HB3	1.97	0.45
1:B:314:PRO:HG2	2:E:2010:PHE:HZ	1.81	0.45
1:C:694:PHE:CZ	1:C:920:HIS:HB3	2.52	0.45
1:C:881:GLN:HE22	1:C:887:GLN:HG2	1.82	0.45
1:A:324:ALA:HB2	1:A:339:LEU:HB2	1.98	0.45
1:C:875:ASN:O	1:C:879:TYR:HD2	2.00	0.45
1:D:518:GLY:O	1:D:521:CYS:HB2	2.17	0.45
1:B:613:LYS:H	1:B:613:LYS:HG2	1.52	0.44
1:C:547:ARG:N	1:C:624:HIS:HD2	1.97	0.44
1:C:897:PRO:O	1:C:898:LYS:C	2.60	0.44
1:C:773:ALA:O	1:C:777:ILE:HG12	2.16	0.44
1:A:844:ASP:HB2	1:A:845:PRO:CD	2.47	0.44
1:A:838:ASN:HB3	1:A:842:LYS:HD2	1.99	0.44
1:B:937:PRO:HG3	1:B:947:ALA:HB2	1.99	0.44
1:C:689:MET:HE2	1:C:1002:TYR:CZ	2.52	0.44
1:A:695:ILE:HG13	1:A:696:GLY:H	1.83	0.44
1:B:895:VAL:HG11	2:F:2009:VAL:CG2	2.47	0.44
1:C:838:ASN:HB3	1:C:842:LYS:HD2	2.00	0.44
1:D:1015:GLU:HA	1:D:1015:GLU:OE1	2.17	0.44
1:A:518:GLY:O	1:A:521:CYS:HB2	2.18	0.44
1:C:514:ALA:O	1:C:515:GLU:C	2.61	0.44
1:C:1015:GLU:HA	1:C:1015:GLU:OE1	2.17	0.44
1:D:940:THR:O	1:D:944:ARG:HG3	2.18	0.44
1:B:564:MET:C	1:B:564:MET:SD	3.01	0.43
1:C:729:ILE:HD13	1:C:729:ILE:HA	1.89	0.43
1:C:777:ILE:HG12	1:C:777:ILE:H	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:HIS:O	1:B:501:MET:HE2	2.18	0.43
1:B:490:ASN:HA	1:B:516:ARG:NH2	2.34	0.43
1:B:1015:GLU:HA	1:B:1015:GLU:OE1	2.17	0.43
1:C:910:VAL:HG12	1:C:911:CYS:N	2.32	0.43
1:D:629:MET:O	1:D:654:GLY:HA3	2.19	0.43
1:C:914:THR:HA	1:C:915:PRO:HD3	1.89	0.43
1:D:384:PHE:CE2	1:D:386:ASP:HB3	2.54	0.43
1:D:426:ALA:HB2	1:D:441:SER:HB2	2.01	0.43
1:A:408:TYR:CZ	1:A:424:ASN:HB3	2.53	0.42
1:B:669:THR:OG1	1:B:670:ASP:N	2.51	0.42
1:A:571:HIS:HA	1:A:1007:GLU:OE2	2.18	0.42
1:B:719:ILE:O	1:B:719:ILE:CG2	2.67	0.42
1:B:514:ALA:O	1:B:515:GLU:C	2.62	0.42
1:D:941:LEU:C	1:D:941:LEU:HD23	2.44	0.42
1:B:410:ARG:HH22	1:C:410:ARG:NH2	2.18	0.42
1:C:324:ALA:HB2	1:C:339:LEU:HB2	2.01	0.42
1:D:694:PHE:CZ	1:D:920:HIS:HB3	2.54	0.42
1:D:850:MET:HE2	1:D:963:ARG:HG2	2.00	0.42
1:B:571:HIS:HA	1:B:1007:GLU:OE2	2.20	0.42
1:A:777:ILE:HG12	1:A:777:ILE:H	1.63	0.42
1:C:678:VAL:O	1:C:681:GLN:HG2	2.20	0.42
1:C:850:MET:HE2	1:C:963:ARG:HG2	2.02	0.42
1:D:713:PHE:N	1:D:713:PHE:HD2	2.18	0.42
1:A:561:SER:O	1:A:565:GLN:HB3	2.20	0.42
1:B:572:ASN:HA	1:B:573:PRO:HD3	1.80	0.42
1:C:910:VAL:CG1	1:C:911:CYS:N	2.82	0.42
1:A:509:PHE:HE1	1:D:859:PRO:HG3	1.85	0.41
1:B:381:SER:O	1:B:384:PHE:HB2	2.20	0.41
1:D:838:ASN:HB3	1:D:842:LYS:HD2	2.02	0.41
1:D:897:PRO:O	1:D:898:LYS:C	2.63	0.41
1:A:941:LEU:HD23	1:A:941:LEU:C	2.45	0.41
1:C:927:LEU:HD23	1:C:927:LEU:HA	1.89	0.41
1:D:498:HIS:O	1:D:501:MET:HE2	2.21	0.41
1:A:589:THR:O	1:A:593:VAL:HG23	2.19	0.41
1:B:607:GLN:HE21	1:B:607:GLN:HB2	1.69	0.41
1:C:541:LEU:HD12	1:C:541:LEU:H	1.85	0.41
1:C:518:GLY:O	1:C:521:CYS:HB2	2.20	0.41
1:A:694:PHE:CZ	1:A:920:HIS:HB3	2.56	0.41
1:C:669:THR:OG1	1:C:670:ASP:N	2.49	0.41
1:C:381:SER:O	1:C:384:PHE:HB2	2.20	0.41
1:C:726:LEU:HD22	1:C:819:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:787:ILE:HG13	1:C:794:ILE:HB	2.02	0.41
1:D:877:GLN:HA	1:D:877:GLN:OE1	2.21	0.41
1:C:384:PHE:CE2	1:C:386:ASP:HB3	2.55	0.41
1:D:324:ALA:HB2	1:D:339:LEU:HB2	2.02	0.41
1:A:876:ILE:O	1:A:877:GLN:C	2.61	0.41
1:C:463:LEU:HD23	1:C:463:LEU:HA	1.94	0.41
1:C:987:VAL:O	1:C:991:ARG:HG2	2.21	0.41
1:D:589:THR:O	1:D:593:VAL:HG23	2.20	0.40
1:C:655:TYR:HA	1:C:656:PRO:HD3	1.96	0.40
1:C:873:GLU:O	1:C:874:PRO:C	2.65	0.40
1:D:678:VAL:O	1:D:681:GLN:HG2	2.21	0.40
1:A:426:ALA:HB2	1:A:441:SER:HB2	2.04	0.40
1:B:384:PHE:CE2	1:B:386:ASP:HB3	2.56	0.40
1:D:488:GLU:C	1:D:490:ASN:H	2.29	0.40
1:D:1014:TRP:O	1:D:1015:GLU:C	2.64	0.40
1:B:936:MET:HA	1:B:937:PRO:HD3	1.91	0.40
1:C:613:LYS:H	1:C:613:LYS:HG2	1.54	0.40
1:A:519:ASN:HA	1:A:522:LEU:HD12	2.02	0.40
1:B:844:ASP:HB2	1:B:845:PRO:HD3	2.04	0.40
1:D:667:ILE:HG22	1:D:684:GLU:HB2	2.03	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	696/723 (96%)	659 (95%)	35 (5%)	2 (0%)	36 68
1	B	696/723 (96%)	654 (94%)	40 (6%)	2 (0%)	36 68
1	C	696/723 (96%)	652 (94%)	42 (6%)	2 (0%)	36 68
1	D	696/723 (96%)	657 (94%)	37 (5%)	2 (0%)	36 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	9/11 (82%)	9 (100%)	0	0	100	100
2	F	9/11 (82%)	9 (100%)	0	0	100	100
2	G	9/11 (82%)	9 (100%)	0	0	100	100
2	H	9/11 (82%)	8 (89%)	1 (11%)	0	100	100
All	All	2820/2936 (96%)	2657 (94%)	155 (6%)	8 (0%)	36	68

