



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:58 AM UTC

PDB ID : 7DPI / pdb_00007dpi
Title : Plasmodium falciparum cytoplasmic Phenylalanyl-tRNA synthetase in complex with BRD7929
Authors : Manmohan, S.; Malhotra, N.; Harlos, K.; Manickam, Y.; Sharma, A.
Deposited on : 2020-12-19
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

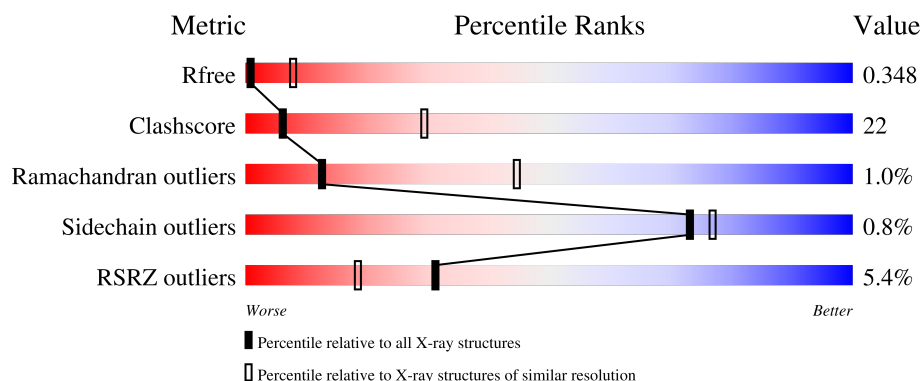
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	308	
1	C	308	
2	B	623	
2	D	623	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11773 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.

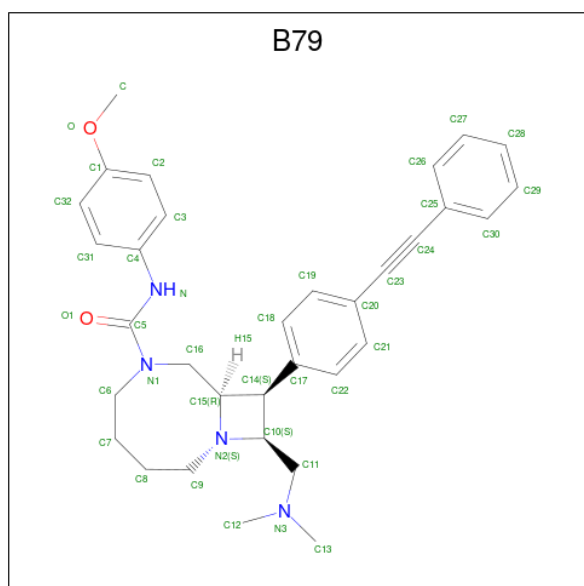
- Molecule 1 is a protein called Phenylalanine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2160	1395	356	399	10			
1	C	292	Total	C	N	O	S	0	0	0
			2161	1388	366	399	8			

- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	536	Total	C	N	O	S	0	0	0
			3776	2361	638	757	20			
2	D	522	Total	C	N	O	S	0	0	0
			3597	2243	615	721	18			

- Molecule 3 is (8R,9S,10S)-10-[(dimethylamino)methyl]-N-(4-methoxyphenyl)-9-[4-(2-phenylethynyl)phenyl]-1,6-diazabicyclo[6.2.0]decane-6-carboxamide (CCD ID: B79) (formula: $C_{33}H_{38}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			39	33	4	2		
3	C	1	Total	C	N	O	0	0
			39	33	4	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.65Å 108.03Å 140.53Å 90.00° 105.11° 90.00°	Depositor
Resolution (Å)	66.14 – 3.60 66.14 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (66.14-3.60) 98.8 (66.14-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.15RC1_3423	Depositor
R, R_{free}	0.294 , 0.330 0.313 , 0.348	Depositor DCC
R_{free} test set	2002 reflections (6.92%)	wwPDB-VP
Wilson B-factor (Å ²)	96.0	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 81.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.094 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.180 for h,-k,-h-l	Depositor
Outliers	1 of 28944 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	11773	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: B79, MG

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	0.69	6/2214 (0.3%)	0.80	6/3010 (0.2%)
1	C	0.65	5/2214 (0.2%)	0.79	4/3011 (0.1%)
2	B	0.53	2/3825 (0.1%)	0.77	7/5228 (0.1%)
2	D	0.61	4/3642 (0.1%)	0.77	6/4981 (0.1%)
All	All	0.61	17/11895 (0.1%)	0.78	23/16230 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	234	SER	CA-C	-8.66	1.42	1.52
1	A	389	HIS	C-O	-7.49	1.14	1.24
1	C	389	HIS	C-O	-7.43	1.17	1.24
2	D	364	ASP	CA-C	-6.32	1.44	1.52
1	A	380	ILE	CA-CB	-6.16	1.46	1.54
1	A	374	PHE	CA-C	-5.82	1.45	1.52
1	C	385	ARG	C-O	-5.61	1.17	1.24
2	D	41	LYS	CA-C	-5.56	1.46	1.52
1	C	388	THR	C-O	-5.55	1.16	1.24
1	C	545	VAL	C-O	-5.52	1.17	1.23
1	A	382	ASN	N-CA	-5.52	1.39	1.46
2	D	493	SER	C-O	-5.30	1.17	1.23
1	A	378	GLU	C-O	-5.28	1.17	1.23
1	A	374	PHE	C-O	-5.28	1.17	1.24
1	C	544	SER	C-O	-5.27	1.17	1.23
2	D	493	SER	CA-C	-5.27	1.46	1.52
2	B	234	SER	N-CA	-5.02	1.39	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	235	LEU	N-CA-C	-11.83	89.36	108.41
2	B	380	TYR	N-CA-C	11.23	126.52	110.23
2	D	545	GLU	N-CA-C	-10.58	91.04	108.49
2	D	360	MET	N-CA-C	9.37	121.09	111.07
2	D	39	GLU	N-CA-C	8.95	123.71	110.46
2	D	41	LYS	N-CA-C	-8.81	94.37	108.73
1	A	388	THR	N-CA-C	8.76	120.60	111.14
2	B	438	ASN	N-CA-C	-7.15	95.33	107.99
1	A	385	ARG	N-CA-C	-7.09	103.49	111.07
2	B	235	LEU	CA-C-N	6.78	134.49	121.54
2	B	235	LEU	C-N-CA	6.78	134.49	121.54
1	A	380	ILE	O-C-N	6.62	130.85	122.57
1	A	377	THR	N-CA-C	-6.36	102.62	111.52
1	C	398	ASN	N-CA-C	6.03	123.64	110.80
1	A	382	ASN	N-CA-C	-5.70	104.97	111.07
2	D	42	ASN	N-CA-C	5.66	122.85	110.80
1	A	387	HIS	N-CA-C	-5.53	104.89	111.03
1	C	386	VAL	N-CA-C	5.37	119.62	111.89
2	D	509	TYR	CA-CB-CG	5.32	123.48	113.90
1	C	543	VAL	CB-CA-C	-5.08	105.14	111.08
2	B	232	LYS	N-CA-C	-5.05	100.03	110.80
2	B	233	ILE	N-CA-C	-5.03	98.88	109.34
1	C	543	VAL	N-CA-C	5.01	115.96	108.54

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	2160	0	1922	118	0
1	C	2161	0	1911	88	0
2	B	3776	0	3207	144	0
2	D	3597	0	2984	164	0
3	A	39	0	0	2	0
3	C	39	0	0	2	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11773	0	10024	490	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 22.

