



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:30 AM UTC

PDB ID : 4AY6 / pdb_00004ay6
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 types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) 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

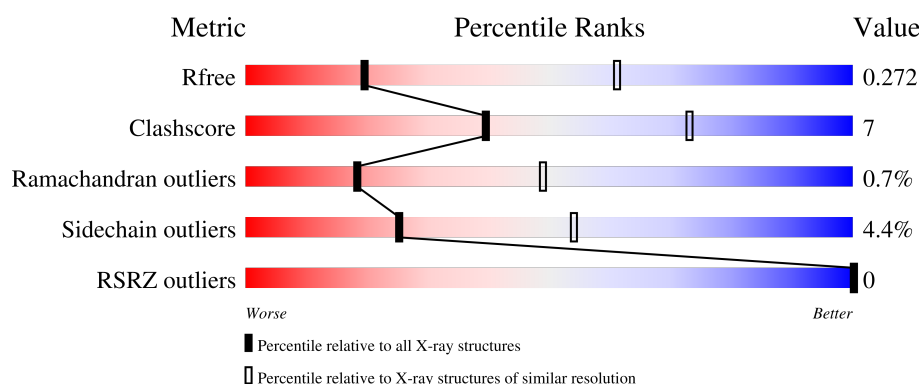
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	
1	B	723	
1	C	723	
1	D	723	
2	E	13	

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Mol	Chain	Length	Quality of chain
2	F	13	 46% 31% 8% 15%
2	G	13	 46% 23% 15% 15%
2	H	13	 54% 23% 8% 15%

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

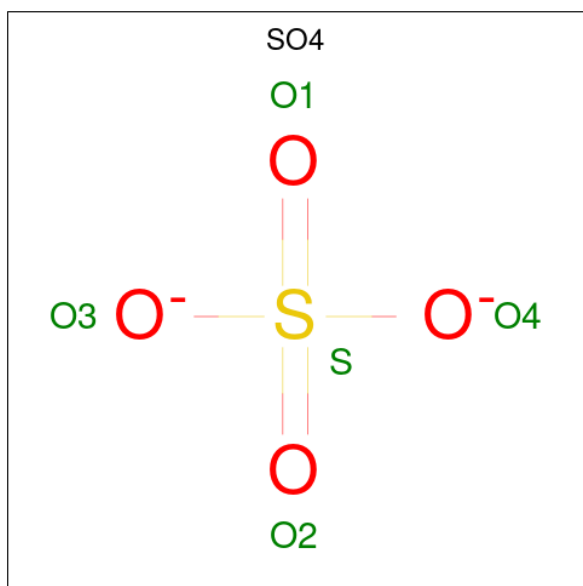
- Molecule 2 is a protein called TGF-BETA-ACTIVATED KINASE 1 AND MAP3K7-BINDING PROTEIN 1.

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:

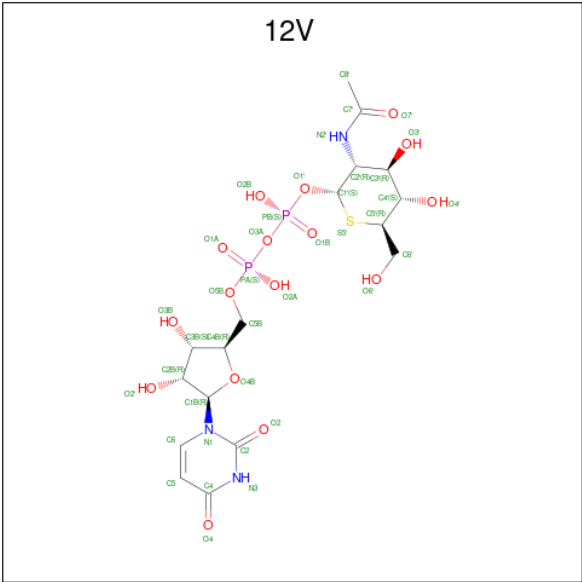
Chain	Residue	Modelled	Actual	Comment	Reference
E	1395	DNP	SER	SEE REMARK 999	UNP Q15750
F	1395	DNP	SER	SEE REMARK 999	UNP Q15750
G	1395	DNP	SER	SEE REMARK 999	UNP Q15750
H	1395	DNP	SER	SEE REMARK 999	UNP Q15750

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



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 (CCD ID: 12V) (formula: C₁₇H₂₇N₃O₁₆P₂S).



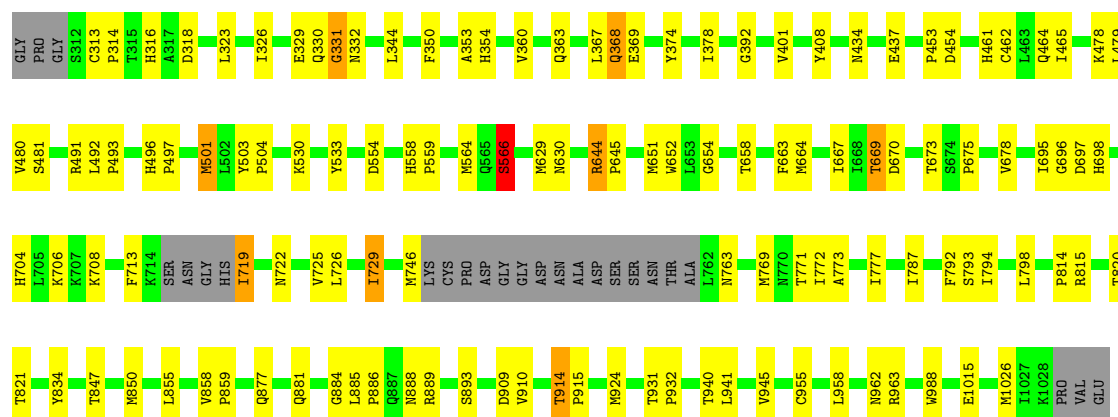
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
4	B	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
4	C	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
4	D	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		

3 Residue-property plots

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.

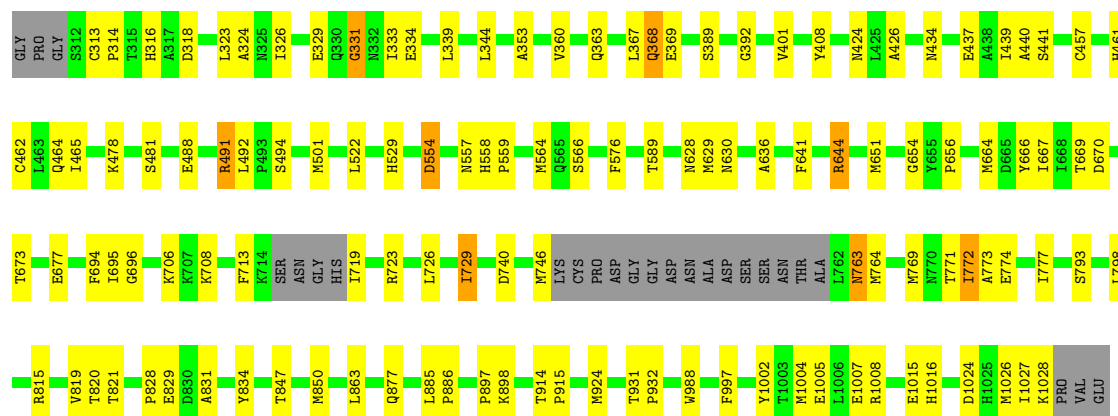
- Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYLTR ANS FERASE 110 KDA SUBUNIT