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	888	ASN
1	C	888	ASN
1	D	719	ILE
1	B	719	ILE
1	B	888	ASN
1	D	888	ASN
1	A	719	ILE
1	C	719	ILE

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	601/618 (97%)	575 (96%)	26 (4%)	26	59
1	B	601/618 (97%)	579 (96%)	22 (4%)	30	63
1	C	601/618 (97%)	579 (96%)	22 (4%)	30	63
1	D	601/618 (97%)	579 (96%)	22 (4%)	30	63
2	E	7/7 (100%)	6 (86%)	1 (14%)	3	16
2	F	7/7 (100%)	6 (86%)	1 (14%)	3	16
2	G	7/7 (100%)	6 (86%)	1 (14%)	3	16
2	H	7/7 (100%)	6 (86%)	1 (14%)	3	16
All	All	2432/2500 (97%)	2336 (96%)	96 (4%)	28	62

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	LEU
1	A	368	GLN
1	A	378	ILE
1	A	410	ARG
1	A	471	ASP
1	A	481	SER
1	A	489	LYS
1	A	501	MET
1	A	541	LEU
1	A	572	ASN
1	A	613	LYS
1	A	644	ARG
1	A	667	ILE
1	A	706	LYS
1	A	713	PHE
1	A	729	ILE
1	A	748	CYS
1	A	771	THR
1	A	772	ILE
1	A	777	ILE
1	A	800	THR
1	A	846	SER
1	A	871	VAL
1	A	898	LYS
1	A	990	GLN
1	A	991	ARG
1	B	367	LEU
1	B	368	GLN
1	B	378	ILE
1	B	481	SER
1	B	489	LYS
1	B	501	MET
1	B	515	GLU
1	B	541	LEU
1	B	572	ASN
1	B	613	LYS
1	B	713	PHE
1	B	729	ILE
1	B	745	LYS
1	B	748	CYS
1	B	772	ILE
1	B	777	ILE

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Mol	Chain	Res	Type
1	B	800	THR
1	B	846	SER
1	B	871	VAL
1	B	926	VAL
1	B	990	GLN
1	B	991	ARG
1	C	367	LEU
1	C	368	GLN
1	C	378	ILE
1	C	481	SER
1	C	489	LYS
1	C	501	MET
1	C	515	GLU
1	C	541	LEU
1	C	572	ASN
1	C	613	LYS
1	C	667	ILE
1	C	706	LYS
1	C	713	PHE
1	C	729	ILE
1	C	772	ILE
1	C	777	ILE
1	C	800	THR
1	C	846	SER
1	C	871	VAL
1	C	926	VAL
1	C	990	GLN
1	C	991	ARG
1	D	367	LEU
1	D	368	GLN
1	D	378	ILE
1	D	481	SER
1	D	489	LYS
1	D	501	MET
1	D	515	GLU
1	D	541	LEU
1	D	566	SER
1	D	572	ASN
1	D	613	LYS
1	D	706	LYS
1	D	713	PHE
1	D	729	ILE

