



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:02 PM UTC

PDB ID : 3MWW / pdb_00003mww
Title : Crystal structure of HCV NS5B polymerase
Authors : Coulombe, R.
Deposited on : 2010-05-06
Resolution : 2.80 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

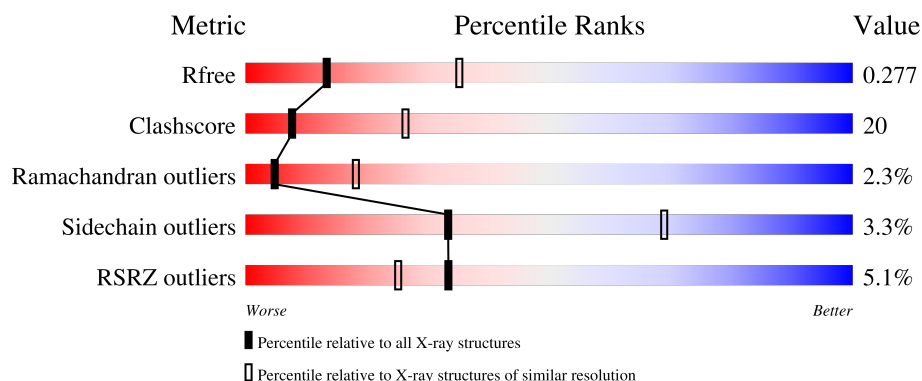
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	576	% 65% 30% . .
1	B	576	9% 52% 36% 5% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8683 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4358	2745	770	811	32			
1	B	541	Total	C	N	O	S	0	0	0
			4210	2652	741	785	32			

There are 12 discrepancies between the modelled and reference sequences:

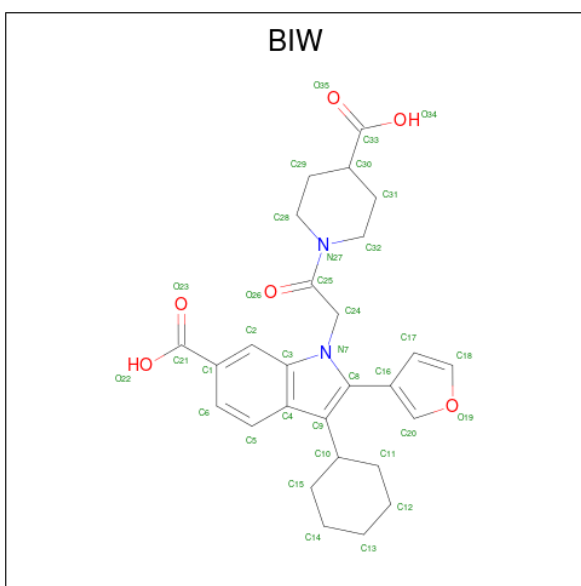
Chain	Residue	Modelled	Actual	Comment	Reference
A	571	HIS	-	expression tag	UNP O92972
A	572	HIS	-	expression tag	UNP O92972
A	573	HIS	-	expression tag	UNP O92972
A	574	HIS	-	expression tag	UNP O92972
A	575	HIS	-	expression tag	UNP O92972
A	576	HIS	-	expression tag	UNP O92972
B	571	HIS	-	expression tag	UNP O92972
B	572	HIS	-	expression tag	UNP O92972
B	573	HIS	-	expression tag	UNP O92972
B	574	HIS	-	expression tag	UNP O92972
B	575	HIS	-	expression tag	UNP O92972
B	576	HIS	-	expression tag	UNP O92972

- 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	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-[2-(4-carboxypiperidin-1-yl)-2-oxoethyl]-3-cyclohexyl-2-furan-3-yl-1H-indole-6-carboxylic acid (CCD ID: BIW) (formula: C₂₇H₃₀N₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			35	27	2	6		

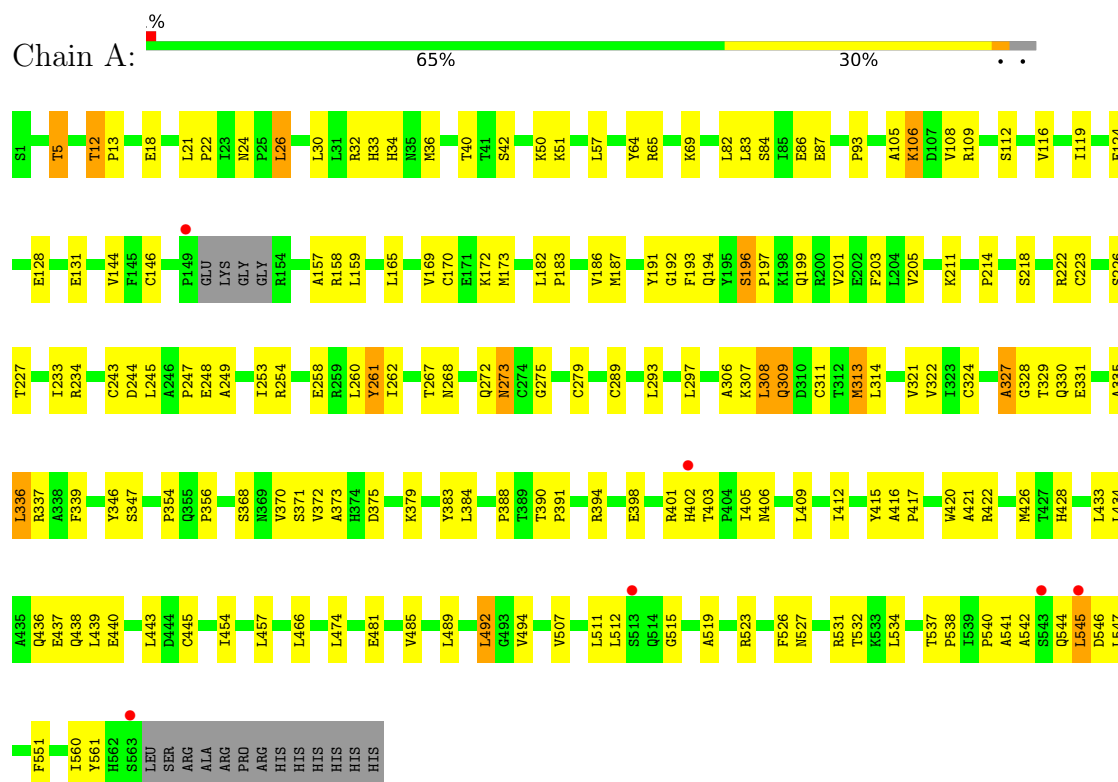
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	22	Total	O	0	0
			22	22		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Genome polypeptide