All (490) 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:A:378:GLU:O	1:A:381:ASP:HB2	1.51	1.11
1:C:540:SER:HB2	1:C:543:VAL:HG23	1.33	1.07
1:C:390:GLY:HA3	1:C:395:PHE:HA	1.50	0.92
2:D:509:TYR:HB3	2:D:613:ASN:HA	1.51	0.91
1:C:411:LEU:HD13	1:C:448:PHE:HE2	1.37	0.87
2:D:462:ILE:HG21	2:D:493:SER:OG	1.74	0.87
1:C:424:PHE:O	1:C:427:ALA:HB3	1.77	0.85
2:B:6:VAL:HB	2:B:47:TYR:H	1.42	0.82
1:A:469:ILE:HG23	1:A:545:VAL:HG12	1.61	0.81
2:D:40:TYR:HD1	2:D:45:LYS:HA	1.46	0.81
2:B:493:SER:HB3	2:B:506:ASN:HD22	1.46	0.80
1:A:438:PRO:HA	1:A:469:ILE:O	1.81	0.80
2:B:597:VAL:HA	2:B:600:ASN:HD22	1.47	0.79
1:A:438:PRO:HB3	1:A:470:ASP:HB3	1.63	0.78
2:D:325:THR:HA	2:D:328:GLU:HG3	1.65	0.77
1:C:395:PHE:O	2:D:360:MET:CB	2.33	0.77
1:C:373:LYS:HB2	1:C:380:ILE:HD11	1.66	0.76
2:D:362:CYS:HB2	2:D:365:ILE:HD12	1.68	0.76
2:B:22:GLU:O	2:B:26:ASP:HB2	1.86	0.75
2:B:512:ILE:HG12	2:B:610:ILE:HG12	1.68	0.75
2:B:258:ILE:O	2:B:262:MET:CB	2.36	0.73
1:A:388:THR:HG22	1:A:399:TYR:O	1.88	0.73
2:B:547:LYS:O	2:B:551:ASN:N	2.20	0.73
2:D:412:THR:N	2:D:488:GLU:OE1	2.21	0.73
2:D:570:PHE:HB2	2:D:575:ILE:HD12	1.69	0.72
1:C:310:HIS:HB3	1:C:313:THR:HG22	1.71	0.72
2:B:389:HIS:ND1	2:B:389:HIS:O	2.22	0.72
1:A:468:ILE:HG22	1:A:546:ILE:HG12	1.72	0.71
2:D:402:LEU:HD21	2:D:532:ILE:HD11	1.70	0.71
1:C:291:ASP:HB3	2:D:573:GLU:HB3	1.72	0.71
1:C:486:TYR:HD2	1:C:491:ILE:HD11	1.54	0.71
1:A:529:PHE:HA	1:A:530:ARG:HH21	1.55	0.71
2:B:613:ASN:OD1	2:B:614:VAL:N	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:ASN:ND2	2:B:302:ILE:O	2.21	0.71
1:A:424:PHE:O	1:A:427:ALA:HB3	1.90	0.71
2:B:264:SER:HB3	2:B:271:TYR:HA	1.72	0.70
1:C:535:ARG:NH2	1:C:541:GLU:O	2.25	0.70
1:A:352:GLN:O	1:A:353:HIS:ND1	2.25	0.70
1:A:409:ASN:ND2	2:D:502:THR:OG1	2.23	0.70
1:A:378:GLU:O	1:A:381:ASP:CB	2.34	0.70
2:D:479:HIS:O	2:D:479:HIS:ND1	2.25	0.70
1:C:335:ASN:O	1:C:412:ARG:NH1	2.26	0.69
2:D:121:ASN:O	2:D:125:TYR:N	2.25	0.69
2:D:434:ASP:O	2:D:437:ILE:N	2.25	0.69
1:A:409:ASN:HD21	2:D:502:THR:HG1	1.41	0.69
1:A:486:TYR:HE2	1:A:523:VAL:HG22	1.58	0.68
1:C:382:ASN:O	1:C:386:VAL:HG23	1.93	0.68
1:C:416:THR:O	1:C:419:SER:HB2	1.94	0.68
1:A:384:LYS:O	1:A:388:THR:HG23	1.93	0.68
2:B:489:ILE:HD13	2:B:510:LEU:HD13	1.75	0.68
2:D:509:TYR:HA	2:D:614:VAL:HG12	1.75	0.68
2:D:152:ASP:HA	2:D:240:VAL:HA	1.77	0.67
1:C:394:SER:HB3	2:D:361:HIS:HA	1.75	0.67
2:B:153:TYR:HA	2:B:156:ILE:HD13	1.75	0.67
1:A:304:ILE:HG22	1:A:305:ASN:H	1.60	0.67
1:C:335:ASN:ND2	1:C:418:ASN:OD1	2.27	0.67
2:D:308:LEU:HD13	2:D:362:CYS:CA	2.25	0.67
1:A:370:CYS:HB3	2:D:502:THR:HA	1.77	0.66
1:A:565:ILE:HG13	1:A:568:LEU:HD21	1.78	0.66
1:A:530:ARG:HD3	1:A:530:ARG:N	2.10	0.66
1:C:540:SER:HB2	1:C:543:VAL:CG2	2.19	0.66
2:D:308:LEU:HD13	2:D:362:CYS:HA	1.78	0.66
1:C:353:HIS:CG	1:C:354:PRO:HD2	2.31	0.66
2:B:309:THR:HG22	2:B:349:LYS:HG2	1.77	0.66
1:A:412:ARG:NH1	1:A:418:ASN:OD1	2.29	0.65
2:D:448:PRO:HG3	2:D:464:THR:HG21	1.78	0.65
2:B:519:THR:OG1	2:B:520:ALA:N	2.28	0.65
2:B:496:THR:HG21	2:B:505:VAL:HB	1.78	0.65
1:A:486:TYR:O	1:A:492:HIS:NE2	2.29	0.65
2:D:361:HIS:C	2:D:363:CYS:H	2.05	0.64
1:C:496:PHE:HD2	1:C:510:ILE:HG22	1.63	0.64
1:C:387:HIS:ND1	1:C:401:TRP:CD1	2.66	0.64
2:D:581:PHE:HB3	2:D:583:HIS:H	1.61	0.64
1:A:282:LEU:HD22	2:B:595:PRO:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:TYR:CE2	2:B:485:ARG:HB3	2.32	0.64
1:C:394:SER:CB	2:D:361:HIS:HA	2.28	0.63
2:B:15:LEU:HD21	2:B:65:CYS:HB2	1.81	0.63
2:D:308:LEU:HD13	2:D:362:CYS:CB	2.29	0.63
1:A:525:ASN:OD1	1:A:526:SER:N	2.29	0.62
2:B:255:ALA:HA	2:B:258:ILE:HG12	1.80	0.62
1:A:539:PHE:HB3	1:A:543:VAL:HG11	1.81	0.62
1:C:438:PRO:HB3	1:C:470:ASP:HB3	1.81	0.62
2:D:175:LEU:O	2:D:230:HIS:N	2.33	0.62
1:A:380:ILE:O	1:A:380:ILE:HG22	1.99	0.61
2:D:540:SER:OG	2:D:541:ASP:N	2.34	0.61
2:B:448:PRO:HB3	2:B:464:THR:HG21	1.83	0.61
1:C:531:PRO:HB3	1:C:535:ARG:HH11	1.65	0.60
1:A:454:ASP:OD1	1:A:456:THR:OG1	2.20	0.60
1:C:470:ASP:OD1	1:C:470:ASP:N	2.33	0.60
2:D:434:ASP:OD1	2:D:434:ASP:N	2.34	0.60
1:A:335:ASN:O	1:A:412:ARG:NH1	2.35	0.60
1:A:362:PHE:CZ	1:A:450:ASN:HB2	2.37	0.60
2:D:613:ASN:OD1	2:D:614:VAL:N	2.35	0.60
1:A:378:GLU:CB	1:A:381:ASP:HB2	2.32	0.59
2:B:4:ILE:O	2:B:48:LYS:HA	2.02	0.59
2:B:425:MET:HB2	2:B:427:ARG:HG2	1.83	0.59
1:C:411:LEU:HD13	1:C:448:PHE:CE2	2.29	0.59
1:A:412:ARG:HG3	1:A:447:VAL:HG13	1.85	0.59
2:B:538:LEU:HB3	2:B:560:TYR:HD1	1.66	0.59
2:D:487:PHE:HB3	2:D:512:ILE:HG23	1.85	0.59
1:C:564:ASN:O	1:C:564:ASN:ND2	2.36	0.59
2:B:309:THR:HA	2:B:348:PHE:O	2.02	0.59
2:D:543:LYS:HD3	2:D:543:LYS:C	2.27	0.59
1:C:370:CYS:C	1:C:371:ILE:HD12	2.28	0.58
1:C:390:GLY:HA3	1:C:395:PHE:CA	2.28	0.58
2:B:76:ASP:OD1	2:B:76:ASP:N	2.36	0.58
2:D:2:PRO:HB2	2:D:50:GLU:O	2.02	0.58
2:D:115:LEU:HA	2:D:273:ILE:HG13	1.86	0.58
2:B:182:ASN:OD1	2:B:183:GLY:N	2.37	0.58
2:B:467:ILE:HA	2:B:470:LEU:HD13	1.86	0.58
2:D:401:VAL:HG21	2:D:535:GLU:HG2	1.84	0.58
2:D:509:TYR:CB	2:D:613:ASN:HA	2.31	0.58
1:C:487:LYS:HA	1:C:491:ILE:O	2.03	0.58
2:B:131:ILE:O	2:B:135:LEU:HB3	2.04	0.58
2:B:362:CYS:HA	2:B:365:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:MET:N	2:D:238:LYS:O	2.37	0.58
2:B:429:HIS:HB2	2:B:448:PRO:HD3	1.86	0.58
2:B:324:ILE:HG21	2:B:327:HIS:HB2	1.85	0.58
2:B:426:LEU:HD12	2:B:568:PRO:HB2	1.86	0.58
2:D:492:VAL:O	2:D:506:ASN:HA	2.04	0.58
1:C:540:SER:CB	1:C:543:VAL:HG23	2.21	0.57
2:B:538:LEU:HB3	2:B:560:TYR:CD1	2.38	0.57
