



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:25 AM UTC

PDB ID : 8XRZ / pdb_00008xrz
Title : Crystal structure of a novel PU plastic degradation enzyme with ligand from *Thermaerobacter marianensis*
Authors : Li, Z.S.; Wang, H.; Zheng, Z.R.; Cong, L.; Chen, Y.Y.; Han, X.; Wei, R.; Uwe, B.; liu, W.D.
Deposited on : 2024-01-08
Resolution : 2.11 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

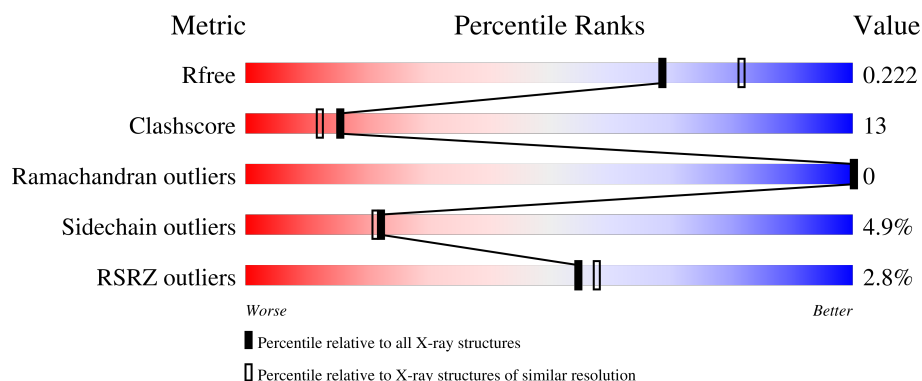
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	527	0% 64% 29% 6%
1	B	527	2% 64% 28% 6%
1	C	527	4% 67% 25% 6%
1	D	527	3% 66% 28% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15514 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 Carboxylic ester hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3748	2382	686	671	9			
1	B	498	Total	C	N	O	S	0	0	0
			3772	2396	690	677	9			
1	C	493	Total	C	N	O	S	0	0	0
			3740	2376	685	670	9			
1	D	495	Total	C	N	O	S	0	0	0
			3757	2387	687	674	9			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP E6SHQ4
A	-5	HIS	-	expression tag	UNP E6SHQ4
A	-4	HIS	-	expression tag	UNP E6SHQ4
A	-3	HIS	-	expression tag	UNP E6SHQ4
A	-2	HIS	-	expression tag	UNP E6SHQ4
A	-1	HIS	-	expression tag	UNP E6SHQ4
A	0	HIS	-	expression tag	UNP E6SHQ4
A	1	GLU	-	expression tag	UNP E6SHQ4
A	2	ASN	-	expression tag	UNP E6SHQ4
A	3	LEU	-	expression tag	UNP E6SHQ4
A	4	TYR	-	expression tag	UNP E6SHQ4
A	5	PHE	-	expression tag	UNP E6SHQ4
A	6	GLN	-	expression tag	UNP E6SHQ4
A	7	GLY	-	expression tag	UNP E6SHQ4
A	8	ALA	-	expression tag	UNP E6SHQ4
A	9	GLY	-	expression tag	UNP E6SHQ4
A	10	ALA	-	expression tag	UNP E6SHQ4
A	11	GLY	-	expression tag	UNP E6SHQ4
A	12	ALA	-	expression tag	UNP E6SHQ4
A	13	GLY	-	expression tag	UNP E6SHQ4
A	14	ALA	-	expression tag	UNP E6SHQ4

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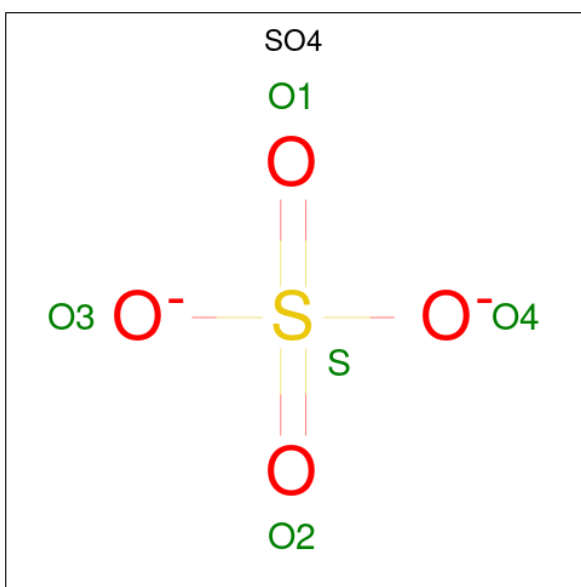
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	expression tag	UNP E6SHQ4
A	16	ALA	-	expression tag	UNP E6SHQ4
A	215	ALA	SER	engineered mutation	UNP E6SHQ4
B	-6	MET	-	initiating methionine	UNP E6SHQ4
B	-5	HIS	-	expression tag	UNP E6SHQ4
B	-4	HIS	-	expression tag	UNP E6SHQ4
B	-3	HIS	-	expression tag	UNP E6SHQ4
B	-2	HIS	-	expression tag	UNP E6SHQ4
B	-1	HIS	-	expression tag	UNP E6SHQ4
B	0	HIS	-	expression tag	UNP E6SHQ4
B	1	GLU	-	expression tag	UNP E6SHQ4
B	2	ASN	-	expression tag	UNP E6SHQ4
B	3	LEU	-	expression tag	UNP E6SHQ4
B	4	TYR	-	expression tag	UNP E6SHQ4
B	5	PHE	-	expression tag	UNP E6SHQ4
B	6	GLN	-	expression tag	UNP E6SHQ4
B	7	GLY	-	expression tag	UNP E6SHQ4
B	8	ALA	-	expression tag	UNP E6SHQ4
B	9	GLY	-	expression tag	UNP E6SHQ4
B	10	ALA	-	expression tag	UNP E6SHQ4
B	11	GLY	-	expression tag	UNP E6SHQ4
B	12	ALA	-	expression tag	UNP E6SHQ4
B	13	GLY	-	expression tag	UNP E6SHQ4
B	14	ALA	-	expression tag	UNP E6SHQ4
B	15	GLY	-	expression tag	UNP E6SHQ4
B	16	ALA	-	expression tag	UNP E6SHQ4
B	215	ALA	SER	engineered mutation	UNP E6SHQ4
C	-6	MET	-	initiating methionine	UNP E6SHQ4
C	-5	HIS	-	expression tag	UNP E6SHQ4
C	-4	HIS	-	expression tag	UNP E6SHQ4
C	-3	HIS	-	expression tag	UNP E6SHQ4
C	-2	HIS	-	expression tag	UNP E6SHQ4
C	-1	HIS	-	expression tag	UNP E6SHQ4
C	0	HIS	-	expression tag	UNP E6SHQ4
C	1	GLU	-	expression tag	UNP E6SHQ4
C	2	ASN	-	expression tag	UNP E6SHQ4
C	3	LEU	-	expression tag	UNP E6SHQ4
C	4	TYR	-	expression tag	UNP E6SHQ4
C	5	PHE	-	expression tag	UNP E6SHQ4
C	6	GLN	-	expression tag	UNP E6SHQ4
C	7	GLY	-	expression tag	UNP E6SHQ4
C	8	ALA	-	expression tag	UNP E6SHQ4

