



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:26 AM UTC

PDB ID : 1VGV / pdb_00001vgv
Title : Crystal structure of UDP-N-acetylglucosamine_2 epimerase
Authors : Structural GenomiX
Deposited on : 2003-11-03
Resolution : 2.31 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

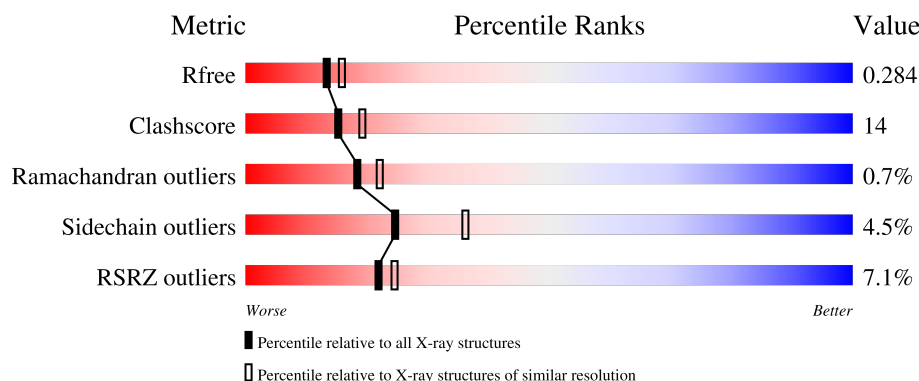
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	384	2% 70% 26% ..
1	B	384	7% 66% 28% ..
1	C	384	9% 61% 31% ..
1	D	384	9% 65% 29% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UD1	B	385	X	-	-	-
2	UD1	C	385	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12241 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 2-epimerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	Se	0	1	0
			2966	1883	519	550	4	10			
1	B	372	Total	C	N	O	S	Se	0	4	0
			2958	1877	520	548	4	9			
1	C	367	Total	C	N	O	S	Se	0	1	0
			2902	1842	511	536	4	9			
1	D	374	Total	C	N	O	S	Se	0	0	0
			2928	1855	514	545	4	10			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	cloning artifact	UNP P27828
A	16	MSE	MET	modified residue	UNP P27828
A	42	MSE	MET	modified residue	UNP P27828
A	61	MSE	MET	modified residue	UNP P27828
A	143	MSE	MET	modified residue	UNP P27828
A	185	MSE	MET	modified residue	UNP P27828
A	207	MSE	MET	modified residue	UNP P27828
A	280	MSE	MET	modified residue	UNP P27828
A	307	MSE	MET	modified residue	UNP P27828
A	349	MSE	MET	modified residue	UNP P27828
A	377	GLY	-	cloning artifact	UNP P27828
A	378	SER	-	cloning artifact	UNP P27828
A	379	HIS	-	cloning artifact	UNP P27828
A	380	HIS	-	cloning artifact	UNP P27828
A	381	HIS	-	cloning artifact	UNP P27828
A	382	HIS	-	cloning artifact	UNP P27828
A	383	HIS	-	cloning artifact	UNP P27828
A	384	HIS	-	cloning artifact	UNP P27828
B	1	MSE	-	cloning artifact	UNP P27828
B	16	MSE	MET	modified residue	UNP P27828
B	42	MSE	MET	modified residue	UNP P27828

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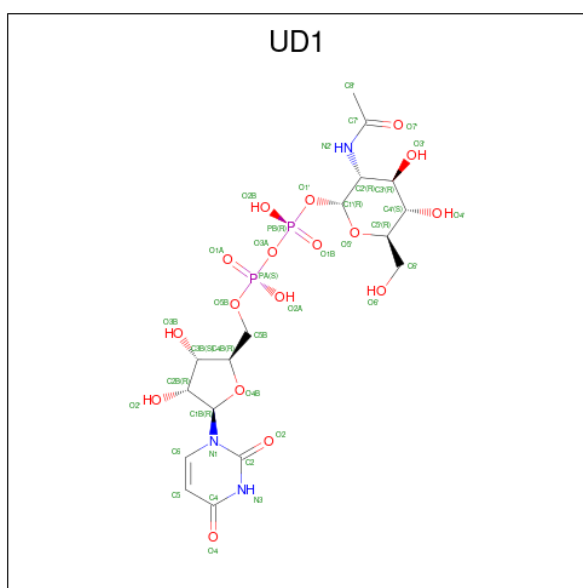
Chain	Residue	Modelled	Actual	Comment	Reference
B	61	MSE	MET	modified residue	UNP P27828
B	143	MSE	MET	modified residue	UNP P27828
B	185	MSE	MET	modified residue	UNP P27828
B	207	MSE	MET	modified residue	UNP P27828
B	280	MSE	MET	modified residue	UNP P27828
B	307	MSE	MET	modified residue	UNP P27828
B	349	MSE	MET	modified residue	UNP P27828
B	377	GLY	-	cloning artifact	UNP P27828
B	378	SER	-	cloning artifact	UNP P27828
B	379	HIS	-	cloning artifact	UNP P27828
B	380	HIS	-	cloning artifact	UNP P27828
B	381	HIS	-	cloning artifact	UNP P27828
B	382	HIS	-	cloning artifact	UNP P27828
B	383	HIS	-	cloning artifact	UNP P27828
B	384	HIS	-	cloning artifact	UNP P27828
C	1	MSE	-	cloning artifact	UNP P27828
C	16	MSE	MET	modified residue	UNP P27828
C	42	MSE	MET	modified residue	UNP P27828
C	61	MSE	MET	modified residue	UNP P27828
C	143	MSE	MET	modified residue	UNP P27828
C	185	MSE	MET	modified residue	UNP P27828
C	207	MSE	MET	modified residue	UNP P27828
C	280	MSE	MET	modified residue	UNP P27828
C	307	MSE	MET	modified residue	UNP P27828
C	349	MSE	MET	modified residue	UNP P27828
C	377	GLY	-	cloning artifact	UNP P27828
C	378	SER	-	cloning artifact	UNP P27828
C	379	HIS	-	cloning artifact	UNP P27828
C	380	HIS	-	cloning artifact	UNP P27828
C	381	HIS	-	cloning artifact	UNP P27828
C	382	HIS	-	cloning artifact	UNP P27828
C	383	HIS	-	cloning artifact	UNP P27828
C	384	HIS	-	cloning artifact	UNP P27828
D	1	MSE	-	cloning artifact	UNP P27828
D	16	MSE	MET	modified residue	UNP P27828
D	42	MSE	MET	modified residue	UNP P27828
D	61	MSE	MET	modified residue	UNP P27828
D	143	MSE	MET	modified residue	UNP P27828
D	185	MSE	MET	modified residue	UNP P27828
D	207	MSE	MET	modified residue	UNP P27828
D	280	MSE	MET	modified residue	UNP P27828
D	307	MSE	MET	modified residue	UNP P27828

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Chain	Residue	Modelled	Actual	Comment	Reference
D	349	MSE	MET	modified residue	UNP P27828
D	377	GLY	-	cloning artifact	UNP P27828
D	378	SER	-	cloning artifact	UNP P27828
D	379	HIS	-	cloning artifact	UNP P27828
D	380	HIS	-	cloning artifact	UNP P27828
D	381	HIS	-	cloning artifact	UNP P27828
D	382	HIS	-	cloning artifact	UNP P27828
D	383	HIS	-	cloning artifact	UNP P27828
D	384	HIS	-	cloning artifact	UNP P27828

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (CCD ID: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	134	Total	O	0	0
			134	134		
3	B	95	Total	O	0	0
			95	95		

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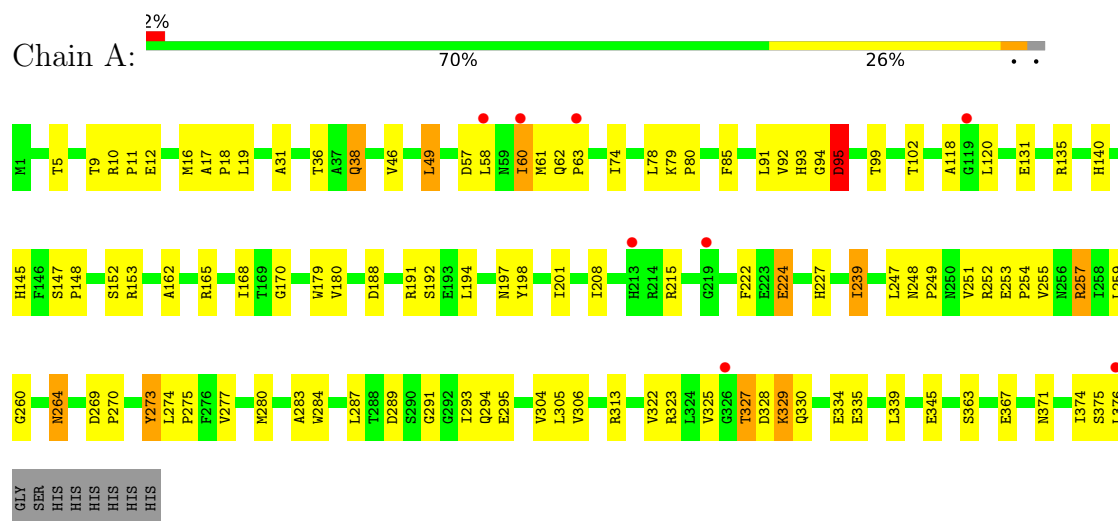
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	84	Total	O	0	0
			84	84		
3	D	96	Total	O	0	0
			96	96		