2:D:338:LEU:O	2:D:351:THR:OG1	2.20	0.57
1:C:362:PHE:HB3	1:C:411:LEU:HB2	1.86	0.57
1:C:386:VAL:HG12	1:C:386:VAL:O	2.02	0.57
2:D:335:ARG:HH12	2:D:371:ILE:HD12	1.68	0.57
1:A:487:LYS:HA	1:A:490:GLY:O	2.05	0.57
2:B:421:ASN:O	2:B:427:ARG:HG3	2.04	0.57
1:C:533:MET:O	1:C:536:SER:OG	2.23	0.57
2:B:472:LYS:O	2:B:475:SER:OG	2.23	0.57
2:D:521:GLY:O	2:D:525:LEU:N	2.27	0.56
1:A:531:PRO:HA	1:A:534:LEU:HB2	1.87	0.56
2:B:419:ASP:HB3	2:B:423:ASN:HB3	1.86	0.56
2:B:516:ASP:OD1	2:B:517:LYS:N	2.39	0.56
1:C:486:TYR:CD2	1:C:491:ILE:HD11	2.38	0.56
2:B:6:VAL:N	2:B:47:TYR:O	2.36	0.56
2:D:489:ILE:HG23	2:D:510:LEU:HB3	1.88	0.56
2:D:573:GLU:O	2:D:574:ARG:HD3	2.04	0.56
2:B:422:TYR:HA	2:B:427:ARG:HB2	1.86	0.56
2:B:540:SER:O	2:B:542:TYR:N	2.38	0.56
2:D:326:VAL:O	2:D:329:VAL:HG12	2.06	0.56
2:D:332:LEU:HB3	2:D:337:MET:HB2	1.86	0.56
1:A:414:HIS:HB3	1:A:416:THR:HG22	1.86	0.56
1:A:362:PHE:HE1	2:D:454:SER:HA	1.70	0.56
1:A:440:LYS:HG2	1:A:468:ILE:HG13	1.87	0.56
2:D:120:ILE:HD11	2:D:236:ASN:H	1.71	0.56
2:D:325:THR:HB	2:D:348:PHE:CZ	2.40	0.56
2:B:267:CYS:SG	2:B:270:LYS:N	2.79	0.56
1:A:503:TYR:O	1:A:530:ARG:HD2	2.05	0.56
2:D:543:LYS:HG3	2:D:546:GLU:HG2	1.88	0.56
1:A:564:ASN:OD1	1:A:565:ILE:N	2.38	0.55
2:D:614:VAL:O	2:D:617:LEU:N	2.32	0.55
2:D:364:ASP:O	2:D:367:GLU:N	2.38	0.55
1:A:348:TYR:HE1	1:A:386:VAL:HG12	1.70	0.55
2:B:334:LYS:HE2	2:B:372:ALA:HB1	1.88	0.55
1:A:467:LEU:HA	1:A:546:ILE:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:398:PHE:O	2:D:402:LEU:N	2.36	0.55
1:A:340:SER:O	1:A:344:PHE:N	2.26	0.55
1:A:553:GLU:O	1:A:556:THR:N	2.39	0.55
2:D:335:ARG:NH1	2:D:371:ILE:HD12	2.22	0.55
1:C:300:SER:OG	1:C:301:GLY:N	2.41	0.54
1:A:380:ILE:C	1:A:382:ASN:N	2.64	0.54
1:C:531:PRO:HA	1:C:534:LEU:HB3	1.90	0.54
1:A:470:ASP:OD1	1:A:470:ASP:N	2.39	0.54
2:B:540:SER:C	2:B:542:TYR:H	2.15	0.54
1:C:473:ILE:H	1:C:544:SER:HB3	1.73	0.54
2:D:364:ASP:O	2:D:367:GLU:HB3	2.07	0.54
2:B:471:LEU:O	2:B:474:VAL:HG12	2.08	0.54
2:D:44:LYS:O	2:D:46:ILE:HG23	2.07	0.54
2:B:434:ASP:O	2:B:436:ASN:N	2.41	0.54
2:B:572:ASN:OD1	2:B:572:ASN:N	2.40	0.54
1:C:387:HIS:ND1	1:C:401:TRP:HD1	2.05	0.53
2:D:315:VAL:HG13	2:D:366:ILE:HG12	1.89	0.53
2:D:415:LEU:HB2	2:D:461:ILE:O	2.08	0.53
2:D:316:ARG:HD3	2:D:322:SER:HA	1.90	0.53
2:D:594:HIS:ND1	2:D:595:PRO:HD2	2.24	0.53
2:D:4:ILE:HA	2:D:49:ILE:O	2.08	0.53
2:D:316:ARG:HD3	2:D:321:ILE:O	2.08	0.53
2:D:490:GLY:O	2:D:508:LYS:HA	2.08	0.53
1:A:331:MET:HG3	1:A:443:SER:HB3	1.89	0.53
1:A:539:PHE:O	1:A:540:SER:OG	2.23	0.53
1:A:507:SER:HA	1:A:527:GLY:HA2	1.91	0.53
1:C:414:HIS:HB3	1:C:416:THR:HG22	1.91	0.53
2:B:342:ILE:O	2:B:344:ASP:N	2.42	0.53
2:D:308:LEU:HD22	2:D:362:CYS:HB3	1.91	0.52
2:D:580:LEU:O	2:D:581:PHE:HB2	2.08	0.52
1:C:491:ILE:HG22	1:C:514:HIS:CD2	2.43	0.52
2:D:515:SER:HB2	2:D:607:VAL:HG12	1.90	0.52
2:B:254:ILE:O	2:B:258:ILE:HG23	2.08	0.52
2:D:534:LYS:HA	2:D:538:LEU:HA	1.91	0.52
1:A:317:ARG:O	1:A:321:GLU:HG2	2.10	0.52
1:C:439:LYS:HD3	1:C:441:TYR:HE1	1.75	0.52
1:C:504:THR:OG1	1:C:528:ILE:O	2.24	0.52
2:D:519:THR:OG1	2:D:520:ALA:O	2.26	0.52
1:A:374:PHE:C	1:A:376:ASP:H	2.17	0.52
2:D:2:PRO:HB3	2:D:51:VAL:O	2.10	0.51
2:B:177:GLU:OE1	2:B:177:GLU:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:TYR:CD2	2:B:485:ARG:HB3	2.45	0.51
2:D:273:ILE:HG12	2:D:274:GLN:O	2.10	0.51
2:D:391:LEU:HG	2:D:392:ASN:H	1.76	0.51
1:C:317:ARG:O	1:C:321:GLU:HG2	2.11	0.51
1:C:504:THR:OG1	1:C:528:ILE:N	2.42	0.51
2:B:501:ASP:OD1	2:B:502:THR:N	2.44	0.51
1:A:412:ARG:NH2	1:A:445:ASP:HB3	2.26	0.51
1:C:526:SER:HA	1:C:548:TRP:HA	1.93	0.51
2:D:115:LEU:HA	2:D:274:GLN:H	1.76	0.51
1:A:475:LEU:O	1:A:478:LEU:N	2.44	0.51
2:B:571:LEU:N	2:B:592:ILE:O	2.38	0.51
1:C:328:PHE:HB3	1:C:442:PHE:HD2	1.76	0.50
1:C:411:LEU:HD11	2:B:451:ILE:HD11	1.93	0.50
2:B:312:ILE:O	2:B:315:VAL:HG22	2.11	0.50
2:B:487:PHE:HB2	2:B:512:ILE:HG22	1.92	0.50
2:D:491:ASP:OD1	2:D:506:ASN:HB3	2.11	0.50
2:B:274:GLN:O	2:B:276:PHE:N	2.43	0.50
1:A:338:GLU:HG3	1:A:342:TRP:HB2	1.92	0.50
2:D:9:ASP:O	2:D:11:LEU:N	2.45	0.50
2:D:233:ILE:O	2:D:234:SER:OG	2.23	0.50
2:D:578:ILE:N	2:D:588:GLY:O	2.37	0.50
2:D:581:PHE:HD2	2:D:583:HIS:HB2	1.76	0.50
1:C:362:PHE:O	1:C:410:VAL:HG22	2.11	0.50
2:B:498:ASN:O	2:B:500:THR:N	2.45	0.50
2:D:572:ASN:OD1	2:D:572:ASN:N	2.42	0.50
1:C:515:GLU:CD	1:C:515:GLU:H	2.20	0.50
2:B:174:PRO:HA	2:B:229:ASP:HA	1.93	0.50
1:C:349:ILE:HD11	1:C:503:TYR:HD1	1.76	0.50
2:B:417:SER:HB2	2:B:420:GLU:HB2	1.93	0.50
2:B:431:SER:OG	2:B:434:ASP:OD1	2.28	0.50
1:A:430:TYR:O	1:A:434:GLY:N	2.41	0.50
1:C:317:ARG:HG3	1:C:321:GLU:OE2	2.11	0.50
2:B:311:ASN:N	2:B:311:ASN:OD1	2.44	0.50
2:B:498:ASN:CG	2:B:499:GLN:H	2.20	0.50
2:D:417:SER:OG	2:D:420:GLU:HB2	2.12	0.50
2:B:578:ILE:HD12	2:B:588:GLY:HA3	1.94	0.49
1:A:310:HIS:O	1:A:313:THR:OG1	2.25	0.49
2:B:274:GLN:C	2:B:276:PHE:H	2.20	0.49
2:B:223:PRO:HG2	2:B:224:PRO:HD3	1.93	0.49
2:B:539:PHE:O	2:B:541:ASP:N	2.45	0.49
1:A:430:TYR:OH	1:A:437:LYS:O	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:SER:OG	1:A:508:MET:N	2.45	0.49
2:B:509:TYR:HD1	2:B:613:ASN:HA	1.77	0.49
2:B:373:TYR:HD2	2:B:373:TYR:O	1.96	0.49
2:D:72:MET:O	2:D:74:LYS:N	2.41	0.49
1:A:394:SER:HB2	2:B:361:HIS:HB2	1.94	0.49
2:B:258:ILE:HG13	2:B:259:LEU:N	2.26	0.49
1:A:374:PHE:C	1:A:376:ASP:N	2.70	0.49
1:C:353:HIS:CD2	1:C:354:PRO:HD2	2.48	0.49
2:D:604:ASP:N	2:D:604:ASP:OD1	2.46	0.49
