



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 07:47 AM EDT

PDB ID : 2NRU / pdb_00002nru
Title : Crystal structure of IRAK-4
Authors : Wang, Z.; Liu, J.; Walker, N.P.C.
Deposited on : 2006-11-02
Resolution : 2.00 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

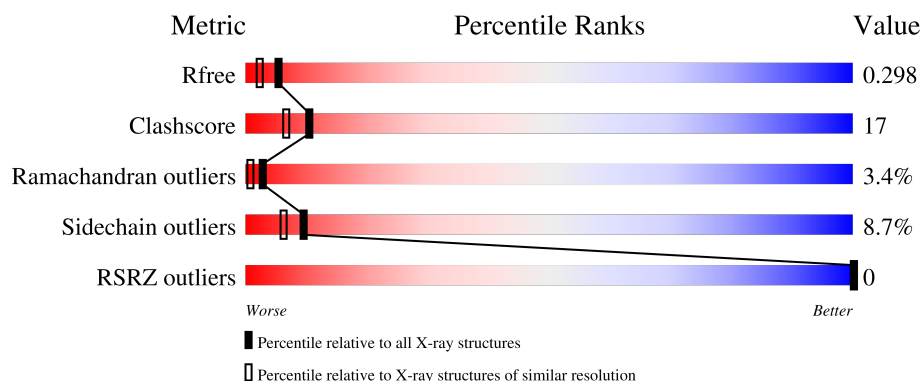
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	307	
1	B	307	
1	C	307	
1	D	307	

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
1	TPO	A	345	X	-	-	-
1	TPO	B	345	X	-	-	-
1	TPO	C	345	X	-	-	-
1	TPO	D	345	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9949 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.

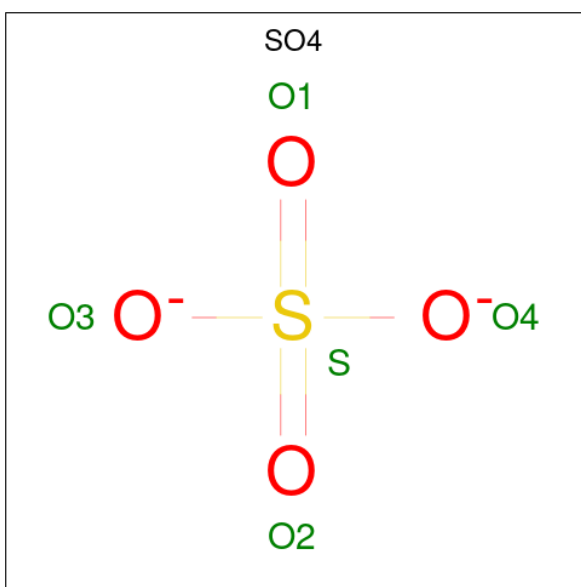
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	P	S	0	0	0
			2329	1462	391	459	2	15			
1	B	296	Total	C	N	O	P	S	0	1	0
			2339	1468	392	461	2	16			
1	C	295	Total	C	N	O	P	S	0	1	0
			2330	1462	391	460	2	15			
1	D	295	Total	C	N	O	P	S	0	1	0
			2330	1462	391	460	2	15			

There are 8 discrepancies between the modelled and reference sequences:

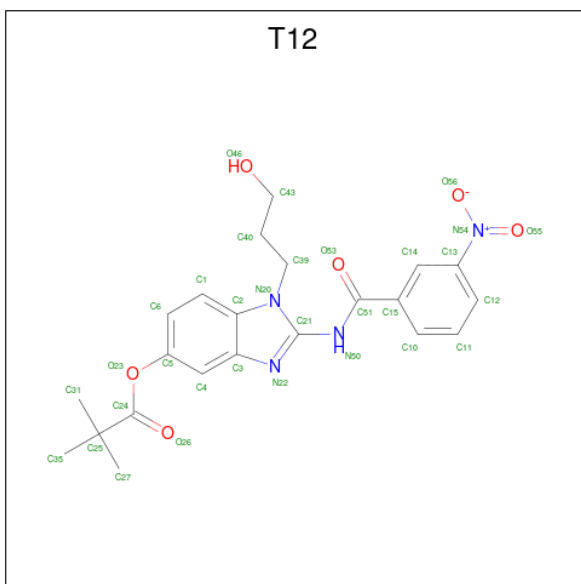
Chain	Residue	Modelled	Actual	Comment	Reference
A	345	TPO	THR	modified residue	UNP Q9NWZ3
A	346	SEP	SER	modified residue	UNP Q9NWZ3
B	345	TPO	THR	modified residue	UNP Q9NWZ3
B	346	SEP	SER	modified residue	UNP Q9NWZ3
C	345	TPO	THR	modified residue	UNP Q9NWZ3
C	346	SEP	SER	modified residue	UNP Q9NWZ3
D	345	TPO	THR	modified residue	UNP Q9NWZ3
D	346	SEP	SER	modified residue	UNP Q9NWZ3

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is 1-(3-HYDROXYPROPYL)-2-[(3-NITROBENZOYL)AMINO]-1H-BENZIMIDAZOL-5-YL PIVALATE (CCD ID: T12) (formula: $C_{22}H_{24}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	22	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			32	22	4	6		
3	C	1	Total	C	N	O	0	0
			32	22	4	6		
3	D	1	Total	C	N	O	0	0
			32	22	4	6		

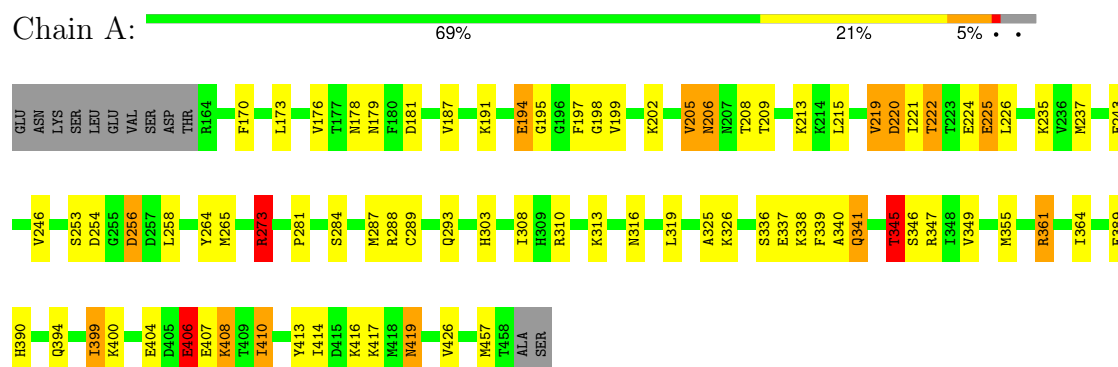
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total	O	0	0
			114	114		
4	B	121	Total	O	0	0
			121	121		
4	C	126	Total	O	0	0
			126	126		
4	D	122	Total	O	0	0
			122	122		

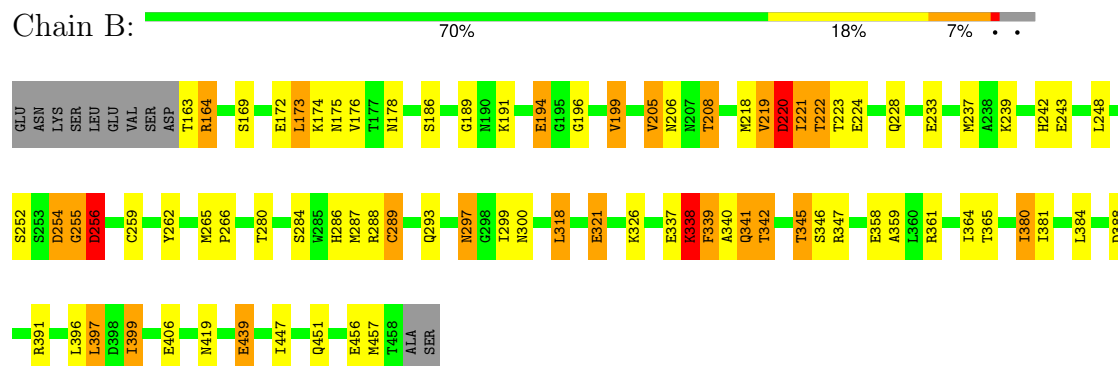
3 Residue-property plots

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.

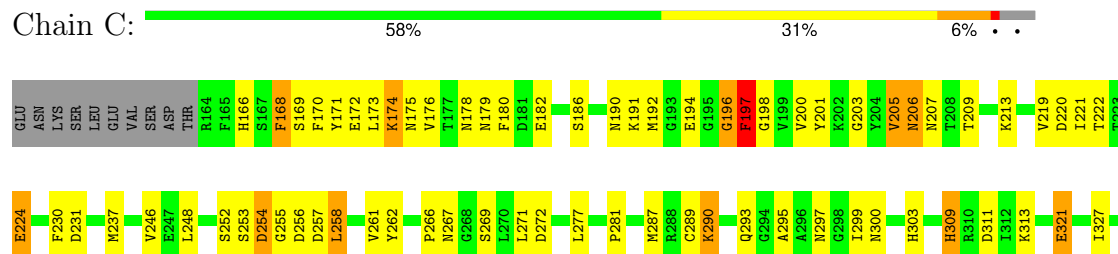
- Molecule 1: Interleukin-1 receptor-associated kinase 4

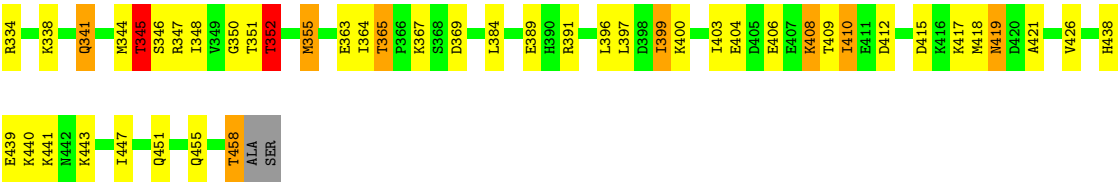


- Molecule 1: Interleukin-1 receptor-associated kinase 4

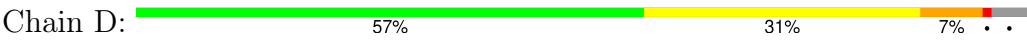


- Molecule 1: Interleukin-1 receptor-associated kinase 4





● Molecule 1: Interleukin-1 receptor-associated kinase 4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.30Å 141.29Å 88.42Å 90.00° 125.80° 90.00°	Depositor
Resolution (Å)	90.29 – 2.00 90.29 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.2 (90.29-2.00) 87.7 (90.29-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.233 , 0.299 0.233 , 0.298	Depositor DCC
R_{free} test set	4644 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.187 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9949	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.38% 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: TPO, SO4, SEP, T12