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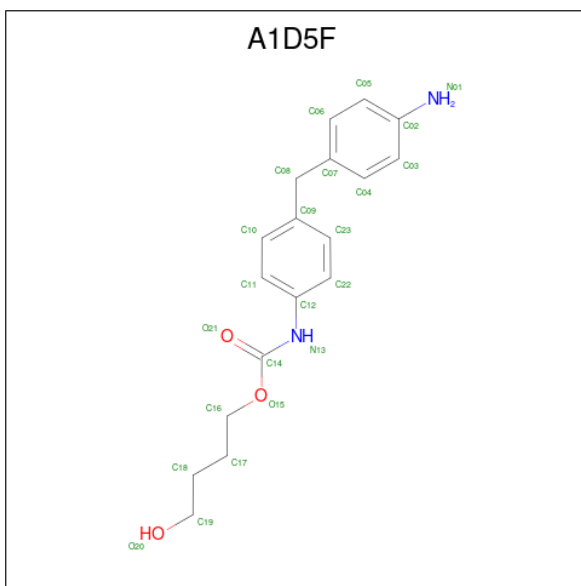
Chain	Residue	Modelled	Actual	Comment	Reference
C	9	GLY	-	expression tag	UNP E6SHQ4
C	10	ALA	-	expression tag	UNP E6SHQ4
C	11	GLY	-	expression tag	UNP E6SHQ4
C	12	ALA	-	expression tag	UNP E6SHQ4
C	13	GLY	-	expression tag	UNP E6SHQ4
C	14	ALA	-	expression tag	UNP E6SHQ4
C	15	GLY	-	expression tag	UNP E6SHQ4
C	16	ALA	-	expression tag	UNP E6SHQ4
C	215	ALA	SER	engineered mutation	UNP E6SHQ4
D	-6	MET	-	initiating methionine	UNP E6SHQ4
D	-5	HIS	-	expression tag	UNP E6SHQ4
D	-4	HIS	-	expression tag	UNP E6SHQ4
D	-3	HIS	-	expression tag	UNP E6SHQ4
D	-2	HIS	-	expression tag	UNP E6SHQ4
D	-1	HIS	-	expression tag	UNP E6SHQ4
D	0	HIS	-	expression tag	UNP E6SHQ4
D	1	GLU	-	expression tag	UNP E6SHQ4
D	2	ASN	-	expression tag	UNP E6SHQ4
D	3	LEU	-	expression tag	UNP E6SHQ4
D	4	TYR	-	expression tag	UNP E6SHQ4
D	5	PHE	-	expression tag	UNP E6SHQ4
D	6	GLN	-	expression tag	UNP E6SHQ4
D	7	GLY	-	expression tag	UNP E6SHQ4
D	8	ALA	-	expression tag	UNP E6SHQ4
D	9	GLY	-	expression tag	UNP E6SHQ4
D	10	ALA	-	expression tag	UNP E6SHQ4
D	11	GLY	-	expression tag	UNP E6SHQ4
D	12	ALA	-	expression tag	UNP E6SHQ4
D	13	GLY	-	expression tag	UNP E6SHQ4
D	14	ALA	-	expression tag	UNP E6SHQ4
D	15	GLY	-	expression tag	UNP E6SHQ4
D	16	ALA	-	expression tag	UNP E6SHQ4
D	215	ALA	SER	engineered mutation	UNP E6SHQ4

- 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		

- Molecule 3 is 4-oxidanylbutyl {N}-[4-[(4-aminophenyl)methyl]phenyl]carbamate (CCD ID: A1D5F) (formula: C₁₈H₂₂N₂O₃) (labeled as "Ligand of Interest" by depositor).



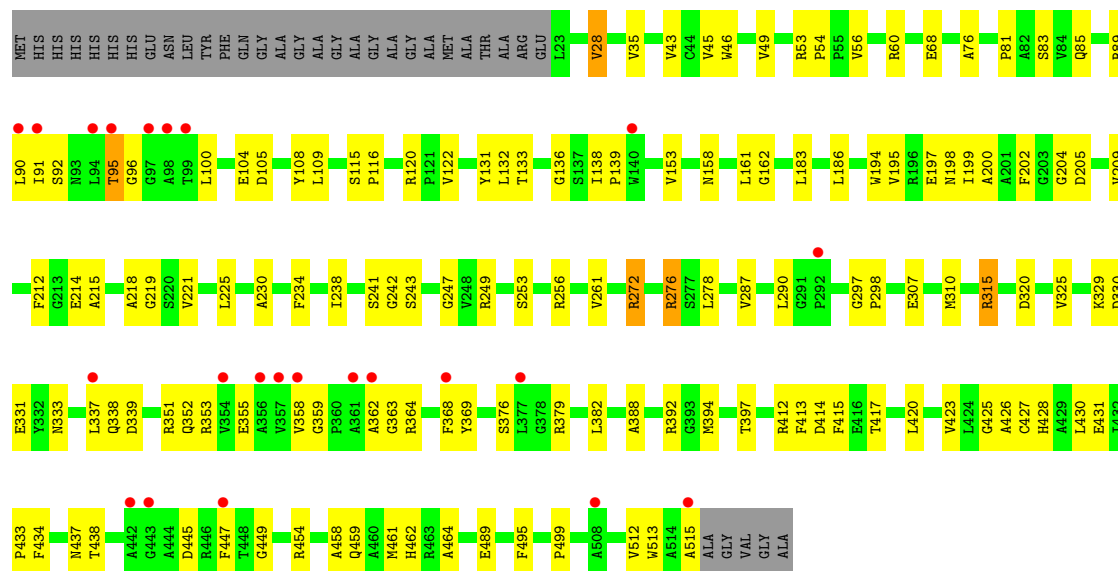
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			23	18	2	3		

- Molecule 4 is water.

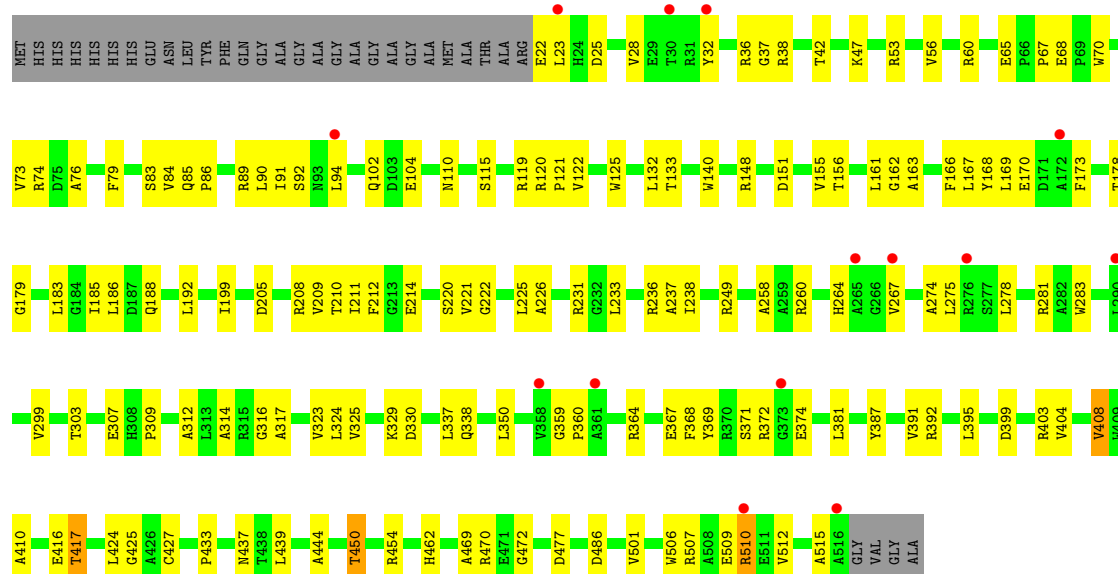
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total 122	O 122	0	0
4	B	115	Total 115	O 115	0	0
4	C	110	Total 110	O 110	0	0
4	D	122	Total 122	O 122	0	0



• Molecule 1: Carboxylic ester hydrolase



• Molecule 1: Carboxylic ester hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	81.57Å 81.57Å 667.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.52 – 2.11 48.52 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.52-2.11) 100.0 (48.52-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.191 , 0.225 0.196 , 0.222	Depositor DCC
R_{free} test set	7260 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.186 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15514	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: A1D5F, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.78	2/3850 (0.1%)	1.02	3/5259 (0.1%)
1	B	0.79	0/3874	1.02	3/5291 (0.1%)
1	C	0.78	0/3842	1.00	0/5248
1	D	0.78	0/3859	1.01	2/5271 (0.0%)
All	All	0.78	2/15425 (0.0%)	1.01	8/21069 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	ALA	C-N	6.88	1.43	1.33
1	A	378	GLY	C-N	-5.57	1.26	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	91	ILE	N-CA-C	-7.31	105.65	112.96
1	A	470	ARG	O-C-N	-6.34	115.25	122.09
1	A	378	GLY	O-C-N	5.81	127.77	122.19
1	B	462	HIS	CA-CB-CG	5.44	119.24	113.80
1	B	212	PHE	CA-CB-CG	5.41	119.21	113.80
1	B	250	THR	CA-CB-OG1	-5.17	101.85	109.60
1	D	417	THR	CA-CB-OG1	-5.06	102.01	109.60
1	A	340	PRO	N-CA-C	5.02	120.63	114.35

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	3748	0	3680	102	0
1	B	3772	0	3701	117	0
1	C	3740	0	3666	87	0
1	D	3757	0	3686	95	0
2	A	5	0	0	0	0
3	C	23	0	0	1	0
4	A	122	0	0	11	0
4	B	115	0	0	11	0
4	C	110	0	0	4	0
4	D	122	0	0	7	0
All	All	15514	0	14733	398	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 13.