S543	S548	S470	S407	K307
Q544	L547	T473	W408	L308
L545	D546	L474	L409	Q309
D546	L547	L474	L412	D310
S548	S548	S478	T413	C311
G549	G549	S478	W414	L314
W550	W550	S478	Y415	L314
Y555	Y555	T482	A416	D318
S556	S556	M483	P417	D318
G557	G557	R484	T418	V321
G558	G558	V485	L419	V322
Y561	Y561	S487	W420	I323
H562	H562	C488	A421	C324
S563	S563	L489	R422	E325
LEU	LEU	V494	I424	S326
SER	SER	R501	L425	A327
ARG	ARG	M426	L425	G328
ALA	ALA	H502	T427	T329
ARG	ARG	R503	H428	Q330
PRQ	PRQ	A504	F429	E331
ARG	ARG	R505	F430	D332
HIS	HIS	S506	S431	A333
HIS	HIS	V507	I432	A334
HIS	HIS	R508	L433	A335
HIS	HIS	A509	L434	L336
HIS	HIS	K510	A435	Y346
HIS	HIS	L511	Q436	S347
HIS	HIS	L512	Q437	S347
HIS	HIS	S513	E438	P356
HIS	HIS	Q514	L439	P356
HIS	HIS	G515	E440	L360
HIS	HIS	G516	R441	L360
HIS	HIS	R517	A442	V372
HIS	HIS	A518	L443	A373
HIS	HIS	A519	D444	H374
HIS	HIS	T520	Y448	D375
HIS	HIS	C521	G449	A376
HIS	HIS	G522	A450	A376
HIS	HIS	R523	C451	T385
HIS	HIS	Y524	Y452	R386
HIS	HIS	L525	S453	D387
HIS	HIS	R526	I454	P388
HIS	HIS	N527	E455	T389
HIS	HIS	W528	P456	T390
HIS	HIS	A529	L457	P391
HIS	HIS	V530	D458	L392
HIS	HIS	R531	L459	A393
HIS	HIS	T532	P460	R394
HIS	HIS	K533	Q461	R394
HIS	HIS	L534	I462	W397
HIS	HIS	K535	I463	E398
HIS	HIS	L536	E464	E398
HIS	HIS	T537	R465	R401
HIS	HIS	P538	L466	H402
HIS	HIS	T539	H467	T403
HIS	HIS	P540	G468	P404
HIS	HIS	A541	L469	I405
HIS	HIS	A542	L469	N406

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.12Å 106.55Å 133.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-2.80) 98.4 (50.00-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.281 0.217 , 0.277	Depositor DCC
R_{free} test set	3704 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8683	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: BIW, 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	0.48	0/4453	0.96	14/6044 (0.2%)
1	B	0.46	0/4299	1.04	21/5831 (0.4%)
All	All	0.47	0/8752	1.00	35/11875 (0.3%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	403	THR	N-CA-C	13.57	139.81	109.81
1	B	12	THR	CA-C-N	11.21	133.85	119.84
1	B	12	THR	C-N-CA	11.21	133.85	119.84
1	B	404	PRO	N-CA-C	-9.68	92.53	112.47
1	B	403	THR	CA-C-N	-9.23	108.31	119.84
1	B	403	THR	C-N-CA	-9.23	108.31	119.84
1	B	531	ARG	N-CA-C	-8.05	101.77	112.72
1	B	261	TYR	N-CA-C	7.81	119.79	111.28
1	A	192	GLY	N-CA-C	7.29	121.72	112.83
1	B	543	SER	N-CA-C	-7.19	104.40	113.02
1	B	78	VAL	N-CA-C	7.11	118.18	109.30
1	B	402	HIS	N-CA-C	6.98	125.66	110.80
1	A	261	TYR	N-CA-C	6.82	118.37	111.07
1	A	196	SER	N-CA-C	-6.66	101.43	110.36
1	B	10	LEU	N-CA-C	6.44	120.06	110.52
1	B	155	LYS	N-CA-C	6.26	117.69	109.93
1	A	131	GLU	N-CA-C	6.22	120.46	112.12
1	A	454	ILE	N-CA-C	6.18	117.59	108.45
1	B	196	SER	N-CA-C	-5.99	102.33	110.36
1	B	12	THR	N-CA-C	5.74	118.05	110.36
1	B	324	CYS	N-CA-C	5.72	117.66	109.14
1	A	327	ALA	N-CA-C	-5.70	103.93	111.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	ALA	N-CA-C	-5.67	107.00	114.04
1	A	193	PHE	N-CA-C	5.64	119.64	112.87
1	A	32	ARG	N-CA-C	5.62	117.49	111.36
1	B	101	PHE	N-CA-C	5.51	118.79	112.57
1	B	92	THR	N-CA-C	5.47	117.55	109.50
1	A	526	PHE	N-CA-C	5.29	119.04	112.59
1	A	186	VAL	N-CA-C	5.25	115.91	110.82
1	A	244	ASP	N-CA-C	-5.23	101.25	109.25
1	B	192	GLY	N-CA-C	5.17	118.49	112.50
1	A	218	SER	N-CA-C	-5.11	102.50	110.42
1	A	12	THR	CA-C-N	5.06	126.17	119.84
1	A	12	THR	C-N-CA	5.06	126.17	119.84
1	B	11	ILE	N-CA-C	-5.00	99.50	107.15

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4358	0	4371	127	0
1	B	4210	0	4218	222	0
2	A	10	0	0	1	0
2	B	5	0	0	0	0
3	B	35	0	28	1	0
4	A	43	0	0	4	0
4	B	22	0	0	0	0
All	All	8683	0	8617	346	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 20.