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	1.13	3/2347 (0.1%)	1.21	9/3164 (0.3%)
1	B	1.20	2/2362 (0.1%)	1.19	11/3184 (0.3%)
1	C	1.22	4/2353 (0.2%)	1.28	9/3172 (0.3%)
1	D	1.28	8/2353 (0.3%)	1.28	13/3172 (0.4%)
All	All	1.21	17/9415 (0.2%)	1.24	42/12692 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	0
1	B	1	2
1	C	2	0
1	D	1	1
All	All	6	3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	280	THR	CA-CB	9.17	1.67	1.53
1	D	313	LYS	N-CA	6.64	1.54	1.46
1	D	280	THR	CA-CB	6.28	1.62	1.53
1	D	311	ASP	CA-CB	6.06	1.57	1.53
1	D	292	ALA	C-O	-6.00	1.17	1.24
1	C	271	LEU	C-O	-5.95	1.17	1.24
1	D	212	VAL	C-O	5.89	1.30	1.24
1	D	399	ILE	CA-CB	5.74	1.62	1.54
1	C	261	VAL	C-O	-5.71	1.17	1.24
1	D	267	ASN	N-CA	-5.61	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	316	ASN	N-CA	5.57	1.52	1.46
1	B	318	LEU	N-CA	5.45	1.52	1.45
1	A	313	LYS	N-CA	5.39	1.52	1.46
1	C	313	LYS	N-CA	5.24	1.52	1.46
1	C	309	HIS	C-O	5.16	1.30	1.24
1	D	386	ALA	CA-CB	5.16	1.61	1.53
1	A	399	ILE	CA-CB	5.03	1.61	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ARG	NE-CZ-NH2	-7.96	112.03	119.20
1	B	189	GLY	N-CA-C	7.16	121.72	112.13
1	B	381	ILE	N-CA-C	7.06	117.20	110.42
1	C	205	VAL	N-CA-C	6.98	116.76	106.85
1	D	281	PRO	O-C-N	6.77	124.33	121.15
1	A	281	PRO	CA-C-N	6.47	126.43	119.76
1	A	281	PRO	C-N-CA	6.47	126.43	119.76
1	C	281	PRO	N-CA-C	6.38	118.48	110.70
1	D	194	GLU	N-CA-C	6.28	118.72	109.24
1	D	281	PRO	N-CA-C	6.17	117.18	110.58
1	A	256	ASP	N-CA-C	6.14	120.35	112.86
1	A	273	ARG	CG-CD-NE	-5.96	98.88	112.00
1	C	352	THR	N-CA-C	5.86	118.14	111.11
1	B	380	ILE	N-CA-C	5.82	116.00	110.42
1	C	269	SER	N-CA-C	5.81	119.11	110.52
1	A	273	ARG	NE-CZ-NH1	5.74	127.24	121.50
1	A	273	ARG	CD-NE-CZ	5.65	132.31	124.40
1	A	406	GLU	N-CA-C	5.65	122.83	110.80
1	B	289	CYS	N-CA-C	5.59	117.05	111.07
1	B	384	LEU	CA-C-N	-5.42	114.37	119.85
1	B	384	LEU	C-N-CA	-5.42	114.37	119.85
1	C	267	ASN	N-CA-C	5.39	118.97	112.93
1	D	219	VAL	N-CA-C	-5.35	98.21	109.34
1	B	242	HIS	CA-C-N	5.35	128.19	120.38
1	B	242	HIS	C-N-CA	5.35	128.19	120.38
1	C	206	ASN	N-CA-C	-5.29	104.00	111.56
1	B	297	ASN	N-CA-C	5.28	117.04	111.28
1	D	166	HIS	N-CA-C	5.28	117.22	108.20
1	D	447	ILE	N-CA-C	5.18	116.53	110.62
1	B	256	ASP	N-CA-C	5.16	121.79	110.80
1	D	175	ASN	N-CA-C	5.14	116.88	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	355	MET	CG-SD-CE	5.14	112.20	100.90
1	D	352	THR	N-CA-C	5.10	116.84	111.28
1	D	265	MET	CA-C-N	5.09	124.70	119.56
1	D	265	MET	C-N-CA	5.09	124.70	119.56
1	A	355	MET	N-CA-C	5.08	118.23	110.20
1	C	203	GLY	CA-C-N	-5.08	115.83	122.99
1	C	203	GLY	C-N-CA	-5.08	115.83	122.99
1	B	208	THR	CB-CA-C	-5.05	101.42	109.75
1	D	183	ARG	CA-C-N	5.04	124.95	119.76
1	D	183	ARG	C-N-CA	5.04	124.95	119.76
1	D	193	GLY	N-CA-C	5.03	120.26	111.46

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	345	TPO	CA,CB
1	B	345	TPO	CB
1	C	345	TPO	CA,CB
1	D	345	TPO	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	255	GLY	Peptide
1	B	256	ASP	Peptide
1	D	222	THR	Peptide

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	2329	0	2293	61	0
1	B	2339	0	2306	56	0
1	C	2330	0	2295	90	0
1	D	2330	0	2295	110	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	32	0	24	0	0
3	B	32	0	24	0	0
3	C	32	0	24	2	0
3	D	32	0	24	3	0
4	A	114	0	0	6	0
4	B	121	0	0	4	0
4	C	126	0	0	11	0
4	D	122	0	0	13	0
All	All	9949	0	9285	316	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 17.