Chain A: 



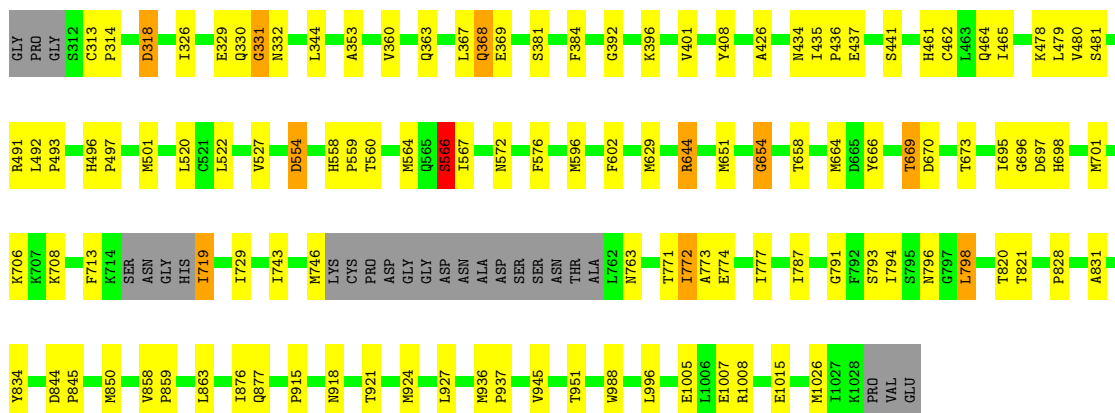
- Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYLTR ANS FERASE 110 KDA SUBUNIT

Chain B: 



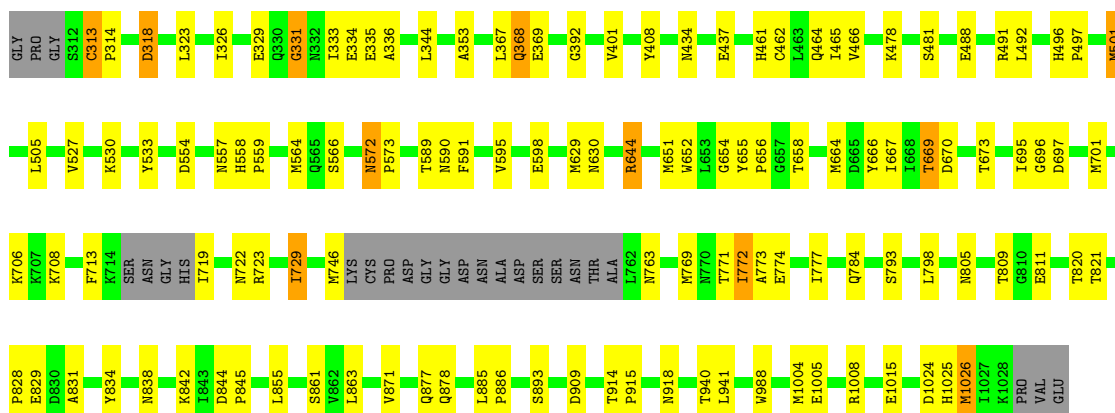
- Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYLTR ANS FERASE 110 KDA SUBUNIT

Chain C:  80% 15% ..

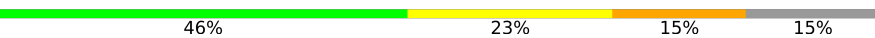


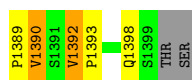
- Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYLTR ANS FERASE 110 KDA SUBUNIT

Chain D:  79% 16% ..

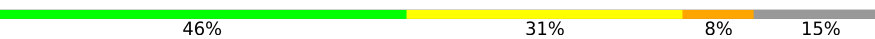


- Molecule 2: TGF-BETA-ACTIVATED KINASE 1 AND MAP3K7-BINDING PROTEIN 1

Chain E:  46% 23% 15% 15%



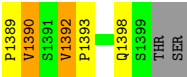
- Molecule 2: TGF-BETA-ACTIVATED KINASE 1 AND MAP3K7-BINDING PROTEIN 1

Chain F:  46% 31% 8% 15%

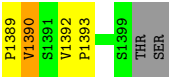


- Molecule 2: TGF-BETA-ACTIVATED KINASE 1 AND MAP3K7-BINDING PROTEIN 1

Chain G:  46% 23% 15% 15%



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



4 Data and refinement statistics

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 40.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (40.00-3.30) 98.3 (40.00-3.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.30Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.227 , 0.272 0.226 , 0.272	Depositor DCC
R_{free} test set	443 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)	0.27 , 6.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.237 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	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.*

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: DNP, 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	0/5641	0.97	4/7650 (0.1%)
1	B	0.88	1/5641 (0.0%)	0.99	3/7650 (0.0%)
1	C	0.86	0/5641	1.00	12/7650 (0.2%)
1	D	0.82	0/5641	0.96	3/7650 (0.0%)
2	E	0.66	0/73	0.93	0/98
2	F	0.60	0/73	0.90	0/98
2	G	0.71	0/73	0.97	0/98
2	H	0.66	0/73	0.92	0/98
All	All	0.86	1/22856 (0.0%)	0.98	22/30992 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	529	HIS	CA-C	-5.58	1.48	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	572	ASN	CA-C-N	6.29	125.99	119.82
1	D	572	ASN	C-N-CA	6.29	125.99	119.82
1	D	652	TRP	N-CA-C	6.27	118.28	107.93
1	A	945	VAL	N-CA-C	5.77	116.41	110.36
1	C	572	ASN	CA-C-N	5.65	125.75	119.87
1	C	572	ASN	C-N-CA	5.65	125.75	119.87
1	C	567	ILE	N-CA-C	5.55	119.01	112.35
1	A	566	SER	CA-C-N	5.54	124.76	120.33
1	A	566	SER	C-N-CA	5.54	124.76	120.33
1	C	996	LEU	N-CA-C	5.50	116.95	111.07
1	C	921	THR	N-CA-C	-5.46	105.33	111.28
1	C	396	LYS	N-CA-C	-5.42	105.06	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	652	TRP	N-CA-C	5.37	116.79	107.93
1	C	743	ILE	N-CA-C	5.25	113.93	106.53
1	B	740	ASP	N-CA-C	5.24	119.22	112.41
1	C	945	VAL	N-CA-C	5.18	115.80	110.36
1	C	566	SER	CA-C-N	5.12	124.43	120.33
1	C	566	SER	C-N-CA	5.12	124.43	120.33
1	C	654	GLY	N-CA-C	5.11	118.43	112.50
1	B	764	MET	CA-C-N	5.11	125.02	119.76
1	B	764	MET	C-N-CA	5.11	125.02	119.76
1	C	326	ILE	N-CA-C	-5.05	105.78	110.53

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	80	0
1	B	5514	0	5489	78	0
1	C	5514	0	5489	66	0
1	D	5514	0	5489	69	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	2	0
All	All	22544	0	22360	300	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 7.