All (346) 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:13:PRO:HB3	1:B:17:GLU:HB2	1.35	1.05
1:B:523:ARG:HG3	1:B:534:LEU:HD23	1.44	0.99
1:B:536:LEU:H	1:B:536:LEU:HD12	1.29	0.95
1:B:434:LEU:H	1:B:434:LEU:HD23	1.37	0.89
1:B:464:GLU:O	1:B:468:GLY:HA2	1.75	0.85
1:B:457:LEU:HD13	1:B:517:ARG:HG2	1.55	0.84
1:B:434:LEU:HD22	1:B:511:LEU:HD21	1.59	0.83
1:B:461:GLN:HG2	1:B:541:ALA:HB3	1.64	0.80
1:A:170:CYS:HA	1:A:173:MET:HE3	1.64	0.78
1:B:46:SER:HA	1:B:49:GLN:HE21	1.47	0.78
1:B:441:LYS:HD3	1:B:443:LEU:HD21	1.65	0.77
1:B:508:ARG:HH12	1:B:530:VAL:HG21	1.49	0.77
1:B:405:ILE:HG13	1:B:443:LEU:HD13	1.66	0.76
1:B:470:SER:O	1:B:474:LEU:HG	1.87	0.75
1:B:13:PRO:CB	1:B:17:GLU:HB2	2.16	0.73
1:A:187:MET:HE2	1:A:293:LEU:HD23	1.70	0.72
1:A:523:ARG:HG3	1:A:534:LEU:HD12	1.71	0.72
1:B:465:ARG:HD3	1:B:547:LEU:HD22	1.70	0.72
1:B:461:GLN:HB3	1:B:541:ALA:O	1.89	0.72
1:B:514:GLN:HB3	1:B:518:ALA:HB3	1.74	0.69
1:B:118:HIS:O	1:B:121:SER:HB3	1.92	0.69
1:B:421:ALA:O	1:B:426:MET:HG3	1.94	0.68
1:B:457:LEU:HD13	1:B:517:ARG:CG	2.25	0.66
1:B:196:SER:OG	1:B:199:GLN:HG3	1.95	0.66
1:B:129:ASP:HB3	1:B:259:ARG:NH1	2.11	0.66
1:B:424:ILE:HD13	1:B:489:LEU:HD21	1.77	0.66
1:B:336:LEU:CD2	1:B:356:PRO:HD3	2.25	0.66
1:A:313:MET:HG3	1:A:322:VAL:HG22	1.78	0.65
1:B:452:TYR:OH	1:B:550:TRP:HA	1.97	0.65
1:A:233:ILE:HD13	1:A:261:TYR:O	1.97	0.65
1:B:346:TYR:O	1:B:347:SER:HB3	1.97	0.65
1:B:517:ARG:H	1:B:517:ARG:CD	2.09	0.65
1:B:418:THR:O	1:B:422:ARG:HG3	1.97	0.65
1:B:465:ARG:HH11	1:B:545:LEU:HB2	1.62	0.64
1:A:254:ARG:HG2	1:B:251:GLN:NE2	2.13	0.63
1:B:454:ILE:HG22	1:B:455:GLU:N	2.12	0.63
1:B:46:SER:HA	1:B:49:GLN:NE2	2.14	0.63
1:B:508:ARG:NH1	1:B:530:VAL:HG11	2.13	0.63
1:A:69:LYS:HD2	1:B:77:THR:HA	1.81	0.63
1:A:466:LEU:HD22	1:A:551:PHE:HE2	1.63	0.63
1:B:401:ARG:HG3	1:B:402:HIS:H	1.63	0.63
1:B:423:MET:HA	1:B:528:TRP:CZ2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ALA:O	1:A:307:LYS:HB2	1.99	0.62
1:A:515:GLY:HA2	1:A:519:ALA:HB2	1.81	0.62
1:B:508:ARG:HH12	1:B:530:VAL:CG2	2.12	0.62
1:B:15:ALA:O	1:B:16:ALA:CB	2.47	0.62
1:B:40:THR:HB	1:B:157:ALA:HB2	1.81	0.62
1:B:433:LEU:HD13	1:B:439:LEU:HD23	1.82	0.62
1:B:372:VAL:HG12	1:B:373:ALA:H	1.65	0.61
1:A:308:LEU:CD1	1:A:335:ALA:HB1	2.30	0.61
1:B:15:ALA:O	1:B:16:ALA:HB3	2.00	0.61
1:B:444:ASP:HA	1:B:453:SER:HA	1.83	0.61
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.81	0.60
1:B:478:SER:O	1:B:482:ILE:HG13	2.00	0.60
1:B:215:MET:HB2	1:B:326:SER:HB2	1.82	0.60
1:A:439:LEU:O	1:A:457:LEU:HG	2.02	0.60
1:A:406:ASN:ND2	1:A:443:LEU:HB3	2.17	0.60
1:B:187:MET:HE3	1:B:296:TYR:CD2	2.37	0.60
1:B:336:LEU:HD22	1:B:356:PRO:HD3	1.84	0.60
1:B:187:MET:HG2	1:B:296:TYR:CD2	2.37	0.59
1:B:372:VAL:HG12	1:B:373:ALA:N	2.17	0.59
1:A:440:GLU:HG2	1:A:457:LEU:HD12	1.84	0.59
1:A:196:SER:OG	1:A:199:GLN:HG3	2.03	0.59
1:B:38:TYR:OH	1:B:155:LYS:HG2	2.03	0.59
1:A:201:VAL:HG22	1:A:384:LEU:HD13	1.85	0.58
1:B:469:LEU:HD23	1:B:469:LEU:H	1.67	0.58
1:B:423:MET:HG2	1:B:528:TRP:CH2	2.38	0.58
1:A:390:THR:HB	1:A:391:PRO:HD3	1.85	0.58
1:B:405:ILE:O	1:B:405:ILE:HG22	2.04	0.58
1:A:182:LEU:HD12	1:A:243:CYS:SG	2.44	0.58
1:B:452:TYR:O	1:B:453:SER:HB2	2.03	0.58
1:B:449:GLY:HA3	1:B:556:SER:HA	1.87	0.57
1:B:36:MET:O	1:B:146:CYS:HA	2.06	0.56
1:B:141:LYS:HG2	1:B:142:SER:N	2.19	0.56
1:B:147:VAL:HG11	1:B:154:ARG:HH21	1.71	0.56
1:B:459:LEU:HB2	1:B:460:PRO:HD3	1.87	0.56
1:A:273:ASN:C	1:A:273:ASN:HD22	2.12	0.56
1:A:108:VAL:HG21	1:A:165:LEU:HD21	1.87	0.55
1:B:187:MET:HE1	1:B:292:THR:HG22	1.89	0.55
1:B:503:ARG:O	1:B:507:VAL:HG23	2.07	0.55
1:A:203:PHE:CE2	1:A:314:LEU:HD13	2.41	0.55
1:B:390:THR:HB	1:B:391:PRO:HD3	1.88	0.55
1:A:5:THR:O	1:A:275:GLY:HA3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LEU:HB3	1:A:439:LEU:HD23	1.89	0.55
1:A:542:ALA:O	1:A:545:LEU:HB2	2.07	0.55
1:B:465:ARG:CD	1:B:547:LEU:HD22	2.37	0.55