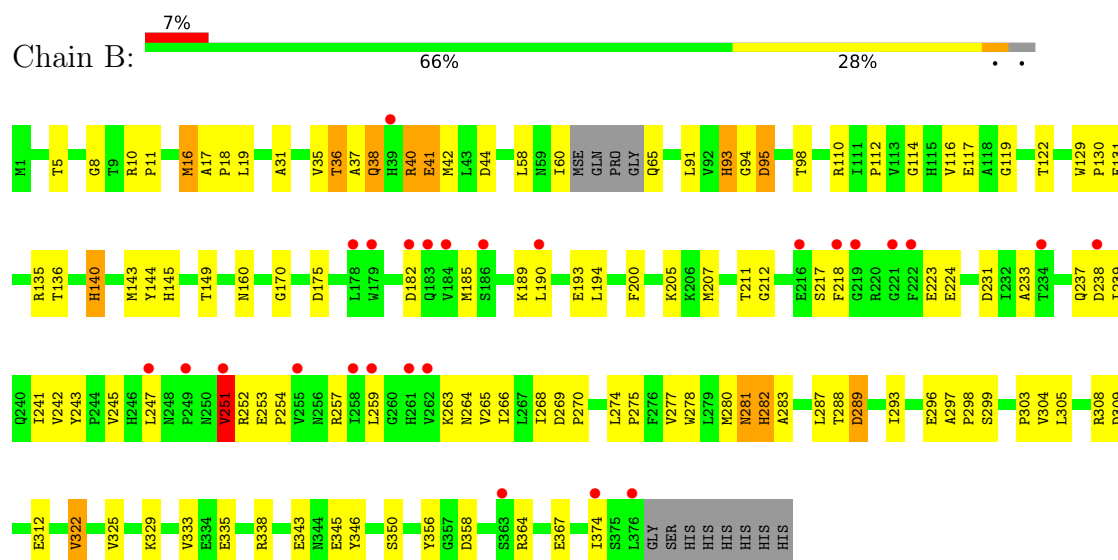
3 Residue-property plots [i](#)

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 2-epimerase

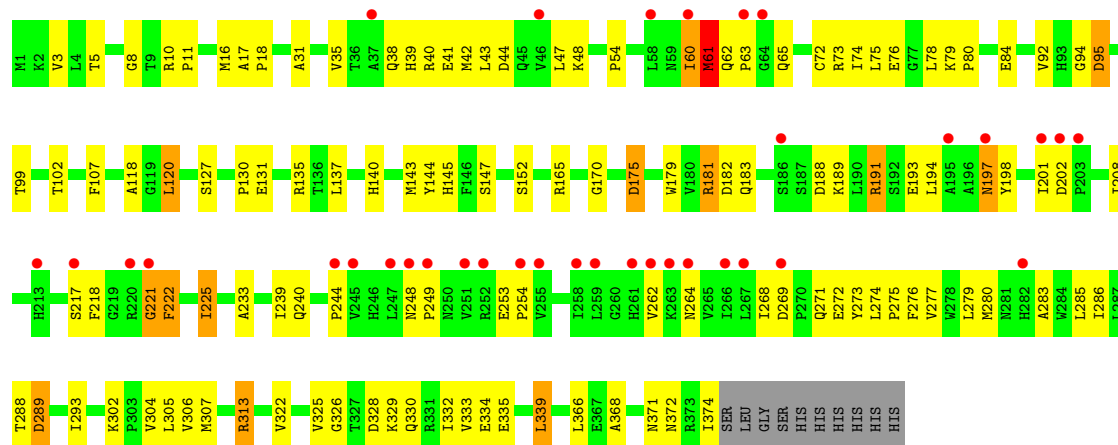


• Molecule 1: UDP-N-acetylglucosamine 2-epimerase



• Molecule 1: UDP-N-acetylglucosamine 2-epimerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.36Å 94.48Å 100.73Å 90.00° 109.29° 90.00°	Depositor
Resolution (Å)	42.47 – 2.31 42.47 – 2.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (42.47-2.31) 92.4 (42.47-2.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.32Å)	Xtriage
Refinement program	REFMAC 4.0	Depositor
R, R_{free}	0.249 , 0.295 (Not available) , 0.284	Depositor DCC
R_{free} test set	3280 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12241	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1310e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: UD1

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	0.61	0/3024	1.30	19/4100 (0.5%)
1	B	0.59	0/3028	1.30	19/4104 (0.5%)
1	C	0.57	0/2959	1.25	15/4010 (0.4%)
1	D	0.60	0/2981	1.31	16/4043 (0.4%)
All	All	0.59	0/11992	1.29	69/16257 (0.4%)

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	313	ARG	CD-NE-CZ	14.14	144.19	124.40
1	A	327	THR	N-CA-C	-10.03	101.38	114.31
1	D	94	GLY	N-CA-C	8.44	126.70	111.34
1	D	175	ASP	CA-CB-CG	8.32	120.92	112.60
1	D	140	HIS	CA-CB-CG	-7.55	106.25	113.80
1	A	94	GLY	N-CA-C	7.53	125.05	111.34
1	C	158	ARG	CD-NE-CZ	7.53	134.94	124.40
1	B	122	THR	N-CA-C	-7.40	104.50	113.97
1	B	95	ASP	N-CA-C	7.23	121.39	111.71
1	D	222	PHE	CA-CB-CG	6.91	120.70	113.80
1	A	264	ASN	CA-CB-CG	6.90	119.50	112.60
1	C	122	THR	N-CA-C	-6.85	105.48	114.31
1	A	31	ALA	N-CA-C	6.74	120.81	109.76
1	C	40	ARG	NE-CZ-NH2	6.67	125.20	119.20
1	C	94	GLY	N-CA-C	6.64	128.92	113.18
1	C	95	ASP	N-CA-C	6.51	120.55	111.56
1	D	131	GLU	N-CA-C	6.46	118.33	111.28
1	B	289	ASP	CA-C-N	6.43	130.00	120.87
1	B	289	ASP	C-N-CA	6.43	130.00	120.87
1	B	237	GLN	CA-C-N	6.28	129.85	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	GLN	C-N-CA	6.28	129.85	120.31
1	C	175	ASP	N-CA-C	-6.26	104.37	111.07
1	B	31	ALA	N-CA-C	6.24	119.99	109.76
1	A	257	ARG	N-CA-C	-6.22	104.58	111.36
1	B	251	VAL	N-CA-C	6.15	119.07	113.10
1	B	182	ASP	N-CA-C	6.12	120.86	112.04
1	D	95	ASP	N-CA-C	6.12	118.72	110.88
1	D	170	GLY	N-CA-C	-6.12	103.75	112.81
1	A	85	PHE	CA-CB-CG	6.07	119.86	113.80
1	D	120	LEU	CB-CA-C	6.00	119.50	109.89
1	B	356	TYR	N-CA-C	5.96	119.51	112.72
1	A	284	TRP	N-CA-C	-5.94	106.17	113.41
1	A	131	GLU	N-CA-C	5.84	117.64	111.28
1	B	93	HIS	CA-CB-CG	-5.82	107.98	113.80
1	A	273	TYR	N-CA-C	5.79	117.26	111.07
1	B	170	GLY	N-CA-C	-5.74	104.31	112.81
1	D	42	MSE	N-CA-C	-5.71	108.11	114.62
1	C	322	VAL	N-CA-CB	-5.70	102.87	112.44
1	B	94	GLY	N-CA-C	5.67	126.63	113.18
1	C	40	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	D	31	ALA	N-CA-C	5.56	119.12	110.17
1	D	3	VAL	N-CA-C	5.44	116.31	108.48
1	C	31	ALA	N-CA-C	5.42	118.31	110.28
1	B	140	HIS	CA-CB-CG	-5.41	108.39	113.80
1	A	95	ASP	N-CA-C	5.37	117.75	110.88
1	C	122	THR	N-CA-CB	5.35	118.02	110.90
1	A	170	GLY	N-CA-C	-5.34	103.75	112.83
1	A	38	GLN	N-CA-C	-5.27	107.02	113.50
1	A	62	GLN	N-CA-C	5.25	116.03	109.57
1	B	119	GLY	N-CA-C	5.19	122.59	115.27
1	A	60	ILE	N-CA-CB	5.19	116.69	110.31
1	D	144	TYR	CA-CB-CG	5.18	123.22	113.90
1	A	140	HIS	CA-CB-CG	-5.16	108.64	113.80
1	A	283	ALA	N-CA-C	5.16	117.36	110.35
1	A	162	ALA	CA-C-N	5.14	127.42	120.38
1	A	162	ALA	C-N-CA	5.14	127.42	120.38
1	D	289	ASP	N-CA-C	-5.13	105.38	113.02
1	C	289	ASP	CA-CB-CG	5.11	117.71	112.60
1	D	262	VAL	N-CA-C	5.10	115.68	109.30
1	B	282	HIS	CA-CB-CG	-5.10	108.70	113.80
1	B	58	LEU	N-CA-C	-5.09	102.95	110.48
1	A	93	HIS	CA-CB-CG	-5.08	108.72	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	GLY	N-CA-C	-5.07	105.31	112.81
1	B	175	ASP	CA-CB-CG	5.07	117.67	112.60
1	C	282	HIS	CA-CB-CG	-5.05	108.75	113.80
1	D	60	ILE	N-CA-CB	5.04	116.60	110.95
1	C	337	THR	CA-C-N	5.02	127.26	120.38
1	C	337	THR	C-N-CA	5.02	127.26	120.38
1	B	149	THR	N-CA-C	5.01	115.92	108.86

