



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:21 AM UTC

PDB ID : 1M2O / pdb_00001m2o
Title : Crystal Structure of the Sec23-Sar1 complex
Authors : Bi, X.; Corpina, R.A.; Goldberg, J.
Deposited on : 2002-06-24
Resolution : 2.50 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

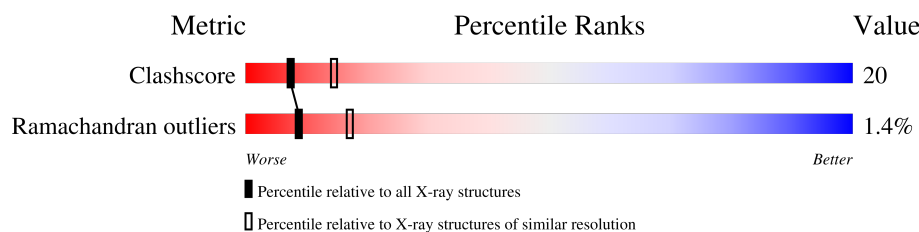
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	768	61% 30% • 7%
1	C	768	55% 37% • 7%
2	B	190	55% 29% • 14%
2	D	190	31% 51% • 17%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14123 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 protein transport protein SEC23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	718	Total	C	N	O	S	0	0	0
			5670	3617	947	1084	22			
1	C	718	Total	C	N	O	S	0	0	0
			5670	3617	947	1084	22			

- Molecule 2 is a protein called GTP-binding protein SAR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	164	Total	C	N	O	S	0	0	0
			1297	836	218	239	4			
2	D	158	Total	C	N	O	S	0	0	0
			1247	803	211	229	4			

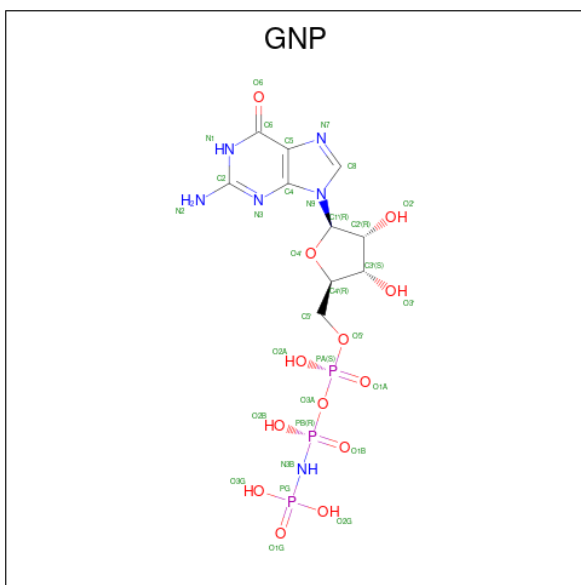
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total 32	C 10	N 6	O 13	P 3	0	0
5	D	1	Total 32	C 10	N 6	O 13	P 3	0	0

- Molecule 6 is water.