1:A:331:GLU:H	1:A:331:GLU:CD	2.15	0.54
1:A:515:GLY:CA	1:A:519:ALA:HB2	2.37	0.54
1:B:93:PRO:HG3	1:B:561:TYR:HB2	1.89	0.54
1:B:505:ARG:NH2	1:B:530:VAL:HG12	2.22	0.54
1:A:21:LEU:HD23	1:A:34:HIS:HA	1.89	0.54
1:A:268:ASN:HD21	1:A:272:GLN:HB2	1.72	0.54
1:B:147:VAL:CG1	1:B:154:ARG:HH21	2.21	0.54
1:B:222:ARG:HH11	1:B:222:ARG:HG2	1.73	0.54
1:A:546:ASP:C	1:A:547:LEU:HD12	2.32	0.54
1:B:450:ALA:HB2	1:B:555:TYR:HD2	1.73	0.54
1:B:212:LYS:HB2	1:B:325:GLU:OE2	2.07	0.54
1:A:51:LYS:HG3	1:A:222:ARG:NH2	2.22	0.53
1:B:71:MET:HE3	1:B:296:TYR:CD1	2.43	0.53
1:B:308:LEU:HB2	1:B:311:CYS:SG	2.47	0.53
1:B:401:ARG:CG	1:B:402:HIS:H	2.21	0.53
1:B:454:ILE:HD11	1:B:550:TRP:CH2	2.44	0.53
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.91	0.53
1:B:268:ASN:HD21	1:B:272:GLN:HB2	1.72	0.53
1:B:401:ARG:HG3	1:B:402:HIS:N	2.22	0.53
1:A:248:GLU:HG3	4:A:616:HOH:O	2.07	0.53
1:A:368:SER:HB3	1:A:384:LEU:HG	1.90	0.53
1:B:109:ARG:HH11	1:B:109:ARG:HG2	1.73	0.53
1:B:464:GLU:O	1:B:468:GLY:CA	2.52	0.52
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.91	0.52
1:B:423:MET:HG2	1:B:528:TRP:CZ3	2.45	0.52
1:B:13:PRO:HG3	1:B:42:SER:OG	2.10	0.52
1:B:532:THR:O	1:B:533:LYS:HB2	2.08	0.52
1:A:327:ALA:HB3	1:A:331:GLU:HB2	1.91	0.52
1:B:434:LEU:HD23	1:B:434:LEU:N	2.17	0.52
1:B:330:GLN:OE1	1:B:330:GLN:N	2.39	0.52
1:B:459:LEU:O	1:B:463:ILE:HG13	2.10	0.52
1:A:336:LEU:HD21	1:A:354:PRO:HB2	1.91	0.52
1:B:454:ILE:HG22	1:B:455:GLU:H	1.75	0.51
1:A:561:TYR:CD1	1:A:561:TYR:O	2.64	0.51
1:B:5:THR:O	1:B:275:GLY:HA3	2.10	0.51
1:B:175:LEU:HD21	1:B:253:ILE:HG12	1.91	0.51
1:B:457:LEU:HD13	1:B:517:ARG:CB	2.40	0.51
1:B:268:ASN:ND2	1:B:272:GLN:HB2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASN:ND2	1:A:272:GLN:HB2	2.26	0.51
1:A:36:MET:O	1:A:146:CYS:HA	2.09	0.51
1:B:420:TRP:H	1:B:420:TRP:CD1	2.29	0.51
1:B:430:PHE:HD2	1:B:511:LEU:HD11	1.75	0.51
1:A:33:HIS:HB2	1:A:492:LEU:O	2.10	0.51
1:B:328:GLY:O	1:B:329:THR:C	2.54	0.51
1:B:330:GLN:CD	1:B:330:GLN:H	2.14	0.51
1:A:82:LEU:HD12	1:A:173:MET:O	2.10	0.51
1:B:86:GLU:HG3	1:B:111:LEU:HD11	1.92	0.50
1:B:309:GLN:OE1	1:B:309:GLN:HA	2.12	0.50
1:B:207:THR:HG22	1:B:323:ILE:HG21	1.92	0.50
1:B:469:LEU:HD23	1:B:469:LEU:N	2.26	0.50
1:B:547:LEU:HA	1:B:550:TRP:NE1	2.27	0.50
1:B:83:LEU:HB2	1:B:173:MET:HA	1.94	0.50
1:B:187:MET:HE3	1:B:296:TYR:HB2	1.93	0.50
1:B:456:PRO:O	1:B:459:LEU:HG	2.12	0.50
1:A:183:PRO:HD2	4:A:586:HOH:O	2.12	0.50
1:A:346:TYR:O	1:A:347:SER:HB3	2.10	0.50
1:B:107:ASP:HB3	1:B:112:SER:OG	2.12	0.49
1:B:419:LEU:HD23	1:B:485:VAL:HG21	1.95	0.49
1:B:457:LEU:O	1:B:460:PRO:HD2	2.12	0.49
1:A:273:ASN:C	1:A:273:ASN:ND2	2.71	0.49
1:A:545:LEU:HD13	1:A:547:LEU:HD11	1.93	0.49
1:A:267:THR:HG23	1:A:272:GLN:O	2.12	0.49
1:B:112:SER:O	1:B:113:SER:C	2.55	0.49
1:B:407:SER:O	1:B:408:TRP:C	2.54	0.49
1:A:57:LEU:HD23	1:A:57:LEU:C	2.38	0.49
1:A:182:LEU:HD23	1:A:182:LEU:C	2.38	0.49
1:A:434:LEU:HD21	1:A:511:LEU:HD23	1.94	0.49
1:B:512:LEU:HD12	1:B:519:ALA:HA	1.94	0.49
1:B:547:LEU:HA	1:B:550:TRP:HE1	1.77	0.49
1:B:434:LEU:C	1:B:436:GLN:H	2.20	0.49
1:A:64:TYR:CZ	1:A:297:LEU:HD21	2.47	0.49
1:A:106:LYS:CE	1:A:106:LYS:HA	2.43	0.49
1:B:336:LEU:HD23	1:B:356:PRO:HD3	1.93	0.49
1:B:388:PRO:C	1:B:391:PRO:HD2	2.38	0.49
1:A:223:CYS:O	1:A:227:THR:HG23	2.13	0.49
1:B:208:TRP:NE1	1:B:214:PRO:HG3	2.28	0.49
1:B:37:VAL:HG21	3:B:577:BIW:H18	1.93	0.48
1:B:441:LYS:CD	1:B:443:LEU:HD21	2.38	0.48
1:A:106:LYS:HA	1:A:106:LYS:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ASP:OD2	1:A:379:LYS:HE2	2.13	0.48
1:B:415:TYR:O	1:B:418:THR:HG23	2.13	0.48
1:A:308:LEU:HB3	1:A:311:CYS:SG	2.54	0.48
1:A:30:LEU:O	1:A:494:VAL:HG22	2.14	0.48
1:A:254:ARG:HG2	1:B:251:GLN:HE22	1.79	0.48
1:A:532:THR:HG22	1:A:532:THR:O	2.14	0.48
1:B:241:GLN:OE1	1:B:250:ARG:HG3	2.13	0.48
1:B:408:TRP:CG	1:B:409:LEU:N	2.82	0.48