All (300) 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:HG3	1:D:644:ARG:HH11	1.25	1.00
1:B:644:ARG:HH11	1:B:644:ARG:HG3	1.24	0.99
1:B:644:ARG:HH11	1:B:644:ARG:CG	1.77	0.98
1:D:644:ARG:HH11	1:D:644:ARG:CG	1.80	0.94
1:A:644:ARG:HG3	1:A:644:ARG:HH11	1.33	0.91
1:C:644:ARG:HG3	1:C:644:ARG:HH11	1.37	0.89
1:A:644:ARG:HH11	1:A:644:ARG:CG	1.91	0.84
1:B:644:ARG:HG3	1:B:644:ARG:NH1	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
1:A:368:GLN:CG	1:A:369:GLU:H	1.95	0.79
1:D:644:ARG:HG3	1:D:644:ARG:NH1	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: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:HG3	1:C:644:ARG:NH1	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:A:651:MET:HG2	1:A:664:MET:HE2	1.83	0.61
1:D:559:PRO:HB2	4:D:1200:12V:H6 ⁺	1.83	0.61
1:C:669:THR:OG1	1:C:670:ASP:N	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE1	1:C:877:GLN:HA	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
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:HA	1:D:877:GLN:OE1	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:HA	1:B:877:GLN:OE1	2.07	0.54
1:C:559:PRO:HB2	4:C:1200:12V:H6'	1.90	0.54
1:B:329:GLU:C	1:B:331:GLY:H	2.15	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:367:LEU:O	1:B:368:GLN:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ARG:CG	1:A:644:ARG:NH1	2.61	0.53
1:D:367:LEU:O	1:D:368:GLN:C	2.52	0.53
1:A:329:GLU:C	1:A:331:GLY:H	2.17	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
1:B:1004:MET:HE3	1:C:791:GLY:C	2.34	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: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:D:564:MET:SD	1:D:564:MET:C	2.93	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:HA	1:C:1015:GLU:OE1	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
1:D:772:ILE:HG22	1:D:773:ALA:N	2.25	0.51
2:F:1392:VAL:CG1	2:F:1393:PRO:HD2	2.41	0.51
1:A:847:THR:HA	1:A:850:MET:HE3	1.93	0.50
2:H:1392:VAL:CG1	2:H:1393:PRO:HD2	2.42	0.50
1:C:367:LEU:O	1:C:368:GLN:C	2.54	0.50
1:D:344:LEU:HD21	1:D:353:ALA:HB3	1.94	0.50
1:B:557:ASN:HB2	1:B:589:THR:HG21	1.93	0.50
1:B:651:MET:HG2	1:B:664:MET:HE2	1.93	0.49
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: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:D:1024:ASP:CG	1:D:1025:HIS:H	2.21	0.49
1:B:636:ALA:HB3	2:F:1398:GLN:NE2	2.29	0.48
1:C:772:ILE:HG22	1:C:773:ALA:N	2.29	0.48
1:D:329:GLU:C	1:D:331:GLY:H	2.21	0.48
2:E:1392:VAL:CG1	2:E:1393:PRO:HD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:636:ALA:HB3	2:F:1398:GLN:HE22	1.78	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:C:329:GLU:C	1:C:331:GLY:H	2.21	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:651:MET:HG2	1:D:664:MET:HE2	1.96	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
1:D:1015:GLU:OE1	1:D:1015:GLU:HA	2.13	0.48
2:G:1392:VAL:HG12	2:G:1393:PRO:HD2	1.94	0.48
1:A:367:LEU:O	1:A:368:GLN:C	2.56	0.48
1:A:962:ASN:O	1:A:963:ARG:C	2.55	0.48
1:C:368:GLN:HG2	1:C:369:GLU:H	1.77	0.48
1:B:439:ILE:O	1:B:440:ALA:C	2.55	0.47
1:B:564:MET:SD	1:B:564:MET:C	2.97	0.47
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: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: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: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:651:MET:HG2	1:C:664:MET:HE2	1.96	0.47
1:C:834:TYR:O	1:C:863:LEU:HD12	2.15	0.47
1:A:564:MET:HE3	1:A:629:MET:HE1	1.97	0.46
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:A:564:MET:SD	1:A:564:MET:C	2.98	0.46
1:A:850:MET:HE1	1:A:915:PRO:HG2	1.97	0.46
1:B:564:MET:HE3	1:B:629:MET:HE1	1.96	0.46
1:B:723:ARG:NE	1:B:829:GLU:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:LEU:O	1:C:480:VAL:C	2.58	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:D:564:MET:HE3	1:D:629:MET:HE1	1.98	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:B:924:MET:HE3	1:B:997:PHE:CE1	2.51	0.46
1:C:496:HIS:CG	1:C:497:PRO:HD2	2.51	0.46
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:666:TYR:OH	1:D:1026:MET:HE3	2.17	0.45
1:D:914:THR:HA	1:D:915:PRO:HD3	1.83	0.45
1:A:479:LEU:O	1:A:480:VAL:C	2.59	0.45
1:A:725:VAL:HG12	1:A:726:LEU:N	2.30	0.45
1:C:564:MET:SD	1:C:564:MET:C	2.99	0.45
1:B:729:ILE:HD13	1:B:729:ILE:HA	1.82	0.45
1:C:564:MET:HE3	1:C:629:MET:HE1	1.99	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:C:666:TYR:OH	1:C:1026:MET:HE3	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:B:897:PRO:O	1:B:898:LYS:C	2.60	0.44
1:A:792:PHE:CE1	1:D:1004:MET:HE1	2.52	0.44
1:A:501:MET:HE3	1:A:501:MET:HB3	1.87	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: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:A:815:ARG:CZ	1:D:598:GLU:HG2	2.48	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:D:885:LEU:HA	1:D:886:PRO:HD2	1.85	0.44
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:HD1	1:B:713:PHE:H	1.65	0.43
3:C:1100:SO4:O1	2:G:1398:GLN:HG3	2.18	0.43
1:D:1005:GLU:OE1	1:D:1008:ARG:HD3	2.18	0.43
1:B:333:ILE:O	1:B:334:GLU:C	2.62	0.43
1:B:914:THR:HA	1:B:915:PRO:HD3	1.80	0.43
1:D:491:ARG:HD2	1:D:491:ARG:HA	1.72	0.43
1:D:784:GLN:HE21	1:D:784:GLN:HB2	1.64	0.43
1:A:644:ARG:N	1:A:645:PRO:HD3	2.33	0.43
1:B:457:CYS:SG	1:B:494:SER:CB	3.07	0.43
1:B:666:TYR:OH	1:B:1026:MET:HE3	2.18	0.43
1:B:1005:GLU:OE1	1:B:1008:ARG:HD3	2.19	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:N	1:D:918:ASN:HD22	2.16	0.42
1:B:726:LEU:CD2	1:B:819:VAL:HG22	2.49	0.42
1:B:850:MET:HE1	1:B:915:PRO:HG2	2.01	0.42
1:D:713:PHE:H	1:D:713:PHE:HD1	1.68	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:B:847:THR:HA	1:B:850:MET:HE3	2.01	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
1:D:335:GLU:O	1:D:336:ALA:C	2.63	0.42
1:D:842:LYS:NZ	4:D:1200:12V:O2B	2.47	0.42
1:B:931:THR:HA	1:B:932:PRO:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:940:THR:O	1:D:941:LEU:C	2.63	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: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:B:1002:TYR:CD1	1:B:1002:TYR:C	2.98	0.41
1:A:675:PRO:O	1:A:678:VAL:HG22	2.20	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:A:940:THR:O	1:A:941:LEU:C	2.62	0.41
1:D:838:ASN:HB3	1:D:842:LYS:HD2	2.01	0.41
1:A:881:GLN:CD	1:B:677:GLU:HA	2.46	0.41
1:A:931:THR:HA	1:A:932:PRO:HD3	1.93	0.41
1:C:435:ILE:O	1:C:436:PRO:C	2.60	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:576:PHE:CZ	1:C:1007:GLU:HG2	2.56	0.41
1:C:1005:GLU:OE1	1:C:1008:ARG:HD3	2.21	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:A:453:PRO:O	1:A:454:ASP:C	2.64	0.41
1:B:313:CYS:HA	1:B:314:PRO:HD2	1.91	0.41
1:B:491:ARG:HA	1:B:491:ARG:HD2	1.68	0.41
1:B:834:TYR:O	1:B:863:LEU:HD12	2.21	0.41
1:B:1015:GLU:OE1	1:B:1015:GLU:HA	2.21	0.41
1:C:559:PRO:O	1:C:560:THR:C	2.64	0.41
1:C:796:ASN:OD1	1:C:798:LEU:HB2	2.21	0.41
1:D:333:ILE:O	1:D:334:GLU:C	2.64	0.41
1:D:697:ASP:HB3	1:D:701:MET:HG3	2.03	0.41
1:D:729:ILE:HD13	1:D:729:ILE:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:501:MET:HE3	1:D:501:MET:HB3	1.92	0.41
1:A:708:LYS:HG2	1:A:988:TRP:CH2	2.56	0.40
1:C:492:LEU:HA	1:C:493:PRO:HD3	1.86	0.40
1:C:850:MET:HE1	1:C:915:PRO:HG2	2.03	0.40
1:C:876:ILE:O	1:C:877:GLN:C	2.65	0.40
1:C:918:ASN:N	1:C:918:ASN:HD22	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:HD13	1:A:729:ILE:HA	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%)	21	52
1	B	692/723 (96%)	641 (93%)	46 (7%)	5 (1%)	18	49
1	C	692/723 (96%)	643 (93%)	46 (7%)	3 (0%)	30	60
1	D	692/723 (96%)	643 (93%)	45 (6%)	4 (1%)	21	52
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	8/13 (62%)	6 (75%)	1 (12%)	1 (12%)	0 1
All	All	2800/2944 (95%)	2599 (93%)	181 (6%)	20 (1%)	18 49