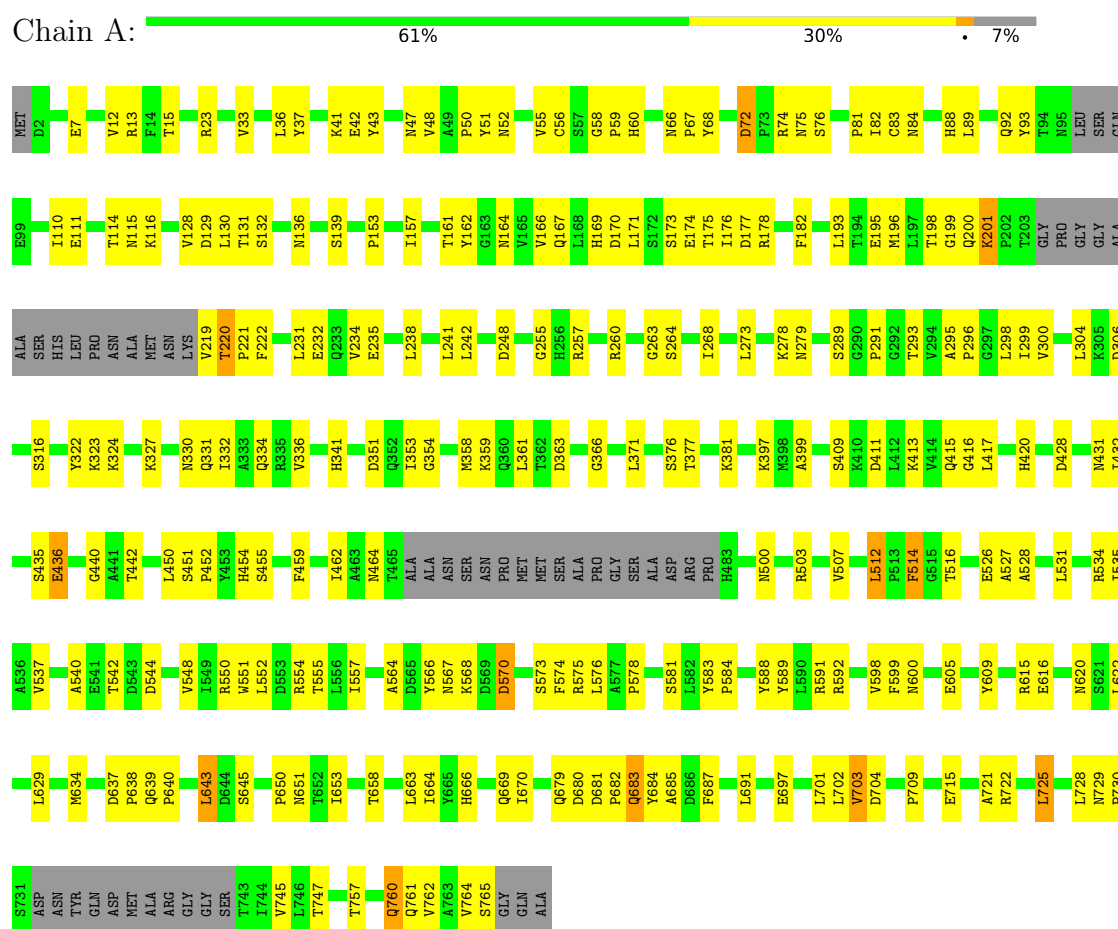
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	114	Total O 114 114	0	0
6	B	24	Total O 24 24	0	0
6	C	33	Total O 33 33	0	0

3 Residue-property plots

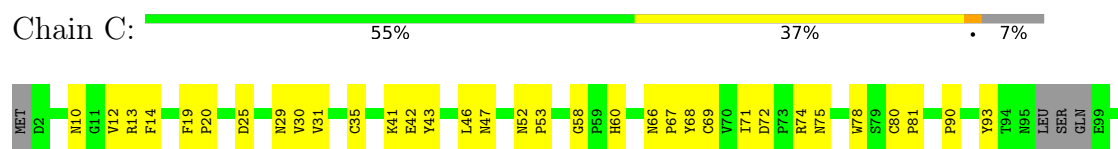
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: protein transport protein SEC23



• Molecule 1: protein transport protein SEC23



V140	S141	E142	A143	E144	L145	R146	S147	A148	L149	G150	L151	L152	W153	T154	T155	G156	SER	GLN	ARG	ILE	GLU	GLY	GLN	R164	P165	V166	E167	V168	F169	M170	C171	S172	V173	V174	M175	R176	M177	G178	Y179	L180	E181	A182	F183	Q184	W185	L186	S187	Q188	TYR	ILE
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4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.20Å 151.16Å 271.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.85 – 2.50	Depositor
% Data completeness (in resolution range)	92.9 (23.85-2.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.238 , 0.294	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	14123	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.49	0/5803	1.03	32/7901 (0.4%)
1	C	0.46	1/5803 (0.0%)	1.01	24/7901 (0.3%)
2	B	0.46	0/1324	0.97	10/1796 (0.6%)
2	D	0.35	0/1273	0.85	3/1727 (0.2%)
All	All	0.47	1/14203 (0.0%)	1.00	69/19325 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	294	VAL	CA-C	5.70	1.59	1.52