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Mol	Chain	Res	Type
1	D	748	CYS
1	D	772	ILE
1	D	777	ILE
1	D	800	THR
1	D	846	SER
1	D	871	VAL
1	D	990	GLN
1	D	991	ARG
2	E	2009	VAL
2	F	2009	VAL
2	G	2009	VAL
2	H	2014	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	363	GLN
1	A	368	GLN
1	A	413	GLN
1	A	434	ASN
1	A	517	HIS
1	A	607	GLN
1	A	620	GLN
1	A	624	HIS
1	A	691	HIS
1	A	763	ASN
1	A	781	ASN
1	A	786	GLN
1	A	881	GLN
1	B	363	GLN
1	B	368	GLN
1	B	413	GLN
1	B	434	ASN
1	B	607	GLN
1	B	620	GLN
1	B	624	HIS
1	B	691	HIS
1	B	700	ASN
1	B	786	GLN
1	B	881	GLN
1	B	1012	GLN
1	C	363	GLN

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Mol	Chain	Res	Type
1	C	368	GLN
1	C	413	GLN
1	C	434	ASN
1	C	607	GLN
1	C	620	GLN
1	C	624	HIS
1	C	691	HIS
1	C	700	ASN
1	C	786	GLN
1	C	881	GLN
1	C	901	HIS
1	C	1012	GLN
1	D	363	GLN
1	D	368	GLN
1	D	434	ASN
1	D	507	HIS
1	D	607	GLN
1	D	620	GLN
1	D	624	HIS
1	D	700	ASN
1	D	763	ASN
1	D	786	GLN
1	D	881	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 oligosaccharides 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
3	SO4	B	1101	-	4,4,4	0.23	0	6,6,6	0.13	0
4	12V	A	1102	-	38,41,41	1.61	5 (13%)	52,62,62	1.99	14 (26%)
4	12V	C	1102	-	38,41,41	1.05	3 (7%)	52,62,62	1.66	12 (23%)
3	SO4	A	1101	-	4,4,4	0.28	0	6,6,6	0.46	0
4	12V	B	1102	-	38,41,41	1.30	4 (10%)	52,62,62	1.78	11 (21%)
3	SO4	H	2101	-	4,4,4	0.23	0	6,6,6	0.17	0
4	12V	D	1200	-	38,41,41	1.35	4 (10%)	52,62,62	1.60	8 (15%)
3	SO4	C	1101	-	4,4,4	0.22	0	6,6,6	0.28	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	D	1200	-	-	6/25/63/63	0/3/3/3
4	12V	A	1102	-	-	5/25/63/63	0/3/3/3
4	12V	C	1102	-	-	4/25/63/63	0/3/3/3
4	12V	B	1102	-	-	6/25/63/63	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1102	12V	PA-O3A	5.82	1.65	1.59
4	D	1200	12V	C4'-C5'	-3.89	1.50	1.53
4	D	1200	12V	C5'-S5'	-3.51	1.76	1.82
4	A	1102	12V	C6'-C5'	3.47	1.55	1.52
4	B	1102	12V	C2-N1	-3.19	1.33	1.38
4	B	1102	12V	PA-O3A	3.17	1.62	1.59
4	C	1102	12V	C5'-S5'	-3.07	1.77	1.82
4	C	1102	12V	C2-N1	-2.81	1.34	1.38
4	A	1102	12V	C2-N1	-2.77	1.34	1.38
4	A	1102	12V	C5'-S5'	-2.56	1.78	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1200	12V	C2-N1	-2.46	1.34	1.38
4	B	1102	12V	C5'-S5'	-2.43	1.78	1.82
4	B	1102	12V	C3'-C2'	2.23	1.57	1.53
4	C	1102	12V	C6-C5	2.21	1.40	1.35
4	A	1102	12V	C3B-C2B	-2.20	1.47	1.53
4	D	1200	12V	C5-C4	-2.03	1.39	1.43