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 ⓘ

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%)	575 (96%)	25 (4%)	26 55
1	B	600/618 (97%)	574 (96%)	26 (4%)	26 54
1	C	600/618 (97%)	574 (96%)	26 (4%)	26 54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	600/618 (97%)	573 (96%)	27 (4%)	24	53
2	E	9/11 (82%)	8 (89%)	1 (11%)	6	22
2	F	9/11 (82%)	9 (100%)	0	100	100
2	G	9/11 (82%)	8 (89%)	1 (11%)	6	22
2	H	9/11 (82%)	9 (100%)	0	100	100
All	All	2436/2516 (97%)	2330 (96%)	106 (4%)	25	54

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	ASP
1	A	360	VAL
1	A	363	GLN
1	A	401	VAL
1	A	434	ASN
1	A	437	GLU
1	A	501	MET
1	A	566	SER
1	A	630	ASN
1	A	644	ARG
1	A	658	THR
1	A	667	ILE
1	A	669	THR
1	A	673	THR
1	A	706	LYS
1	A	719	ILE
1	A	729	ILE
1	A	771	THR
1	A	793	SER
1	A	798	LEU
1	A	820	THR
1	A	821	THR
1	A	893	SER
1	A	914	THR
1	A	1026	MET
1	B	318	ASP
1	B	360	VAL
1	B	363	GLN
1	B	401	VAL
1	B	434	ASN

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Mol	Chain	Res	Type
1	B	437	GLU
1	B	488	GLU
1	B	491	ARG
1	B	501	MET
1	B	522	LEU
1	B	554	ASP
1	B	566	SER
1	B	630	ASN
1	B	644	ARG
1	B	667	ILE
1	B	673	THR
1	B	694	PHE
1	B	706	LYS
1	B	719	ILE
1	B	729	ILE
1	B	771	THR
1	B	772	ILE
1	B	793	SER
1	B	798	LEU
1	B	820	THR
1	B	821	THR
1	C	318	ASP
1	C	360	VAL
1	C	363	GLN
1	C	381	SER
1	C	401	VAL
1	C	434	ASN
1	C	437	GLU
1	C	501	MET
1	C	522	LEU
1	C	527	VAL
1	C	554	ASP
1	C	566	SER
1	C	644	ARG
1	C	658	THR
1	C	669	THR
1	C	673	THR
1	C	706	LYS
1	C	719	ILE
1	C	729	ILE
1	C	771	THR
1	C	772	ILE

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Mol	Chain	Res	Type
1	C	793	SER
1	C	798	LEU
1	C	820	THR
1	C	821	THR
1	C	951	THR
1	D	313	CYS
1	D	318	ASP
1	D	401	VAL
1	D	434	ASN
1	D	437	GLU
1	D	488	GLU
1	D	501	MET
1	D	505	LEU
1	D	527	VAL
1	D	566	SER
1	D	630	ASN
1	D	644	ARG
1	D	658	THR
1	D	667	ILE
1	D	669	THR
1	D	673	THR
1	D	706	LYS
1	D	719	ILE
1	D	729	ILE
1	D	771	THR
1	D	772	ILE
1	D	793	SER
1	D	798	LEU
1	D	820	THR
1	D	821	THR
1	D	893	SER
1	D	1026	MET
2	E	1392	VAL
2	G	1392	VAL