2:D:40:TYR:CD1	2:D:45:LYS:HA	2.37	0.49
2:D:418:ARG:HG3	2:D:419:ASP:H	1.78	0.49
1:A:557:MET:SD	1:A:565:ILE:HB	2.53	0.48
2:B:6:VAL:HG21	2:B:47:TYR:HD1	1.78	0.48
2:D:520:ALA:HB1	2:D:608:SER:HB3	1.95	0.48
1:A:458:LEU:HD12	1:A:459:ALA:H	1.78	0.48
1:C:375:VAL:HG22	1:C:380:ILE:HD12	1.95	0.48
1:A:315:GLN:HA	1:A:315:GLN:OE1	2.13	0.48
2:B:517:LYS:O	2:B:517:LYS:HD3	2.13	0.48
1:C:475:LEU:O	1:C:478:LEU:N	2.47	0.48
2:D:324:ILE:O	2:D:325:THR:OG1	2.29	0.48
1:A:560:TYR:CG	1:A:560:TYR:O	2.67	0.48
2:D:579:VAL:HG23	2:D:585:LEU:C	2.39	0.48
2:B:467:ILE:O	2:B:470:LEU:HB2	2.13	0.48
1:A:352:GLN:H	1:A:352:GLN:CD	2.20	0.48
1:C:510:ILE:HD12	1:C:510:ILE:O	2.13	0.48
2:B:596:LYS:NZ	2:B:600:ASN:OD1	2.47	0.48
2:D:434:ASP:O	2:D:435:PRO:C	2.57	0.48
1:A:446:ARG:HH11	1:A:460:GLU:HG3	1.79	0.48
2:D:361:HIS:C	2:D:363:CYS:N	2.72	0.48
2:D:540:SER:HA	2:D:560:TYR:CE1	2.49	0.48
1:A:380:ILE:C	1:A:382:ASN:H	2.22	0.47
2:B:492:VAL:O	2:B:506:ASN:HA	2.14	0.47
1:A:442:PHE:HA	1:A:465:GLU:O	2.14	0.47
2:B:489:ILE:CD1	2:B:510:LEU:HD13	2.44	0.47
2:D:421:ASN:OD1	2:D:468:VAL:HG11	2.14	0.47
2:B:488:GLU:O	2:B:510:LEU:HA	2.14	0.47
1:C:286:GLU:N	1:C:286:GLU:OE1	2.48	0.47
2:B:509:TYR:HE1	2:B:613:ASN:ND2	2.13	0.47
2:D:470:LEU:O	2:D:474:VAL:HG23	2.14	0.47
2:D:570:PHE:CD2	2:D:591:GLY:HA3	2.49	0.47
2:D:534:LYS:HA	2:D:538:LEU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:471:LEU:O	2:D:475:SER:N	2.42	0.47
1:A:348:TYR:HB2	1:A:533:MET:HB3	1.96	0.47
1:A:385:ARG:O	1:A:389:HIS:N	2.38	0.47
2:B:400:ASN:O	2:B:404:GLU:HG3	2.15	0.47
2:B:513:ILE:HG22	2:B:609:ALA:CB	2.45	0.47
2:D:464:THR:O	2:D:509:TYR:OH	2.25	0.47
2:D:538:LEU:HD23	2:D:538:LEU:O	2.14	0.47
1:A:331:MET:CG	1:A:443:SER:HB3	2.44	0.47
1:C:328:PHE:HB3	1:C:442:PHE:CD2	2.49	0.47
2:B:316:ARG:HB3	2:B:322:SER:HB3	1.97	0.47
2:B:509:TYR:CD1	2:B:613:ASN:HA	2.50	0.47
2:B:35:VAL:HG11	2:B:48:LYS:O	2.15	0.47
2:D:424:CYS:O	2:D:597:VAL:HG23	2.15	0.47
1:A:464:VAL:HG22	1:A:550:LEU:HG	1.96	0.46
2:B:418:ARG:HG3	2:B:460:GLU:HB3	1.96	0.46
2:B:451:ILE:HG23	2:B:452:LYS:O	2.15	0.46
2:B:594:HIS:CG	2:B:595:PRO:HD2	2.50	0.46
2:D:308:LEU:CD1	2:D:362:CYS:HA	2.45	0.46
1:A:387:HIS:O	1:A:396:GLY:HA3	2.15	0.46
2:B:429:HIS:O	2:B:446:ALA:HB1	2.15	0.46
2:D:8:GLU:H	2:D:8:GLU:CD	2.23	0.46
2:D:579:VAL:HA	2:D:586:LYS:HA	1.98	0.46
1:A:333:THR:HG23	1:A:445:ASP:HB2	1.98	0.46
1:A:340:SER:OG	1:A:406:SER:O	2.33	0.46
1:C:560:TYR:CG	1:C:560:TYR:O	2.68	0.46
2:D:51:VAL:O	2:D:51:VAL:HG12	2.16	0.46
1:C:309:ILE:HG22	1:C:310:HIS:O	2.16	0.46
2:B:440:ASP:HB3	2:B:443:ASN:CB	2.45	0.46
2:D:125:TYR:O	2:D:129:ILE:HG13	2.15	0.46
2:D:412:THR:OG1	2:D:413:ASN:N	2.45	0.46
1:C:365:LYS:HA	1:C:368:GLU:HB3	1.97	0.46
2:B:412:THR:HG21	2:B:470:LEU:HD12	1.97	0.46
2:D:543:LYS:HG3	2:D:546:GLU:CG	2.46	0.46
1:A:420:CYS:O	1:A:423:LEU:HB2	2.16	0.45
1:C:550:LEU:HA	3:C:701:B79:C21	2.47	0.45
2:B:425:MET:HB2	2:B:427:ARG:CG	2.46	0.45
1:A:363:PHE:O	2:D:452:LYS:HG2	2.15	0.45
1:C:529:PHE:HB3	1:C:533:MET:HE1	1.98	0.45
1:C:535:ARG:HE	1:C:541:GLU:HA	1.81	0.45
2:B:253:GLN:O	2:B:257:ASN:ND2	2.50	0.45
1:A:552:LEU:O	1:A:555:PRO:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:ASN:OD1	2:B:176:ASN:N	2.49	0.45
2:D:521:GLY:N	2:D:608:SER:OG	2.36	0.45
1:C:371:ILE:HG22	1:C:372:ASP:N	2.31	0.45
2:D:54:ASN:HB3	2:D:357:SER:HB2	1.98	0.45
2:D:501:ASP:OD1	2:D:502:THR:N	2.50	0.45
2:D:509:TYR:HB2	2:D:612:ILE:O	2.16	0.45
1:A:380:ILE:HG21	1:A:383:ILE:HD12	1.98	0.45
1:A:523:VAL:HG23	3:A:701:B79:C32	2.47	0.45
1:A:531:PRO:HD2	2:B:363:CYS:SG	2.56	0.45
2:B:7:TYR:HA	2:B:44:LYS:HD3	1.98	0.45
2:D:490:GLY:O	2:D:508:LYS:CB	2.64	0.45
2:D:399:ARG:O	2:D:403:VAL:HG23	2.17	0.45
1:A:492:HIS:HB3	1:A:513:TYR:O	2.17	0.45
1:C:373:LYS:O	1:C:375:VAL:N	2.49	0.45
1:C:394:SER:HB3	2:D:361:HIS:CA	2.43	0.45
2:B:28:CYS:HB3	2:B:33:LEU:CD1	2.46	0.44
2:D:13:GLU:O	2:D:16:GLY:N	2.50	0.44
2:B:498:ASN:C	2:B:500:THR:H	2.25	0.44
2:B:540:SER:O	2:B:540:SER:OG	2.20	0.44
2:B:571:LEU:HD12	2:B:594:HIS:CE1	2.53	0.44
2:D:412:THR:HB	2:D:488:GLU:OE2	2.17	0.44
2:B:151:HIS:HA	2:B:241:PHE:O	2.17	0.44
2:D:490:GLY:O	2:D:508:LYS:CA	2.65	0.44
1:A:394:SER:CB	2:B:361:HIS:HB2	2.48	0.44
2:D:126:ASN:OD1	2:D:127:ASN:N	2.50	0.44
1:A:463:GLN:HA	1:A:550:LEU:O	2.17	0.44
2:B:442:TYR:HB2	2:B:585:LEU:HD21	1.99	0.44
2:D:115:LEU:CA	2:D:273:ILE:HG13	2.47	0.44
2:D:318:LEU:C	2:D:318:LEU:HD12	2.43	0.44
2:D:393:ASN:N	2:D:393:ASN:OD1	2.51	0.44
2:D:492:VAL:HG21	2:D:509:TYR:CE2	2.53	0.44
1:A:319:PHE:HD1	1:A:464:VAL:HG11	1.82	0.44
1:C:531:PRO:HD2	2:D:361:HIS:HD2	1.83	0.44
2:D:564:PRO:HA	2:D:576:VAL:HG12	1.99	0.44
2:D:11:LEU:O	2:D:15:LEU:HG	2.18	0.44
1:A:312:LEU:HD21	1:A:568:LEU:HD12	1.99	0.44
1:A:505:GLU:HB3	2:B:364:ASP:OD1	2.17	0.43
2:B:263:LEU:O	2:B:266:TYR:N	2.49	0.43
2:D:402:LEU:HD23	2:D:402:LEU:HA	1.78	0.43
1:A:351:GLN:HG2	1:A:352:GLN:OE1	2.18	0.43
1:A:364:ILE:HG21	2:D:449:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:ILE:HA	2:B:451:ILE:HD12	1.99	0.43
2:B:431:SER:O	2:B:434:ASP:N	2.51	0.43
1:A:511:TYR:HB2	1:A:521:LEU:O	2.18	0.43
2:B:33:LEU:HD12	2:B:33:LEU:O	2.19	0.43
2:D:391:LEU:HG	2:D:392:ASN:N	2.33	0.43
2:B:538:LEU:HA	2:B:559:TYR:HB3	2.01	0.43
1:A:362:PHE:CE1	1:A:450:ASN:HB2	2.52	0.43
1:A:420:CYS:HA	1:A:423:LEU:HG	2.01	0.43
1:C:444:ILE:HD11	1:C:552:LEU:HD22	2.00	0.43
2:B:180:ASN:OD1	2:B:180:ASN:N	2.52	0.43
2:B:354:PHE:C	2:B:356:ARG:H	2.25	0.43