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	12V	C4-N3-C2	-6.42	118.64	126.61
4	B	1102	12V	C1'-C2'-N2'	-6.15	99.88	111.07
4	A	1102	12V	N3-C2-N1	5.38	121.89	114.89
4	C	1102	12V	N3-C2-N1	5.21	121.67	114.89
4	C	1102	12V	C4-N3-C2	-4.75	120.71	126.61
4	D	1200	12V	C4-N3-C2	-4.62	120.88	126.61
4	B	1102	12V	C4-N3-C2	-4.27	121.31	126.61
4	D	1200	12V	O1'-C1'-C2'	4.25	113.98	107.52
4	A	1102	12V	C5-C4-N3	4.22	120.71	114.80
4	C	1102	12V	C1'-C2'-N2'	-4.03	103.74	111.07
4	A	1102	12V	C3B-C2B-C1B	-3.91	94.07	101.46
4	A	1102	12V	C4B-O4B-C1B	-3.87	100.92	109.47
4	D	1200	12V	N3-C2-N1	3.57	119.54	114.89
4	D	1200	12V	C5-C4-N3	3.54	119.76	114.80
4	B	1102	12V	N3-C2-N1	3.48	119.43	114.89
4	A	1102	12V	O1'-C1'-C2'	3.48	112.81	107.52
4	B	1102	12V	C5-C4-N3	3.29	119.41	114.80
4	B	1102	12V	O1'-C1'-C2'	3.25	112.47	107.52
4	D	1200	12V	C1'-C2'-N2'	-2.99	105.63	111.07
4	C	1102	12V	O4B-C1B-N1	2.79	114.69	108.36
4	A	1102	12V	O4B-C1B-N1	2.75	114.59	108.36
4	B	1102	12V	O3'-C3'-C4'	-2.71	103.98	110.38
4	B	1102	12V	O4-C4-C5	-2.62	120.65	125.16
4	D	1200	12V	O3A-PB-O1B	-2.56	103.00	110.70
4	B	1102	12V	O3'-C3'-C2'	2.55	114.66	109.58
4	B	1102	12V	C3'-C2'-N2'	2.54	115.29	110.62
4	C	1102	12V	O2-C2-N1	-2.50	119.55	122.80
4	D	1200	12V	C3B-C2B-C1B	-2.49	96.76	101.46
4	A	1102	12V	C1'-C2'-N2'	-2.47	106.58	111.07
4	A	1102	12V	C5-C6-N1	-2.45	117.86	121.84
4	B	1102	12V	O2-C2-N1	-2.42	119.65	122.80
4	A	1102	12V	C5B-C4B-C3B	-2.41	106.52	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1200	12V	O4-C4-C5	-2.38	121.06	125.16
4	A	1102	12V	O2B-PB-O3A	2.30	113.50	107.27
4	C	1102	12V	O3A-PB-O1B	-2.26	103.91	110.70
4	B	1102	12V	C6'-C5'-C4'	-2.23	104.94	114.44
4	C	1102	12V	O4B-C4B-C5B	-2.14	102.48	109.33
4	C	1102	12V	O4B-C1B-C2B	-2.10	102.12	106.62
4	A	1102	12V	O2-C2-N1	-2.10	120.07	122.80
4	C	1102	12V	C5-C4-N3	2.09	117.73	114.80
4	C	1102	12V	O2B-PB-O3A	2.08	112.89	107.27
4	A	1102	12V	O4B-C1B-C2B	-2.08	102.17	106.62
4	A	1102	12V	O4-C4-C5	-2.05	121.63	125.16
4	C	1102	12V	O2A-PA-O1A	2.03	121.87	112.44
4	C	1102	12V	C5B-C4B-C3B	-2.01	107.98	115.21

There are no chirality outliers.

All (21) torsion outliers are listed below:

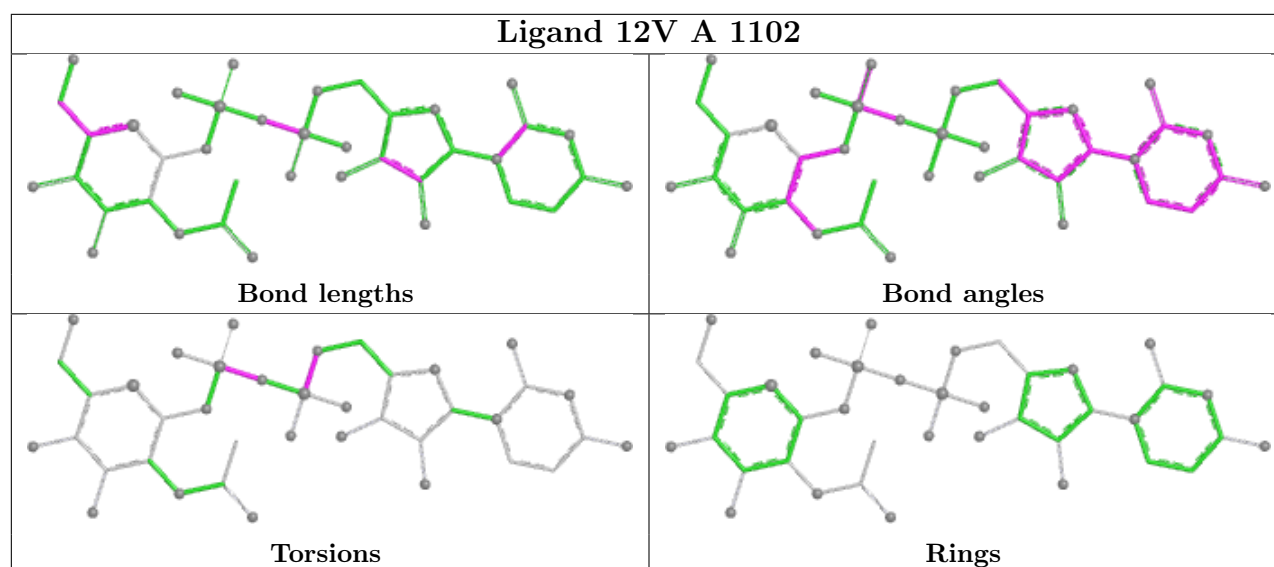
Mol	Chain	Res	Type	Atoms
4	A	1102	12V	C5B-O5B-PA-O1A
4	A	1102	12V	C5B-O5B-PA-O2A
4	B	1102	12V	C3B-C4B-C5B-O5B
4	B	1102	12V	C4'-C5'-C6'-O6'
4	B	1102	12V	S5'-C5'-C6'-O6'
4	D	1200	12V	C5B-O5B-PA-O3A
4	D	1200	12V	C3B-C4B-C5B-O5B
4	B	1102	12V	O4B-C4B-C5B-O5B
4	C	1102	12V	C3B-C4B-C5B-O5B
4	C	1102	12V	O4B-C4B-C5B-O5B
4	D	1200	12V	O4B-C4B-C5B-O5B
4	A	1102	12V	PA-O3A-PB-O1B
4	B	1102	12V	PA-O3A-PB-O2B
4	A	1102	12V	C5B-O5B-PA-O3A
4	A	1102	12V	PA-O3A-PB-O2B
4	C	1102	12V	PA-O3A-PB-O1B
4	B	1102	12V	PA-O3A-PB-O1B
4	D	1200	12V	PA-O3A-PB-O1B
4	C	1102	12V	PA-O3A-PB-O2B
4	D	1200	12V	PA-O3A-PB-O2B
4	D	1200	12V	C1'-C2'-N2'-C7'