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

Mol	Chain	Res	Type
1	A	354	HIS
1	A	356	ASN
1	A	363	GLN
1	A	406	GLN

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Mol	Chain	Res	Type
1	A	424	ASN
1	A	786	GLN
1	A	824	GLN
1	A	888	ASN
1	A	1012	GLN
1	B	321	ASN
1	B	354	HIS
1	B	363	GLN
1	B	406	GLN
1	B	424	ASN
1	B	557	ASN
1	B	763	ASN
1	B	784	GLN
1	B	901	HIS
1	B	1012	GLN
1	C	321	ASN
1	C	363	GLN
1	C	406	GLN
1	C	424	ASN
1	C	784	GLN
1	C	901	HIS
1	C	1012	GLN
1	D	356	ASN
1	D	363	GLN
1	D	406	GLN
1	D	422	HIS
1	D	784	GLN
1	D	901	HIS
1	D	1012	GLN
2	E	1398	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	4,5,6	0.58	0	1,5,7	0.19	0
2	DNP	H	1395	2	4,5,6	0.60	0	1,5,7	0.11	0
2	DNP	E	1395	2	4,5,6	0.82	0	1,5,7	0.02	0
2	DNP	F	1395	2	4,5,6	0.75	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	H	1395	2	-	1/2/4/6	-
2	DNP	E	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	E	1395	DNP	N-CA-CB-NG
2	F	1395	DNP	N-CA-CB-NG
2	G	1395	DNP	N-CA-CB-NG
2	H	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 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	1100	-	4,4,4	0.37	0	6,6,6	0.26	0
3	SO4	C	1100	-	4,4,4	0.41	0	6,6,6	0.20	0
3	SO4	A	1100	-	4,4,4	0.43	0	6,6,6	0.19	0
3	SO4	D	1100	-	4,4,4	0.27	0	6,6,6	0.25	0
4	12V	C	1200	-	38,41,41	1.41	6 (15%)	52,62,62	1.71	11 (21%)
4	12V	B	1200	-	38,41,41	1.27	4 (10%)	52,62,62	1.57	11 (21%)
4	12V	D	1200	-	38,41,41	1.16	3 (7%)	52,62,62	1.71	10 (19%)
4	12V	A	1200	-	38,41,41	1.76	5 (13%)	52,62,62	1.73	9 (17%)

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1200	12V	PA-O3A	7.76	1.67	1.59
4	C	1200	12V	PA-O3A	4.40	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1200	12V	C5'-S5'	-3.85	1.76	1.82
4	A	1200	12V	C5'-S5'	-3.76	1.76	1.82
4	C	1200	12V	C5'-S5'	-3.07	1.77	1.82
4	B	1200	12V	C2-N1	-3.05	1.33	1.38
4	A	1200	12V	PB-O3A	3.04	1.62	1.59
4	B	1200	12V	C5'-S5'	-2.80	1.78	1.82
4	B	1200	12V	C5-C4	-2.70	1.37	1.43
4	C	1200	12V	C4'-C5'	-2.55	1.51	1.53
4	C	1200	12V	PB-O3A	2.27	1.61	1.59
4	B	1200	12V	O4B-C1B	2.27	1.47	1.42
4	C	1200	12V	C2-N1	-2.21	1.35	1.38
4	D	1200	12V	PB-O3A	2.19	1.61	1.59
4	D	1200	12V	C2-N1	-2.14	1.35	1.38
4	A	1200	12V	C5-C4	-2.12	1.39	1.43
4	A	1200	12V	C6-N1	2.11	1.43	1.38
4	C	1200	12V	C5-C4	-2.06	1.39	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1200	12V	C4-N3-C2	-6.07	119.08	126.61
4	D	1200	12V	C4-N3-C2	-5.95	119.23	126.61
4	A	1200	12V	C4-N3-C2	-5.38	119.94	126.61
4	D	1200	12V	N3-C2-N1	4.83	121.18	114.89
4	A	1200	12V	C5-C4-N3	4.80	121.53	114.80
4	C	1200	12V	N3-C2-N1	4.72	121.03	114.89
4	B	1200	12V	O1'-C1'-C2'	4.30	114.06	107.52
4	B	1200	12V	C4-N3-C2	-4.18	121.42	126.61
4	A	1200	12V	O1'-C1'-C2'	4.12	113.78	107.52
4	C	1200	12V	C5-C4-N3	4.06	120.49	114.80
4	B	1200	12V	N3-C2-N1	4.00	120.10	114.89
4	A	1200	12V	N3-C2-N1	3.95	120.04	114.89
4	D	1200	12V	C5-C4-N3	3.76	120.07	114.80
4	A	1200	12V	O4B-C1B-C2B	-3.42	99.29	106.62
4	B	1200	12V	C5-C4-N3	2.90	118.86	114.80
4	A	1200	12V	O4-C4-C5	-2.80	120.33	125.16
4	C	1200	12V	C1'-C2'-N2'	-2.77	106.04	111.07
4	A	1200	12V	O2-C2-N3	-2.76	116.41	121.49
4	B	1200	12V	C1'-C2'-N2'	-2.73	106.11	111.07
4	D	1200	12V	C1'-C2'-N2'	-2.68	106.20	111.07
4	C	1200	12V	O1'-C1'-C2'	2.66	111.56	107.52
4	D	1200	12V	O4B-C1B-N1	-2.63	102.39	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1200	12V	O1'-C1'-C2'	2.63	111.52	107.52
4	D	1200	12V	C5-C6-N1	-2.46	117.84	121.84
4	C	1200	12V	O4-C4-C5	-2.44	120.96	125.16
4	B	1200	12V	O4B-C1B-C2B	-2.43	101.42	106.62
4	A	1200	12V	C1'-C2'-N2'	-2.36	106.79	111.07
4	C	1200	12V	O4B-C1B-N1	-2.35	103.02	108.36
4	B	1200	12V	O3B-C3B-C4B	-2.27	104.56	111.08
4	B	1200	12V	C3B-C2B-C1B	-2.25	97.21	101.46
4	C	1200	12V	C5-C6-N1	-2.25	118.19	121.84
4	C	1200	12V	O4B-C1B-C2B	-2.21	101.88	106.62
4	A	1200	12V	C2B-C1B-N1	2.18	119.33	113.25
4	B	1200	12V	C2B-C1B-N1	2.18	119.32	113.25
4	D	1200	12V	O4B-C1B-C2B	-2.18	101.96	106.62
4	B	1200	12V	O4-C4-C5	-2.16	121.44	125.16
4	C	1200	12V	C3B-C2B-C1B	-2.12	97.46	101.46
4	C	1200	12V	C2B-C1B-N1	2.07	119.01	113.25
4	B	1200	12V	O4'-C4'-C3'	-2.06	105.53	110.38
4	D	1200	12V	O4'-C4'-C3'	-2.03	105.58	110.38
4	D	1200	12V	C3B-C2B-C1B	-2.03	97.63	101.46

There are no chirality outliers.