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	2966	0	2983	68	0
1	B	2958	0	2968	79	0
1	C	2902	0	2913	96	0
1	D	2928	0	2924	77	0
2	B	39	0	25	4	0
2	C	39	0	25	3	0
3	A	134	0	0	8	0
3	B	95	0	0	3	0
3	C	84	0	0	4	0
3	D	96	0	0	3	0
All	All	12241	0	11838	322	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 14.

All (322) 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:C:37:ALA:HB2	1:C:43:LEU:HD23	1.35	1.07
1:C:253:GLU:H	1:C:254:PRO:HD2	1.28	0.96
1:A:208:ILE:HD12	1:A:239:ILE:HD13	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:MSE:HE1	1:B:93:HIS:HB2	1.46	0.95
1:D:233:ALA:HB1	1:D:264:ASN:HB2	1.50	0.92
1:B:259:LEU:HD23	1:B:265:VAL:HG11	1.54	0.86
1:C:10:ARG:HB3	1:C:11:PRO:HD3	1.58	0.86
1:A:95:ASP:HB3	1:A:135:ARG:HB3	1.56	0.85
1:D:95:ASP:HB3	1:D:135:ARG:HB3	1.61	0.83
1:C:37:ALA:HB3	1:C:40:ARG:HG2	1.62	0.80
1:B:190:LEU:HD21	1:B:274:LEU:HD21	1.64	0.80
1:D:208:ILE:HD12	1:D:239:ILE:HD13	1.63	0.79
1:C:233:ALA:HB1	1:C:264:ASN:HB2	1.64	0.79
1:D:60:ILE:HD11	1:D:74:ILE:HD11	1.65	0.78
1:B:16:MSE:HE1	1:B:93:HIS:CB	2.13	0.78
1:C:40:ARG:HH11	1:C:40:ARG:HB3	1.50	0.77
1:D:307:MSE:HE3	1:D:332:ILE:HG21	1.66	0.77
1:C:40:ARG:HD2	1:C:59:ASN:OD1	1.85	0.76
2:B:385:UD1:H1'	2:B:385:UD1:H8'3	1.68	0.76
1:C:247:LEU:HB3	1:C:252:ARG:HB3	1.66	0.75
1:C:16:MSE:HE1	1:C:19:LEU:HD23	1.69	0.75
1:B:16:MSE:CE	1:B:93:HIS:HB2	2.17	0.74
1:B:297:ALA:HB3	1:B:298:PRO:HD3	1.69	0.74
1:B:247:LEU:HB3	1:B:252:ARG:HB3	1.70	0.73
1:A:325:VAL:HG12	1:A:335:GLU:HG3	1.69	0.72
1:D:274:LEU:HB3	1:D:275:PRO:HD3	1.71	0.71
1:D:61:MSE:H	1:D:73:ARG:NH1	1.89	0.71
1:B:274:LEU:HB3	1:B:275:PRO:HD3	1.73	0.70
1:B:10:ARG:HB3	1:B:11:PRO:HD3	1.74	0.69
1:C:17:ALA:HB3	1:C:18:PRO:HD3	1.75	0.69
1:C:36:THR:HG22	1:C:58:LEU:HD12	1.73	0.69
1:A:291:GLY:HA2	1:A:294:GLN:HE21	1.58	0.68
1:C:40:ARG:NH2	1:C:57:ASP:OD2	2.26	0.68
1:B:8:GLY:HA3	1:B:36:THR:HB	1.75	0.67
1:D:201:ILE:HA	1:D:240:GLN:HE22	1.59	0.67
1:C:268:ILE:HD12	1:C:271:GLN:NE2	2.10	0.66
1:C:229:LEU:HG	1:C:241:ILE:HG21	1.78	0.66
1:D:143:MSE:HB3	1:D:374:ILE:HG13	1.77	0.66
1:A:36:THR:HG22	1:A:58:LEU:HB2	1.78	0.64
1:B:131:GLU:HG2	2:B:385:UD1:C7'	2.28	0.64
1:B:16:MSE:HE1	1:B:93:HIS:CG	2.32	0.64
1:D:221:GLY:O	1:D:225:ILE:HD13	1.98	0.64
1:C:190:LEU:HD21	1:C:274:LEU:HD21	1.80	0.64
1:B:40:ARG:HG3	1:B:40:ARG:HH11	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ALA:HB1	1:B:264:ASN:HB3	1.79	0.63
1:C:253:GLU:H	1:C:254:PRO:CD	2.06	0.63
1:D:120:LEU:HD22	3:D:417:HOH:O	1.97	0.63
1:A:215:ARG:HG3	1:A:222:PHE:CZ	2.34	0.62
1:A:198:TYR:HB2	1:A:201:ILE:HD12	1.80	0.62
1:A:10:ARG:HB3	1:A:11:PRO:HD3	1.81	0.62
1:C:65:GLN:HG2	1:C:69:GLU:HG2	1.82	0.62
1:B:17:ALA:HB3	1:B:18:PRO:HD3	1.82	0.62
1:D:5:THR:HG23	1:D:16:MSE:HE3	1.81	0.61
1:A:49:LEU:O	1:A:179:TRP:HZ3	1.82	0.61
1:B:10:ARG:HD3	1:B:42:MSE:HB3	1.82	0.61
1:C:274:LEU:HB3	1:C:275:PRO:HD3	1.83	0.61
1:C:211:THR:HG21	1:C:293:ILE:HD13	1.82	0.61
1:C:188:ASP:HA	1:C:191:ARG:HH11	1.66	0.61
1:C:5:THR:HG21	1:C:16:MSE:HE2	1.83	0.60
1:C:22:ALA:HB1	1:C:366:LEU:HD11	1.83	0.60
1:C:37:ALA:HB2	1:C:43:LEU:CD2	2.23	0.60
1:D:248:ASN:HB3	1:D:249:PRO:HD2	1.82	0.60
1:B:37:ALA:HB2	1:B:40:ARG:NH2	2.17	0.60
1:D:328:ASP:O	1:D:332:ILE:HG12	2.00	0.60
1:A:5:THR:HG23	1:A:16:MSE:HE3	1.84	0.60
1:B:254:PRO:HA	1:B:257:ARG:HD3	1.84	0.60
1:A:153:ARG:HB2	1:A:168:ILE:HD11	1.83	0.60
1:A:253:GLU:O	1:A:257:ARG:HG3	2.02	0.59
1:B:268:ILE:HG22	1:B:269:ASP:N	2.17	0.59
1:A:375:SER:O	1:A:376:LEU:HB3	2.02	0.59
1:D:10:ARG:HB3	1:D:11:PRO:HD3	1.85	0.59
1:C:325:VAL:CG1	1:C:335:GLU:HG3	2.33	0.59
1:D:201:ILE:HA	1:D:240:GLN:NE2	2.17	0.59
1:A:60:ILE:HD11	1:A:74:ILE:HD11	1.84	0.58
1:C:214:ARG:HG3	1:C:246:HIS:HB3	1.84	0.58
1:A:153:ARG:CB	1:A:168:ILE:HD11	2.35	0.57
1:C:79:LYS:HB3	1:C:80:PRO:HD3	1.85	0.57
1:C:131:GLU:HG2	2:C:385:UD1:C7'	2.34	0.57
1:C:37:ALA:CB	1:C:40:ARG:HG2	2.34	0.57
1:C:206:LYS:HB2	1:C:239:ILE:HG22	1.87	0.57
1:A:145:HIS:HD2	3:A:386:HOH:O	1.88	0.56
1:A:38:GLN:NE2	1:A:63:PRO:HB3	2.20	0.56
1:A:79:LYS:HB3	1:A:80:PRO:HD3	1.87	0.56
1:D:92:VAL:HB	1:D:99:THR:HG23	1.86	0.56
1:B:278:TRP:O	1:B:282:HIS:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG23	3:A:444:HOH:O	2.04	0.56
1:C:224:GLU:HG3	1:C:329:LYS:HB3	1.87	0.56
1:A:306:VAL:HG23	1:A:322:VAL:HG13	1.87	0.56
1:C:21[A]:HIS:NE2	1:C:50:PHE:O	2.39	0.55
1:A:9:THR:OG1	1:A:12[B]:GLU:HG2	2.05	0.55
1:B:112:PRO:HG3	1:B:374:ILE:HD11	1.89	0.55
1:C:5:THR:CG2	1:C:16:MSE:HE2	2.36	0.55
1:C:306:VAL:HB	1:C:324:LEU:HD23	1.89	0.55
1:A:330:GLN:O	1:A:334:GLU:HG3	2.07	0.55
1:D:145:HIS:HD2	3:D:385:HOH:O	1.90	0.55
1:C:308:ARG:HG3	1:C:308:ARG:HH11	1.72	0.55
1:B:36:THR:HG22	1:B:38:GLN:N	2.23	0.54
1:C:40:ARG:HH12	1:C:44:ASP:CG	2.15	0.54
1:A:118:ALA:HB1	3:A:386:HOH:O	2.07	0.54
1:C:243:TYR:CE1	1:C:245:VAL:HB	2.42	0.54
1:B:338:ARG:HG2	1:B:345:GLU:OE1	2.07	0.54
1:C:16:MSE:SE	1:C:93:HIS:HB2	2.58	0.54
1:B:325:VAL:HG12	1:B:335:GLU:HG3	1.90	0.54