All (398) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ARG:HH11	1:B:236:ARG:CG	1.66	1.07
1:B:236:ARG:HH11	1:B:236:ARG:HG2	1.25	1.01
1:A:439:LEU:HD13	1:A:454:ARG:HG3	1.49	0.92
1:C:461:MET:HA	4:C:716:HOH:O	1.82	0.78
1:C:352:GLN:OE1	1:C:353:ARG:NH1	2.17	0.77
1:B:236:ARG:HH11	1:B:236:ARG:HG3	1.50	0.76
1:D:121:PRO:HG2	1:D:470:ARG:HG2	1.67	0.76
1:A:370:ARG:HG2	1:A:377:LEU:HD11	1.65	0.76
1:B:151:ASP:HB3	1:B:470:ARG:HH21	1.53	0.73
1:A:302:GLY:HA2	1:A:306:PRO:HA	1.70	0.72
1:C:153:VAL:HG11	1:C:199:ILE:HD11	1.71	0.71
1:B:357:VAL:HG12	1:B:358:VAL:HG13	1.73	0.71
1:C:337:LEU:HD21	1:C:420:LEU:HD13	1.72	0.71
1:D:507:ARG:O	1:D:510:ARG:HG3	1.92	0.69
1:A:42:THR:HG22	1:A:43:VAL:HG23	1.73	0.69
1:D:329:LYS:NZ	1:D:330:ASP:OD2	2.26	0.69
1:A:307:GLU:OE1	1:A:315:ARG:NH2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:TRP:HZ3	1:A:113:SER:HB3	1.58	0.68
1:B:236:ARG:HG2	1:B:236:ARG:NH1	2.01	0.68
1:C:28:VAL:HG11	1:C:202:PHE:CE1	2.28	0.68
1:B:49:VAL:HB	1:B:109:LEU:HD12	1.76	0.68
1:D:102:GLN:OE1	1:D:281:ARG:NH2	2.27	0.67
1:A:230:ALA:N	4:A:702:HOH:O	2.29	0.66
1:C:329:LYS:HB3	1:C:426:ALA:HB3	1.78	0.66
1:C:249:ARG:NH1	1:C:253:SER:OG	2.28	0.65
1:B:387:TYR:HA	1:B:391:VAL:HB	1.80	0.65
1:A:350:LEU:HB3	1:A:381:LEU:HD12	1.80	0.64
1:B:88:ASP:HB2	1:B:133:THR:HG21	1.80	0.64
1:C:331:GLU:OE1	1:C:428:HIS:ND1	2.30	0.64
1:B:236:ARG:CG	1:B:236:ARG:NH1	2.38	0.64
1:B:488:GLU:HG2	1:B:489:GLU:HG2	1.79	0.64
1:B:85:GLN:O	1:B:281:ARG:NH2	2.31	0.64
1:C:464:ALA:HB3	4:C:716:HOH:O	1.97	0.64
1:D:120:ARG:NE	1:D:151:ASP:OD1	2.25	0.63
1:A:327:VAL:HG21	1:A:391:VAL:HG22	1.80	0.63
1:D:368:PHE:CZ	1:D:372:ARG:HD3	2.33	0.63
1:D:132:LEU:HD23	1:D:162:GLY:HA2	1.81	0.62
1:D:56:VAL:HG12	1:D:104:GLU:HG2	1.81	0.62
1:A:500:ARG:NH2	1:A:502:GLU:OE2	2.31	0.61
1:B:140:TRP:HE1	1:B:444:ALA:HB2	1.65	0.61
1:D:316:GLY:HA2	1:D:404:VAL:HG11	1.81	0.61
1:A:370:ARG:HG2	1:A:377:LEU:CD1	2.31	0.61
1:C:28:VAL:HG11	1:C:202:PHE:CZ	2.36	0.61
1:C:219:GLY:HA2	1:C:243:SER:O	2.01	0.61
1:B:332:TYR:HE1	1:B:389:VAL:HG21	1.65	0.61
1:D:122:VAL:HB	1:D:209:VAL:HG22	1.81	0.61
1:D:433:PRO:HB2	1:D:439:LEU:HD23	1.83	0.61
1:D:231:ARG:NH1	1:D:317:ALA:O	2.34	0.60
1:A:112:TRP:CD1	1:A:144:THR:HG1	2.19	0.60
1:D:90:LEU:HD13	1:D:338:GLN:HG3	1.83	0.60
1:D:437:ASN:HB2	1:D:462:HIS:CG	2.37	0.60
1:B:248:VAL:HG22	1:B:298:PRO:HB2	1.84	0.59
1:C:120:ARG:O	1:C:205:ASP:N	2.29	0.59
1:A:162:GLY:O	1:A:166:PHE:N	2.32	0.58
1:A:248:VAL:HG21	1:A:309:PRO:HG2	1.86	0.58
1:A:479:LEU:HD13	1:A:493:MET:HE3	1.85	0.58
1:A:249:ARG:NH1	1:A:294:LEU:O	2.37	0.58
1:A:489:GLU:OE1	1:A:503:ARG:NE	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:TYR:CE1	1:B:389:VAL:HG21	2.39	0.57
1:C:261:VAL:HG22	1:C:290:LEU:HD11	1.86	0.56
1:B:419:VAL:HG11	1:B:446:ARG:O	2.05	0.56
1:B:507:ARG:HA	1:B:510:ARG:HE	1.70	0.56
1:A:357:VAL:HG12	1:A:358:VAL:HG13	1.87	0.56
1:D:192:LEU:HB3	1:D:233:LEU:HB3	1.88	0.56
1:D:74:ARG:NH1	4:D:614:HOH:O	2.39	0.56
1:A:95:THR:HG22	1:A:97:GLY:H	1.71	0.56
1:D:506:TRP:O	1:D:510:ARG:HG2	2.05	0.56
1:B:236:ARG:HG3	1:B:236:ARG:NH1	2.15	0.56
1:C:351:ARG:HH22	1:C:363:GLY:HA2	1.70	0.56
1:B:370:ARG:HG3	1:B:380:ARG:HH12	1.70	0.56
1:C:131:TYR:CZ	1:C:298:PRO:HD3	2.41	0.56
1:C:132:LEU:HD22	1:C:287:VAL:HG11	1.88	0.55
1:A:186:LEU:HA	1:A:189:ILE:HD12	1.86	0.55
1:B:29:GLU:HA	1:B:34:ALA:HA	1.88	0.55
1:D:367:GLU:O	1:D:371:SER:OG	2.24	0.55
1:D:387:TYR:HA	1:D:391:VAL:HB	1.88	0.55
1:B:144:THR:HB	1:B:441:ARG:HH22	1.70	0.55
1:D:350:LEU:HB3	1:D:381:LEU:HD12	1.87	0.55
1:A:154:VAL:HB	4:A:710:HOH:O	2.07	0.55
1:D:125:TRP:HB3	1:D:156:THR:HG22	1.89	0.55
1:A:420:LEU:HB3	1:A:423:VAL:HG22	1.89	0.55
1:D:509:GLU:HA	1:D:512:VAL:HG12	1.89	0.54
1:C:307:GLU:OE2	1:C:315:ARG:NH2	2.40	0.54
1:D:60:ARG:NH1	1:D:283:TRP:HE1	2.05	0.54
1:B:331:GLU:HB3	1:B:390:PHE:CD2	2.41	0.54
1:C:83:SER:HB3	1:C:161:LEU:HD12	1.88	0.54
1:C:499:PRO:HD2	1:D:403:ARG:NH2	2.21	0.54
1:B:508:ALA:O	1:B:512:VAL:HG12	2.08	0.54
1:B:370:ARG:O	1:B:380:ARG:NH1	2.34	0.54
1:A:229:ALA:HB3	4:A:702:HOH:O	2.08	0.54
1:A:319:ARG:HA	1:A:406:ALA:HB2	1.90	0.54
1:B:370:ARG:NH1	4:B:603:HOH:O	2.25	0.54
1:A:143:GLY:HA3	4:A:710:HOH:O	2.08	0.53
1:D:450:THR:HG22	4:D:615:HOH:O	2.08	0.53
1:A:215:ALA:HB2	1:A:428:HIS:HE2	1.72	0.53
1:A:366:ILE:O	1:A:370:ARG:HG3	2.09	0.53
1:A:163:ALA:HB1	1:A:167:LEU:HD22	1.91	0.53
1:C:413:PHE:CZ	1:C:415:PHE:HB3	2.44	0.53
1:D:364:ARG:NH1	1:D:515:ALA:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:VAL:N	1:B:210:THR:O	2.34	0.52
1:B:302:GLY:HA2	1:B:306:PRO:HA	1.91	0.52
1:C:132:LEU:HD23	1:C:162:GLY:HA2	1.92	0.52
1:C:358:VAL:HG23	1:C:362:ALA:HB2	1.90	0.52
1:A:62:ARG:NH2	1:A:276:ARG:HH22	2.08	0.52
1:C:325:VAL:HG22	1:C:394:MET:HG3	1.90	0.52
1:B:460:ALA:HB1	1:B:479:LEU:HD21	1.90	0.52
1:C:355:GLU:O	1:C:359:GLY:N	2.37	0.52
1:D:236:ARG:HD3	1:D:472:GLY:HA2	1.91	0.52
1:B:505:PRO:HG2	1:B:506:TRP:CE3	2.45	0.52
1:C:214:GLU:HG3	1:C:431:GLU:OE1	2.10	0.52
1:D:125:TRP:HH2	1:D:214:GLU:HB2	1.75	0.52
1:B:148:ARG:CD	4:B:702:HOH:O	2.56	0.52
1:B:412:ARG:NH2	1:B:414:ASP:OD2	2.37	0.51
1:D:501:VAL:HG23	4:D:643:HOH:O	2.11	0.51
1:D:86:PRO:HD2	1:D:132:LEU:O	2.11	0.51
1:D:260:ARG:O	1:D:264:HIS:ND1	2.43	0.51
1:D:330:ASP:O	1:D:427:CYS:HA	2.11	0.51
1:A:58:PRO:O	1:A:62:ARG:NH1	2.42	0.51
1:A:351:ARG:HG2	1:A:366:ILE:HD13	1.93	0.51
1:A:62:ARG:CZ	1:A:276:ARG:HH22	2.24	0.51
1:D:25:ASP:OD1	1:D:38:ARG:NE	2.42	0.51
1:D:395:LEU:O	1:D:399:ASP:OD2	2.28	0.51
1:B:463:ARG:HH22	1:B:477:ASP:CG	2.19	0.50
1:C:35:VAL:HG11	1:C:49:VAL:HG13	1.93	0.50
1:C:412:ARG:NH2	1:C:414:ASP:OD2	2.27	0.50
1:B:388:ALA:HB2	1:B:513:TRP:HH2	1.76	0.50
1:C:434:PHE:HB3	1:C:458:ALA:HA	1.94	0.50
1:A:46:TRP:CZ3	1:A:113:SER:HB3	2.43	0.50
1:A:380:ARG:O	1:A:383:PRO:HD2	2.11	0.50
1:A:504:ASP:N	1:A:505:PRO:HD3	2.27	0.50
1:B:53:ARG:HG3	1:B:66:PRO:O	2.11	0.50
1:B:461:MET:HG2	1:B:495:PHE:CD1	2.46	0.50
1:C:85:GLN:HB2	1:C:133:THR:HA	1.94	0.50
1:B:24:HIS:N	1:B:39:SER:O	2.26	0.50
1:B:512:VAL:HG13	1:B:513:TRP:HD1	1.77	0.50