2:B:478:LYS:NZ	2:B:602:SER:O	2.34	0.43
2:B:538:LEU:HA	2:B:559:TYR:CG	2.53	0.43
2:D:127:ASN:O	2:D:131:ILE:HG13	2.19	0.43
2:D:477:ASN:OD1	2:D:477:ASN:N	2.50	0.43
2:D:544:ILE:HB	2:D:545:GLU:H	1.32	0.43
1:A:348:TYR:CE1	1:A:386:VAL:HG12	2.53	0.43
1:C:498:PRO:HB3	2:D:375:TYR:CE2	2.53	0.43
2:B:367:GLU:O	2:B:371:ILE:HG13	2.18	0.43
2:B:392:ASN:O	2:B:392:ASN:ND2	2.37	0.43
2:D:533:LEU:O	2:D:538:LEU:N	2.51	0.43
2:B:43:ASP:OD1	2:B:43:ASP:N	2.51	0.43
2:B:388:LYS:H	2:B:388:LYS:HG2	1.49	0.43
2:D:39:GLU:O	2:D:46:ILE:HG12	2.19	0.43
1:A:441:TYR:HB2	1:A:467:LEU:HG	2.01	0.43
1:A:485:PHE:O	1:A:488:HIS:N	2.52	0.43
1:C:412:ARG:HB3	1:C:447:VAL:HG13	2.00	0.43
2:D:332:LEU:HB3	2:D:337:MET:O	2.18	0.43
1:C:287:TYR:N	1:C:287:TYR:CD2	2.87	0.43
1:C:533:MET:HE3	1:C:533:MET:HB3	1.84	0.43
2:B:138:ASN:OD1	2:B:138:ASN:N	2.51	0.43
2:B:263:LEU:C	2:B:265:GLU:N	2.77	0.43
2:B:483:PRO:HA	2:B:515:SER:O	2.19	0.43
2:B:594:HIS:CD2	2:B:595:PRO:HD2	2.54	0.43
2:D:153:TYR:HB3	2:D:239:ASN:CB	2.49	0.42
2:D:491:ASP:HA	2:D:508:LYS:HA	1.99	0.42
1:A:352:GLN:OE1	1:A:352:GLN:N	2.39	0.42
1:A:372:ASP:OD1	2:D:501:ASP:HA	2.18	0.42
1:A:386:VAL:HG22	1:A:391:ASP:HB3	2.01	0.42
1:C:339:SER:HA	1:C:409:ASN:HA	2.01	0.42
1:C:387:HIS:HA	1:C:397:TRP:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:CYS:O	1:C:423:LEU:HB2	2.19	0.42
2:B:528:VAL:O	2:B:532:ILE:HG13	2.19	0.42
2:D:543:LYS:HD2	2:D:546:GLU:HB3	2.01	0.42
2:D:581:PHE:CD1	2:D:582:PRO:HD2	2.54	0.42
1:C:400:LYS:O	1:C:402:LYS:N	2.51	0.42
2:B:488:GLU:O	2:B:510:LEU:HD12	2.19	0.42
2:D:64:LEU:O	2:D:68:LEU:HG	2.18	0.42
1:A:306:LYS:NZ	1:A:308:ASN:HB3	2.33	0.42
1:A:362:PHE:CE1	2:D:454:SER:HA	2.51	0.42
1:C:283:LYS:O	1:C:285:GLU:N	2.52	0.42
2:B:315:VAL:HG12	2:B:366:ILE:CD1	2.50	0.42
2:D:362:CYS:O	2:D:362:CYS:SG	2.75	0.42
2:D:535:GLU:O	2:D:536:TYR:HD1	2.02	0.42
1:A:484:ALA:O	1:A:487:LYS:HB3	2.19	0.42
1:A:461:PHE:HB2	1:A:553:GLU:OE1	2.20	0.42
1:A:568:LEU:H	1:A:568:LEU:HD23	1.84	0.42
2:B:223:PRO:CG	2:B:224:PRO:HD3	2.50	0.42
2:B:253:GLN:H	2:B:253:GLN:CD	2.27	0.42
2:B:315:VAL:HG12	2:B:366:ILE:HD11	2.00	0.42
2:B:540:SER:C	2:B:542:TYR:N	2.78	0.42
2:D:312:ILE:HD13	2:D:312:ILE:HA	1.76	0.42
2:D:581:PHE:HD2	2:D:583:HIS:CB	2.32	0.42
2:D:9:ASP:O	2:D:11:LEU:HG	2.19	0.42
1:A:314:LYS:HA	1:A:317:ARG:HD2	2.02	0.42
2:B:186:LEU:HD12	2:B:186:LEU:HA	1.86	0.42
1:A:539:PHE:CB	1:A:543:VAL:HG11	2.48	0.42
1:C:411:LEU:HD23	1:C:411:LEU:HA	1.84	0.42
1:A:453:LEU:HA	1:A:453:LEU:HD23	1.72	0.41
1:C:283:LYS:H	1:C:283:LYS:HG3	1.57	0.41
1:C:504:THR:HG23	1:C:507:SER:HB3	2.02	0.41
2:B:35:VAL:HG21	2:B:49:ILE:HA	2.01	0.41
2:B:112:CYS:CB	2:B:243:GLU:HB2	2.49	0.41
1:A:514:HIS:O	1:A:514:HIS:ND1	2.53	0.41
1:C:385:ARG:O	1:C:389:HIS:N	2.52	0.41
2:B:50:GLU:H	2:B:50:GLU:HG2	1.65	0.41
1:C:485:PHE:O	1:C:488:HIS:N	2.52	0.41
1:A:446:ARG:HD2	1:A:448:PHE:HE1	1.85	0.41
2:B:433:ASP:N	2:B:433:ASP:OD1	2.53	0.41
2:D:450:GLN:C	2:D:451:ILE:HD12	2.44	0.41
2:D:516:ASP:C	2:D:518:PHE:H	2.29	0.41
1:A:475:LEU:N	2:B:318:LEU:O	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:VAL:HG12	2:B:8:GLU:N	2.36	0.41
2:B:35:VAL:HG13	2:B:36:ASP:O	2.19	0.41
2:B:438:ASN:OD1	2:B:438:ASN:N	2.53	0.41
2:D:496:THR:HG22	2:D:498:ASN:O	2.20	0.41
1:A:371:ILE:HG23	1:A:372:ASP:OD1	2.21	0.41
1:A:561:ASN:O	1:A:562:ILE:HD13	2.21	0.41
1:C:535:ARG:HH21	1:C:541:GLU:CA	2.34	0.41
2:D:462:ILE:HG23	2:D:463:ARG:O	2.20	0.41
1:C:368:GLU:H	1:C:368:GLU:HG2	1.63	0.41
1:C:457:HIS:ND1	1:C:554:ARG:NH1	2.69	0.41
1:A:282:LEU:HD11	2:B:606:PRO:HB3	2.03	0.41
1:A:475:LEU:O	1:A:476:SER:C	2.64	0.41
1:C:475:LEU:O	1:C:476:SER:C	2.62	0.41
1:C:499:THR:OG1	1:C:500:PHE:N	2.53	0.41
2:D:319:SER:OG	2:D:321:ILE:HG12	2.21	0.41
2:D:517:LYS:HA	2:D:606:PRO:HD2	2.03	0.41
2:D:521:GLY:H	2:D:608:SER:HG	1.63	0.41
1:A:319:PHE:CD1	1:A:464:VAL:HG11	2.56	0.41
1:A:331:MET:SD	1:A:443:SER:HB3	2.61	0.41
1:A:372:ASP:HB2	2:D:501:ASP:CB	2.51	0.41
1:A:521:LEU:O	1:A:523:VAL:N	2.53	0.41
3:A:701:B79:C16	3:A:701:B79:C22	2.98	0.41
2:B:316:ARG:HD3	2:B:322:SER:HB2	2.03	0.41
2:B:514:PHE:O	2:B:607:VAL:HG23	2.20	0.41
2:B:572:ASN:C	2:B:574:ARG:H	2.29	0.41
2:D:118:MET:O	2:D:238:LYS:HA	2.21	0.41
2:D:489:ILE:HG12	2:D:510:LEU:HB2	2.03	0.41
2:D:533:LEU:HD13	2:D:533:LEU:HA	1.67	0.41
2:D:560:TYR:HB2	2:D:579:VAL:O	2.20	0.41
1:A:486:TYR:O	1:A:489:ILE:HG22	2.21	0.41
2:D:70:ASN:HD22	2:D:70:ASN:C	2.29	0.41
2:D:543:LYS:O	2:D:543:LYS:CG	2.69	0.41
1:C:345:ASP:OD2	1:C:401:TRP:NE1	2.54	0.40
2:B:544:ILE:HD11	2:B:559:TYR:HD2	1.85	0.40
2:D:124:VAL:O	2:D:128:ILE:HG23	2.21	0.40
2:D:335:ARG:HD3	2:D:368:ASP:HB3	2.04	0.40
2:D:585:LEU:HD12	2:D:585:LEU:HA	1.77	0.40
1:A:535:ARG:HD2	1:A:541:GLU:HA	2.03	0.40
3:C:701:B79:C16	3:C:701:B79:C22	2.99	0.40
2:B:451:ILE:HD12	2:B:451:ILE:HA	1.81	0.40
2:D:114:VAL:HA	2:D:241:PHE:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:TYR:C	1:A:381:ASP:H	2.28	0.40
1:A:498:PRO:HB3	2:B:375:TYR:CE2	2.57	0.40
2:D:397:LEU:HD12	2:D:536:TYR:OH	2.22	0.40
1:A:335:ASN:ND2	1:A:338:GLU:OE1	2.55	0.40
2:B:483:PRO:HB2	2:B:485:ARG:HE	1.86	0.40
2:D:314:TYR:OH	2:D:361:HIS:NE2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	286/308 (93%)	230 (80%)	54 (19%)	2 (1%)	18	51
1	C	288/308 (94%)	223 (77%)	65 (23%)	0	100	100
2	B	518/623 (83%)	411 (79%)	97 (19%)	10 (2%)	6	33
2	D	508/623 (82%)	410 (81%)	94 (18%)	4 (1%)	16	49
All	All	1600/1862 (86%)	1274 (80%)	310 (19%)	16 (1%)	12	45