All (316) 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:287:MET:HE1	4:D:615:HOH:O	1.23	1.31
1:D:287:MET:CE	4:D:615:HOH:O	1.74	1.26
1:D:323:PHE:HB2	4:D:615:HOH:O	1.13	1.26
1:B:191:LYS:HE3	1:B:194:GLU:HB2	1.30	1.14
1:B:284:SER:N	1:B:287[A]:MET:HE3	1.65	1.11
1:A:237:MET:HE1	1:A:246:VAL:HG23	1.37	1.07
1:B:284:SER:H	1:B:287[A]:MET:CE	1.71	1.04
1:B:266:PRO:HG2	1:B:321:GLU:HG3	1.43	1.00
1:B:284:SER:H	1:B:287[A]:MET:HE3	0.84	0.97
1:C:290:LYS:HG2	4:C:724:HOH:O	1.65	0.96
1:A:361:ARG:HH11	1:A:361:ARG:HG2	1.26	0.96
1:D:237:MET:HE1	1:D:246:VAL:HG23	1.43	0.95
1:D:288:ARG:NE	1:D:418:MET:HE1	1.84	0.91
1:B:196:GLY:HA2	4:B:727:HOH:O	1.71	0.89
1:D:345:TPO:HG23	1:D:364:ILE:HD11	1.53	0.88
1:A:345:TPO:HG23	1:A:364:ILE:HD11	1.55	0.87
1:C:178:ASN:HD22	1:C:190:ASN:HD21	1.21	0.86
1:B:297:ASN:ND2	1:B:451:GLN:HE21	1.74	0.85
1:C:237:MET:HE1	1:C:246:VAL:HG23	1.57	0.85
1:A:284:SER:H	1:A:287:MET:HE3	1.45	0.80
1:C:309:HIS:HD2	1:C:311:ASP:H	1.29	0.80
1:D:345:TPO:HG23	1:D:364:ILE:CD1	2.11	0.79
1:D:266:PRO:HG2	1:D:321:GLU:HG3	1.65	0.79
1:A:361:ARG:HH11	1:A:361:ARG:CG	1.95	0.79
1:D:199:VAL:HG12	4:D:650:HOH:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:TPO:HG23	1:A:364:ILE:CD1	2.14	0.78
1:D:309:HIS:HD2	1:D:311:ASP:H	1.32	0.77
1:D:214:LYS:NZ	1:D:257:ASP:OD1	2.18	0.77
1:D:438:HIS:HD2	1:D:440:LYS:H	1.30	0.77
1:A:191:LYS:HE2	1:A:194:GLU:HG2	1.66	0.76
1:B:191:LYS:CE	1:B:194:GLU:HB2	2.13	0.76
1:C:266:PRO:HG2	1:C:321:GLU:HG3	1.68	0.76
1:D:288:ARG:CZ	1:D:418:MET:HE1	2.16	0.75
1:D:345:TPO:CG2	1:D:364:ILE:HD11	2.16	0.75
2:A:612:SO4:O3	1:C:207:ASN:ND2	2.20	0.74
1:A:345:TPO:CG2	1:A:364:ILE:HD11	2.17	0.74
1:D:408:LYS:HG2	1:D:413:TYR:HE2	1.53	0.74
1:D:219:VAL:O	1:D:220:ASP:HB2	1.86	0.73
1:B:173:LEU:HA	1:B:176:VAL:HG22	1.70	0.73
1:D:399:ILE:O	1:D:403:ILE:HG13	1.88	0.73
1:C:191:LYS:CE	1:C:194:GLU:HG2	2.19	0.72
1:C:191:LYS:HE3	1:C:194:GLU:HG2	1.71	0.72
1:C:341:GLN:HE22	1:C:365:THR:HB	1.54	0.72
1:D:288:ARG:CZ	1:D:418:MET:CE	2.68	0.72
1:A:408:LYS:HG2	1:A:413:TYR:HE2	1.55	0.71
1:D:199:VAL:HG13	1:D:201:TYR:CE1	2.25	0.70
1:C:253:SER:HA	1:C:258:LEU:HD22	1.74	0.70
1:C:303:HIS:HD2	4:C:651:HOH:O	1.75	0.69
1:A:340:ALA:O	1:A:341:GLN:HB2	1.93	0.69
1:B:297:ASN:HD22	1:B:451:GLN:HE21	1.38	0.69
1:B:220:ASP:O	1:B:222:THR:N	2.24	0.69
1:D:220:ASP:O	1:D:221:ILE:HG12	1.93	0.68
1:D:178:ASN:HD22	1:D:190:ASN:HD21	1.42	0.68
1:B:287[B]:MET:HE3	4:D:689:HOH:O	1.94	0.67
1:D:237:MET:CE	1:D:246:VAL:HG23	2.21	0.66
1:D:323:PHE:CB	4:D:615:HOH:O	1.95	0.66
1:A:390:HIS:HE1	4:A:668:HOH:O	1.77	0.66
1:D:180:PHE:CD2	1:D:214:LYS:HD2	2.30	0.66
1:C:237:MET:CE	1:C:262:TYR:HE1	2.09	0.66
1:C:290:LYS:CG	4:C:724:HOH:O	2.35	0.66
1:D:223:THR:O	1:D:224:GLU:C	2.38	0.66
1:B:252:SER:HB3	1:B:259:CYS:HB2	1.77	0.65
1:D:288:ARG:NH2	1:D:418:MET:HE3	2.11	0.65
1:D:265:MET:HE1	1:D:320:ASP:HB3	1.79	0.65
1:D:197:PHE:CD1	1:D:198:GLY:N	2.65	0.65
1:C:438:HIS:HD2	1:C:440:LYS:H	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:HIS:HE1	1:C:369:ASP:OD2	1.80	0.65
1:D:171:TYR:HB2	4:D:679:HOH:O	1.97	0.64
1:B:265:MET:HE1	1:B:326:LYS:HG3	1.80	0.64
1:C:205:VAL:O	1:C:206:ASN:HB3	1.98	0.64
1:C:438:HIS:CD2	1:C:440:LYS:H	2.15	0.64
1:D:287:MET:HE2	1:D:323:PHE:CB	2.28	0.63
1:A:361:ARG:CG	1:A:361:ARG:NH1	2.57	0.63
1:D:256:ASP:O	1:D:257:ASP:HB2	1.98	0.62
1:A:410:ILE:HD11	1:A:426:VAL:HG12	1.81	0.62
1:A:205:VAL:O	1:A:208:THR:HB	1.99	0.62
1:C:178:ASN:HD22	1:C:190:ASN:ND2	1.95	0.62
1:D:410:ILE:HD11	1:D:426:VAL:HG12	1.81	0.62
1:A:191:LYS:HE2	1:A:194:GLU:CG	2.30	0.61
1:C:363:GLU:OE1	1:C:441:LYS:NZ	2.26	0.61
1:A:408:LYS:HG2	1:A:413:TYR:CE2	2.35	0.61
1:B:289:CYS:O	1:B:293:GLN:HG3	2.00	0.61
1:B:266:PRO:CG	1:B:321:GLU:HG3	2.24	0.61
1:C:438:HIS:HB2	4:C:620:HOH:O	1.99	0.61
1:A:191:LYS:HE3	1:A:199:VAL:CG1	2.31	0.60
1:D:224:GLU:O	1:D:227:LYS:N	2.34	0.60
1:A:237:MET:CE	1:A:246:VAL:HG23	2.22	0.60
1:C:170:PHE:CB	1:C:255:GLY:HA3	2.32	0.60
1:D:216:ALA:HB3	1:D:218:MET:HE2	1.84	0.60
1:D:185:ILE:HG13	1:D:192:MET:HG2	1.84	0.59
1:D:408:LYS:HG2	1:D:413:TYR:CE2	2.37	0.59
1:B:233:GLU:OE1	1:B:262:TYR:OH	2.19	0.59
1:C:295:ALA:O	1:C:299:ILE:HG13	2.03	0.59
1:D:408:LYS:NZ	1:D:412:ASP:OD2	2.36	0.58
1:C:400:LYS:O	1:C:404:GLU:HB2	2.03	0.58
1:B:321:GLU:CD	1:B:321:GLU:H	2.12	0.58
1:B:169:SER:OG	1:B:172:GLU:HB2	2.04	0.57
1:D:180:PHE:CD2	1:D:214:LYS:CD	2.86	0.57
1:A:308:ILE:HD11	1:A:336:SER:HB3	1.85	0.57
1:C:396:LEU:O	1:C:399:ILE:HB	2.04	0.57
1:C:179:ASN:O	1:C:180:PHE:C	2.49	0.56
1:C:351:THR:O	1:C:355:MET:HG3	2.05	0.56
1:D:265:MET:HE3	1:D:320:ASP:N	2.21	0.56
1:C:352:THR:HA	1:C:355:MET:HE3	1.87	0.56
1:D:182:GLU:OE2	1:D:201:TYR:OH	2.19	0.56
1:C:166:HIS:HB3	1:C:168:PHE:HE1	1.70	0.55
1:D:303:HIS:HE1	1:D:369:ASP:OD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:VAL:HG22	1:A:187:VAL:O	2.06	0.55
1:D:199:VAL:HG13	1:D:201:TYR:HE1	1.68	0.55
1:C:367:LYS:HD2	1:C:441:LYS:HD2	1.88	0.55
1:A:195:GLY:HA3	1:A:197:PHE:CE2	2.42	0.55
1:D:287:MET:HE2	4:D:615:HOH:O	1.71	0.55
1:C:409:THR:O	1:C:412:ASP:HB2	2.07	0.55
1:B:254:ASP:O	1:B:256:ASP:HA	2.06	0.54
1:C:168:PHE:O	1:C:252:SER:HB3	2.07	0.54
1:C:345:TPO:CG2	1:C:364:ILE:HD11	2.38	0.54
1:D:254:ASP:OD1	1:D:254:ASP:O	2.26	0.54
1:D:322:ALA:O	1:D:323:PHE:HB2	2.06	0.54
1:C:169[B]:SER:HB2	1:C:172:GLU:HG3	1.89	0.54
1:C:438:HIS:CD2	1:C:439:GLU:N	2.75	0.54
1:D:321:GLU:CD	1:D:321:GLU:H	2.15	0.54
1:C:169[A]:SER:HB3	1:C:172:GLU:HG3	1.89	0.54
1:C:321:GLU:HB3	4:C:717:HOH:O	2.08	0.54
1:D:340:ALA:O	1:D:341:GLN:HB2	2.07	0.54
1:D:438:HIS:CD2	1:D:440:LYS:H	2.19	0.54
1:C:172:GLU:O	1:C:176:VAL:HG13	2.07	0.54
1:C:438:HIS:HD2	1:C:439:GLU:N	2.06	0.54
1:D:288:ARG:CZ	1:D:418:MET:HE3	2.38	0.54
1:B:345:TPO:HG23	1:B:364:ILE:HG13	1.88	0.53
1:B:361:ARG:HD2	4:B:647:HOH:O	2.08	0.53
1:A:170:PHE:HB2	1:A:254:ASP:O	2.08	0.53
1:A:303:HIS:HD2	4:A:692:HOH:O	1.91	0.53
1:C:345:TPO:HG23	1:C:364:ILE:HD11	1.91	0.53
1:D:438:HIS:CE1	1:D:443:LYS:HD2	2.43	0.53
1:A:284:SER:O	1:A:288:ARG:HG3	2.09	0.53
1:C:418:MET:HE3	1:C:421:ALA:HB2	1.90	0.53
1:D:258:LEU:HD21	4:D:721:HOH:O	2.09	0.53
1:B:340:ALA:O	1:B:341:GLN:HB2	2.09	0.53
1:C:237:MET:HE3	1:C:248:LEU:HB2	1.91	0.53
1:A:197:PHE:CD1	1:A:198:GLY:N	2.78	0.52
1:A:202:LYS:HE2	1:A:209:THR:HG21	1.91	0.52
1:D:287:MET:CE	1:D:323:PHE:CB	2.87	0.52
1:A:205:VAL:O	1:A:206:ASN:HB2	2.08	0.52
1:B:239:LYS:HE2	4:B:646:HOH:O	2.09	0.52
1:B:191:LYS:HE3	1:B:194:GLU:CB	2.21	0.52
1:D:180:PHE:CG	1:D:214:LYS:HD2	2.44	0.52
1:C:166:HIS:HB3	1:C:168:PHE:CE1	2.44	0.52
1:C:192:MET:HB3	3:C:602:T12:C1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:VAL:O	1:A:220:ASP:HB2	2.09	0.52
1:C:287:MET:HG2	4:C:723:HOH:O	2.09	0.52
1:D:181:ASP:HB3	1:D:190:ASN:HB2	1.90	0.52
1:B:288:ARG:HB3	1:B:380:ILE:HG23	1.92	0.52
1:B:338:LYS:HD3	1:B:338:LYS:C	2.35	0.51
1:A:361:ARG:HG2	1:A:361:ARG:NH1	2.06	0.51
1:C:272:ASP:CG	1:C:277:LEU:HD23	2.34	0.51
1:D:262:TYR:O	1:D:263:VAL:C	2.53	0.51
1:D:224:GLU:O	1:D:228:GLN:N	2.37	0.51