1:C:339:ASP:OD2	1:C:353:ARG:NH2	2.41	0.50
1:D:260:ARG:NH1	4:D:621:HOH:O	2.43	0.49
1:C:215:ALA:HB1	3:C:601:A1D5F:N13	2.27	0.49
1:B:445:ASP:HB2	1:B:450:THR:HG22	1.95	0.49
1:D:36:ARG:HB2	1:D:73:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:LYS:HB3	1:D:79:PHE:HA	1.94	0.49
1:D:170:GLU:HG2	1:D:178:THR:HA	1.94	0.49
1:A:236:ARG:HG2	1:A:322:ALA:HB3	1.94	0.49
1:A:445:ASP:OD1	1:A:445:ASP:N	2.45	0.49
1:A:110:ASN:ND2	1:A:156:THR:OG1	2.43	0.49
1:C:28:VAL:CG1	1:C:202:PHE:CZ	2.94	0.49
1:B:53:ARG:NH1	1:B:68:GLU:OE2	2.46	0.49
1:C:351:ARG:NH2	1:C:363:GLY:HA2	2.27	0.49
1:B:249:ARG:N	1:B:298:PRO:O	2.46	0.49
1:C:445:ASP:OD1	1:C:445:ASP:N	2.46	0.49
1:B:36:ARG:HB2	1:B:73:VAL:CG1	2.43	0.48
1:D:307:GLU:HG3	1:D:312:ALA:HB2	1.95	0.48
1:D:119:ARG:HG2	1:D:205:ASP:HB2	1.96	0.48
1:A:32:TYR:OH	1:A:66:PRO:HB3	2.13	0.48
1:C:272:ARG:CZ	1:C:276:ARG:NH1	2.77	0.48
1:C:212:PHE:HB2	1:C:238:ILE:HB	1.96	0.48
1:C:54:PRO:HB3	1:C:105:ASP:HB2	1.96	0.48
1:B:148:ARG:HD3	4:B:702:HOH:O	2.12	0.48
1:B:249:ARG:NH2	1:B:294:LEU:O	2.45	0.48
1:C:200:ALA:HA	1:C:204:GLY:O	2.13	0.48
1:D:53:ARG:N	1:D:65:GLU:O	2.38	0.48
1:D:226:ALA:HB2	1:D:309:PRO:HA	1.96	0.48
1:C:417:THR:HG22	1:C:425:GLY:O	2.13	0.48
1:D:168:TYR:CD2	1:D:299:VAL:HG11	2.49	0.48
1:B:434:PHE:CD2	1:B:457:VAL:HG22	2.49	0.47
1:C:136:GLY:N	1:C:158:ASN:OD1	2.32	0.47
1:B:214:GLU:HG3	1:B:431:GLU:OE2	2.14	0.47
1:C:199:ILE:N	4:C:707:HOH:O	2.47	0.47
1:C:218:ALA:HB3	1:C:242:GLY:HA3	1.95	0.47
1:D:278:LEU:HD23	1:D:283:TRP:CD2	2.49	0.47
1:B:504:ASP:OD1	1:B:510:ARG:NE	2.48	0.47
1:C:109:LEU:HD11	1:C:194:TRP:CZ3	2.48	0.47
1:A:196:ARG:NH1	4:A:715:HOH:O	2.46	0.47
1:C:122:VAL:HB	1:C:209:VAL:HG22	1.95	0.47
1:D:267:VAL:HG13	1:D:274:ALA:HB3	1.97	0.47
1:A:168:TYR:OH	1:A:251:ALA:HB1	2.15	0.47
1:D:163:ALA:HB3	1:D:283:TRP:HB3	1.96	0.47
1:A:398:ALA:HA	1:A:408:VAL:HG21	1.97	0.47
1:B:60:ARG:O	1:B:276:ARG:NH1	2.42	0.47
1:B:119:ARG:HB3	1:B:205:ASP:HB2	1.96	0.47
1:B:223:VAL:HG13	1:B:305:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ARG:HA	1:A:276:ARG:HD2	1.78	0.47
1:B:138:ILE:HB	1:B:141:TYR:CD2	2.50	0.47
1:A:214:GLU:HG3	1:A:431:GLU:OE2	2.15	0.46
1:A:273:GLU:O	1:A:277:SER:OG	2.27	0.46
1:B:506:TRP:O	1:B:510:ARG:N	2.40	0.46
1:D:454:ARG:NH2	4:D:615:HOH:O	2.40	0.46
1:B:28:VAL:HG13	1:B:201:ALA:HB1	1.97	0.46
1:B:32:TYR:CD2	1:B:67:PRO:HG2	2.51	0.46
1:C:60:ARG:NH1	1:C:278:LEU:O	2.46	0.46
1:B:163:ALA:O	1:B:167:LEU:HB2	2.16	0.46
1:B:460:ALA:HA	1:B:476:HIS:CE1	2.51	0.46
1:C:91:ILE:O	1:C:95:THR:OG1	2.33	0.46
1:D:211:ILE:HD12	1:D:221:VAL:HG13	1.97	0.46
1:A:53:ARG:HD3	1:A:59:LEU:HD11	1.97	0.46
1:B:208:ARG:NE	4:B:609:HOH:O	2.38	0.46
1:D:507:ARG:HA	1:D:510:ARG:HD3	1.98	0.46
1:C:89:ARG:H	1:C:89:ARG:HE	1.63	0.46
1:A:351:ARG:NH2	1:D:367:GLU:OE2	2.49	0.46
1:B:377:LEU:O	1:B:381:LEU:HG	2.15	0.46
1:A:387:TYR:HA	1:A:391:VAL:HB	1.98	0.46
1:D:369:TYR:HD1	1:D:372:ARG:HH21	1.62	0.46
1:A:320:ASP:CG	4:A:705:HOH:O	2.59	0.45
1:A:507:ARG:HA	1:A:510:ARG:HE	1.80	0.45
1:B:411:TYR:HA	1:B:493:MET:O	2.15	0.45
1:C:430:LEU:HA	1:C:447:PHE:HE1	1.80	0.45
1:D:170:GLU:OE2	1:D:179:GLY:N	2.36	0.45
1:A:107:LEU:HD21	1:A:160:ARG:HG3	1.97	0.45
1:C:90:LEU:HD11	1:C:337:LEU:HB2	1.97	0.45
1:A:349:ALA:O	1:A:353:ARG:NH1	2.49	0.45
1:A:131:TYR:N	4:A:720:HOH:O	2.49	0.45
1:D:275:LEU:HD12	1:D:283:TRP:HH2	1.82	0.45
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.79	0.45
1:B:96:GLY:H	1:B:446:ARG:HH12	1.63	0.45
1:D:70:TRP:NE1	1:D:74:ARG:HB2	2.32	0.45
1:A:54:PRO:HD2	4:A:733:HOH:O	2.17	0.45
1:A:95:THR:HG23	1:A:443:GLY:O	2.16	0.45
1:A:129:GLY:O	1:A:130:ALA:HB3	2.16	0.45
1:A:326:GLY:HA3	1:A:411:TYR:CE2	2.52	0.45
1:A:329:LYS:NZ	1:A:416:GLU:OE2	2.49	0.45
1:C:329:LYS:NZ	1:C:330:ASP:OD2	2.50	0.45
1:A:119:ARG:NH1	4:A:721:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:VAL:O	1:B:462:HIS:ND1	2.50	0.45
1:C:60:ARG:NH2	1:C:278:LEU:O	2.47	0.45
1:C:212:PHE:CB	1:C:238:ILE:HB	2.47	0.45
1:A:331:GLU:HB3	1:A:390:PHE:CD2	2.52	0.45
1:A:514:ALA:HB2	4:A:752:HOH:O	2.17	0.45
1:B:177:PHE:HA	4:B:602:HOH:O	2.16	0.45
1:C:90:LEU:HD13	1:C:338:GLN:HG3	1.98	0.45
1:D:337:LEU:HD21	1:D:424:LEU:HD21	1.99	0.45
1:C:364:ARG:HH22	1:C:515:ALA:HB3	1.82	0.45
1:C:445:ASP:O	1:C:449:GLY:N	2.46	0.44
1:D:36:ARG:O	1:D:76:ALA:HB3	2.17	0.44
1:B:35:VAL:HG12	1:B:74:ARG:HB3	1.99	0.44
1:B:163:ALA:HB2	1:B:287:VAL:CG2	2.46	0.44
1:B:170:GLU:HG2	1:B:178:THR:HA	1.98	0.44
1:A:272:ARG:HD3	1:A:276:ARG:NH1	2.33	0.44
1:B:362:ALA:O	1:B:366:ILE:HG13	2.17	0.44
1:D:210:THR:OG1	1:D:236:ARG:HB2	2.18	0.44
1:A:199:ILE:HD12	1:A:199:ILE:HA	1.88	0.44
1:C:388:ALA:HB2	1:C:513:TRP:HH2	1.82	0.44
1:D:140:TRP:CZ2	1:D:444:ALA:HA	2.52	0.44
1:B:507:ARG:NH1	4:B:607:HOH:O	2.36	0.44
1:D:53:ARG:HD2	1:D:68:GLU:HG3	2.00	0.44
1:D:325:VAL:O	1:D:410:ALA:HA	2.16	0.44
1:C:392:ARG:NH1	4:C:720:HOH:O	2.51	0.44
1:B:445:ASP:O	1:B:449:GLY:N	2.50	0.44
1:A:23:LEU:HA	1:A:39:SER:O	2.17	0.44
1:B:194:TRP:O	1:B:198:ASN:N	2.49	0.44
1:C:362:ALA:O	1:C:363:GLY:C	2.61	0.44
1:D:121:PRO:HG3	1:D:208:ARG:NH2	2.33	0.44
1:A:247:GLY:HA2	1:A:294:LEU:HD23	2.00	0.43
1:A:445:ASP:O	1:A:449:GLY:N	2.51	0.43
1:B:180:SER:HA	1:B:183:LEU:HG	2.00	0.43
1:B:482:TRP:NE1	4:B:621:HOH:O	2.48	0.43
1:C:35:VAL:HB	1:C:76:ALA:HB2	2.00	0.43
1:C:368:PHE:CD2	1:C:512:VAL:HG11	2.52	0.43
1:B:368:PHE:HD1	1:B:369:TYR:CD2	2.36	0.43
1:B:430:LEU:O	1:B:433:PRO:HD2	2.17	0.43
1:B:504:ASP:OD2	1:B:510:ARG:NH2	2.51	0.43
1:A:330:ASP:O	1:A:427:CYS:HA	2.18	0.43
1:A:350:LEU:O	1:A:354:VAL:HG23	2.19	0.43
1:A:408:VAL:HG13	1:A:485:TYR:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLY:HA3	1:B:70:TRP:CE2	2.53	0.43
1:B:140:TRP:NE1	1:B:444:ALA:HB2	2.32	0.43
1:B:505:PRO:HB2	4:B:691:HOH:O	2.18	0.43
1:A:302:GLY:CA	1:A:306:PRO:HA	2.45	0.43
1:C:230:ALA:HB1	1:C:234:PHE:HE2	1.82	0.43
1:D:166:PHE:HE1	1:D:185:ILE:HG12	1.84	0.43
1:B:151:ASP:HB3	1:B:470:ARG:NH2	2.28	0.43
1:B:327:VAL:HG21	1:B:391:VAL:HG22	2.01	0.43
1:B:463:ARG:NH2	4:B:616:HOH:O	2.42	0.43
1:C:138:ILE:HG23	1:C:139:PRO:HD2	1.99	0.43