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	295	ALA	CA-C-N	17.00	167.79	127.00
1	C	295	ALA	C-N-CA	17.00	167.79	127.00
1	C	295	ALA	C-N-CD	-14.93	87.76	120.60
1	A	295	ALA	CA-C-N	14.29	161.30	127.00
1	A	295	ALA	C-N-CA	14.29	161.30	127.00
1	A	295	ALA	C-N-CD	-13.83	90.18	120.60
1	C	598	VAL	N-CA-C	8.13	119.14	111.91
1	A	257	ARG	N-CA-C	-6.86	101.42	110.40
1	A	72	ASP	CA-C-N	6.76	126.28	119.24
1	A	72	ASP	C-N-CA	6.76	126.28	119.24
1	C	162	TYR	N-CA-C	6.67	118.90	108.96
1	C	570	ASP	CA-C-N	6.42	125.91	119.24
1	C	570	ASP	C-N-CA	6.42	125.91	119.24
1	C	52	ASN	CA-C-N	6.38	126.14	119.76
1	C	52	ASN	C-N-CA	6.38	126.14	119.76
1	C	294	VAL	CA-C-N	6.33	131.43	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	294	VAL	C-N-CA	6.33	131.43	121.17
1	C	484	LEU	N-CA-C	6.29	119.39	108.76
1	A	220	THR	N-CA-C	6.27	118.61	110.40
1	A	162	TYR	N-CA-C	6.19	118.48	109.07
1	A	58	GLY	CA-C-N	6.13	127.50	119.84
1	A	58	GLY	C-N-CA	6.13	127.50	119.84
1	A	416	GLY	N-CA-C	5.99	118.09	110.96
1	C	512	LEU	CA-C-N	5.99	127.33	119.84
1	C	512	LEU	C-N-CA	5.99	127.33	119.84
2	B	66	ASN	N-CA-C	-5.99	105.56	112.92
1	A	306	ASP	N-CA-C	-5.98	100.57	109.42
2	B	184	GLN	N-CA-C	-5.97	104.69	111.14
1	C	128	VAL	N-CA-C	5.94	116.41	107.80
1	A	512	LEU	CA-C-N	5.80	127.09	119.84
1	A	512	LEU	C-N-CA	5.80	127.09	119.84
1	C	257	ARG	N-CA-C	-5.76	101.74	110.50
1	C	103	LEU	N-CA-C	5.75	118.29	111.33
1	C	616	GLU	N-CA-C	5.74	117.93	110.53
1	A	643	LEU	N-CA-C	-5.66	100.39	109.39
1	A	581	SER	N-CA-C	5.65	118.21	111.71
1	A	570	ASP	CA-C-N	5.65	126.90	119.84
1	A	570	ASP	C-N-CA	5.65	126.90	119.84
1	C	280	ILE	N-CA-C	-5.60	100.95	107.61
1	A	136	ASN	N-CA-C	-5.57	105.21	111.28
1	A	760	GLN	N-CA-C	5.50	117.28	111.28
2	B	171	CYS	N-CA-C	5.46	115.75	108.38
2	B	177	ASN	N-CA-C	5.44	117.53	108.99
2	D	125	VAL	CA-C-N	5.43	125.69	119.83
2	D	125	VAL	C-N-CA	5.43	125.69	119.83
1	A	36	LEU	N-CA-C	-5.41	100.42	109.24
1	A	316	SER	N-CA-C	-5.41	106.73	113.38
1	A	33	VAL	N-CA-C	-5.40	101.76	108.89
1	A	322	TYR	N-CA-C	5.39	117.60	111.02
1	A	658	THR	N-CA-C	-5.35	105.98	112.88
2	B	69	PHE	N-CA-C	5.33	117.42	108.73
2	B	102	ASP	CA-C-N	5.30	125.11	119.28
2	B	102	ASP	C-N-CA	5.30	125.11	119.28
2	D	69	PHE	N-CA-C	5.26	117.31	107.99
2	B	164	ARG	CA-C-N	5.21	125.46	119.83
2	B	164	ARG	C-N-CA	5.21	125.46	119.83
1	A	436	GLU	N-CA-C	5.21	117.91	109.06
1	A	128	VAL	N-CA-C	5.19	115.32	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	58	GLY	CA-C-N	5.17	126.30	119.84
1	C	58	GLY	C-N-CA	5.17	126.30	119.84
1	A	82	ILE	N-CA-C	5.11	115.34	110.53
2	B	67	ILE	N-CA-C	5.10	115.32	108.17
1	C	119	THR	N-CA-C	5.09	121.65	110.80
1	A	598	VAL	N-CA-C	5.08	118.64	112.80
1	A	725	LEU	N-CA-C	5.08	117.20	111.11
1	A	685	ALA	N-CA-C	-5.06	105.95	111.82
1	C	296	PRO	CA-N-CD	-5.06	104.41	111.50
1	C	292	GLY	N-CA-C	-5.04	104.68	111.54
1	A	431	ASN	N-CA-C	5.01	118.23	112.57