1:B:465:ARG:NH1	1:B:545:LEU:O	2.47	0.48
1:B:263:GLY:HA3	1:B:277:ARG:O	2.14	0.47
1:B:428:HIS:O	1:B:431:SER:HB2	2.14	0.47
1:B:454:ILE:CG2	1:B:455:GLU:N	2.77	0.47
1:B:461:GLN:CG	1:B:541:ALA:HB3	2.38	0.47
1:B:508:ARG:NH1	1:B:530:VAL:CG1	2.76	0.47
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.97	0.47
1:B:113:SER:O	1:B:114:ARG:C	2.56	0.47
1:B:129:ASP:HB3	1:B:259:ARG:HH12	1.79	0.47
1:A:544:GLN:O	1:A:544:GLN:HG2	2.15	0.47
1:B:187:MET:HE1	1:B:292:THR:CG2	2.44	0.47
1:A:201:VAL:O	1:A:205:VAL:HG23	2.14	0.47
1:B:13:PRO:O	1:B:14:CYS:CB	2.62	0.47
1:B:68:LEU:O	1:B:72:LYS:HG3	2.14	0.47
1:B:309:GLN:O	1:B:310:ASP:C	2.57	0.47
1:B:375:ASP:HA	1:B:473:THR:O	2.15	0.47
1:B:424:ILE:CD1	1:B:489:LEU:HD21	2.43	0.47
1:A:24:ASN:OD1	1:A:26:LEU:HB2	2.15	0.47
1:A:512:LEU:HA	1:A:519:ALA:HA	1.97	0.47
1:A:523:ARG:HG3	1:A:534:LEU:CD1	2.44	0.47
1:B:208:TRP:CE3	1:B:360:LEU:HD13	2.49	0.47
1:B:385:THR:OG1	1:B:386:ARG:N	2.48	0.47
1:B:405:ILE:O	1:B:405:ILE:CG2	2.63	0.47
1:B:530:VAL:C	1:B:532:THR:H	2.22	0.47
1:A:40:THR:HB	1:A:157:ALA:HB2	1.96	0.47
1:B:13:PRO:O	1:B:14:CYS:HB3	2.15	0.47
1:B:524:TYR:CE2	1:B:536:LEU:HB3	2.50	0.46
1:A:308:LEU:HD12	1:A:335:ALA:HB1	1.96	0.46
1:B:12:THR:HA	1:B:13:PRO:HD3	1.58	0.46
1:B:388:PRO:O	1:B:392:LEU:HG	2.16	0.46
1:B:438:GLN:C	1:B:440:GLU:H	2.23	0.46
1:B:454:ILE:HD11	1:B:550:TRP:HH2	1.77	0.46
1:B:38:TYR:CZ	1:B:154:ARG:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLU:HA	4:A:596:HOH:O	2.15	0.46
1:A:308:LEU:HD11	1:A:335:ALA:HB1	1.96	0.46
1:A:328:GLY:O	1:A:329:THR:C	2.58	0.46
1:A:93:PRO:HG3	1:A:561:TYR:HB2	1.97	0.46
1:A:211:LYS:HB2	1:A:214:PRO:HB3	1.98	0.46
1:B:187:MET:HE3	1:B:296:TYR:HD2	1.79	0.46
1:B:416:ALA:HB3	1:B:417:PRO:HD3	1.98	0.46
1:A:21:LEU:HD12	1:A:22:PRO:HD2	1.97	0.46
1:B:388:PRO:HB3	1:B:420:TRP:CD2	2.51	0.46
1:B:407:SER:OG	1:B:408:TRP:N	2.50	0.46
1:B:374:HIS:O	1:B:474:LEU:HA	2.17	0.45
1:A:336:LEU:O	1:A:339:PHE:HB3	2.16	0.45
1:A:485:VAL:O	1:A:489:LEU:HG	2.17	0.45
1:B:109:ARG:HG2	1:B:109:ARG:NH1	2.31	0.45
1:B:222:ARG:HG2	1:B:222:ARG:NH1	2.31	0.45
1:A:416:ALA:N	1:A:417:PRO:CD	2.80	0.45
1:B:14:CYS:O	1:B:14:CYS:SG	2.75	0.45
1:A:330:GLN:OE1	1:A:330:GLN:HA	2.16	0.45
1:A:434:LEU:CD2	1:A:439:LEU:HD11	2.47	0.45
1:B:328:GLY:HA3	1:B:331:GLU:OE1	2.16	0.45
1:A:65:ARG:O	1:A:69:LYS:HG2	2.16	0.45
1:A:398:GLU:HG2	1:A:403:THR:OG1	2.17	0.45
1:B:280:ARG:NE	1:B:291:ASN:OD1	2.46	0.45
1:B:501:ARG:O	1:B:505:ARG:HG3	2.16	0.45
1:A:13:PRO:HG3	1:A:42:SER:OG	2.16	0.45
1:A:105:ALA:O	1:A:109:ARG:HG3	2.17	0.45
1:A:196:SER:O	1:A:197:PRO:C	2.59	0.45
1:A:314:LEU:HB3	1:A:321:VAL:CG1	2.47	0.45
1:B:517:ARG:H	1:B:517:ARG:NE	2.14	0.45
1:A:183:PRO:HG3	1:A:289:CYS:SG	2.56	0.44
1:B:233:ILE:HD13	1:B:261:TYR:O	2.17	0.44
1:A:18:GLU:HB3	1:A:401:ARG:NH2	2.32	0.44
1:B:224:PHE:CD2	1:B:318:ASP:HB2	2.53	0.44
1:B:540:PRO:O	1:B:541:ALA:C	2.61	0.44
1:A:422:ARG:HA	1:A:426:MET:HE3	2.00	0.44
1:B:408:TRP:CD2	1:B:409:LEU:N	2.85	0.44
1:B:506:SER:O	1:B:510:LYS:HG3	2.18	0.44
1:B:508:ARG:HH12	1:B:530:VAL:HG11	1.78	0.44
1:B:13:PRO:HB3	1:B:17:GLU:CB	2.26	0.44
1:A:372:VAL:HG12	1:A:373:ALA:N	2.32	0.44
1:A:336:LEU:CD1	1:A:356:PRO:HD3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:MET:SD	1:B:215:MET:C	3.01	0.44
1:B:405:ILE:HG23	1:B:408:TRP:NE1	2.33	0.44
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.83	0.44
1:A:383:TYR:OH	1:A:481:GLU:HG2	2.18	0.44
1:B:514:GLN:HB3	1:B:518:ALA:CB	2.46	0.44
1:B:138:ILE:O	1:B:139:MET:HG2	2.18	0.43
1:B:434:LEU:C	1:B:436:GLN:N	2.76	0.43
1:B:438:GLN:C	1:B:440:GLU:N	2.76	0.43
1:A:406:ASN:HD22	1:A:443:LEU:HB3	1.83	0.43
1:A:415:TYR:C	1:A:417:PRO:CD	2.91	0.43
1:A:420:TRP:CD1	1:A:420:TRP:H	2.35	0.43
1:A:421:ALA:O	1:A:426:MET:HG3	2.17	0.43
1:B:97:ALA:O	1:B:168:ARG:NH2	2.48	0.43
1:B:532:THR:O	1:B:533:LYS:CB	2.67	0.43
1:B:170:CYS:HA	1:B:173:MET:HE3	2.00	0.43