All (20) torsion outliers are listed below:

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

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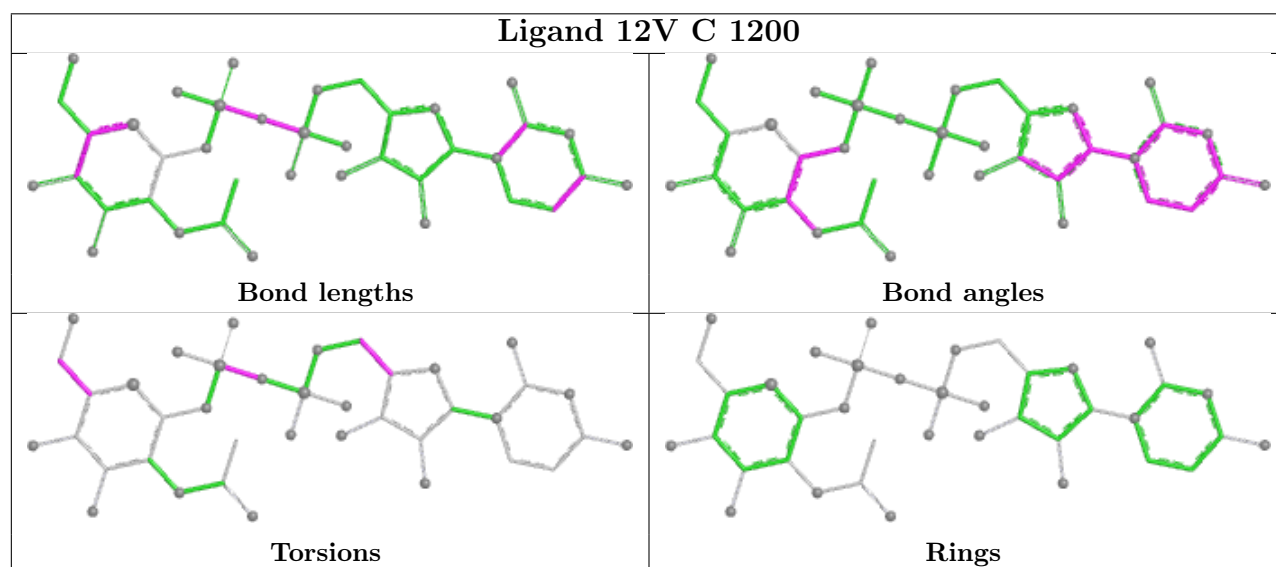
Mol	Chain	Res	Type	Atoms
4	B	1200	12V	PA-O3A-PB-O1B
4	D	1200	12V	PA-O3A-PB-O1B

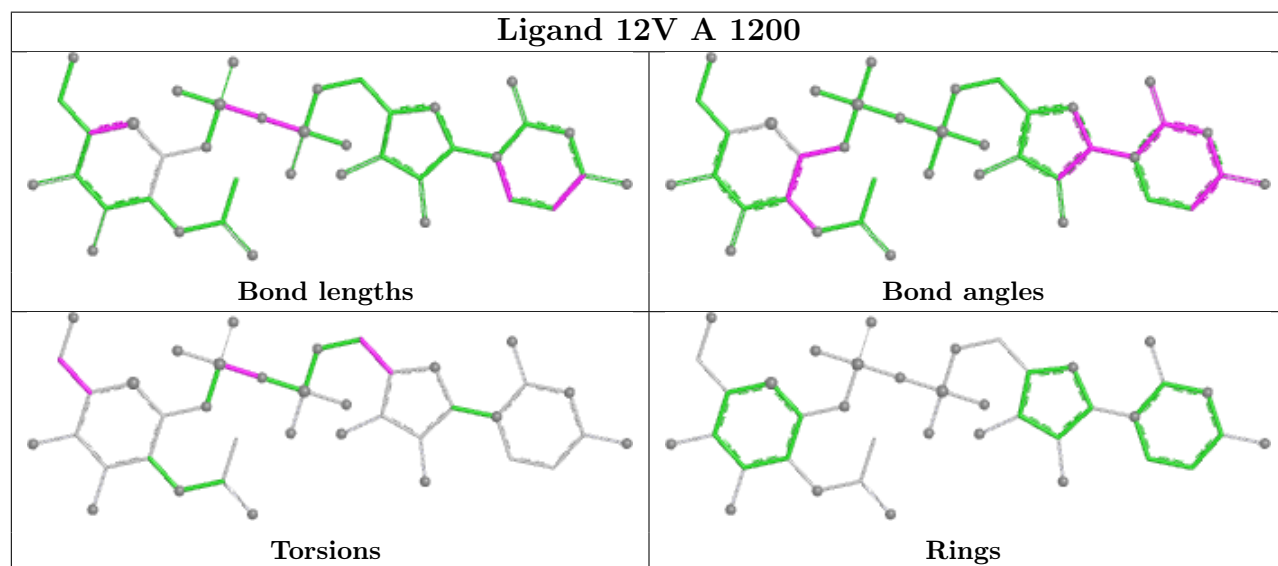
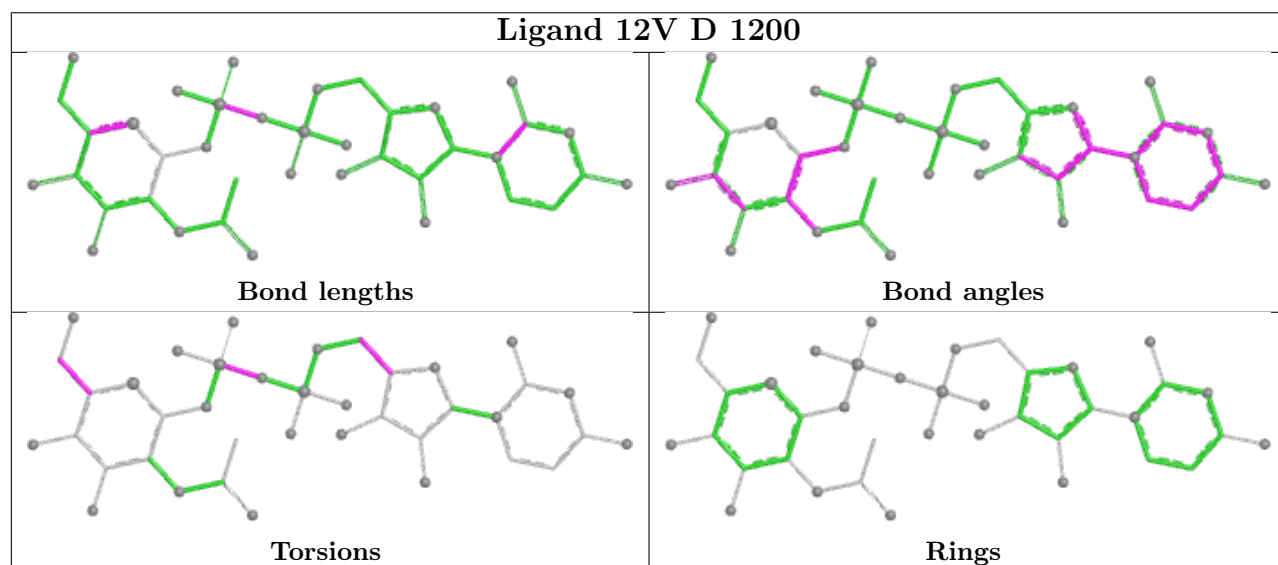
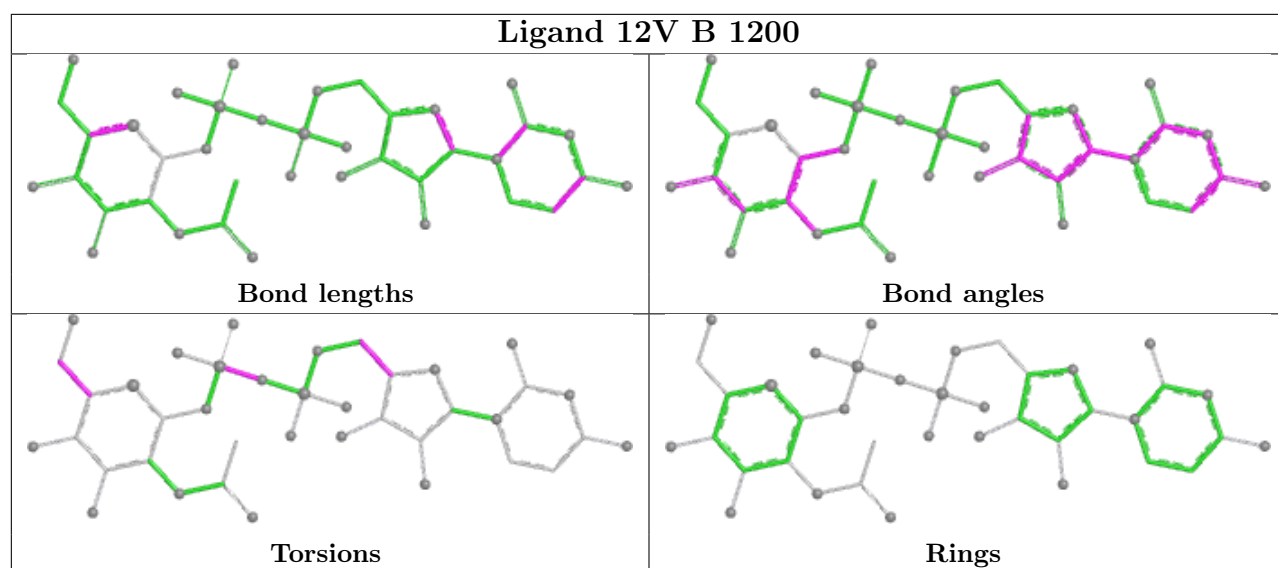
There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1100	SO4	1	0
3	A	1100	SO4	1	0
4	C	1200	12V	2	0
4	B	1200	12V	2	0
4	D	1200	12V	2	0
4	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, 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	698/723 (96%)	-1.73	0 100 100	22, 41, 74, 115	0
1	B	698/723 (96%)	-1.71	0 100 100	21, 43, 77, 109	0
1	C	698/723 (96%)	-1.72	0 100 100	22, 42, 74, 119	0
1	D	698/723 (96%)	-1.71	0 100 100	26, 50, 81, 136	0
2	E	10/13 (76%)	-1.41	0 100 100	45, 63, 86, 91	0
2	F	10/13 (76%)	-1.53	0 100 100	52, 63, 83, 98	0
2	G	10/13 (76%)	-1.61	0 100 100	46, 62, 70, 82	0
2	H	10/13 (76%)	-1.58	0 100 100	47, 62, 73, 81	0
All	All	2832/2944 (96%)	-1.72	0 100 100	21, 44, 77, 136	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DNP	E	1395	6/7	1.00	0.02	48,52,55,59	0
2	DNP	F	1395	6/7	1.00	0.03	54,55,57,57	0
2	DNP	G	1395	6/7	1.00	0.02	54,55,57,57	0
2	DNP	H	1395	6/7	1.00	0.03	54,56,57,57	0