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	236	ASN
2	B	275	SER
2	B	439	LEU
2	B	540	SER
2	D	42	ASN
2	B	499	GLN
2	D	362	CYS
2	B	232	LYS
2	B	174	PRO

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Mol	Chain	Res	Type
2	D	544	ILE
2	B	274	GLN
2	D	51	VAL
2	B	435	PRO
1	A	375	VAL
2	B	233	ILE
1	A	380	ILE

5.3.2 Protein sidechains [i](#)

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	204/282 (72%)	201 (98%)	3 (2%)	57	70
1	C	201/282 (71%)	200 (100%)	1 (0%)	81	80
2	B	348/588 (59%)	347 (100%)	1 (0%)	86	83
2	D	315/588 (54%)	311 (99%)	4 (1%)	61	72
All	All	1068/1740 (61%)	1059 (99%)	9 (1%)	73	77

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	ILE
1	A	380	ILE
1	A	381	ASP
1	C	545	VAL
2	B	261	SER
2	D	492	VAL
2	D	543	LYS
2	D	544	ILE
2	D	546	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	ASN
1	C	353	HIS
2	B	70	ASN
2	B	450	GLN
2	D	185	ASN
2	D	331	ASN
2	D	469	ASN
2	D	499	GLN
2	D	503	ASN
2	D	537	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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	B79	C	701	-	41,43,43	0.68	1 (2%)	46,59,59	0.73	2 (4%)
3	B79	A	701	-	41,43,43	0.64	1 (2%)	46,59,59	0.65	2 (4%)