1:D:437:ASN:HB2	1:D:462:HIS:CD2	2.53	0.43
1:A:110:ASN:HB2	1:A:112:TRP:CZ3	2.53	0.43
1:A:146:LEU:HG	1:A:462:HIS:HE1	1.84	0.43
1:B:512:VAL:HG13	1:B:513:TRP:CD1	2.52	0.43
1:C:56:VAL:HG12	1:C:104:GLU:HB3	2.01	0.43
1:D:211:ILE:O	1:D:237:ALA:HA	2.19	0.43
1:B:347:GLU:HG2	1:B:377:LEU:HD22	1.99	0.43
1:C:272:ARG:NE	1:C:276:ARG:NH1	2.67	0.43
1:C:437:ASN:HB2	1:C:462:HIS:ND1	2.34	0.43
1:B:78:ARG:HA	1:B:78:ARG:HD3	1.78	0.43
1:A:329:LYS:HB3	1:A:329:LYS:HE3	1.57	0.43
1:D:486:ASP:OD1	1:D:486:ASP:N	2.52	0.43
1:A:411:TYR:HA	1:A:493:MET:O	2.19	0.42
1:B:86:PRO:HA	4:B:626:HOH:O	2.19	0.42
1:B:89:ARG:HD2	1:B:93:ASN:OD1	2.19	0.42
1:B:388:ALA:HB2	1:B:513:TRP:CH2	2.52	0.42
1:B:395:LEU:HD13	1:B:510:ARG:HG2	1.99	0.42
1:B:502:GLU:OE1	1:B:505:PRO:HB3	2.19	0.42
1:A:445:ASP:HB2	1:A:450:THR:HG22	2.01	0.42
1:B:248:VAL:HG11	1:B:309:PRO:HD2	2.01	0.42
1:C:46:TRP:CZ2	1:C:116:PRO:HG3	2.54	0.42
1:C:459:GLN:HG3	1:D:314:ALA:HB3	2.00	0.42
1:D:32:TYR:CG	1:D:67:PRO:HG2	2.54	0.42
1:D:477:ASP:N	1:D:477:ASP:OD1	2.52	0.42
1:A:182:ASN:HD22	1:A:304:VAL:HB	1.84	0.42
1:B:330:ASP:OD2	1:B:426:ALA:N	2.47	0.42
1:D:83:SER:HB3	1:D:161:LEU:HD12	2.01	0.42
1:A:214:GLU:HA	1:A:240:GLN:O	2.20	0.42
1:B:281:ARG:NH2	4:B:626:HOH:O	2.51	0.42
1:B:503:ARG:HG2	1:B:503:ARG:HH11	1.85	0.42
1:D:25:ASP:HA	1:D:37:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:507:ARG:HA	1:D:510:ARG:CD	2.50	0.42
1:A:189:ILE:O	1:A:193:ARG:HG3	2.20	0.42
1:A:248:VAL:HG11	1:A:309:PRO:CD	2.50	0.42
1:C:310:MET:HE1	1:C:397:THR:HA	2.00	0.42
1:A:273:GLU:O	1:A:277:SER:N	2.44	0.42
1:B:90:LEU:HD11	1:B:338:GLN:CD	2.44	0.42
1:C:333:ASN:ND2	1:C:423:VAL:O	2.38	0.42
1:C:430:LEU:O	1:C:433:PRO:HD2	2.20	0.42
1:D:359:GLY:HA3	1:D:360:PRO:HD3	1.91	0.42
1:A:239:LEU:HB2	1:A:325:VAL:HG23	2.02	0.42
1:A:492:VAL:HG21	1:A:506:TRP:HZ3	1.85	0.42
1:B:461:MET:HE2	1:B:461:MET:HB3	1.86	0.42
1:C:195:VAL:O	1:C:199:ILE:HB	2.20	0.42
1:C:369:TYR:OH	1:C:513:TRP:NE1	2.42	0.42
1:D:417:THR:HG22	1:D:425:GLY:O	2.20	0.42
1:A:89:ARG:O	1:A:93:ASN:HB2	2.20	0.42
1:A:165:GLY:O	1:A:183:LEU:HB2	2.20	0.42
1:D:278:LEU:HD23	1:D:283:TRP:CE2	2.55	0.42
1:D:403:ARG:HA	1:D:403:ARG:HD3	1.83	0.42
1:A:294:LEU:HD12	1:A:294:LEU:HA	1.87	0.41
1:B:248:VAL:HG21	1:B:309:PRO:HG2	2.01	0.41
1:D:416:GLU:HB3	1:D:425:GLY:HA2	2.01	0.41
1:C:183:LEU:HD23	1:C:186:LEU:HD12	2.02	0.41
1:C:330:ASP:O	1:C:427:CYS:HA	2.19	0.41
1:D:183:LEU:HD23	1:D:186:LEU:HD12	2.01	0.41
1:D:222:GLY:HA2	1:D:225:LEU:HD12	2.02	0.41
1:A:428:HIS:O	1:A:429:ALA:HB3	2.19	0.41
1:C:221:VAL:O	1:C:225:LEU:HG	2.20	0.41
1:C:253:SER:HA	1:C:256:ARG:NH2	2.35	0.41
1:D:148:ARG:NH1	4:D:629:HOH:O	2.52	0.41
1:D:249:ARG:HG3	4:D:609:HOH:O	2.20	0.41
1:A:62:ARG:HH22	1:A:272:ARG:NH1	2.18	0.41
1:B:64:PRO:HD2	1:B:186:LEU:HB3	2.02	0.41
1:B:364:ARG:HD2	1:B:516:ALA:HA	2.00	0.41
1:A:249:ARG:O	1:A:299:VAL:HA	2.20	0.41
1:A:451:ALA:O	1:A:454:ARG:NE	2.41	0.41
1:B:460:ALA:HB1	1:B:479:LEU:CD2	2.50	0.41
1:A:486:ASP:CG	1:A:489:GLU:H	2.28	0.41
1:B:121:PRO:HB2	1:B:152:VAL:HG12	2.02	0.41
1:B:328:ASN:O	1:B:331:GLU:HG2	2.21	0.41
1:D:125:TRP:CH2	1:D:214:GLU:HB2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:TYR:CE1	1:D:392:ARG:HB3	2.55	0.41
1:A:82:ALA:O	1:A:102:GLN:HA	2.20	0.41
1:B:61:PHE:HE1	1:B:163:ALA:O	2.03	0.41
1:B:326:GLY:HA3	1:B:411:TYR:CE2	2.55	0.41
1:C:81:PRO:HD2	1:C:108:TYR:CE2	2.55	0.41
1:A:53:ARG:N	1:A:65:GLU:O	2.32	0.41
1:A:261:VAL:O	1:A:286:ALA:HB1	2.20	0.41
1:A:506:TRP:O	1:A:510:ARG:HG3	2.21	0.41
1:B:195:VAL:O	1:B:199:ILE:HB	2.20	0.41
1:B:337:LEU:HD21	1:B:424:LEU:HD21	2.03	0.41
1:B:391:VAL:HG11	1:B:506:TRP:CD1	2.56	0.41
1:C:92:SER:O	1:C:96:GLY:N	2.39	0.41
1:D:210:THR:OG1	1:D:469:ALA:HA	2.21	0.41
1:A:112:TRP:HB2	4:A:710:HOH:O	2.20	0.41
1:A:119:ARG:HB3	1:A:205:ASP:HB2	2.03	0.41
1:B:37:GLY:HA3	1:B:46:TRP:CD1	2.56	0.41
1:B:60:ARG:HG2	1:B:61:PHE:N	2.35	0.41
1:B:327:VAL:O	1:B:412:ARG:HA	2.21	0.41
1:B:357:VAL:HG21	1:B:385:MET:HE1	2.02	0.41
1:B:370:ARG:HG3	1:B:380:ARG:NH1	2.36	0.41
1:C:364:ARG:HH21	1:C:515:ALA:C	2.29	0.41
1:C:414:ASP:HB2	1:C:495:PHE:O	2.20	0.41
1:C:434:PHE:HE2	1:C:454:ARG:HB2	1.86	0.41
1:D:85:GLN:HB2	1:D:133:THR:HA	2.03	0.41
1:D:140:TRP:NE1	1:D:444:ALA:HB2	2.36	0.41
1:D:169:LEU:HD13	1:D:275:LEU:HD21	2.02	0.41
1:D:173:PHE:CE2	1:D:275:LEU:HD22	2.56	0.41
1:D:199:ILE:HD12	1:D:199:ILE:HA	1.90	0.41
1:D:236:ARG:NE	1:D:469:ALA:O	2.53	0.41
1:D:110:ASN:O	1:D:155:VAL:HA	2.21	0.41
1:B:36:ARG:NH1	1:B:75:ASP:OD1	2.53	0.40
1:B:214:GLU:HA	1:B:240:GLN:O	2.21	0.40
1:B:413:PHE:CZ	1:B:415:PHE:HB3	2.57	0.40
1:C:215:ALA:HA	1:C:241:SER:O	2.21	0.40
1:C:379:ARG:HA	1:C:382:LEU:HD12	2.03	0.40
1:D:188:GLN:OE1	1:D:220:SER:HB3	2.21	0.40
1:D:238:ILE:HA	1:D:324:LEU:O	2.21	0.40
1:A:420:LEU:HD13	1:A:420:LEU:HA	1.80	0.40
1:D:167:LEU:HD11	1:D:258:ALA:HA	2.03	0.40
1:A:230:ALA:HA	1:A:233:LEU:HD12	2.03	0.40
1:A:409:TRP:HB3	1:A:482:TRP:CZ2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LEU:HD23	1:B:313:LEU:HA	1.88	0.40
1:B:464:ALA:HA	1:B:474:PRO:O	2.21	0.40
1:C:197:GLU:HG3	1:C:198:ASN:ND2	2.35	0.40
1:D:167:LEU:HD23	1:D:169:LEU:HD21	2.04	0.40
1:D:323:VAL:O	1:D:408:VAL:HA	2.22	0.40
1:A:51:PHE:HD2	1:A:109:LEU:HG	1.86	0.40
1:A:196:ARG:HA	1:A:206:PRO:HB3	2.04	0.40
1:B:503:ARG:HH11	1:B:503:ARG:CG	2.34	0.40
1:C:247:GLY:O	1:C:297:GLY:HA3	2.22	0.40
1:B:36:ARG:HB2	1:B:73:VAL:HG11	2.03	0.40
1:C:53:ARG:HH11	1:C:68:GLU:HG3	1.86	0.40
1:C:339:ASP:CG	1:C:353:ARG:HE	2.30	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	492/527 (93%)	482 (98%)	10 (2%)	0	100	100
1	B	496/527 (94%)	488 (98%)	8 (2%)	0	100	100
1	C	491/527 (93%)	481 (98%)	10 (2%)	0	100	100
1	D	493/527 (94%)	484 (98%)	9 (2%)	0	100	100
All	All	1972/2108 (94%)	1935 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	364/382 (95%)	342 (94%)	22 (6%)	17	15
1	B	366/382 (96%)	344 (94%)	22 (6%)	17	15
1	C	363/382 (95%)	350 (96%)	13 (4%)	31	33
1	D	365/382 (96%)	350 (96%)	15 (4%)	27	27
All	All	1458/1528 (95%)	1386 (95%)	72 (5%)	22	21