6.3 Carbohydrates [i](#)

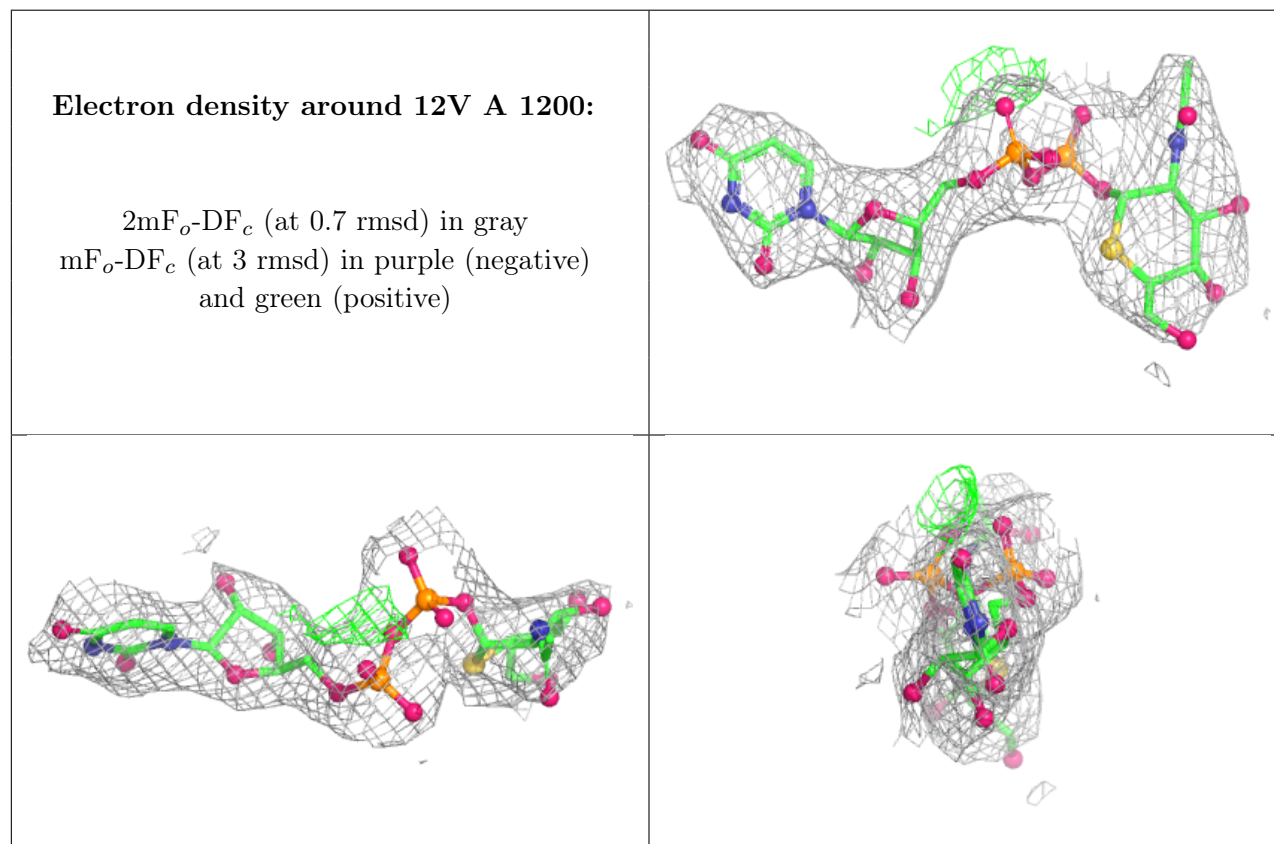
There are no oligosaccharides in this entry.