1:B:254:ASP:O	1:B:256:ASP:N	2.43	0.51
1:B:219:VAL:O	1:B:221:ILE:N	2.44	0.51
1:C:196:GLY:O	1:C:198:GLY:N	2.44	0.51
1:D:237:MET:HE3	1:D:262:TYR:HE1	1.76	0.51
1:A:191:LYS:HE3	1:A:199:VAL:HG13	1.92	0.51
1:D:288:ARG:NH2	1:D:418:MET:CE	2.73	0.51
1:A:265:MET:HE3	1:A:319:LEU:C	2.36	0.51
1:C:410:ILE:HD11	1:C:426:VAL:HG12	1.93	0.51
1:D:198:GLY:HA3	1:D:214:LYS:O	2.11	0.51
1:A:191:LYS:HE3	1:A:199:VAL:HG11	1.92	0.50
1:C:197:PHE:HB3	4:C:643:HOH:O	2.11	0.50
1:C:350:GLY:C	1:C:355:MET:HE2	2.37	0.50
1:D:233:GLU:OE1	4:D:619:HOH:O	2.20	0.50
1:C:289:CYS:O	1:C:293:GLN:HG3	2.12	0.50
1:C:297:ASN:OD1	1:C:451:GLN:NE2	2.28	0.49
1:D:192:MET:HB3	3:D:603:T12:C1	2.42	0.49
1:C:254:ASP:OD1	1:C:254:ASP:C	2.55	0.49
1:D:218:MET:O	1:D:219:VAL:HG23	2.13	0.49
1:B:345:TPO:CG2	1:B:364:ILE:HD11	2.42	0.49
1:D:174:LYS:HG2	1:D:179:ASN:HD22	1.78	0.49
1:B:224:GLU:O	1:B:228:GLN:HG3	2.12	0.49
1:B:284:SER:CB	1:B:287[A]:MET:HE3	2.43	0.49
1:C:334:ARG:NH2	1:C:345:TPO:O2P	2.36	0.49
1:C:300:ASN:HA	1:C:447:ILE:HG21	1.95	0.48
1:B:345:TPO:HG23	1:B:364:ILE:CG1	2.43	0.48
1:C:196:GLY:C	1:C:198:GLY:H	2.21	0.48
1:C:237:MET:HE3	1:C:262:TYR:HE1	1.77	0.48
1:C:309:HIS:HD2	1:C:311:ASP:N	2.04	0.48
1:D:167:SER:HB2	4:D:720:HOH:O	2.13	0.48
1:A:178:ASN:O	1:A:181:ASP:HB2	2.14	0.48
1:C:206:ASN:O	1:C:207:ASN:HB2	2.14	0.48
1:A:173:LEU:HA	1:A:176:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:PHE:CD1	1:C:168:PHE:N	2.81	0.48
1:D:265:MET:HE3	1:D:319:LEU:C	2.39	0.47
1:D:291:ILE:HG23	1:D:325:ALA:HB2	1.96	0.47
1:D:287:MET:CE	1:D:323:PHE:HB3	2.44	0.47
1:D:309:HIS:CD2	1:D:311:ASP:H	2.22	0.47
1:A:400:LYS:O	1:A:404:GLU:CB	2.63	0.47
1:A:400:LYS:O	1:A:404:GLU:HB2	2.14	0.47
1:D:251:PHE:CD1	1:D:251:PHE:C	2.92	0.47
1:A:265:MET:HE2	1:A:326:LYS:HB2	1.96	0.47
1:D:399:ILE:O	1:D:400:LYS:C	2.57	0.47
1:A:222:THR:HB	1:A:225:GLU:H	1.80	0.47
1:D:224:GLU:O	1:D:225:GLU:C	2.57	0.47
1:D:309:HIS:HD2	1:D:311:ASP:N	2.07	0.47
1:A:406:GLU:O	1:A:406:GLU:HG2	2.13	0.47
1:A:416:LYS:HB2	4:A:669:HOH:O	2.14	0.47
1:D:179:ASN:O	1:D:180:PHE:C	2.58	0.47
1:A:221:ILE:HD12	1:A:226:LEU:HB2	1.97	0.47
1:A:310:ARG:NH1	1:A:349:VAL:CG2	2.77	0.47
1:B:266:PRO:HG2	1:B:321:GLU:CG	2.30	0.47
1:B:345:TPO:HG21	1:B:364:ILE:HD11	1.97	0.47
1:A:414:ILE:CD1	1:A:426:VAL:HG11	2.45	0.47
1:D:344:MET:HE3	1:D:344:MET:HB3	1.86	0.47
1:A:419:ASN:ND2	4:A:625:HOH:O	2.48	0.46
1:C:321:GLU:H	1:C:321:GLU:CD	2.22	0.46
1:D:183:ARG:NH1	4:D:618:HOH:O	2.47	0.46
1:A:419:ASN:ND2	4:A:672:HOH:O	2.43	0.46
1:B:265:MET:CE	1:B:326:LYS:HG3	2.46	0.46
1:C:237:MET:CE	1:C:262:TYR:CE1	2.95	0.46
1:D:205:VAL:HG23	4:D:640:HOH:O	2.14	0.46
1:D:220:ASP:C	1:D:221:ILE:HG12	2.41	0.46
1:A:289:CYS:O	1:A:293:GLN:HG3	2.15	0.46
1:A:389:GLU:HA	1:A:394:GLN:NE2	2.31	0.46
1:B:358:GLU:HG2	1:B:359:ALA:N	2.31	0.46
1:B:284:SER:CA	1:B:287[A]:MET:HE3	2.45	0.45
1:C:171:TYR:N	4:C:719:HOH:O	2.48	0.45
1:D:169[B]:SER:OG	1:D:172:GLU:HG3	2.16	0.45
1:D:414:ILE:HG12	1:D:426:VAL:HG11	1.98	0.45
1:C:173:LEU:HA	1:C:176:VAL:HG22	1.98	0.45
1:A:336:SER:O	1:A:337:GLU:HG2	2.17	0.45
1:C:205:VAL:O	1:C:205:VAL:HG12	2.17	0.45
1:D:185:ILE:HD13	1:D:189:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:PHE:HD1	1:C:197:PHE:N	2.15	0.45
1:A:178:ASN:O	1:A:179:ASN:CG	2.60	0.45
1:C:297:ASN:HA	1:C:451:GLN:NE2	2.32	0.45
1:C:192:MET:HE3	1:C:200:VAL:HG12	1.98	0.44
1:B:388:ASP:HB3	1:B:391:ARG:HB3	2.00	0.44
1:B:396:LEU:O	1:B:399:ILE:HB	2.18	0.44
1:C:197:PHE:N	1:C:197:PHE:CD1	2.85	0.44
1:D:197:PHE:CG	1:D:198:GLY:N	2.86	0.44
1:D:265:MET:CE	1:D:320:ASP:N	2.81	0.44
1:D:262:TYR:HB3	3:D:603:T12:H11	1.99	0.44
1:C:258:LEU:N	1:C:258:LEU:HD23	2.32	0.44
1:B:341:GLN:O	1:B:342:THR:O	2.36	0.44
1:A:319:LEU:HD23	1:A:325:ALA:HA	1.99	0.43
1:C:168:PHE:O	1:C:252:SER:CB	2.65	0.43
1:D:418:MET:HE2	1:D:418:MET:HB3	1.35	0.43
1:C:192:MET:HE2	1:C:201:TYR:C	2.43	0.43
1:C:419:ASN:H	1:C:419:ASN:HD22	1.66	0.43
1:D:192:MET:HE2	1:D:202:LYS:N	2.33	0.43
1:C:186:SER:HB3	4:C:678:HOH:O	2.18	0.43
1:D:181:ASP:OD1	1:D:183:ARG:HG3	2.17	0.43
1:D:208:THR:O	1:D:210:VAL:HG13	2.18	0.43
1:A:206:ASN:C	1:A:208:THR:N	2.76	0.43
1:C:191:LYS:CE	1:C:194:GLU:CG	2.92	0.43
1:D:213:LYS:O	1:D:259:CYS:HA	2.19	0.43
1:D:257:ASP:O	1:D:258:LEU:O	2.36	0.43
1:C:174:LYS:HG3	1:C:180:PHE:CE1	2.53	0.43
1:C:309:HIS:CD2	1:C:311:ASP:H	2.20	0.43
1:A:287:MET:HG2	4:A:721:HOH:O	2.18	0.43
1:B:286:HIS:HE1	1:D:247:GLU:OE2	2.01	0.43
1:C:295:ALA:O	1:C:327:ILE:HD11	2.19	0.43
1:D:192:MET:HE3	1:D:200:VAL:HG12	1.99	0.43
1:A:407:GLU:O	1:A:407:GLU:HG2	2.18	0.43
1:C:417:LYS:HE2	4:C:610:HOH:O	2.19	0.43
1:C:196:GLY:C	1:C:198:GLY:N	2.77	0.42
1:B:456:GLU:O	1:B:457:MET:C	2.59	0.42
1:D:300:ASN:HA	1:D:447:ILE:HG21	2.00	0.42
1:D:227:LYS:HD3	1:D:231:ASP:OD1	2.19	0.42
1:D:431:SER:O	1:D:435:GLN:HG3	2.19	0.42
1:D:287:MET:HE2	1:D:323:PHE:HB2	2.00	0.42
1:A:215:LEU:HB3	1:A:226:LEU:HD11	2.02	0.42
1:A:337:GLU:C	1:A:339:PHE:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ARG:HG2	1:B:164:ARG:HH11	1.84	0.42
1:B:318:LEU:N	1:B:318:LEU:HD23	2.35	0.42
1:C:384:LEU:HB3	1:C:391:ARG:NH1	2.35	0.42
1:C:415:ASP:OD2	1:C:417:LYS:NZ	2.45	0.42
1:D:400:LYS:O	1:D:404:GLU:HG3	2.19	0.42
1:D:206:ASN:O	1:D:207:ASN:HB2	2.20	0.42
1:D:253:SER:HA	1:D:258:LEU:HD23	2.02	0.42
1:A:202:LYS:HE3	1:A:264:TYR:CZ	2.55	0.42
1:C:196:GLY:C	1:C:197:PHE:HD1	2.27	0.42
1:A:273:ARG:HD3	1:A:273:ARG:HA	1.50	0.41
1:B:237:MET:HE3	1:B:248:LEU:HB2	2.02	0.41
1:B:439:GLU:HB2	4:B:699:HOH:O	2.21	0.41
1:A:419:ASN:C	1:A:419:ASN:HD22	2.29	0.41
1:B:299:ILE:HG22	1:B:447:ILE:HG12	2.02	0.41
1:D:172:GLU:O	1:D:176:VAL:HG22	2.20	0.41
1:D:262:TYR:CG	3:D:603:T12:C12	3.03	0.41
1:C:192:MET:HB3	3:C:602:T12:C2	2.51	0.41
1:B:219:VAL:O	1:B:220:ASP:C	2.62	0.41
1:C:170:PHE:O	1:C:173:LEU:N	2.48	0.41
1:C:293:GLN:HE22	1:C:458:THR:HG21	1.84	0.41
1:C:352:THR:CA	1:C:355:MET:HE3	2.49	0.41
1:A:197:PHE:CD1	1:A:213:LYS:HD3	2.55	0.41
1:B:205:VAL:O	1:B:206:ASN:HB2	2.19	0.41
1:D:180:PHE:CD2	1:D:214:LYS:HD3	2.54	0.41
1:A:170:PHE:CB	1:A:254:ASP:O	2.69	0.41
1:C:403:ILE:HA	1:C:408:LYS:O	2.21	0.41
1:D:287:MET:HE2	1:D:323:PHE:HB3	1.99	0.41
1:D:337:GLU:O	1:D:338:LYS:C	2.63	0.41
1:D:375:VAL:HG22	1:D:397:LEU:HD13	2.03	0.41
1:C:352:THR:HG22	4:C:606:HOH:O	2.20	0.41
1:B:218:MET:HB3	1:B:219:VAL:H	1.74	0.40
1:B:237:MET:HE3	1:B:248:LEU:H	1.87	0.40
1:B:300:ASN:HA	1:B:447:ILE:HG21	2.04	0.40
1:D:404:GLU:C	1:D:406:GLU:H	2.29	0.40
1:A:457:MET:HE2	1:A:457:MET:HB3	1.91	0.40
1:B:194:GLU:HG3	1:B:199:VAL:HB	2.03	0.40
1:D:358:GLU:O	1:D:363:GLU:HB3	2.21	0.40
1:D:406:GLU:C	1:D:408:LYS:H	2.29	0.40
1:B:339:PHE:HE1	1:B:365:THR:OG1	2.04	0.40
1:D:309:HIS:O	1:D:310:ARG:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	291/307 (95%)	268 (92%)	16 (6%)	7 (2%)	4	2
1	B	293/307 (95%)	268 (92%)	13 (4%)	12 (4%)	2	0
1	C	292/307 (95%)	266 (91%)	16 (6%)	10 (3%)	3	1
1	D	292/307 (95%)	257 (88%)	24 (8%)	11 (4%)	2	1
All	All	1168/1228 (95%)	1059 (91%)	69 (6%)	40 (3%)	3	1