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	THR
1	A	65	GLU
1	A	71	SER
1	A	78	ARG
1	A	126	ILE
1	A	180	SER
1	A	212	PHE
1	A	243	SER
1	A	250	THR
1	A	287	VAL
1	A	329	LYS
1	A	371	SER
1	A	374	GLU
1	A	376	SER
1	A	381	LEU
1	A	394	MET
1	A	419	VAL
1	A	420	LEU
1	A	435	VAL
1	A	454	ARG
1	A	459	GLN
1	A	481	GLU
1	B	29	GLU
1	B	91	ILE
1	B	92	SER
1	B	94	LEU
1	B	95	THR
1	B	148	ARG

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Mol	Chain	Res	Type
1	B	157	LEU
1	B	186	LEU
1	B	210	THR
1	B	212	PHE
1	B	236	ARG
1	B	243	SER
1	B	320	ASP
1	B	329	LYS
1	B	357	VAL
1	B	364	ARG
1	B	371	SER
1	B	408	VAL
1	B	441	ARG
1	B	457	VAL
1	B	470	ARG
1	B	498	GLU
1	C	28	VAL
1	C	43	VAL
1	C	45	VAL
1	C	95	THR
1	C	100	LEU
1	C	115	SER
1	C	272	ARG
1	C	276	ARG
1	C	315	ARG
1	C	320	ASP
1	C	376	SER
1	C	438	THR
1	C	489	GLU
1	D	22	GLU
1	D	23	LEU
1	D	28	VAL
1	D	42	THR
1	D	84	VAL
1	D	89	ARG
1	D	92	SER
1	D	94	LEU
1	D	115	SER
1	D	212	PHE
1	D	303	THR
1	D	374	GLU
1	D	408	VAL