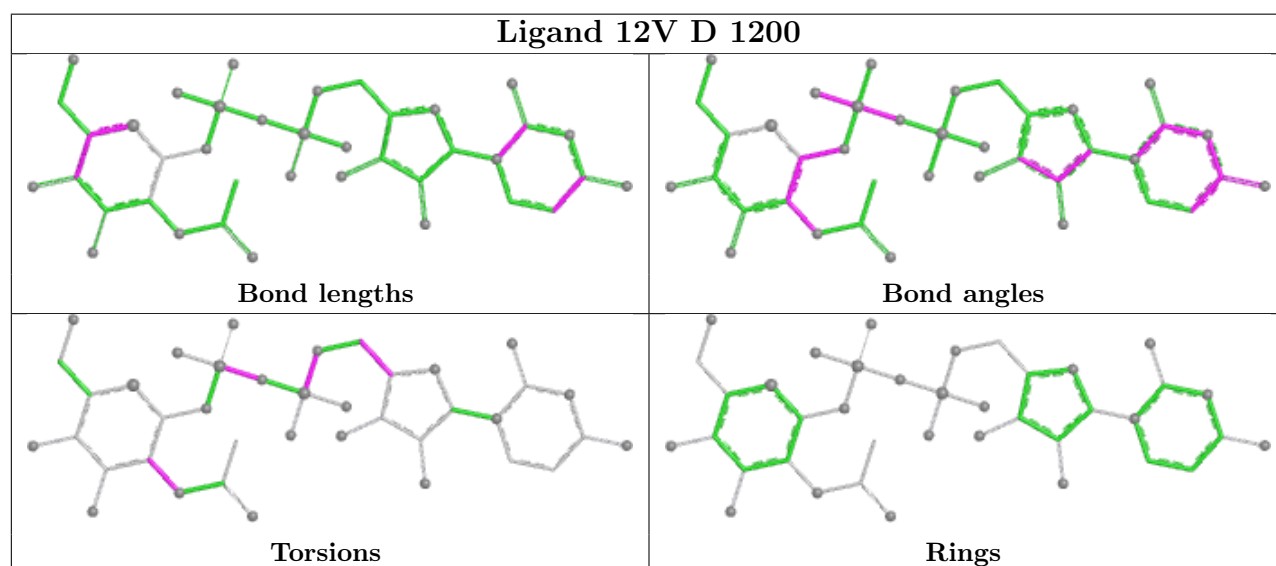
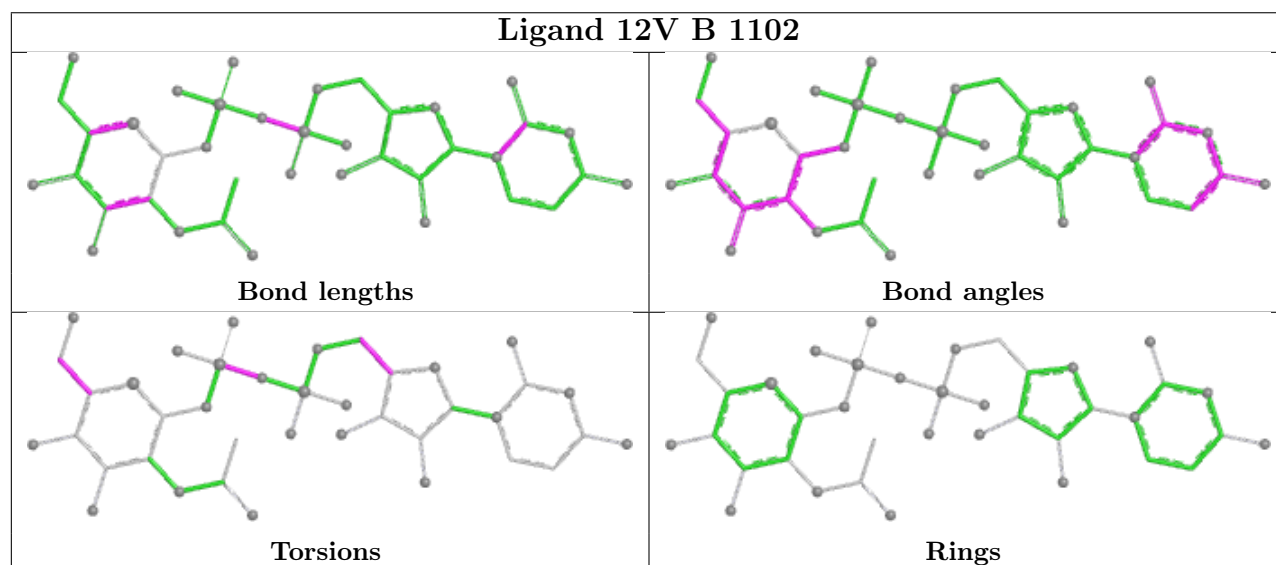
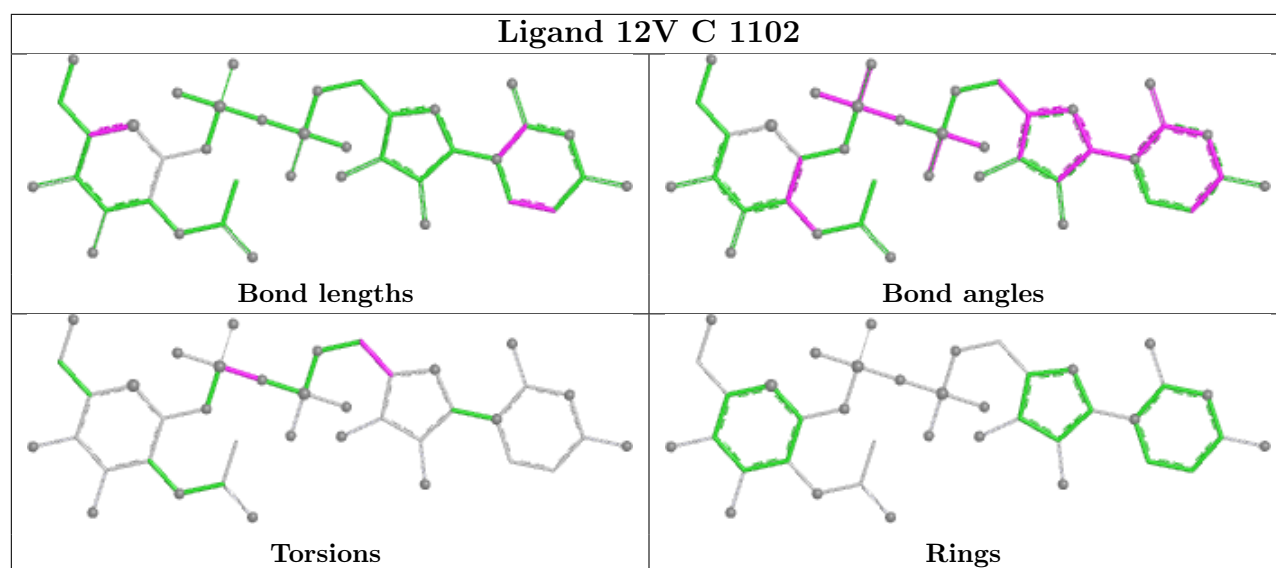
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1102	12V	1	0
4	C	1102	12V	1	0
4	D	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å ²)	Q<0.9
1	A	702/723 (97%)	0.01	21 (2%) 52 33	35, 51, 78, 113	0
1	B	702/723 (97%)	-0.03	16 (2%) 61 41	35, 51, 78, 113	0
1	C	702/723 (97%)	-0.06	4 (0%) 85 73	36, 51, 78, 113	0
1	D	702/723 (97%)	0.09	26 (3%) 45 28	35, 51, 78, 113	0
2	E	11/11 (100%)	1.70	4 (36%) 1 1	49, 69, 83, 85	0
2	F	11/11 (100%)	1.12	1 (9%) 15 9	49, 69, 83, 85	0
2	G	11/11 (100%)	1.51	1 (9%) 15 9	49, 69, 83, 85	0
2	H	11/11 (100%)	1.48	4 (36%) 1 1	49, 69, 83, 85	0
All	All	2852/2936 (97%)	0.03	77 (2%) 56 36	35, 52, 79, 113	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	2017	GLY	5.4
2	G	2017	GLY	4.6
1	D	312	SER	4.4
1	D	718	HIS	4.4
2	F	2017	GLY	4.2
2	H	2017	GLY	4.1
1	B	312	SER	4.0
1	A	523	ASP	3.9
1	A	888	ASN	3.7
1	C	718	HIS	3.6
1	B	1028	LYS	3.6
1	B	860	ASN	3.4
1	D	368	GLN	3.4
1	D	762	LEU	3.4
1	D	313	CYS	3.4
1	B	746	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	859	PRO	3.4
1	B	718	HIS	3.4
1	A	718	HIS	3.4
1	B	747	LYS	3.3
1	D	523	ASP	3.3
1	B	714	LYS	3.2
1	D	747	LYS	3.2
1	C	761	ALA	3.2
1	B	315	THR	3.2
1	C	762	LEU	3.0
1	A	489	LYS	3.0
1	D	334	GLU	3.0
1	C	714	LYS	3.0
1	A	761	ALA	2.9
1	B	748	CYS	2.8
2	H	2008	PRO	2.8
1	B	762	LEU	2.7
1	D	474	GLU	2.7
1	A	860	ASN	2.7
1	A	714	LYS	2.6
2	E	2007	GLY	2.6
1	B	1024	ASP	2.5
1	B	680	GLU	2.4
2	H	2013	ARG	2.4
1	D	761	ALA	2.4
1	A	515	GLU	2.4
1	D	713	PHE	2.4
1	A	740	ASP	2.4
1	D	748	CYS	2.4
2	E	2016	ALA	2.4
1	D	881	GLN	2.4
1	D	338	ARG	2.4
1	D	372	MET	2.3
1	B	314	PRO	2.3
1	D	746	MET	2.3
1	D	680	GLU	2.3
1	A	748	CYS	2.3
1	A	386	ASP	2.3
1	D	515	GLU	2.3
1	D	719	ILE	2.3
2	H	2016	ALA	2.3
1	D	316	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	747	LYS	2.2
1	A	313	CYS	2.2
1	A	329	GLU	2.2
1	D	345	GLU	2.2
1	A	506	SER	2.2
1	D	714	LYS	2.2
1	B	677	GLU	2.2
1	A	1028	LYS	2.1
1	A	491	ARG	2.1
1	B	939	GLU	2.1
1	D	830	ASP	2.1
1	D	1020	GLY	2.1
2	E	2008	PRO	2.1
1	D	335	GLU	2.1
1	A	680	GLU	2.1
1	A	713	PHE	2.1
1	B	1027	ILE	2.0
1	D	963	ARG	2.0
1	A	762	LEU	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	SO4	A	1101	5/5	0.86	0.14	92,92,93,93	0
3	SO4	C	1101	5/5	0.88	0.09	106,107,107,108	0
3	SO4	H	2101	5/5	0.92	0.10	93,93,94,94	0
3	SO4	B	1101	5/5	0.93	0.11	98,98,99,99	0