1:C:358:ASP:OD2	1:C:364:ARG:NH2	2.40	0.54
1:D:72:CYS:O	1:D:76:GLU:HG3	2.08	0.54
1:C:262:VAL:HG11	1:C:265:VAL:HG23	1.91	0.53
1:D:202:ASP:H	1:D:240:GLN:HE22	1.54	0.53
1:D:325:VAL:HG23	1:D:332:ILE:HD12	1.91	0.53
1:C:287:LEU:HD23	1:C:305:LEU:HB2	1.89	0.53
1:D:189:LYS:O	1:D:193:GLU:HG3	2.09	0.53
1:A:287:LEU:HD12	1:A:305:LEU:HB2	1.90	0.53
1:A:224:GLU:OE2	1:A:328:ASP:HA	2.09	0.53
1:D:269:ASP:O	1:D:271:GLN:NE2	2.42	0.53
1:B:17:ALA:HB3	1:B:18:PRO:CD	2.38	0.52
1:C:10:ARG:HB3	1:C:11:PRO:CD	2.35	0.52
1:C:233:ALA:HB2	1:C:241:ILE:HD12	1.92	0.52
1:D:188:ASP:HA	1:D:191:ARG:HD3	1.91	0.52
1:A:249:PRO:HA	3:A:456:HOH:O	2.08	0.52
1:C:218:PHE:HB2	1:C:251:VAL:HG12	1.90	0.52
1:D:305:LEU:HD11	1:D:339:LEU:HD22	1.92	0.52
1:B:37:ALA:HB2	1:B:40:ARG:HH21	1.75	0.52
1:B:247:LEU:HB3	1:B:252:ARG:CB	2.38	0.52
1:C:178:LEU:O	1:C:182:ASP:HB2	2.09	0.52
1:C:40:ARG:HB3	1:C:40:ARG:NH1	2.22	0.52
1:B:243:TYR:CE1	1:B:245:VAL:HB	2.45	0.52
1:B:114:GLY:HA2	1:B:144:TYR:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ARG:O	1:C:41:GLU:C	2.53	0.52
1:C:114:GLY:HA2	1:C:144:TYR:HB2	1.92	0.52
1:D:218:PHE:CZ	1:D:254:PRO:HB2	2.45	0.52
1:C:274:LEU:HB3	1:C:275:PRO:CD	2.40	0.51
1:B:280:MSE:CE	1:B:297:ALA:HB2	2.40	0.51
1:D:38:GLN:HB3	1:D:63:PRO:HD3	1.93	0.51
1:B:212:GLY:HA2	1:B:289:ASP:OD1	2.10	0.51
1:B:296:GLU:O	1:B:299:SER:HB2	2.11	0.51
1:A:95:ASP:HA	3:A:486:HOH:O	2.10	0.51
1:A:227:HIS:HB2	1:A:329:LYS:HE2	1.93	0.51
1:C:9:THR:OG1	1:C:12:GLU:HB2	2.11	0.51
1:A:57:ASP:HB2	3:A:494:HOH:O	2.10	0.51
1:B:112:PRO:CG	1:B:374:ILE:HD11	2.41	0.51
1:C:200:PHE:CD1	1:C:266:ILE:HD13	2.45	0.51
1:D:276:PHE:CE2	1:D:280:MSE:HE2	2.46	0.51
1:C:269:ASP:HB3	1:C:270:PRO:HD2	1.93	0.50
1:A:17:ALA:N	1:A:18:PRO:HD2	2.27	0.50
2:B:385:UD1:HI'	2:B:385:UD1:C8'	2.39	0.50
1:C:325:VAL:HG12	1:C:335:GLU:HG3	1.92	0.50
1:A:248:ASN:H	1:A:251:VAL:CG1	2.25	0.50
1:B:36:THR:HG22	1:B:38:GLN:H	1.77	0.50
1:B:19:LEU:HD21	1:B:91:LEU:HD13	1.93	0.50
1:B:36:THR:O	1:B:60:ILE:HG12	2.11	0.50
1:B:211:THR:O	1:B:288:THR:HA	2.12	0.50
1:C:211:THR:O	1:C:288:THR:HA	2.12	0.50
1:D:306:VAL:HG23	1:D:322:VAL:HG13	1.94	0.50
1:C:338:ARG:NE	1:C:345:GLU:OE2	2.46	0.49
1:C:44:ASP:HA	1:C:47:LEU:HD12	1.94	0.49
1:D:304:VAL:HB	1:D:322:VAL:HG22	1.93	0.49
1:C:11:PRO:HB2	2:C:385:UD1:O6'	2.12	0.49
1:B:308:ARG:NH2	1:B:312:GLU:OE2	2.46	0.49
1:A:188:ASP:HA	1:A:191:ARG:NH1	2.28	0.49
1:B:207:MSE:HE3	1:B:283:ALA:HB2	1.94	0.49
1:D:307:MSE:HE3	1:D:332:ILE:HG13	1.94	0.49
1:A:375:SER:O	1:A:376:LEU:CB	2.60	0.49
1:C:308:ARG:NH2	1:C:312:GLU:OE2	2.43	0.49
1:C:107:PHE:HB2	3:C:462:HOH:O	2.13	0.49
1:D:194:LEU:HD21	1:D:274:LEU:HD23	1.95	0.49
1:C:255:VAL:HG12	1:C:259:LEU:HD11	1.95	0.48
1:B:217:SER:O	1:B:251:VAL:HG11	2.13	0.48
1:B:268:ILE:HG22	1:B:269:ASP:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LEU:HD23	1:B:305:LEU:HB2	1.94	0.48
1:D:253:GLU:HB2	1:D:254:PRO:CD	2.43	0.48
1:B:38:GLN:HG3	3:B:387:HOH:O	2.13	0.48
1:B:253:GLU:N	1:B:254:PRO:HD2	2.28	0.48
1:B:211:THR:HG21	1:B:293:ILE:CD1	2.44	0.48
1:C:145:HIS:HE1	3:C:413:HOH:O	1.96	0.48
1:B:303:PRO:HG2	1:B:346:TYR:CE2	2.49	0.48
1:A:92:VAL:HB	1:A:99:THR:HG23	1.95	0.48
1:B:40:ARG:NH1	1:B:44:ASP:OD1	2.47	0.48
1:C:95:ASP:HB3	1:C:135:ARG:HB3	1.96	0.47
1:D:253:GLU:HB2	1:D:254:PRO:HD3	1.95	0.47
1:A:78:LEU:CD1	1:A:102:THR:HG23	2.44	0.47
1:A:323:ARG:NH1	1:A:335:GLU:OE2	2.47	0.47
1:B:269:ASP:HB3	1:B:270:PRO:HD2	1.97	0.47
1:B:36:THR:HG21	1:B:98:THR:OG1	2.15	0.47
1:C:262:VAL:HG12	1:C:264:ASN:H	1.79	0.47
1:C:210:VAL:O	1:C:244:PRO:HD2	2.14	0.47
1:D:244:PRO:HA	1:D:268:ILE:O	2.14	0.47
1:D:288:THR:HG21	1:D:293:ILE:CG2	2.45	0.47
1:B:200:PHE:HE2	1:B:242:VAL:HG22	1.79	0.47
1:D:244:PRO:HA	1:D:268:ILE:HG13	1.96	0.47
1:D:307:MSE:HE3	1:D:332:ILE:CG2	2.38	0.47
1:A:147:SER:HB2	1:A:168:ILE:HD13	1.97	0.47
1:A:280:MSE:SE	1:A:293:ILE:HD11	2.66	0.47
1:A:259:LEU:O	1:A:260:GLY:C	2.58	0.46
1:D:329:LYS:O	1:D:333:VAL:HG23	2.16	0.46
1:B:5:THR:CG2	1:B:16:MSE:HG2	2.46	0.46
1:B:117:GLU:O	1:B:117:GLU:HG2	2.16	0.46
1:A:49:LEU:O	1:A:179:TRP:CZ3	2.66	0.46
1:A:145:HIS:HE1	3:A:457:HOH:O	1.98	0.46
1:C:189:LYS:O	1:C:193:GLU:HG3	2.15	0.46
1:C:179:TRP:O	1:C:183:GLN:HB3	2.16	0.46
1:D:35:VAL:HG23	1:D:54:PRO:HB3	1.97	0.46
1:D:285:LEU:HG	1:D:286:ILE:N	2.31	0.46
1:B:143:MSE:HG3	1:B:374:ILE:HD13	1.97	0.46
1:C:1:MSE:HE1	1:C:369:LEU:O	2.16	0.46
1:B:268:ILE:CG2	1:B:269:ASP:N	2.78	0.46
1:B:358:ASP:CG	1:B:364:ARG:HH22	2.24	0.46
1:A:79:LYS:HB3	1:A:80:PRO:CD	2.46	0.45
1:A:339:LEU:CD2	1:A:345:GLU:HG2	2.46	0.45
1:C:358:ASP:CG	1:C:364:ARG:HH22	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:ARG:HG3	1:C:308:ARG:NH1	2.30	0.45
1:D:330:GLN:O	1:D:334:GLU:HG3	2.17	0.45
1:D:202:ASP:H	1:D:240:GLN:NE2	2.14	0.45
1:A:198:TYR:CB	1:A:201:ILE:HD12	2.45	0.45
1:A:251:VAL:O	1:A:255:VAL:HG23	2.17	0.45
1:B:189:LYS:O	1:B:193:GLU:HG3	2.17	0.45
1:C:35:VAL:CG1	1:C:43:LEU:HD21	2.46	0.45
1:C:253:GLU:N	1:C:254:PRO:HD2	2.09	0.45