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.

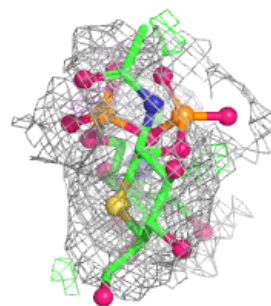
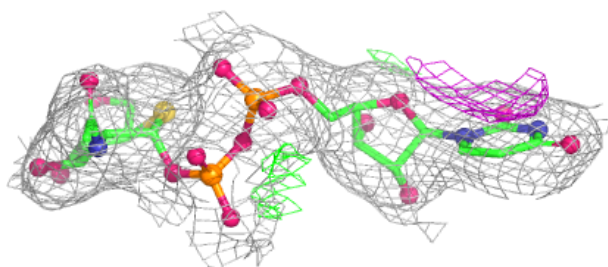
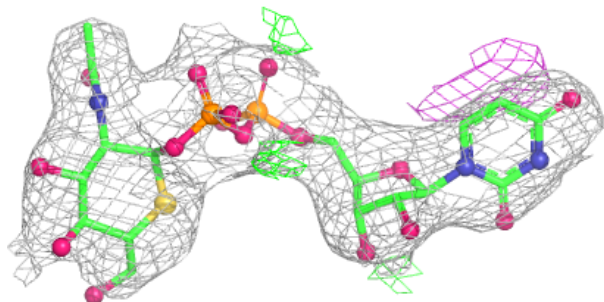
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	1100	5/5	1.00	0.02	63,64,68,73	0
3	SO4	B	1100	5/5	1.00	0.02	58,60,61,68	0
3	SO4	C	1100	5/5	1.00	0.01	60,62,62,63	0
3	SO4	D	1100	5/5	1.00	0.01	63,63,67,69	0
4	12V	A	1200	39/39	1.00	0.03	28,34,63,70	0
4	12V	B	1200	39/39	1.00	0.03	31,45,67,70	0
4	12V	C	1200	39/39	1.00	0.02	32,38,56,65	0
4	12V	D	1200	39/39	1.00	0.02	41,48,71,79	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.

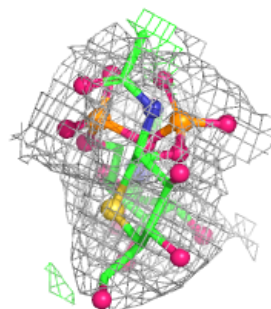
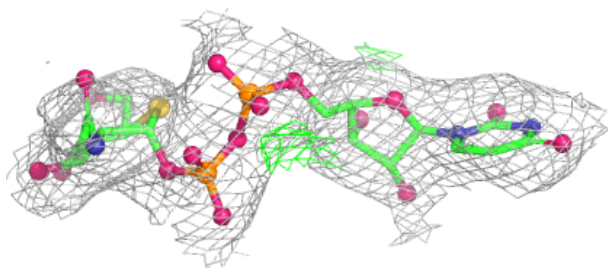
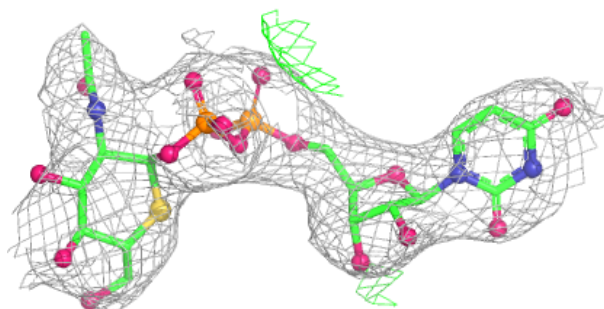


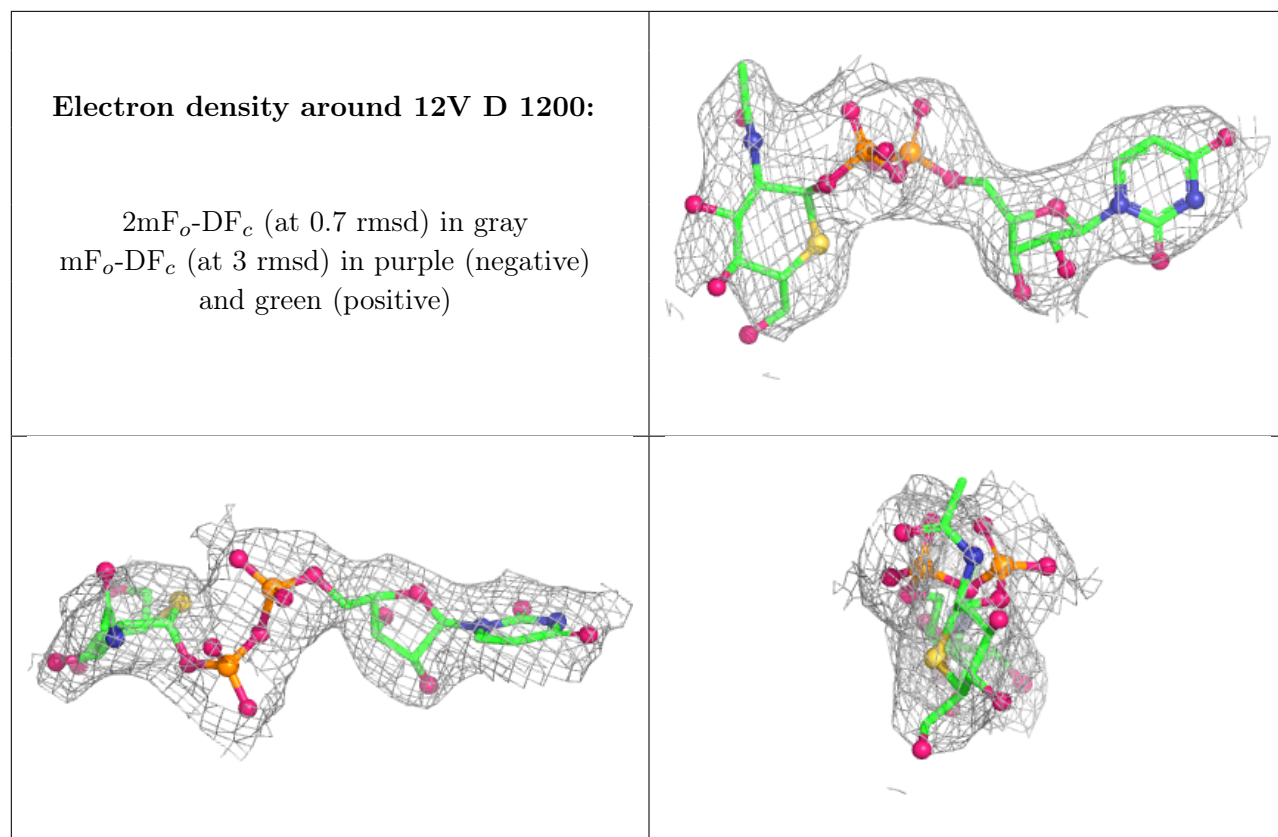
Electron density around 12V B 1200:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.