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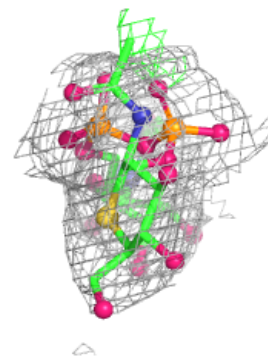
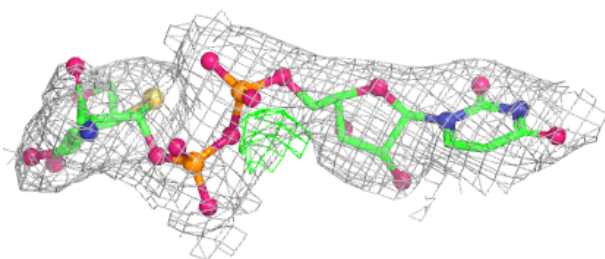
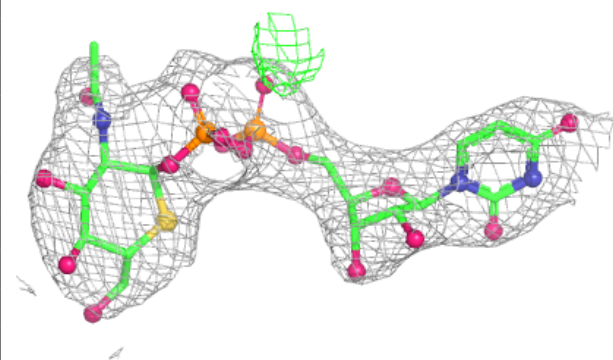
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	12V	C	1102	39/39	0.96	0.07	56,58,63,65	0
4	12V	A	1102	39/39	0.97	0.08	38,43,47,49	0
4	12V	B	1102	39/39	0.98	0.06	37,39,44,47	0
4	12V	D	1200	39/39	0.98	0.06	37,39,48,51	0