1:D:78:LEU:CD1	1:D:102:THR:HG23	2.46	0.45
1:A:304:VAL:HB	1:A:322:VAL:HG22	1.98	0.45
1:C:303:PRO:HG2	1:C:346:TYR:CE2	2.52	0.45
1:D:43:LEU:O	1:D:47:LEU:HG	2.17	0.45
1:D:326:GLY:O	1:D:332:ILE:HD11	2.17	0.45
1:D:368:ALA:HA	1:D:372:ASN:HD22	1.81	0.45
1:A:215:ARG:NH2	1:A:289:ASP:OD1	2.43	0.45
1:B:185:MSE:HE2	1:B:194:LEU:CD1	2.47	0.45
1:B:329:LYS:O	1:B:333:VAL:HG23	2.16	0.45
3:C:386:HOH:O	1:D:107:PHE:HA	2.16	0.45
1:A:165:ARG:CZ	1:A:374:ILE:HD11	2.47	0.44
1:B:143:MSE:HG3	1:B:374:ILE:CD1	2.47	0.44
1:A:224:GLU:HG3	1:A:329:LYS:HE3	2.00	0.44
1:D:179:TRP:O	1:D:183:GLN:HG2	2.18	0.44
1:B:268:ILE:CG2	1:B:269:ASP:H	2.29	0.44
1:D:120:LEU:HD12	1:D:120:LEU:N	2.32	0.44
1:D:368:ALA:O	1:D:372:ASN:HB2	2.17	0.44
1:B:304:VAL:HB	1:B:322:VAL:HG22	1.98	0.44
1:B:257:ARG:HH11	1:B:257:ARG:HG3	1.83	0.44
1:C:243:TYR:HB3	1:C:267:LEU:HD23	1.99	0.44
1:D:197:ASN:N	1:D:197:ASN:HD22	2.15	0.44
1:A:291:GLY:HA2	1:A:294:GLN:NE2	2.27	0.44
1:B:112:PRO:HB3	1:B:374:ILE:HD11	1.99	0.44
1:A:269:ASP:HB3	1:A:270:PRO:HD2	1.98	0.44
3:A:471:HOH:O	1:C:158:ARG:HD3	2.18	0.44
1:D:65:GLN:HE22	1:D:73:ARG:CZ	2.31	0.44
1:D:273:TYR:O	1:D:277:VAL:HG23	2.17	0.44
1:C:1:MSE:HE2	1:C:373:ARG:HD3	1.99	0.43
1:C:127:SER:HA	1:C:128:PRO:HA	1.89	0.43
1:D:283:ALA:O	1:D:302:LYS:NZ	2.40	0.43
1:D:118:ALA:HB1	3:D:385:HOH:O	2.18	0.43
1:D:201:ILE:O	1:D:201:ILE:HG13	2.17	0.43
1:C:79:LYS:HB3	1:C:80:PRO:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ALA:N	1:C:298:PRO:HD2	2.33	0.43
1:D:17:ALA:N	1:D:18:PRO:HD2	2.33	0.43
1:B:129:TRP:HA	1:B:130:PRO:HA	1.75	0.43
1:C:21[A]:HIS:CE1	1:C:50:PHE:O	2.72	0.43
1:B:16:MSE:HE1	1:B:93:HIS:CD2	2.53	0.43
1:B:218:PHE:CE1	1:B:223:GLU:HB2	2.53	0.43
1:D:5:THR:CG2	1:D:16:MSE:HE3	2.47	0.43
1:D:202:ASP:N	1:D:240:GLN:HE22	2.17	0.43
1:D:268:ILE:HD12	1:D:271:GLN:NE2	2.34	0.43
1:A:19:LEU:HD21	1:A:91:LEU:HD13	2.00	0.43
1:C:298:PRO:HG2	1:C:354:ASN:ND2	2.34	0.43
1:A:10:ARG:N	1:A:11:PRO:CD	2.82	0.43
1:A:148:PRO:HD2	1:A:152:SER:OG	2.18	0.43
1:B:200:PHE:CE1	1:B:268:ILE:HD11	2.53	0.43
1:A:274:LEU:N	1:A:275:PRO:HD2	2.34	0.42
1:B:145:HIS:HE1	3:B:441:HOH:O	2.02	0.42
1:C:10:ARG:CB	1:C:11:PRO:HD3	2.35	0.42
1:B:224:GLU:HG3	1:B:329:LYS:N	2.33	0.42
1:C:253:GLU:N	1:C:254:PRO:CD	2.73	0.42
1:C:323:ARG:HD2	1:C:349:MSE:SE	2.69	0.42
2:C:385:UD1:H5'	3:C:427:HOH:O	2.19	0.42
1:D:38:GLN:OE1	1:D:63:PRO:HA	2.19	0.42
1:A:273:TYR:O	1:A:277:VAL:HG23	2.20	0.42
1:B:263:LYS:HB2	3:B:454:HOH:O	2.18	0.42
1:D:41:GLU:HA	1:D:44:ASP:OD2	2.19	0.42
1:C:13:ALA:HB2	1:C:43:LEU:HD13	2.01	0.42
1:C:211:THR:HG21	1:C:293:ILE:CD1	2.48	0.42
1:C:288:THR:OG1	1:C:290:SER:HB3	2.19	0.42
1:A:147:SER:HA	1:A:148:PRO:HD3	1.91	0.42
1:B:116:VAL:O	1:B:117:GLU:HB3	2.19	0.42
1:C:122:THR:HG23	1:C:312:GLU:HB3	2.02	0.42
1:D:39:HIS:CD2	1:D:63:PRO:HG3	2.55	0.42
1:A:78:LEU:HD11	1:A:102:THR:HG23	2.02	0.42
2:B:385:UD1:O2B	2:B:385:UD1:H5'2	2.20	0.42
1:C:40:ARG:NH1	1:C:44:ASP:OD1	2.46	0.42
1:A:180:VAL:HG21	1:A:273:TYR:CE2	2.55	0.41
1:B:95:ASP:HB3	1:B:135:ARG:HB3	2.02	0.41
1:D:272:GLU:O	1:D:275:PRO:HD2	2.20	0.41
1:A:5:THR:CG2	1:A:16:MSE:HE3	2.49	0.41
1:B:239:ILE:CD1	1:B:241:ILE:HG13	2.49	0.41
1:C:160:ASN:HD22	1:C:160:ASN:HA	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:GLU:O	1:C:299:SER:HB2	2.20	0.41
1:A:247:LEU:HB2	1:A:252:ARG:HG2	2.01	0.41
1:C:232:ILE:HD13	1:C:336:VAL:HG21	2.02	0.41
1:A:374:ILE:HA	1:A:374:ILE:HD13	1.85	0.41
1:B:277:VAL:O	1:B:281:ASN:HB2	2.20	0.41
1:D:325:VAL:HG12	1:D:335:GLU:HG3	2.02	0.41
1:A:227:HIS:CB	1:A:329:LYS:HE2	2.50	0.41
1:A:295:GLU:OE2	1:A:313:ARG:NE	2.53	0.41
1:B:200:PHE:CE2	1:B:266:ILE:HG21	2.56	0.41
1:C:325:VAL:HG11	1:C:335:GLU:HG3	2.03	0.41
1:A:253:GLU:HB3	1:A:254:PRO:HD3	2.02	0.41
1:D:147:SER:HB3	1:D:152:SER:HB2	2.02	0.41
1:A:9:THR:HB	1:A:11:PRO:HD2	2.03	0.41
1:B:136:THR:O	1:B:140:HIS:HD2	2.04	0.41
1:C:137:LEU:HD13	1:D:137:LEU:HD13	2.02	0.41
1:D:61:MSE:CB	1:D:73:ARG:HH12	2.33	0.41
1:D:197:ASN:N	1:D:197:ASN:ND2	2.68	0.41
1:A:367:GLU:HG3	1:A:371:ASN:ND2	2.36	0.41
1:B:40:ARG:HG3	1:B:40:ARG:NH1	2.30	0.41
1:C:68:THR:HG23	1:D:75:LEU:HB3	2.02	0.41
1:B:205:LYS:HB3	1:B:238:ASP:O	2.21	0.40
1:B:280:MSE:HE3	1:B:293:ILE:HG23	2.01	0.40
1:D:181:ARG:NH1	1:D:182:ASP:OD1	2.48	0.40
1:D:62:GLN:HA	1:D:63:PRO:HD2	1.91	0.40
1:A:194:LEU:HA	1:A:197:ASN:HD22	1.87	0.40
1:D:79:LYS:N	1:D:80:PRO:HD2	2.35	0.40
1:C:35:VAL:HG13	1:C:43:LEU:HD21	2.02	0.40
1:C:153:ARG:HD3	1:C:168:ILE:HD11	2.02	0.40
1:D:165:ARG:NH2	1:D:374:ILE:HG12	2.37	0.40
1:D:198:TYR:CE2	1:D:279:LEU:HG	2.56	0.40
1:D:244:PRO:HB3	1:D:268:ILE:HG13	2.03	0.40
1:C:205:LYS:HE3	1:C:237:GLN:O	2.21	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	375/384 (98%)	362 (96%)	12 (3%)	1 (0%)	36	45
1	B	330/384 (86%)	313 (95%)	16 (5%)	1 (0%)	36	45
1	C	362/384 (94%)	341 (94%)	17 (5%)	4 (1%)	11	12
1	D	372/384 (97%)	347 (93%)	21 (6%)	4 (1%)	11	12
All	All	1439/1536 (94%)	1363 (95%)	66 (5%)	10 (1%)	18	22