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ASP
1	A	406	GLU
1	B	219	VAL
1	B	220	ASP
1	B	221	ILE
1	B	256	ASP
1	B	341	GLN
1	B	342	THR
1	C	197	PHE
1	C	220	ASP
1	D	197	PHE
1	D	224	GLU
1	D	225	GLU
1	D	257	ASP
1	D	258	LEU
1	A	341	GLN
1	B	255	GLY
1	B	338	LYS
1	C	256	ASP
1	D	219	VAL
1	D	223	THR
1	D	338	LYS

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Mol	Chain	Res	Type
1	A	219	VAL
1	B	186	SER
1	B	339	PHE
1	C	224	GLU
1	C	257	ASP
1	C	338	LYS
1	D	179	ASN
1	D	221	ILE
1	D	222	THR
1	A	206	ASN
1	A	224	GLU
1	A	258	LEU
1	B	254	ASP
1	B	397	LEU
1	C	219	VAL
1	C	258	LEU
1	C	341	GLN
1	C	196	GLY

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	255/266 (96%)	238 (93%)	17 (7%)	15	11
1	B	257/266 (97%)	233 (91%)	24 (9%)	8	5
1	C	256/266 (96%)	226 (88%)	30 (12%)	5	3
1	D	256/266 (96%)	238 (93%)	18 (7%)	14	10
All	All	1024/1064 (96%)	935 (91%)	89 (9%)	9	6

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	GLU
1	A	205	VAL
1	A	222	THR

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Mol	Chain	Res	Type
1	A	225	GLU
1	A	235	LYS
1	A	243	GLU
1	A	253	SER
1	A	256	ASP
1	A	273	ARG
1	A	338	LYS
1	A	347	ARG
1	A	361	ARG
1	A	399	ILE
1	A	408	LYS
1	A	410	ILE
1	A	417	LYS
1	A	419	ASN
1	B	163	THR
1	B	164	ARG
1	B	173	LEU
1	B	174	LYS
1	B	175	ASN
1	B	178	ASN
1	B	194	GLU
1	B	199	VAL
1	B	205	VAL
1	B	208	THR
1	B	220	ASP
1	B	222	THR
1	B	223	THR
1	B	243	GLU
1	B	256	ASP
1	B	321	GLU
1	B	337	GLU
1	B	338	LYS
1	B	347	ARG
1	B	397	LEU
1	B	399	ILE
1	B	406	GLU
1	B	419	ASN
1	B	439	GLU
1	C	168	PHE
1	C	174	LYS
1	C	175	ASN
1	C	182	GLU

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Mol	Chain	Res	Type
1	C	197	PHE
1	C	209	THR
1	C	213	LYS
1	C	221	ILE
1	C	222	THR
1	C	224	GLU
1	C	230	PHE
1	C	231	ASP
1	C	254	ASP
1	C	290	LYS
1	C	321	GLU
1	C	344	MET
1	C	347	ARG
1	C	348	ILE
1	C	352	THR
1	C	365	THR
1	C	389	GLU
1	C	397	LEU
1	C	399	ILE
1	C	406	GLU
1	C	408	LYS
1	C	410	ILE
1	C	419	ASN
1	C	443	LYS
1	C	455	GLN
1	C	458	THR
1	D	164	ARG
1	D	194	GLU
1	D	214	LYS
1	D	222	THR
1	D	225	GLU
1	D	239	LYS
1	D	241	GLN
1	D	256	ASP
1	D	339	PHE
1	D	341	GLN
1	D	347	ARG
1	D	365	THR
1	D	397	LEU
1	D	406	GLU
1	D	408	LYS
1	D	410	ILE

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Mol	Chain	Res	Type
1	D	422	ASP
1	D	423	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	175	ASN
1	A	190	ASN
1	A	228	GLN
1	A	303	HIS
1	A	306	HIS
1	A	307	HIS
1	A	394	GLN
1	A	419	ASN
1	B	166	HIS
1	B	175	ASN
1	B	179	ASN
1	B	207	ASN
1	B	228	GLN
1	B	229	GLN
1	B	286	HIS
1	B	293	GLN
1	B	297	ASN
1	B	305	ASN
1	B	394	GLN
1	B	419	ASN
1	C	178	ASN
1	C	206	ASN
1	C	286	HIS
1	C	293	GLN
1	C	303	HIS
1	C	305	ASN
1	C	309	HIS
1	C	341	GLN
1	C	394	GLN
1	C	419	ASN
1	C	438	HIS
1	D	166	HIS
1	D	179	ASN
1	D	190	ASN
1	D	241	GLN

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Mol	Chain	Res	Type
1	D	303	HIS
1	D	309	HIS
1	D	394	GLN
1	D	438	HIS
1	D	442	ASN
1	D	452	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	$\# Z > 2$
1	SEP	A	346	1	8,9,10	1.87	2 (25%)	7,12,14	1.29	1 (14%)
1	TPO	B	345	1	8,10,11	1.37	1 (12%)	10,14,16	2.11	3 (30%)
1	SEP	B	346	1	8,9,10	1.76	1 (12%)	7,12,14	1.01	1 (14%)
1	SEP	C	346	1	8,9,10	1.80	3 (37%)	7,12,14	2.50	2 (28%)
1	TPO	D	345	1	8,10,11	1.87	1 (12%)	10,14,16	2.01	4 (40%)
1	TPO	A	345	1	8,10,11	1.66	1 (12%)	10,14,16	2.26	3 (30%)
1	TPO	C	345	1	8,10,11	1.40	1 (12%)	10,14,16	2.21	4 (40%)
1	SEP	D	346	1	8,9,10	1.76	3 (37%)	7,12,14	1.35	1 (14%)

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
1	SEP	A	346	1	-	0/6/8/10	-
1	TPO	B	345	1	1/1/3/4	5/9/11/13	-
1	SEP	B	346	1	-	1/6/8/10	-
1	SEP	C	346	1	-	5/6/8/10	-
1	TPO	D	345	1	1/1/3/4	6/9/11/13	-
1	TPO	A	345	1	2/2/3/4	5/9/11/13	-
1	TPO	C	345	1	2/2/3/4	1/9/11/13	-
1	SEP	D	346	1	-	1/6/8/10	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	345	TPO	P-OG1	-4.79	1.51	1.59
1	A	345	TPO	P-OG1	-4.50	1.51	1.59
1	A	346	SEP	P-O1P	4.13	1.63	1.50
1	B	346	SEP	P-O1P	3.88	1.62	1.50
1	C	346	SEP	P-O1P	3.84	1.62	1.50
1	D	346	SEP	P-O1P	3.80	1.62	1.50
1	B	345	TPO	P-OG1	-3.31	1.53	1.59
1	C	345	TPO	P-OG1	-3.01	1.54	1.59
1	A	346	SEP	P-O2P	2.14	1.62	1.54
1	D	346	SEP	P-O3P	2.14	1.62	1.54
1	C	346	SEP	P-O3P	2.10	1.62	1.54
1	D	346	SEP	P-O2P	2.09	1.62	1.54
1	C	346	SEP	P-O2P	2.07	1.62	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	346	SEP	OG-CB-CA	6.17	114.15	108.14
1	A	345	TPO	P-OG1-CB	5.41	138.04	123.33
1	B	345	TPO	P-OG1-CB	4.77	136.28	123.33
1	D	345	TPO	P-OG1-CB	4.38	135.23	123.33
1	C	345	TPO	CG2-CB-CA	-4.37	104.75	113.26
1	C	345	TPO	P-OG1-CB	-3.18	114.68	123.33
1	D	346	SEP	OG-CB-CA	3.05	111.12	108.14
1	B	345	TPO	O-C-CA	-3.04	116.94	124.77
1	A	346	SEP	OG-CB-CA	2.99	111.06	108.14
1	D	345	TPO	O-C-CA	-2.87	117.39	124.77
1	A	345	TPO	O-C-CA	-2.81	117.54	124.77
1	B	345	TPO	CB-CA-N	2.64	131.41	114.17
1	A	345	TPO	CB-CA-N	2.43	130.02	114.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	345	TPO	CB-CA-N	2.31	129.25	114.17
1	C	345	TPO	O2P-P-OG1	2.31	114.84	105.85
1	C	345	TPO	O-C-CA	-2.27	118.93	124.77
1	C	346	SEP	O3P-P-OG	2.18	112.36	106.67
1	D	345	TPO	O3P-P-OG1	2.18	114.33	105.85
1	B	346	SEP	OG-CB-CA	2.04	110.13	108.14

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	345	TPO	CA
1	A	345	TPO	CB
1	B	345	TPO	CB
1	C	345	TPO	CA
1	C	345	TPO	CB
1	D	345	TPO	CB