1:B:523:ARG:O	1:B:527:ASN:HB2	2.18	0.43
1:B:375:ASP:O	1:B:376:ALA:C	2.62	0.43
1:B:448:TYR:C	1:B:450:ALA:H	2.26	0.43
1:B:48:ARG:HD3	1:B:52:VAL:HG13	2.01	0.43
1:B:85:ILE:CD1	1:B:120:ARG:HG2	2.49	0.43
1:B:296:TYR:CD1	1:B:296:TYR:C	2.96	0.43
1:A:313:MET:CG	1:A:322:VAL:HG22	2.48	0.43
1:B:542:ALA:C	1:B:544:GLN:H	2.26	0.43
1:B:432:ILE:O	1:B:432:ILE:HG22	2.18	0.43
1:B:321:VAL:O	1:B:321:VAL:HG13	2.18	0.43
1:A:440:GLU:HG2	1:A:457:LEU:CD1	2.46	0.43
1:B:38:TYR:CE2	1:B:154:ARG:HG3	2.52	0.43
1:B:328:GLY:O	1:B:331:GLU:N	2.52	0.43
1:B:518:ALA:O	1:B:519:ALA:C	2.61	0.43
1:B:412:ILE:O	1:B:416:ALA:N	2.52	0.42
1:A:112:SER:O	1:A:116:VAL:HG23	2.18	0.42
1:B:401:ARG:HE	1:B:401:ARG:HA	1.84	0.42
1:A:545:LEU:HB3	1:A:547:LEU:CD1	2.48	0.42
1:B:56:ARG:N	1:B:56:ARG:HD3	2.34	0.42
1:A:412:ILE:O	1:A:416:ALA:N	2.52	0.42
1:B:155:LYS:HE2	1:B:155:LYS:HB3	1.90	0.42
1:B:398:GLU:CD	1:B:407:SER:HG	2.26	0.42
1:A:523:ARG:CG	1:A:534:LEU:HD12	2.47	0.42
1:B:182:LEU:HD12	1:B:243:CYS:SG	2.59	0.42
1:B:223:CYS:O	1:B:227:THR:HG23	2.18	0.42
1:B:426:MET:O	1:B:430:PHE:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:THR:HA	1:A:13:PRO:HD3	1.75	0.42
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.49	0.42
1:B:440:GLU:O	1:B:441:LYS:C	2.63	0.42
1:A:84:SER:OG	1:A:87:GLU:HG3	2.20	0.42
1:B:433:LEU:C	1:B:435:ALA:N	2.77	0.42
1:B:144:VAL:HG21	1:B:397:TRP:CG	2.55	0.42
1:B:415:TYR:HB3	1:B:418:THR:CG2	2.49	0.42
1:A:30:LEU:HB2	1:A:428:HIS:CE1	2.55	0.42
1:A:309:GLN:O	1:A:324:CYS:HB2	2.19	0.42
1:B:113:SER:HB2	1:B:117:ASN:ND2	2.35	0.42
1:B:207:THR:O	1:B:211:LYS:HG2	2.20	0.42
1:B:414:MET:O	1:B:467:HIS:HE1	2.03	0.42
1:A:409:LEU:HB3	1:A:445:CYS:HB3	2.02	0.41
1:B:405:ILE:HD13	1:B:405:ILE:HA	1.96	0.41
1:A:234:ARG:NH1	1:A:258:GLU:OE2	2.53	0.41
1:A:531:ARG:HD3	1:A:531:ARG:HA	1.65	0.41
1:A:537:THR:O	1:A:538:PRO:C	2.63	0.41
1:B:489:LEU:HD22	1:B:494:VAL:HB	2.02	0.41
1:A:405:ILE:HG22	1:A:406:ASN:N	2.35	0.41
1:A:436:GLN:O	1:A:437:GLU:C	2.63	0.41
1:B:99:SER:HB2	1:B:165:LEU:HB3	2.02	0.41
1:B:505:ARG:CZ	1:B:530:VAL:HG12	2.51	0.41
1:B:307:LYS:HE2	1:B:307:LYS:HB3	1.92	0.41
1:B:207:THR:HG22	1:B:323:ILE:CG2	2.51	0.41
1:B:536:LEU:H	1:B:536:LEU:CD1	2.07	0.41
1:A:13:PRO:HG3	1:A:42:SER:CB	2.50	0.41
1:A:388:PRO:C	1:A:391:PRO:HD2	2.45	0.41
1:B:401:ARG:CG	1:B:402:HIS:N	2.83	0.41
1:A:507:VAL:O	1:A:511:LEU:HG	2.21	0.41
1:A:191:TYR:O	1:A:194:GLN:HG2	2.20	0.41
1:A:260:LEU:HA	4:A:580:HOH:O	2.21	0.41
1:B:402:HIS:HB2	1:B:403:THR:H	1.71	0.41
1:A:201:VAL:CG2	1:A:384:LEU:HB2	2.51	0.41
1:A:226:SER:HA	1:A:279:CYS:SG	2.60	0.41
1:B:547:LEU:O	1:B:548:SER:O	2.38	0.41
1:A:233:ILE:CD1	1:A:262:ILE:HA	2.51	0.41
1:A:245:LEU:HD13	1:A:253:ILE:HD12	2.03	0.41
1:B:442:ALA:HB2	1:B:455:GLU:HG2	2.02	0.41
1:B:508:ARG:HH12	1:B:530:VAL:CG1	2.33	0.41
1:B:540:PRO:O	1:B:542:ALA:N	2.53	0.41
1:A:370:VAL:HG12	1:A:371:SER:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ALA:O	1:B:247:PRO:C	2.63	0.40
1:B:332:ASP:O	1:B:333:ALA:C	2.64	0.40
1:B:454:ILE:CG2	1:B:455:GLU:H	2.33	0.40
1:B:483:ASN:O	1:B:484:ARG:C	2.63	0.40
1:A:158:ARG:NH2	2:A:577:SO4:O3	2.55	0.40
1:A:436:GLN:O	1:A:438:GLN:HG3	2.22	0.40
1:B:430:PHE:O	1:B:433:LEU:HB2	2.20	0.40
1:B:197:PRO:HG3	1:B:414:MET:HE3	2.03	0.40
1:A:144:VAL:HB	1:A:394:ARG:HG2	2.04	0.40
1:A:336:LEU:HD12	1:A:356:PRO:HD3	2.04	0.40
1:A:527:ASN:HD21	1:A:534:LEU:H	1.69	0.40
1:B:197:PRO:O	1:B:201:VAL:HG23	2.22	0.40
1:B:308:LEU:CD2	1:B:335:ALA:HB1	2.52	0.40
1:B:465:ARG:HB2	1:B:545:LEU:HD12	2.02	0.40
1:A:124:GLU:OE1	1:A:124:GLU:HA	2.21	0.40
1:A:561:TYR:CD1	1:A:561:TYR:C	2.99	0.40
1:B:511:LEU:O	1:B:514:GLN:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	555/576 (96%)	515 (93%)	38 (7%)	2 (0%)	30	60
1	B	535/576 (93%)	449 (84%)	63 (12%)	23 (4%)	2	7
All	All	1090/1152 (95%)	964 (88%)	101 (9%)	25 (2%)	5	18