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	41	GLU
1	A	61	MSE
1	D	61	MSE
1	D	217	SER
1	B	41	GLU
1	C	253	GLU
1	C	59	ASN
1	D	8	GLY
1	D	221	GLY
1	C	268	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	326/324 (101%)	316 (97%)	10 (3%)	35	51
1	B	326/324 (101%)	308 (94%)	18 (6%)	19	27
1	C	318/324 (98%)	304 (96%)	14 (4%)	25	37
1	D	318/324 (98%)	301 (95%)	17 (5%)	20	29
All	All	1288/1296 (99%)	1229 (95%)	59 (5%)	24	35

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	95	ASP
1	A	120	LEU
1	A	192	SER
1	A	224	GLU
1	A	239	ILE
1	A	264	ASN
1	A	327	THR
1	A	329	LYS
1	A	363	SER
1	B	16	MSE
1	B	35	VAL
1	B	36	THR
1	B	38	GLN
1	B	40	ARG
1	B	41	GLU
1	B	65	GLN
1	B	110[A]	ARG
1	B	110[B]	ARG
1	B	160	ASN
1	B	231	ASP
1	B	251	VAL
1	B	281	ASN
1	B	309	ASP
1	B	322	VAL
1	B	343	GLU
1	B	350	SER
1	B	367	GLU
1	C	35	VAL
1	C	40	ARG
1	C	41	GLU
1	C	84	GLU
1	C	120	LEU
1	C	130	PRO
1	C	137	LEU
1	C	160	ASN
1	C	214	ARG
1	C	235	THR
1	C	240	GLN
1	C	281	ASN
1	C	299	SER
1	C	322	VAL

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Mol	Chain	Res	Type
1	D	40	ARG
1	D	48	LYS
1	D	61	MSE
1	D	84	GLU
1	D	127	SER
1	D	130	PRO
1	D	175	ASP
1	D	181	ARG
1	D	191	ARG
1	D	197	ASN
1	D	222	PHE
1	D	225	ILE
1	D	289	ASP
1	D	313	ARG
1	D	339	LEU
1	D	366	LEU
1	D	371	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	145	HIS
1	A	154	GLN
1	A	197	ASN
1	A	256	ASN
1	A	294	GLN
1	A	371	ASN
1	B	39	HIS
1	B	145	HIS
1	B	160	ASN
1	B	237	GLN
1	B	281	ASN
1	B	282	HIS
1	C	145	HIS
1	C	160	ASN
1	C	197	ASN
1	C	213	HIS
1	C	227	HIS
1	C	237	GLN
1	C	256	ASN
1	C	371	ASN

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Mol	Chain	Res	Type
1	D	140	HIS
1	D	145	HIS
1	D	197	ASN
1	D	213	HIS
1	D	240	GLN
1	D	248	ASN
1	D	372	ASN

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UD1	B	385	-	40,41,41	1.45	5 (12%)	59,62,62	1.84	14 (23%)
2	UD1	C	385	-	40,41,41	1.47	4 (10%)	59,62,62	2.09	16 (27%)

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	UD1	B	385	-	1/1/12/13	9/26/63/63	0/3/3/3
2	UD1	C	385	-	1/1/12/13	8/26/63/63	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	385	UD1	PB-O3A	-5.69	1.53	1.59
2	B	385	UD1	PB-O3A	-5.61	1.53	1.59
2	C	385	UD1	O5'-C1'	3.43	1.50	1.41
2	C	385	UD1	PB-O1'	-3.21	1.49	1.59
2	B	385	UD1	PB-O1'	-3.02	1.50	1.59
2	B	385	UD1	O5'-C1'	2.87	1.49	1.41
2	C	385	UD1	PA-O3A	-2.15	1.57	1.59
2	B	385	UD1	PA-O3A	-2.11	1.57	1.59
2	B	385	UD1	C2'-N2'	2.09	1.49	1.45