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-CG2
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	C-CA-CB-CG2
1	A	345	TPO	CA-CB-OG1-P
1	B	345	TPO	N-CA-CB-CG2
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	C-CA-CB-CG2
1	B	345	TPO	CA-CB-OG1-P
1	C	345	TPO	C-CA-CB-CG2
1	C	346	SEP	N-CA-CB-OG
1	C	346	SEP	C-CA-CB-OG
1	C	346	SEP	CB-OG-P-O2P
1	C	346	SEP	CB-OG-P-O3P
1	D	345	TPO	N-CA-CB-CG2
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	C-CA-CB-CG2
1	D	345	TPO	CA-CB-OG1-P
1	D	346	SEP	C-CA-CB-OG
1	B	346	SEP	CB-OG-P-O1P
1	C	346	SEP	CB-OG-P-O1P
1	D	345	TPO	CB-OG1-P-O1P
1	A	345	TPO	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	B	345	TPO	O-C-CA-CB
1	D	345	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	345	TPO	4	0
1	D	345	TPO	3	0
1	A	345	TPO	3	0
1	C	345	TPO	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	SO4	B	611	-	4,4,4	0.30	0	6,6,6	0.53	0
3	T12	D	603	-	33,34,34	2.82	9 (27%)	44,49,49	1.80	9 (20%)
3	T12	B	601	-	33,34,34	2.89	9 (27%)	44,49,49	1.45	7 (15%)
3	T12	A	600	-	33,34,34	2.96	9 (27%)	44,49,49	1.79	11 (25%)
3	T12	C	602	-	33,34,34	2.62	8 (24%)	44,49,49	2.12	15 (34%)
2	SO4	A	612	-	4,4,4	0.29	0	6,6,6	1.20	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
3	T12	A	600	-	-	0/24/26/26	0/3/3/3
3	T12	D	603	-	-	1/24/26/26	0/3/3/3
3	T12	C	602	-	-	0/24/26/26	0/3/3/3
3	T12	B	601	-	-	0/24/26/26	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	T12	O55-N54	11.44	1.42	1.22
3	B	601	T12	O55-N54	10.91	1.41	1.22
3	D	603	T12	O55-N54	10.14	1.40	1.22
3	C	602	T12	O55-N54	9.21	1.38	1.22
3	B	601	T12	O23-C5	-7.79	1.24	1.41
3	A	600	T12	O23-C5	-7.66	1.24	1.41
3	C	602	T12	O23-C5	-6.84	1.26	1.41
3	D	603	T12	O23-C5	-6.46	1.27	1.41
3	D	603	T12	O26-C24	5.75	1.33	1.20
3	C	602	T12	O26-C24	5.02	1.31	1.20
3	B	601	T12	O26-C24	4.68	1.31	1.20
3	A	600	T12	C51-N50	-4.68	1.29	1.37
3	A	600	T12	O26-C24	4.03	1.29	1.20
3	D	603	T12	C39-N20	-3.97	1.38	1.47
3	C	602	T12	C39-N20	-3.87	1.38	1.47
3	A	600	T12	C21-N22	3.77	1.38	1.32
3	B	601	T12	C2-N20	-3.73	1.32	1.39
3	C	602	T12	O23-C24	3.66	1.46	1.35
3	D	603	T12	O53-C51	3.59	1.31	1.23
3	B	601	T12	C51-N50	-3.59	1.31	1.37
3	D	603	T12	O23-C24	3.51	1.45	1.35
3	B	601	T12	O53-C51	3.38	1.31	1.23
3	D	603	T12	C2-N20	-3.27	1.33	1.39
3	C	602	T12	C4-C5	3.06	1.44	1.39
3	C	602	T12	O53-C51	3.00	1.30	1.23
3	C	602	T12	C2-N20	-2.96	1.34	1.39
3	A	600	T12	O23-C24	2.86	1.44	1.35
3	A	600	T12	C39-N20	-2.83	1.40	1.47
3	B	601	T12	O23-C24	2.79	1.43	1.35
3	D	603	T12	C4-C5	2.71	1.43	1.39
3	A	600	T12	O53-C51	2.58	1.29	1.23
3	D	603	T12	C13-N54	-2.23	1.39	1.45
3	B	601	T12	C21-N22	2.18	1.35	1.32
3	B	601	T12	C11-C10	2.18	1.42	1.38
3	A	600	T12	C2-N20	-2.04	1.35	1.39

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	T12	C40-C39-N20	6.09	125.66	112.45
3	D	603	T12	C15-C51-N50	5.78	124.58	116.25
3	C	602	T12	C5-O23-C24	5.77	132.36	117.97
3	C	602	T12	C15-C51-N50	5.35	123.96	116.25
3	D	603	T12	O23-C24-C25	4.79	122.40	111.78
3	C	602	T12	O23-C24-C25	4.63	122.05	111.78
3	A	600	T12	O23-C24-O26	-3.93	115.40	123.13
3	C	602	T12	C4-C3-C2	-3.92	116.57	120.16
3	B	601	T12	O23-C24-C25	3.72	120.03	111.78
3	C	602	T12	C12-C13-N54	3.58	122.47	119.34
3	B	601	T12	C5-O23-C24	3.58	126.88	117.97
3	A	600	T12	C15-C51-N50	3.52	121.33	116.25
3	C	602	T12	O53-C51-C15	-3.40	114.16	120.90
3	B	601	T12	O23-C24-O26	-3.36	116.53	123.13
3	B	601	T12	C4-C3-C2	-3.23	117.20	120.16
3	D	603	T12	C5-O23-C24	3.23	126.02	117.97
3	A	600	T12	O23-C24-C25	3.02	118.47	111.78
3	D	603	T12	C4-C3-C2	-2.94	117.46	120.16
3	A	600	T12	O53-C51-N50	-2.83	118.14	122.27
3	D	603	T12	O53-C51-C15	-2.72	115.51	120.90
3	B	601	T12	C40-C39-N20	2.67	118.23	112.45
3	C	602	T12	C4-C3-N22	2.65	135.01	129.31
3	A	600	T12	O55-N54-C13	2.58	122.36	118.82
3	D	603	T12	C40-C39-N20	2.53	117.93	112.45
3	C	602	T12	C3-C2-N20	-2.49	103.58	105.55
3	C	602	T12	C5-C4-C3	2.47	122.06	118.21
3	C	602	T12	C40-C39-N20	2.44	117.75	112.45
3	D	603	T12	C5-C4-C3	2.41	121.97	118.21
3	C	602	T12	C3-N22-C21	2.36	107.73	104.06
3	B	601	T12	C6-C5-C4	2.31	123.61	120.50
3	C	602	T12	C1-C2-N20	2.26	135.11	130.42
3	D	603	T12	C4-C3-N22	2.22	134.09	129.31
3	A	600	T12	C12-C13-N54	2.20	121.26	119.34
3	C	602	T12	C1-C6-C5	-2.20	117.22	119.73
3	A	600	T12	C35-C25-C24	2.19	115.19	109.14
3	A	600	T12	C6-C5-C4	2.17	123.43	120.50
3	A	600	T12	C10-C15-C14	2.17	121.76	119.25
3	B	601	T12	C15-C51-N50	2.15	119.35	116.25
3	A	600	T12	C31-C25-C24	-2.15	103.22	109.14
3	C	602	T12	C39-C40-C43	-2.13	107.30	112.69
3	D	603	T12	C1-C2-N20	2.08	134.75	130.42
3	C	602	T12	C6-C1-C2	2.02	123.15	119.10

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	603	T12	C39-C40-C43-O46

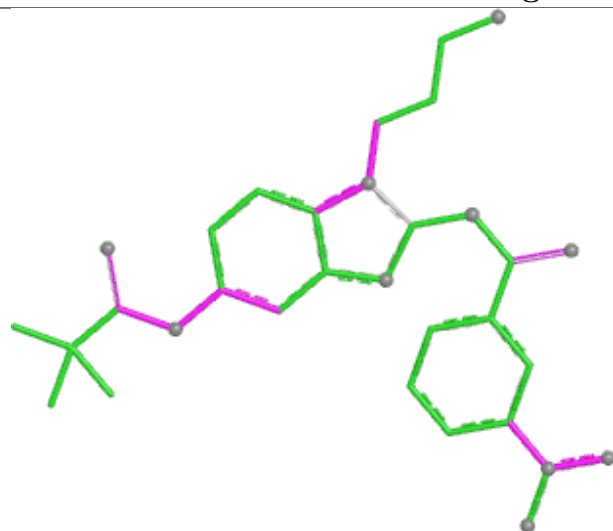
There are no ring outliers.

3 monomers are involved in 6 short contacts:

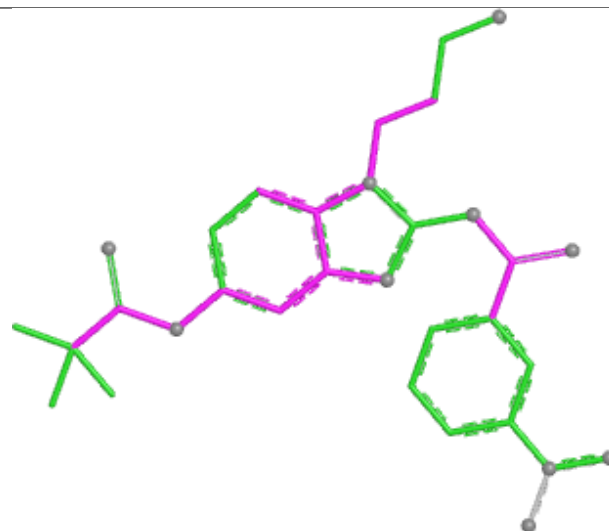
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	603	T12	3	0
3	C	602	T12	2	0
2	A	612	SO4	1	0