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.

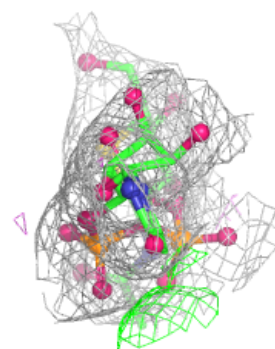
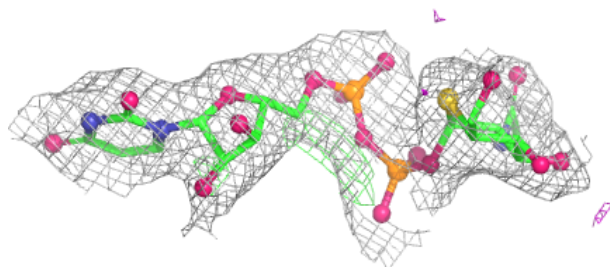
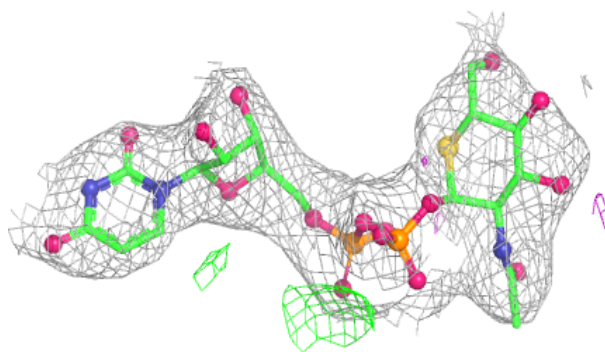
Electron density around 12V C 1102:

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

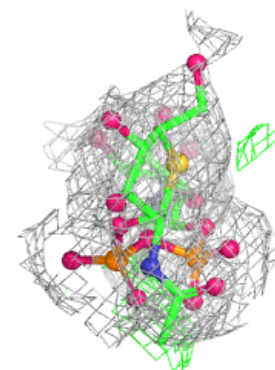
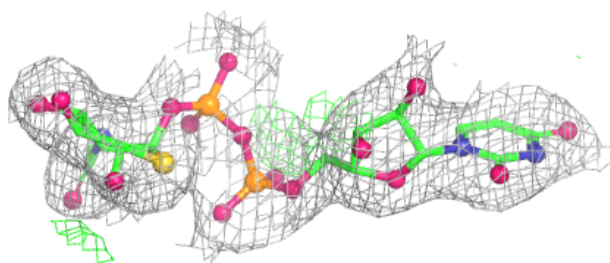
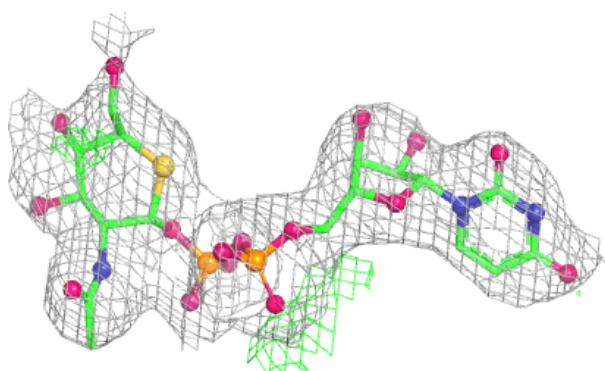


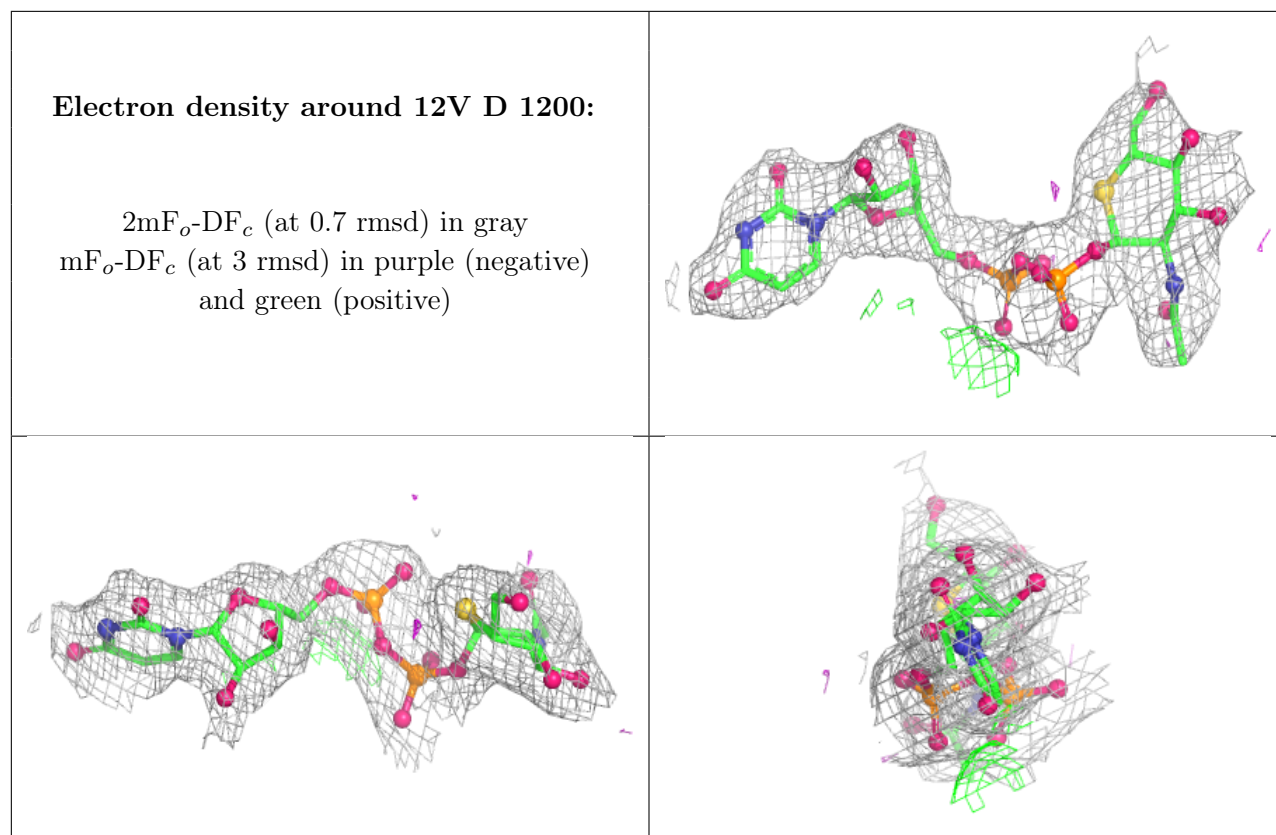
Electron density around 12V A 1102:

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

**Electron density around 12V B 1102:**

$2mF_o-DF_c$ (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.