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	385	UD1	O5'-C1'-O1'	-8.86	99.79	111.36
2	B	385	UD1	O5'-C1'-O1'	-6.63	102.70	111.36
2	B	385	UD1	O3A-PA-O1A	-4.76	96.39	110.70
2	C	385	UD1	O3A-PA-O1A	-4.63	96.78	110.70
2	C	385	UD1	O4-C4-C5	3.95	131.98	125.16
2	C	385	UD1	O4-C4-N3	-3.93	113.57	119.27
2	C	385	UD1	O2A-PA-O3A	3.58	116.94	107.27
2	B	385	UD1	C2'-N2'-C7'	-3.41	115.12	123.11
2	B	385	UD1	O4-C4-N3	-3.24	114.58	119.27
2	B	385	UD1	C1'-C2'-C3'	3.09	118.72	110.19
2	B	385	UD1	O2A-PA-O3A	2.99	115.35	107.27
2	C	385	UD1	C3'-C4'-C5'	-2.98	104.83	110.23
2	C	385	UD1	C2B-C1B-N1	2.90	121.32	113.25
2	B	385	UD1	O4-C4-C5	2.86	130.10	125.16
2	B	385	UD1	C3'-C2'-N2'	-2.81	105.44	110.62
2	B	385	UD1	O5'-C1'-C2'	-2.75	105.39	110.59
2	B	385	UD1	C1'-C2'-N2'	-2.68	106.42	110.92
2	C	385	UD1	C4B-O4B-C1B	2.54	115.07	109.47
2	C	385	UD1	C1'-O5'-C5'	-2.49	108.85	113.72
2	C	385	UD1	C1'-C2'-C3'	2.45	116.96	110.19
2	C	385	UD1	C1'-C2'-N2'	-2.44	106.83	110.92
2	C	385	UD1	O3A-PB-O1B	-2.29	103.82	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	385	UD1	C4B-O4B-C1B	2.22	114.38	109.47
2	B	385	UD1	C2B-C1B-N1	2.20	119.39	113.25
2	C	385	UD1	C2'-N2'-C7'	-2.17	118.03	123.11
2	C	385	UD1	O2'-C2B-C3B	-2.16	104.91	111.82
2	B	385	UD1	O3'-C3'-C2'	-2.15	105.30	109.58
2	C	385	UD1	O5'-C1'-C2'	-2.15	106.53	110.59
2	B	385	UD1	O3A-PB-O1B	-2.06	104.50	110.70
2	C	385	UD1	C3B-C2B-C1B	2.04	105.33	101.46

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	385	UD1	C2'
2	C	385	UD1	C2'

All (17) torsion outliers are listed below:

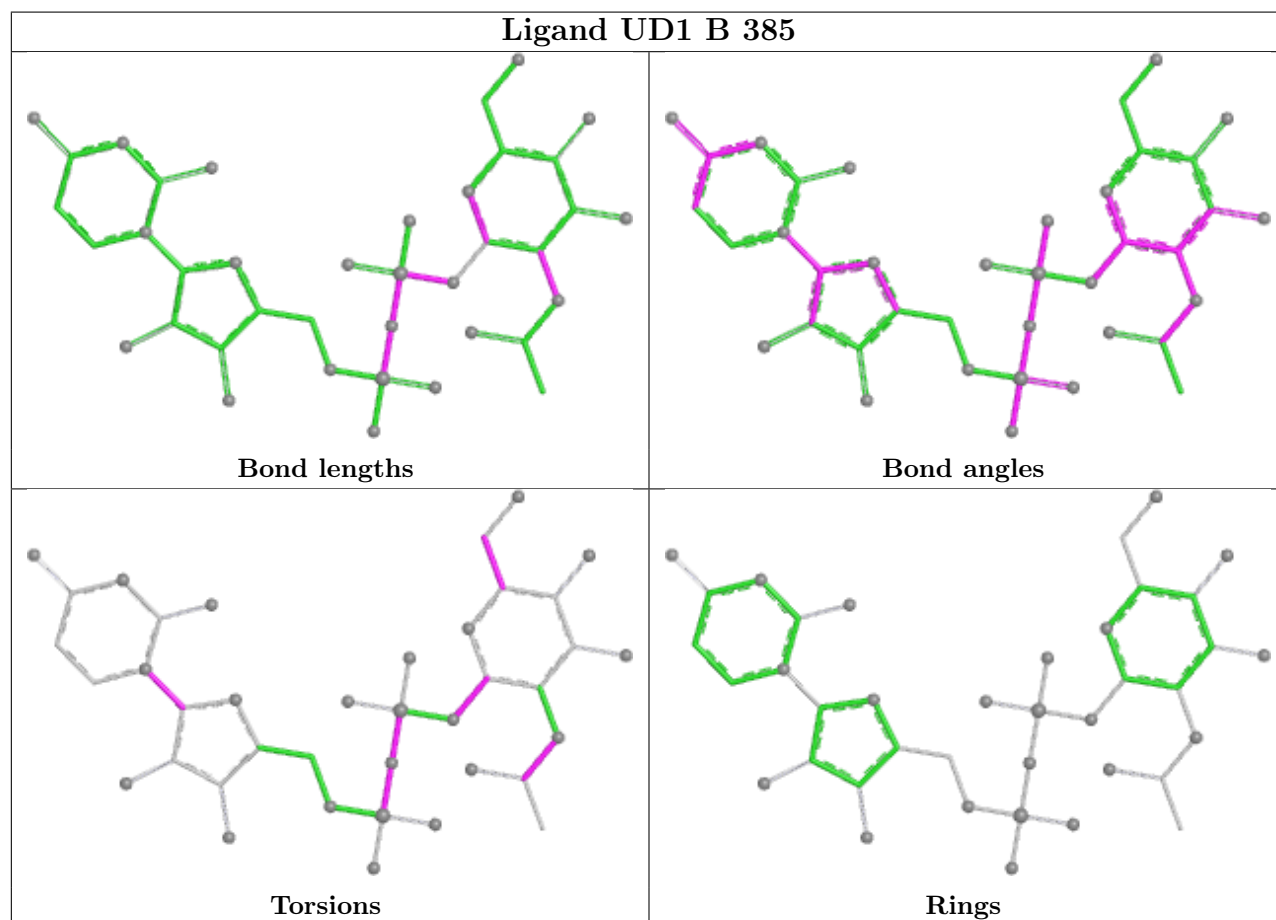
Mol	Chain	Res	Type	Atoms
2	B	385	UD1	O5'-C1'-O1'-PB
2	B	385	UD1	C8'-C7'-N2'-C2'
2	B	385	UD1	O7'-C7'-N2'-C2'
2	B	385	UD1	PB-O3A-PA-O5B
2	C	385	UD1	O5'-C1'-O1'-PB
2	C	385	UD1	C8'-C7'-N2'-C2'
2	C	385	UD1	O7'-C7'-N2'-C2'
2	C	385	UD1	PB-O3A-PA-O5B
2	C	385	UD1	O5'-C5'-C6'-O6'
2	B	385	UD1	O5'-C5'-C6'-O6'
2	C	385	UD1	C4'-C5'-C6'-O6'
2	B	385	UD1	C4'-C5'-C6'-O6'
2	B	385	UD1	PA-O3A-PB-O2B
2	C	385	UD1	PA-O3A-PB-O2B
2	B	385	UD1	C2B-C1B-N1-C6
2	C	385	UD1	PA-O3A-PB-O1B
2	B	385	UD1	O4B-C1B-N1-C6