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	B79	C	701	-	-	3/20/50/50	0/4/5/5
3	B79	A	701	-	-	3/20/50/50	0/4/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	701	B79	C16-N1	-3.74	1.43	1.47
3	A	701	B79	C16-N1	-3.64	1.43	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	B79	C17-C14-C15	2.67	124.39	118.21
3	A	701	B79	C17-C14-C10	2.65	124.34	118.21
3	C	701	B79	C17-C14-C10	2.43	123.84	118.21
3	A	701	B79	C17-C14-C15	2.33	123.61	118.21

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	B79	C32-C1-O-C
3	C	701	B79	C2-C1-O-C
3	C	701	B79	C32-C1-O-C
3	A	701	B79	C2-C1-O-C
3	C	701	B79	C15-C14-C17-C22
3	A	701	B79	C15-C14-C17-C18

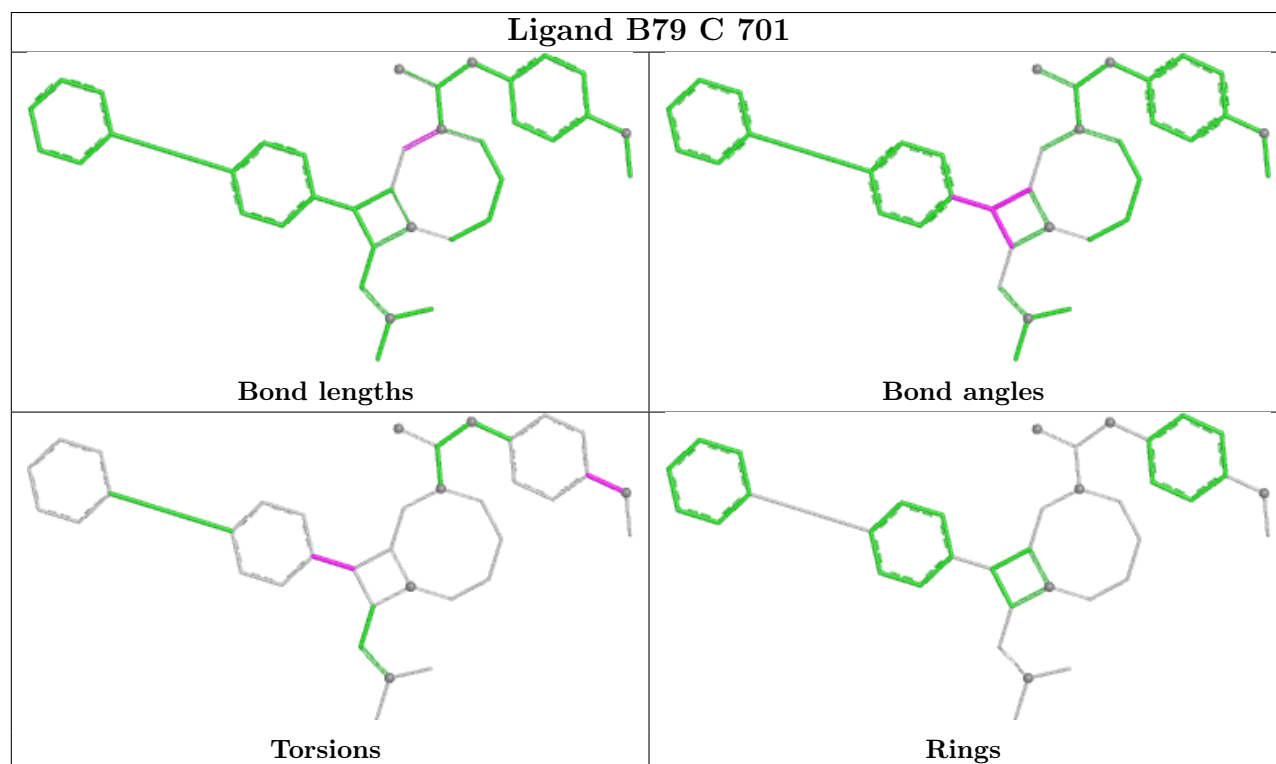
There are no ring outliers.

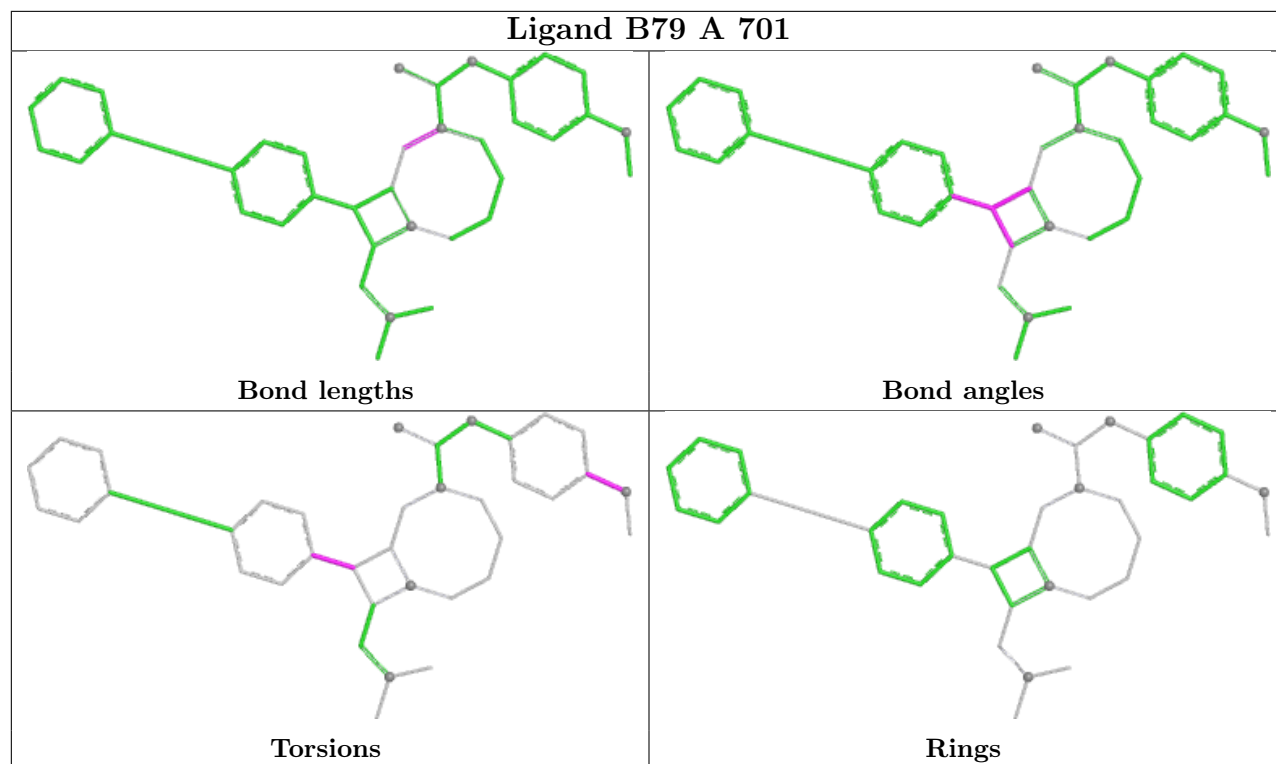
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	701	B79	2	0
3	A	701	B79	2	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	290/308 (94%)	0.57	21 (7%)	21 14	49, 79, 128, 153	0
1	C	292/308 (94%)	0.65	20 (6%)	23 15	48, 79, 125, 177	0
2	B	536/623 (86%)	0.54	23 (4%)	40 22	50, 87, 135, 191	0
2	D	522/623 (83%)	0.54	25 (4%)	35 20	48, 87, 140, 203	0
All	All	1640/1862 (88%)	0.57	89 (5%)	31 18	48, 84, 134, 203	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	520	TRP	8.7
2	B	280	TYR	5.8
2	D	136	HIS	5.4
2	D	348	PHE	5.0
2	D	47	TYR	4.9
2	B	340	CYS	4.7
1	C	391	ASP	4.7
2	B	348	PHE	4.5
2	D	60	CYS	4.3
2	D	494	TYR	4.3
2	D	5	SER	4.1
2	D	323	HIS	4.1
1	A	503	TYR	4.1
2	B	343	MET	3.9
2	B	450	GLN	3.8
2	B	341	ASP	3.8
1	A	501	ASN	3.8
1	A	539	PHE	3.7
2	B	130	GLU	3.6
2	D	390	SER	3.4
1	C	464	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	360	ASP	3.3
2	D	141	LYS	3.3
1	C	392	TYR	3.3
2	D	138	ASN	3.3
1	C	456	THR	3.3
2	D	406	GLY	3.2
2	D	405	CYS	3.2
2	D	427	ARG	3.2
1	C	336	TYR	3.1
2	B	351	THR	3.0
2	D	422	TYR	3.0
2	B	199	TYR	2.9
1	A	413	THR	2.9
2	D	349	LYS	2.9
1	A	570	GLY	2.8
1	C	521	LEU	2.8
1	A	279	TYR	2.8
1	C	343	CYS	2.7
2	B	375	TYR	2.7
2	B	435	PRO	2.6
1	A	365	LYS	2.6
1	C	508	MET	2.6
2	D	152	ASP	2.6
2	D	190	TYR	2.6
2	D	398	PHE	2.6
1	C	490	GLY	2.6
2	B	355	TYR	2.6
1	A	356	ARG	2.5
1	A	448	PHE	2.5
1	A	568	LEU	2.5
2	B	120	ILE	2.5
1	C	442	PHE	2.4
2	D	59	ILE	2.4
1	C	443	SER	2.4
1	C	370	CYS	2.4
1	A	557	MET	2.4
1	A	330	GLU	2.4
1	A	505	GLU	2.4
2	B	453	ASN	2.3
2	B	28	CYS	2.3
2	D	375	TYR	2.3
1	C	509	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	449	ARG	2.3
1	C	459	ALA	2.3
1	C	530	ARG	2.3
1	A	569	PHE	2.3
1	A	391	ASP	2.3
1	A	451	GLU	2.2
1	A	511	TYR	2.2
1	A	414	HIS	2.2
2	D	391	LEU	2.2
1	A	560	TYR	2.2
2	B	494	TYR	2.2
2	B	611	GLU	2.2
2	B	305	ASN	2.2
2	B	252	ALA	2.1
1	A	348	TYR	2.1
2	D	237	THR	2.1
2	B	136	HIS	2.1
2	D	335	ARG	2.1
2	B	451	ILE	2.1
2	B	198	PRO	2.0
2	D	123	SER	2.0
1	C	451	GLU	2.0
1	C	484	ALA	2.0
1	C	447	VAL	2.0
2	D	485	ARG	2.0
2	B	439	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