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

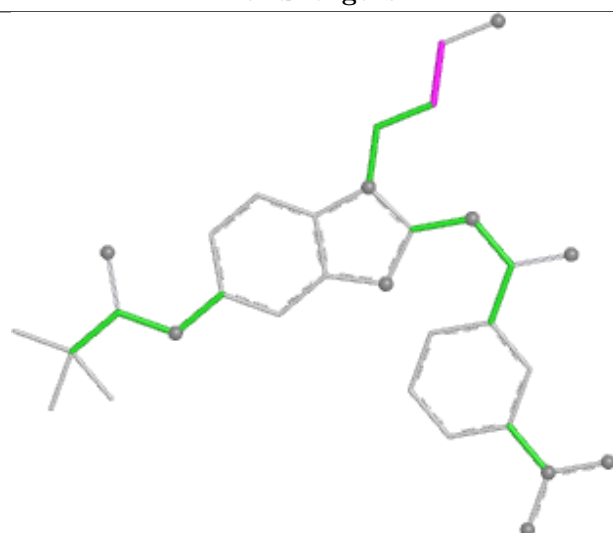
Ligand T12 D 603



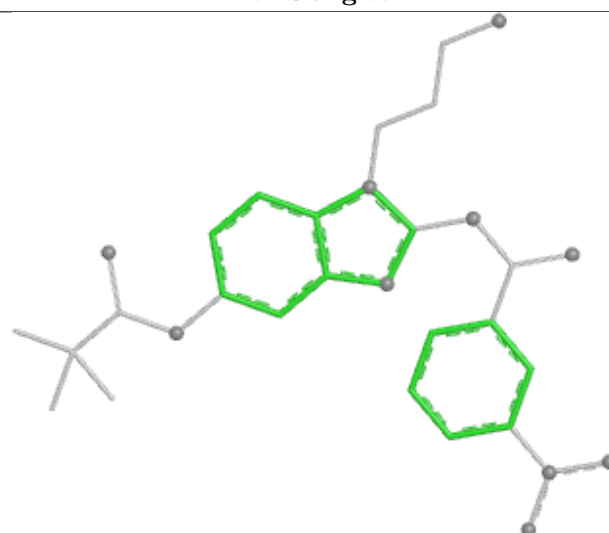
Bond lengths



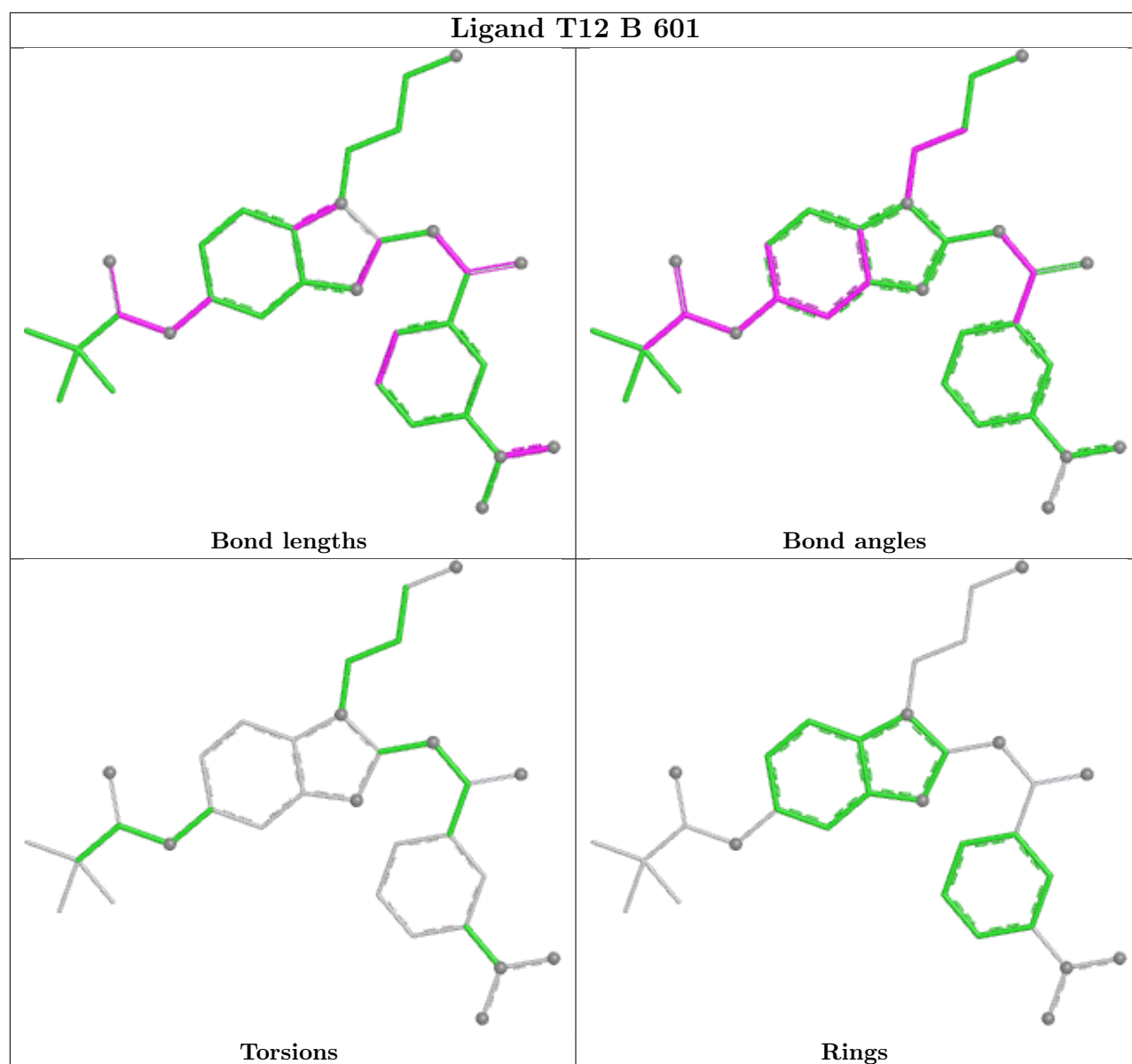
Bond angles



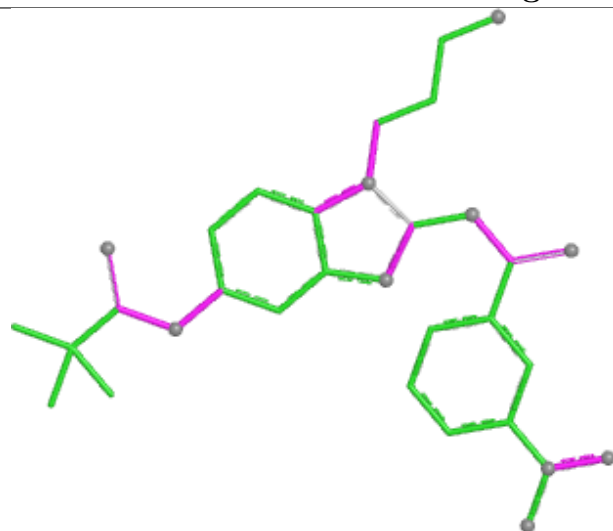
Torsions



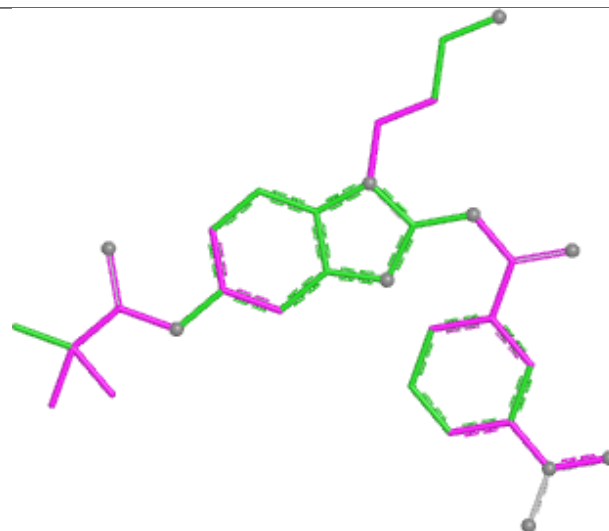
Rings



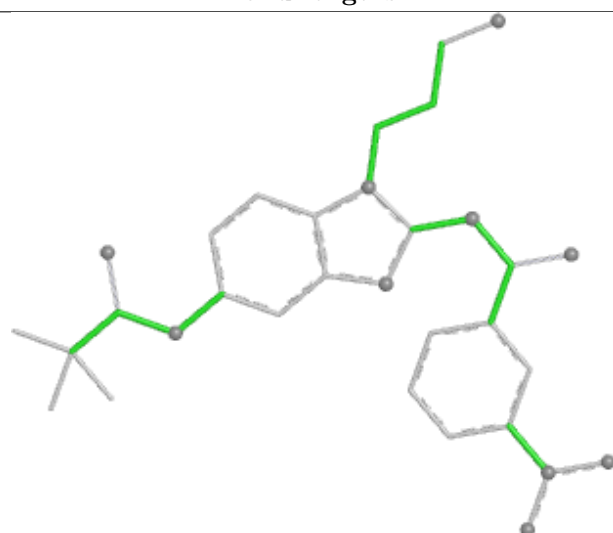
Ligand T12 A 600



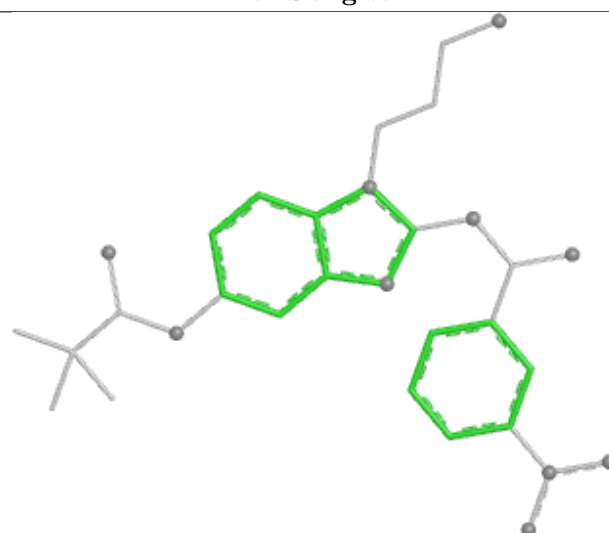
Bond lengths



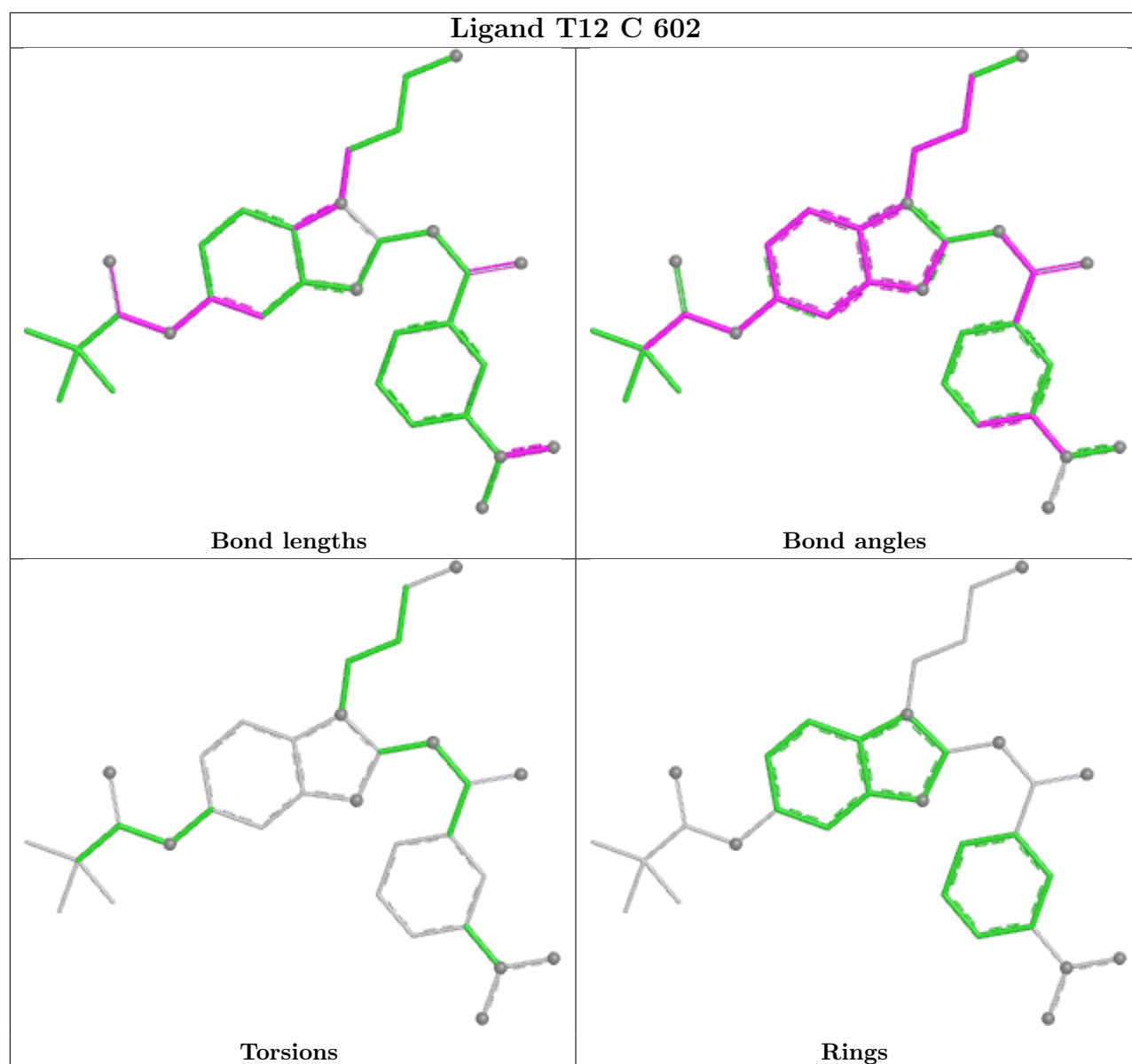
Bond angles



Torsions



Rings



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	293/307 (95%)	-0.93	0 100 100	22, 39, 74, 89	0
1	B	294/307 (95%)	-0.96	0 100 100	16, 38, 70, 87	1 (0%)
1	C	293/307 (95%)	-0.79	0 100 100	21, 39, 73, 95	1 (0%)
1	D	293/307 (95%)	-0.83	0 100 100	20, 39, 69, 88	1 (0%)
All	All	1173/1228 (95%)	-0.88	0 100 100	16, 39, 73, 95	3 (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
1	SEP	A	346	10/11	0.97	0.05	55,56,65,65	0
1	TPO	A	345	11/12	0.98	0.06	55,56,56,58	0
1	SEP	B	346	10/11	0.98	0.05	53,55,62,64	0
1	SEP	C	346	10/11	0.98	0.06	56,60,65,67	0
1	SEP	D	346	10/11	0.98	0.05	47,51,63,64	0
1	TPO	B	345	11/12	0.99	0.05	50,54,56,56	0
1	TPO	D	345	11/12	0.99	0.05	42,47,48,48	0
1	TPO	C	345	11/12	0.99	0.06	57,60,61,62	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