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	16	ALA

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Mol	Chain	Res	Type
1	B	113	SER
1	B	406	ASN
1	B	453	SER
1	B	469	LEU
1	B	538	PRO
1	B	540	PRO
1	B	548	SER
1	B	13	PRO
1	B	14	CYS
1	B	407	SER
1	B	468	GLY
1	B	470	SER
1	B	534	LEU
1	B	535	LYS
1	B	541	ALA
1	B	542	ALA
1	A	541	ALA
1	B	441	LYS
1	B	533	LYS
1	A	540	PRO
1	B	310	ASP
1	B	329	THR
1	B	389	THR
1	B	403	THR

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	477/491 (97%)	459 (96%)	18 (4%)	29	64
1	B	458/491 (93%)	445 (97%)	13 (3%)	38	73
All	All	935/982 (95%)	904 (97%)	31 (3%)	33	69

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	26	LEU
1	A	50	LYS
1	A	83	LEU
1	A	86	GLU
1	A	106	LYS
1	A	159	LEU
1	A	247	PRO
1	A	273	ASN
1	A	308	LEU
1	A	309	GLN
1	A	313	MET
1	A	336	LEU
1	A	337	ARG
1	A	402	HIS
1	A	474	LEU
1	A	492	LEU
1	A	545	LEU
1	B	41	THR
1	B	147	VAL
1	B	247	PRO
1	B	434	LEU
1	B	444	ASP
1	B	469	LEU
1	B	487	SER
1	B	513	SER
1	B	517	ARG
1	B	536	LEU
1	B	539	ILE
1	B	546	ASP
1	B	547	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	194	GLN
1	A	273	ASN
1	A	406	ASN
1	A	428	HIS
1	A	527	ASN
1	A	544	GLN
1	B	49	GLN

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Mol	Chain	Res	Type
1	B	251	GLN
1	B	273	ASN
1	B	438	GLN
1	B	446	GLN
1	B	544	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](#)

4 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	577	-	4,4,4	0.43	0	6,6,6	0.12	0
2	SO4	B	578	-	4,4,4	0.44	0	6,6,6	0.14	0
2	SO4	A	578	-	4,4,4	0.38	0	6,6,6	0.12	0
3	BIW	B	577	-	39,39,39	1.88	10 (25%)	51,56,56	1.02	2 (3%)

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	BIW	B	577	-	-	0/24/42/42	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	577	BIW	C25-N27	4.73	1.44	1.35
3	B	577	BIW	C8-C9	4.48	1.42	1.37
3	B	577	BIW	C10-C9	3.65	1.55	1.49
3	B	577	BIW	C2-C1	2.98	1.44	1.39
3	B	577	BIW	C5-C4	2.92	1.44	1.39
3	B	577	BIW	C2-C3	2.76	1.44	1.39
3	B	577	BIW	C6-C1	2.48	1.43	1.39
3	B	577	BIW	C30-C33	2.40	1.55	1.51
3	B	577	BIW	C6-C5	2.38	1.42	1.38
3	B	577	BIW	C8-N7	2.03	1.41	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	577	BIW	C16-C8-N7	2.92	126.16	121.74
3	B	577	BIW	C32-N27-C28	2.89	118.58	112.68

There are no chirality outliers.

There are no torsion outliers.

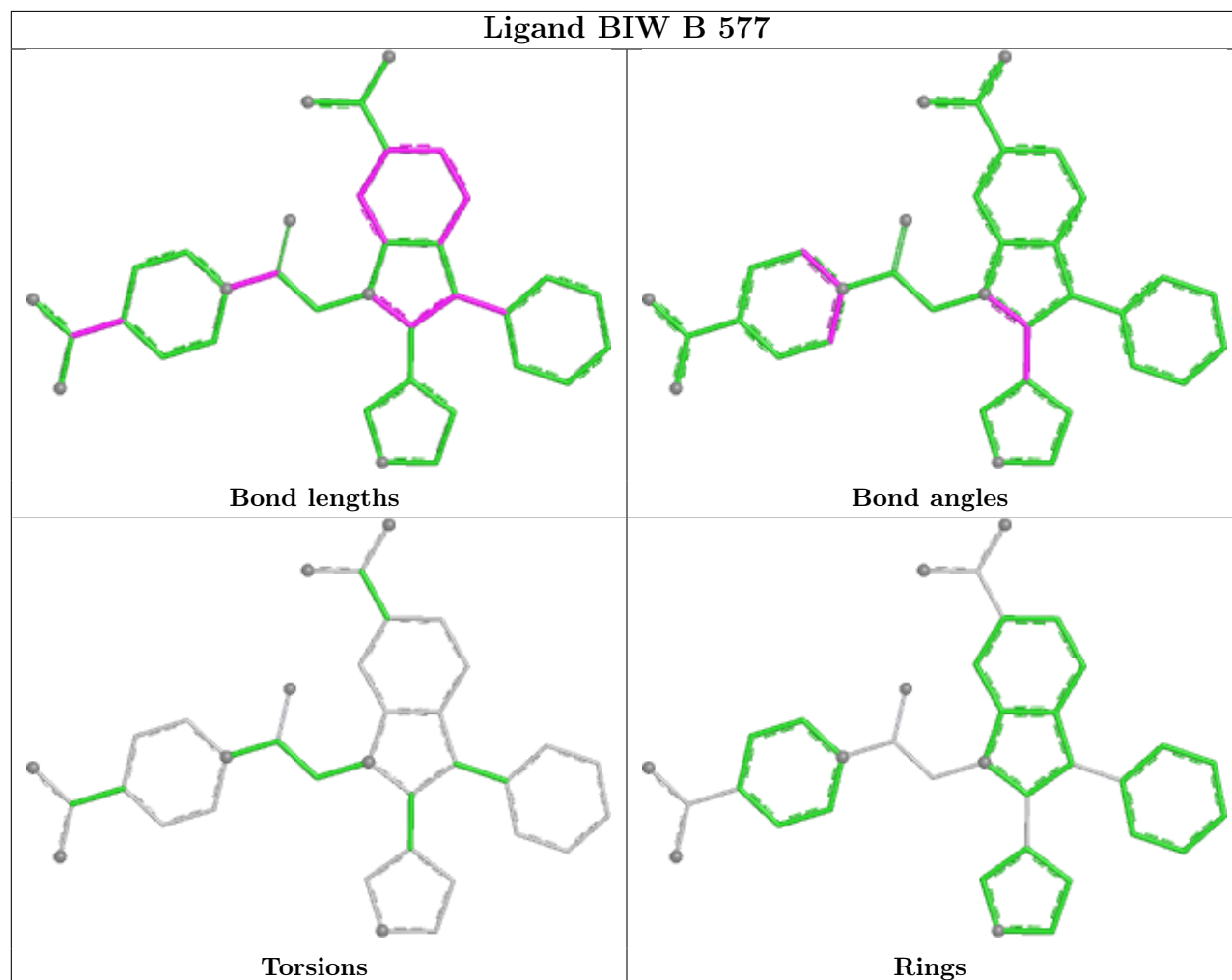
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	577	SO4	1	0
3	B	577	BIW	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	559/576 (97%)	-0.31	6 (1%) 78 70	15, 28, 50, 80	0
1	B	541/576 (93%)	0.38	50 (9%) 14 10	14, 47, 92, 99	0
All	All	1100/1152 (95%)	0.03	56 (5%) 33 25	14, 34, 87, 99	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	469	LEU	4.4
1	B	406	ASN	4.0
1	A	149	PRO	3.8
1	B	16	ALA	3.8
1	B	407	SER	3.6
1	B	520	THR	3.5
1	B	541	ALA	3.5
1	B	405	ILE	3.4
1	B	563	SER	3.4
1	B	543	SER	3.4
1	B	403	THR	3.3
1	A	545	LEU	3.2
1	B	453	SER	3.0
1	B	404	PRO	3.0
1	B	511	LEU	3.0
1	B	558	GLY	3.0
1	B	540	PRO	2.9
1	B	468	GLY	2.9
1	B	402	HIS	2.9
1	B	450	ALA	2.8
1	B	531	ARG	2.8
1	B	148	GLN	2.8
1	B	542	ALA	2.7
1	B	442	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	518	ALA	2.7
1	B	457	LEU	2.7
1	B	443	LEU	2.6
1	B	525	LEU	2.6
1	B	15	ALA	2.6
1	B	430	PHE	2.6
1	B	17	GLU	2.5
1	B	561	TYR	2.5
1	B	512	LEU	2.5
1	B	147	VAL	2.5
1	B	536	LEU	2.4
1	B	533	LYS	2.4
1	B	516	GLY	2.4
1	A	402	HIS	2.4
1	B	515	GLY	2.3
1	B	439	LEU	2.3
1	B	534	LEU	2.3
1	B	153	GLY	2.3
1	B	519	ALA	2.3
1	B	526	PHE	2.2
1	B	506	SER	2.2
1	B	449	GLY	2.2
1	B	535	LYS	2.1
1	B	522	GLY	2.1
1	B	532	THR	2.1
1	A	543	SER	2.1
1	B	549	GLY	2.1
1	B	539	ILE	2.0
1	A	513	SER	2.0
1	A	563	SER	2.0
1	B	214	PRO	2.0
1	B	521	CYS	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](#)