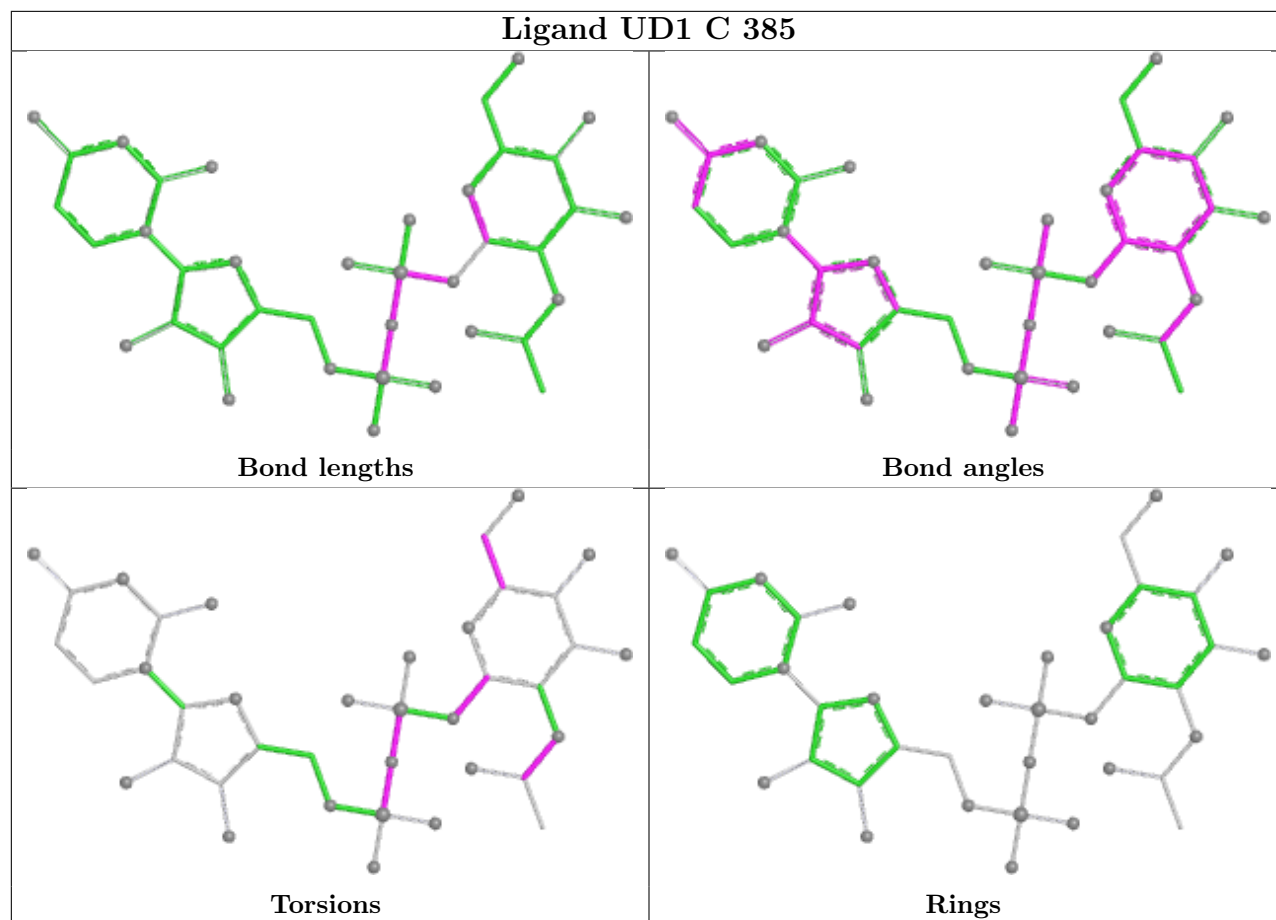
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	385	UD1	4	0
2	C	385	UD1	3	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	366/384 (95%)	0.19	8 (2%) 62 65	18, 32, 59, 71	1 (0%)
1	B	363/384 (94%)	0.45	26 (7%) 21 24	15, 35, 71, 86	4 (1%)
1	C	358/384 (93%)	0.68	34 (9%) 14 16	21, 43, 82, 90	1 (0%)
1	D	364/384 (94%)	0.51	35 (9%) 13 15	18, 37, 81, 91	0
All	All	1451/1536 (94%)	0.45	103 (7%) 22 24	15, 37, 73, 91	6 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	247	LEU	5.0
1	B	251	VAL	4.5
1	C	38	GLN	4.1
1	C	249	PRO	4.1
1	B	376	LEU	4.0
1	D	249	PRO	3.7
1	B	247	LEU	3.6
1	C	214	ARG	3.4
1	D	258	ILE	3.4
1	D	201	ILE	3.4
1	D	251	VAL	3.4
1	C	184	VAL	3.3
1	C	251	VAL	3.2
1	B	255	VAL	3.2
1	B	178	LEU	3.2
1	C	218	PHE	3.2
1	D	195	ALA	3.2
1	D	255	VAL	3.1
1	C	260	GLY	3.1
1	D	64	GLY	3.0
1	C	60	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	266	ILE	3.0
1	A	60	ILE	2.9
1	B	249	PRO	2.9
1	C	213	HIS	2.9
1	D	259	LEU	2.9
1	D	245	VAL	2.9
1	B	190	LEU	2.8
1	D	203	PRO	2.8
1	D	46	VAL	2.8
1	B	221	GLY	2.8
1	C	248	ASN	2.7
1	C	187	SER	2.7
1	D	262	VAL	2.7
1	D	60	ILE	2.7
1	B	216	GLU	2.7
1	C	255	VAL	2.7
1	D	252	ARG	2.7
1	A	63	PRO	2.6
1	B	222	PHE	2.6
1	D	264	ASN	2.6
1	C	265	VAL	2.6
1	C	258	ILE	2.6
1	A	326	GLY	2.6
1	B	218	PHE	2.6
1	D	217	SER	2.6
1	D	248	ASN	2.5
1	C	222	PHE	2.5
1	B	39	HIS	2.5
1	B	182	ASP	2.5
1	A	219	GLY	2.5
1	D	63	PRO	2.5
1	B	258	ILE	2.5
1	D	269	ASP	2.5
1	D	213	HIS	2.5
1	D	221	GLY	2.5
1	B	262	VAL	2.5
1	C	191	ARG	2.5
1	C	49	LEU	2.4
1	C	254	PRO	2.4
1	A	376	LEU	2.4
1	C	36	THR	2.4
1	C	274	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	58	LEU	2.4
1	B	183	GLN	2.4
1	B	219	GLY	2.3
1	D	220	ARG	2.3
1	A	119	GLY	2.3
1	B	261	HIS	2.3
1	C	261	HIS	2.3
1	C	245	VAL	2.3
1	C	372	ASN	2.2
1	C	35	VAL	2.2
1	D	244	PRO	2.2
1	C	180	VAL	2.2
1	B	234	THR	2.2
1	B	259	LEU	2.1
1	D	254	PRO	2.1
1	D	261	HIS	2.1
1	B	363	SER	2.1
1	C	195	ALA	2.1
1	B	238	ASP	2.1
1	C	281	ASN	2.1
1	D	202	ASP	2.1
1	C	199	PRO	2.1
1	C	359	GLY	2.1
1	C	58	LEU	2.1
1	D	267	LEU	2.1
1	C	262	VAL	2.1
1	D	186	SER	2.1
1	C	37	ALA	2.1
1	A	58	LEU	2.1
1	A	213	HIS	2.1
1	C	39	HIS	2.1
1	C	259	LEU	2.1
1	D	197	ASN	2.1
1	B	184	VAL	2.1
1	B	186	SER	2.0
1	D	37	ALA	2.0
1	B	179	TRP	2.0
1	D	282	HIS	2.0
1	B	374	ILE	2.0
1	D	263	LYS	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](#)

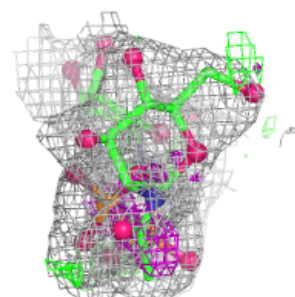
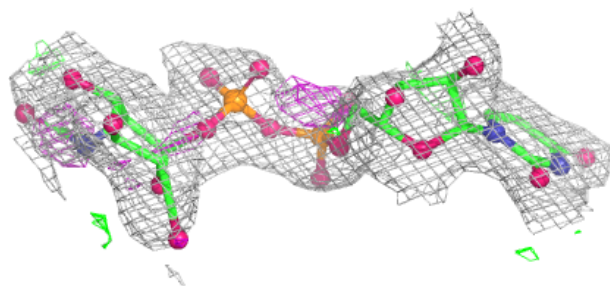
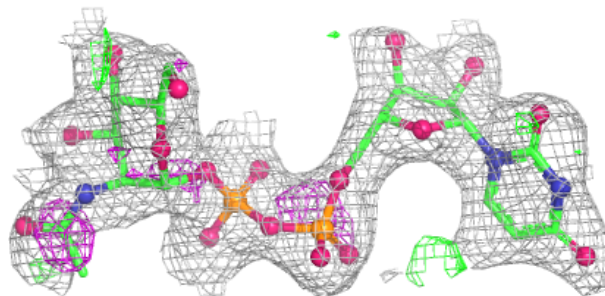
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	UD1	C	385	39/39	0.85	0.11	46,51,54,54	0
2	UD1	B	385	39/39	0.89	0.10	41,45,50,51	0

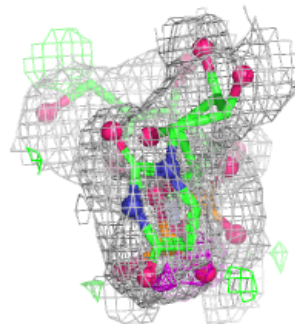
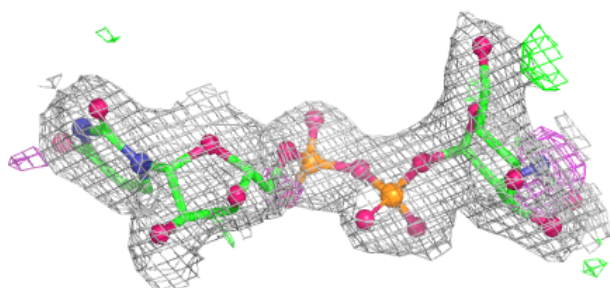
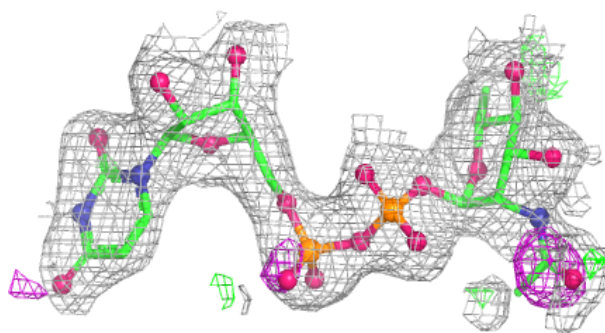
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UD1 C 385:

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

**Electron density around UD1 B 385:**

$2mF_o-DF_c$ (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.