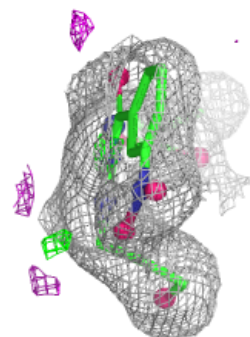
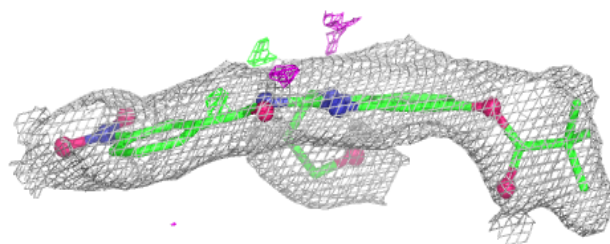
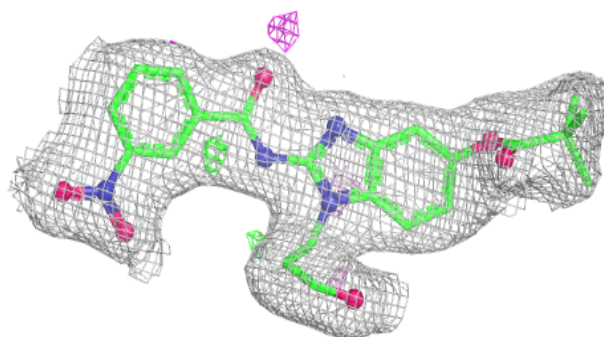
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	SO4	A	612	5/5	0.98	0.05	50,51,56,58	0
3	T12	D	603	32/32	0.98	0.04	34,38,45,49	0
3	T12	A	600	32/32	0.99	0.04	22,28,39,48	0
3	T12	B	601	32/32	0.99	0.03	22,26,38,40	0
3	T12	C	602	32/32	0.99	0.04	27,33,38,45	0
2	SO4	B	611	5/5	0.99	0.04	42,43,47,51	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.

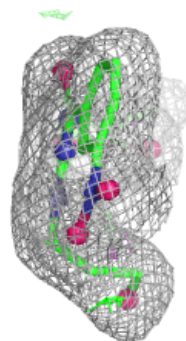
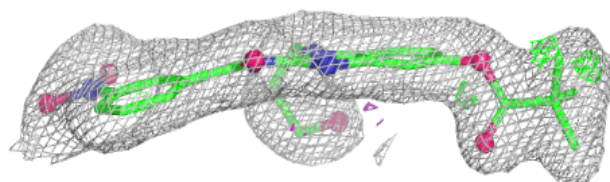
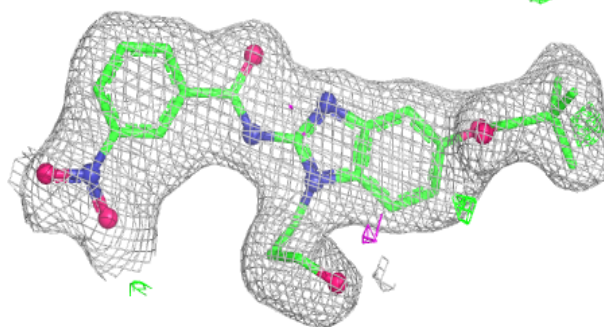
Electron density around T12 D 603:

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

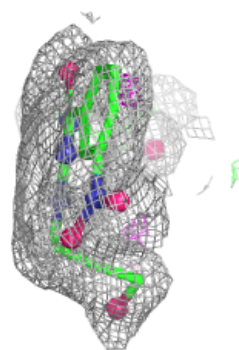
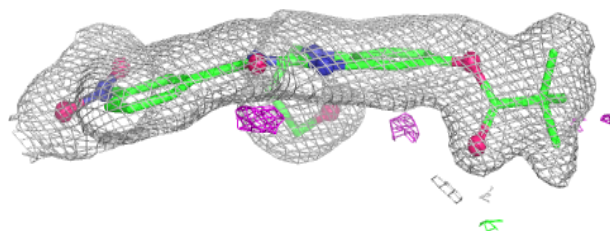
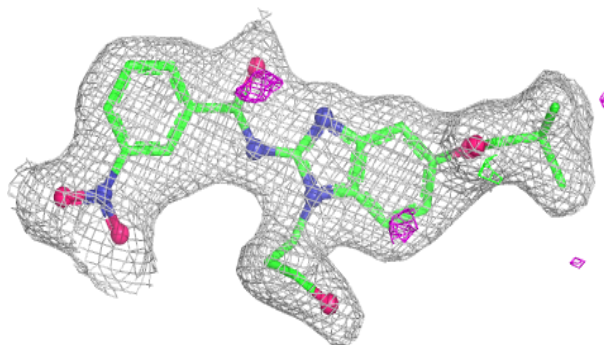


Electron density around T12 A 600:

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

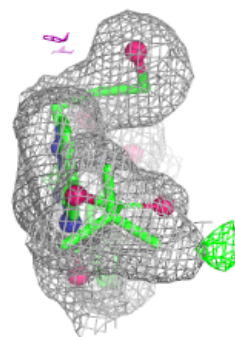
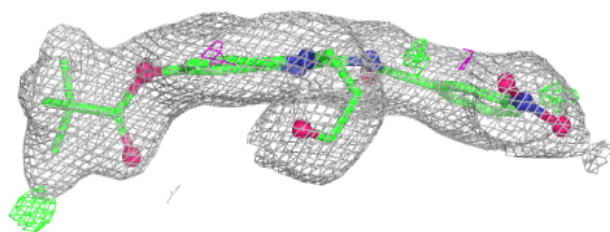
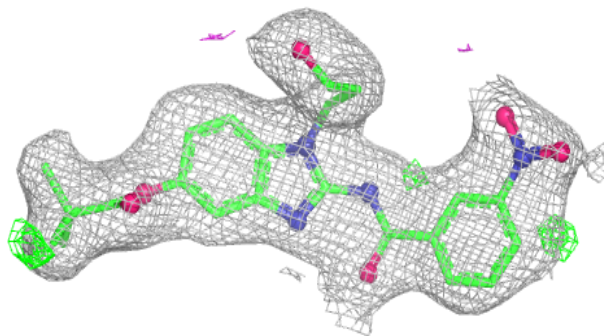
**Electron density around T12 B 601:**

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



Electron density around T12 C 602:

$2mF_o-DF_c$ (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.