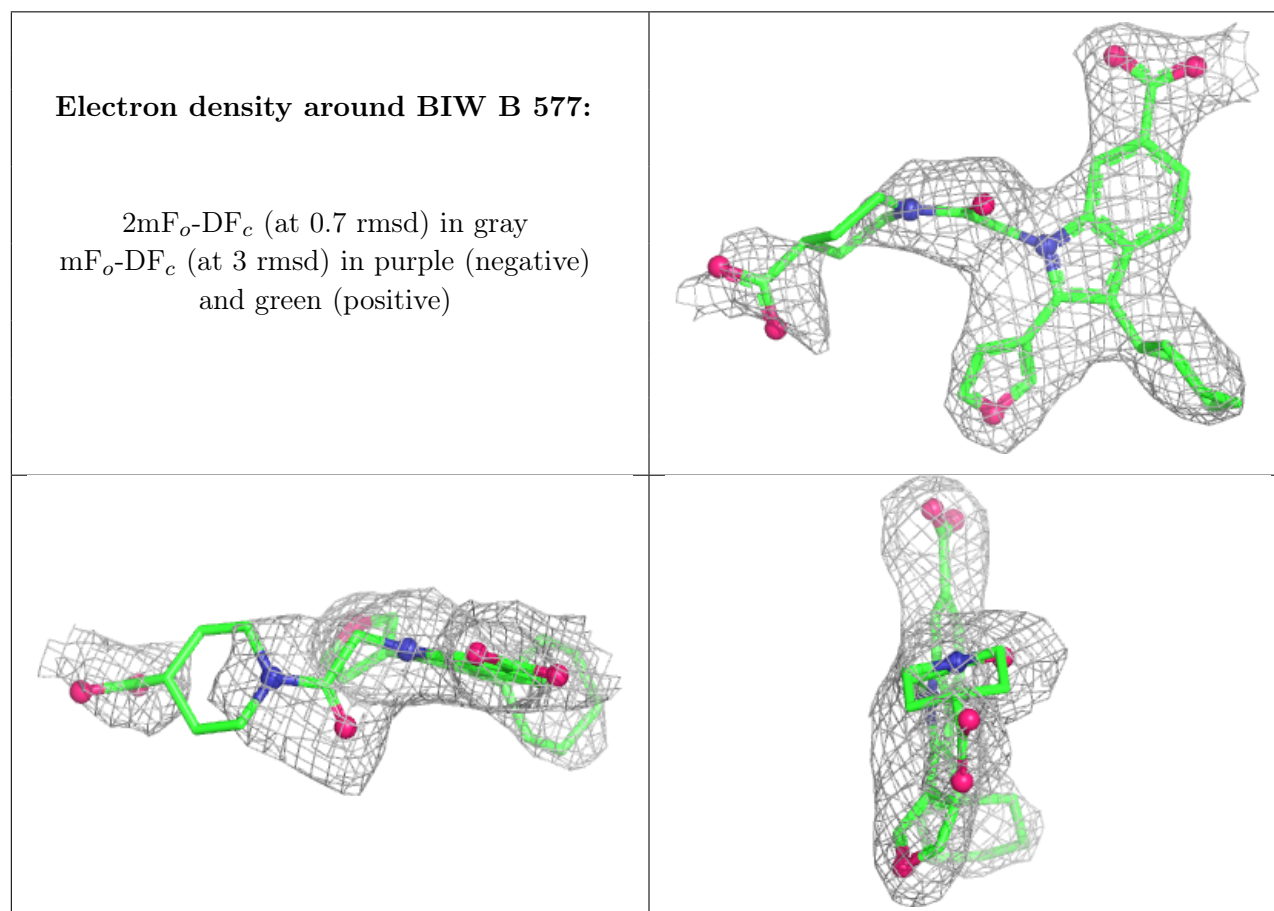
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
2	SO4	B	578	5/5	0.76	0.19	93,93,94,94	0
3	BIW	B	577	35/35	0.89	0.16	76,81,88,89	0
2	SO4	A	577	5/5	0.91	0.14	89,89,89,89	0
2	SO4	A	578	5/5	0.92	0.14	73,73,73,73	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.