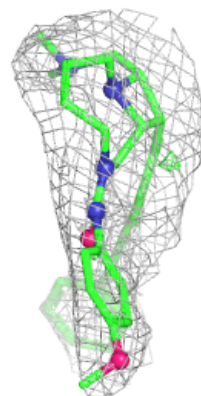
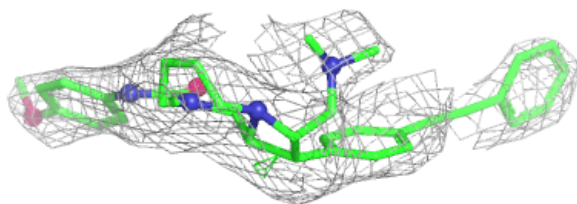
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	B79	A	701	39/39	0.83	0.19	57,72,91,93	0
3	B79	C	701	39/39	0.83	0.23	49,61,84,105	39
4	MG	B	701	1/1	0.86	0.14	88,88,88,88	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.

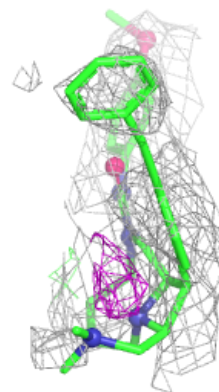
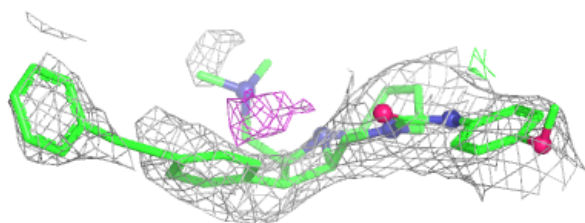
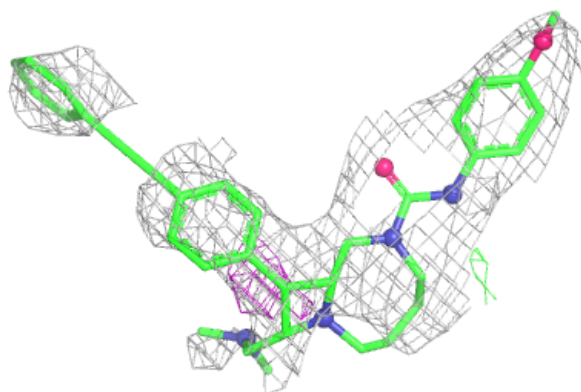
Electron density around B79 A 701:

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



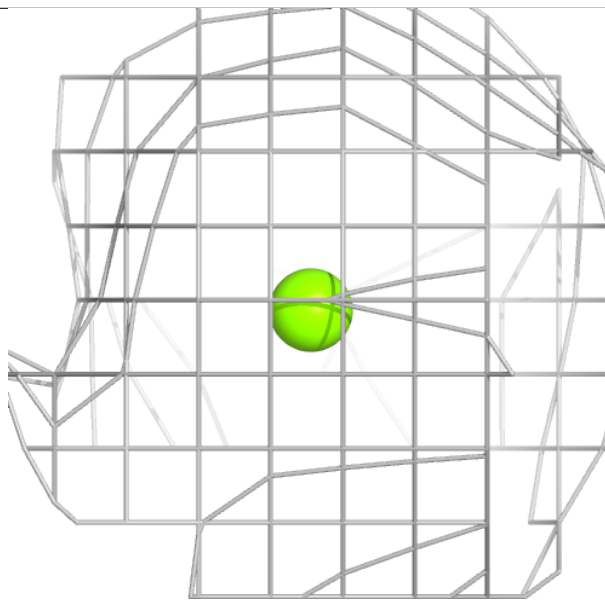
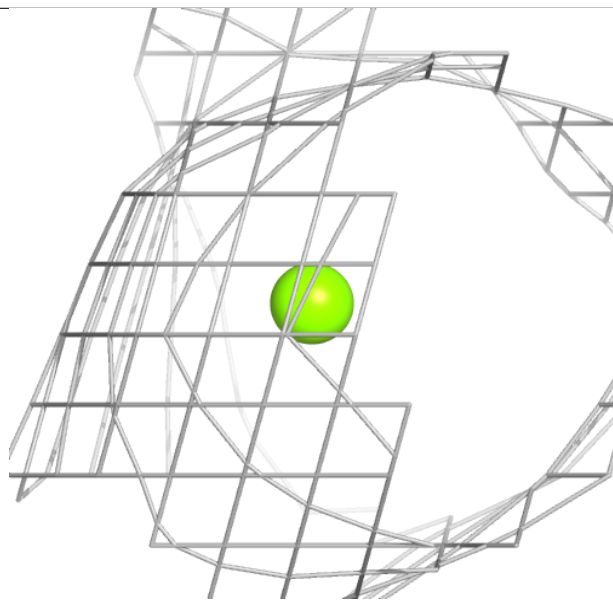
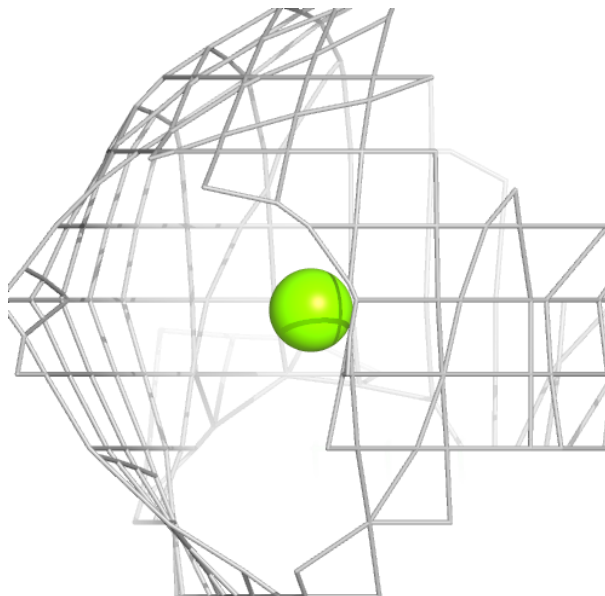
Electron density around B79 C 701:

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



Electron density around MG B 701:

$2mF_o-DF_c$ (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.