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Mol	Chain	Res	Type
1	D	450	THR
1	D	510	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	338	GLN
1	B	240	GLN
1	C	102	GLN
1	C	264	HIS
1	D	240	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	SO4	A	601	-	4,4,4	0.64	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1D5F	C	601	-	24,24,24	1.57	4 (16%)	30,30,30	1.84	7 (23%)

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	A1D5F	C	601	-	-	6/14/14/14	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	A1D5F	C14-N13	3.94	1.44	1.36
3	C	601	A1D5F	O21-C14	-3.72	1.15	1.21
3	C	601	A1D5F	C22-C12	-2.78	1.34	1.39
3	C	601	A1D5F	C08-C07	2.25	1.59	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	A1D5F	O15-C14-N13	6.34	119.31	109.35
3	C	601	A1D5F	C12-N13-C14	-3.74	120.47	126.39
3	C	601	A1D5F	C08-C07-C06	-2.75	113.89	120.95
3	C	601	A1D5F	O21-C14-N13	-2.68	120.43	126.12
3	C	601	A1D5F	C05-C02-N01	-2.49	116.32	120.90
3	C	601	A1D5F	C08-C07-C04	2.46	127.25	120.95
3	C	601	A1D5F	O15-C14-O21	-2.09	120.26	124.26

There are no chirality outliers.

All (6) torsion outliers are listed below:

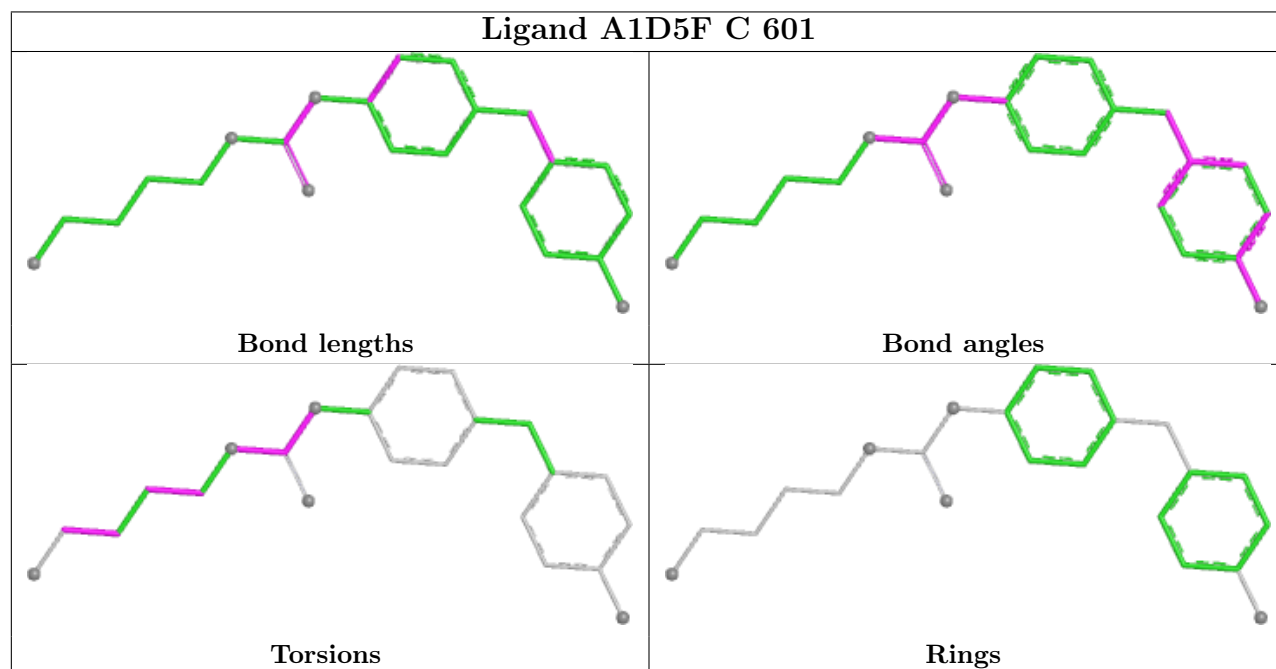
Mol	Chain	Res	Type	Atoms
3	C	601	A1D5F	O15-C14-N13-C12
3	C	601	A1D5F	O21-C14-N13-C12
3	C	601	A1D5F	O15-C16-C17-C18
3	C	601	A1D5F	N13-C14-O15-C16
3	C	601	A1D5F	O21-C14-O15-C16
3	C	601	A1D5F	C17-C18-C19-O20

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	A1D5F	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	494/527 (93%)	0.35	6 (1%) 76 79	25, 37, 57, 78	0
1	B	498/527 (94%)	0.27	13 (2%) 57 60	24, 36, 56, 90	0
1	C	493/527 (93%)	0.33	23 (4%) 36 39	26, 36, 58, 88	0
1	D	495/527 (93%)	0.34	14 (2%) 55 58	26, 37, 56, 75	0
All	All	1980/2108 (93%)	0.32	56 (2%) 55 58	24, 37, 57, 90	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	94	LEU	6.1
1	B	94	LEU	5.5
1	C	91	ILE	5.0
1	D	358	VAL	4.1
1	C	356	ALA	3.9
1	C	95	THR	3.7
1	D	265	ALA	3.5
1	B	96	GLY	3.5
1	A	454	ARG	3.4
1	C	98	ALA	3.2
1	B	90	LEU	3.2
1	D	30	THR	3.2
1	C	447	PHE	3.0
1	A	420	LEU	3.0
1	B	266	GLY	2.9
1	C	97	GLY	2.9
1	B	95	THR	2.9
1	B	371	SER	2.8
1	D	172	ALA	2.7
1	C	377	LEU	2.7
1	D	510	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	443	GLY	2.6
1	D	94	LEU	2.6
1	A	289	ALA	2.5
1	C	515	ALA	2.5
1	C	90	LEU	2.5
1	D	267	VAL	2.5
1	C	357	VAL	2.4
1	C	358	VAL	2.4
1	C	99	THR	2.4
1	B	91	ILE	2.4
1	A	98	ALA	2.4
1	A	516	ALA	2.4
1	C	508	ALA	2.4
1	B	378	GLY	2.4
1	D	373	GLY	2.4
1	D	516	ALA	2.3
1	B	98	ALA	2.3
1	C	362	ALA	2.3
1	C	140	TRP	2.3
1	B	92	SER	2.2
1	C	292	PRO	2.2
1	C	361	ALA	2.2
1	D	361	ALA	2.2
1	A	275	LEU	2.1
1	C	368	PHE	2.1
1	C	337	LEU	2.1
1	D	23	LEU	2.1
1	B	344	GLY	2.1
1	D	290	LEU	2.0
1	B	89	ARG	2.0
1	D	276	ARG	2.0
1	B	358	VAL	2.0
1	C	354	VAL	2.0
1	C	442	ALA	2.0
1	D	32	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

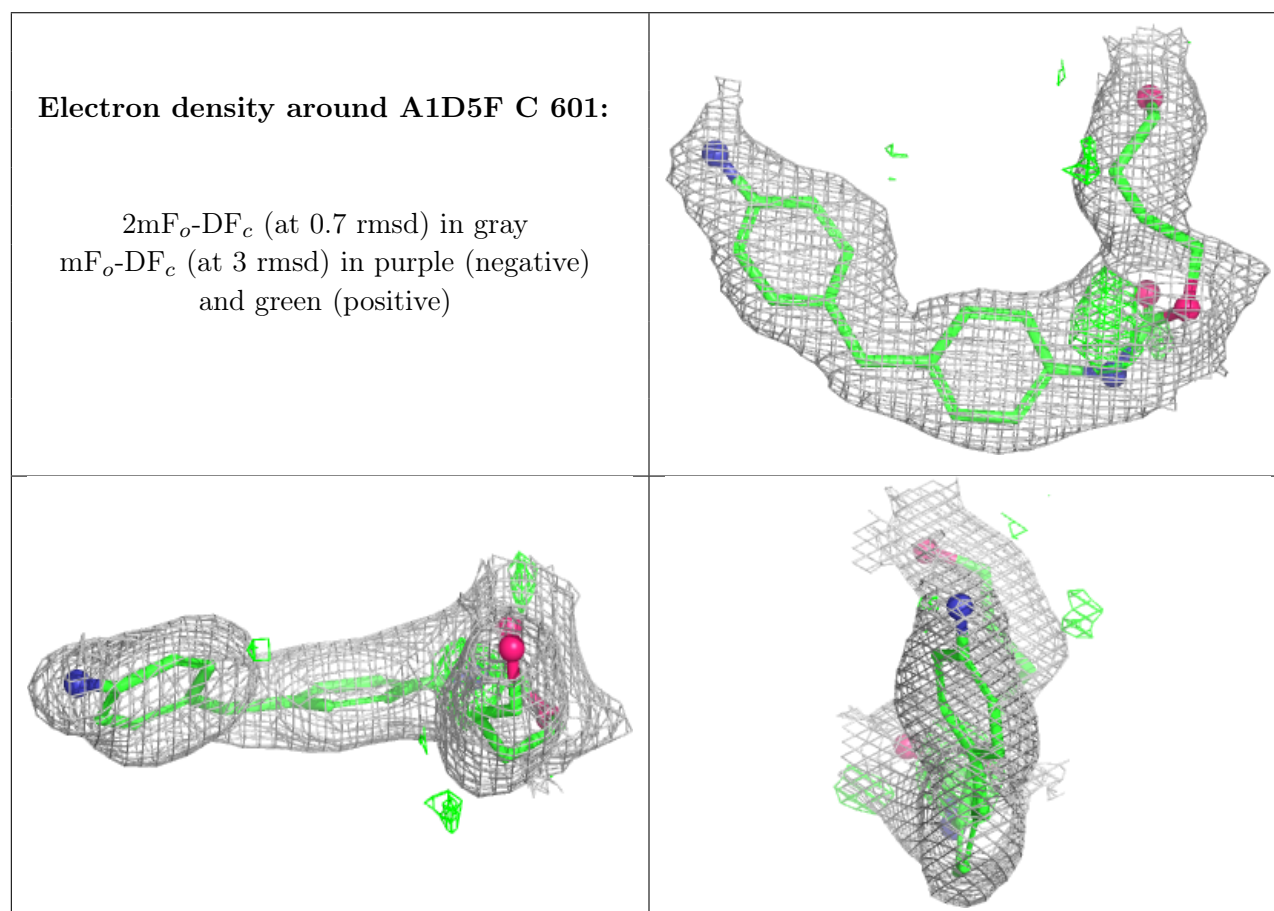
There are no oligosaccharides in this entry.

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	SO4	A	601	5/5	0.89	0.18	27,47,49,58	0
3	A1D5F	C	601	23/23	0.90	0.14	45,50,57,64	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.