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	5670	0	5566	178	0
1	C	5670	0	5566	238	0
2	B	1297	0	1291	49	0
2	D	1247	0	1245	114	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	32	0	13	5	0
5	D	32	0	13	2	0
6	A	114	0	0	8	0
6	B	24	0	0	1	0
6	C	33	0	0	3	0
All	All	14123	0	13694	564	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 (564) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:THR:HG22	1:C:116:LYS:H	1.15	1.09
1:A:114:THR:HG22	1:A:116:LYS:H	1.22	1.02
2:B:140:VAL:HG13	2:B:144:GLU:HB2	1.44	0.98
1:C:722:ARG:HH12	5:D:7200:GNP:HNB3	1.08	0.98
1:A:682:PRO:O	1:A:683:GLN:HG2	1.71	0.90
1:C:598:VAL:HA	1:C:601:ASN:HD22	1.36	0.89
1:C:651:ASN:H	1:C:651:ASN:HD22	1.24	0.86
1:C:714:THR:HG21	1:C:721:ALA:HA	1.57	0.85
1:C:171:LEU:HB3	1:C:237:LYS:HE3	1.58	0.84
1:C:327:LYS:O	1:C:331:GLN:HG3	1.77	0.84
1:A:722:ARG:HH12	5:B:5200:GNP:HNB3	1.23	0.84
1:A:220:THR:HG22	1:A:222:PHE:H	1.42	0.83
2:D:155:THR:HG23	2:D:156:GLY:H	1.43	0.83
1:C:114:THR:HB	1:C:500:ASN:O	1.79	0.82
1:A:166:VAL:CG2	1:A:182:PHE:HB2	2.10	0.81
1:A:60:HIS:HD2	1:A:428:ASP:HB2	1.46	0.81
1:A:371:LEU:HD21	2:B:56:HIS:HE1	1.46	0.80
1:A:193:LEU:HA	1:A:196:MET:HE3	1.63	0.80
2:B:57:PRO:HB3	2:B:74:LEU:HD22	1.62	0.80
1:A:74:ARG:HG3	1:A:75:ASN:H	1.47	0.79
2:D:140:VAL:CG1	2:D:144:GLU:HB2	2.12	0.79
2:D:117:PHE:HA	2:D:164:ARG:HH12	1.48	0.78
1:C:324:LYS:HA	1:C:327:LYS:HE3	1.66	0.78
1:C:600:ASN:HB2	2:D:51:LEU:HD23	1.66	0.77
1:C:153:PRO:HB3	1:C:232:GLU:HG3	1.66	0.76
2:D:155:THR:CG2	2:D:166:VAL:H	2.00	0.75
1:C:164:ASN:HD22	1:C:164:ASN:H	1.33	0.74
1:C:588:TYR:O	1:C:591:ARG:HG2	1.87	0.74
2:D:140:VAL:HG13	2:D:144:GLU:HB2	1.68	0.74
1:C:166:VAL:HG22	1:C:182:PHE:HB2	1.69	0.73
2:B:140:VAL:CG1	2:B:144:GLU:HB2	2.18	0.73
1:C:191:GLU:CD	1:C:202:PRO:HG3	2.15	0.72
1:C:201:LYS:HG3	1:C:202:PRO:HA	1.71	0.71
2:D:117:PHE:HD2	2:D:164:ARG:NH1	1.88	0.71
1:C:574:PHE:O	1:C:575:ARG:HG3	1.90	0.71
1:A:220:THR:HG23	1:A:221:PRO:HD2	1.73	0.70
2:D:45:ASN:O	2:D:47:ARG:HG3	1.91	0.70
2:B:154:THR:HB	2:B:166:VAL:O	1.91	0.70
1:A:682:PRO:C	1:A:684:TYR:H	1.98	0.70
2:D:41:HIS:CE1	2:D:45:ASN:HD22	2.09	0.70
1:A:651:ASN:H	1:A:651:ASN:HD22	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ASN:O	1:A:110:ILE:HG13	1.92	0.69
1:C:634:MET:SD	1:C:686:ASP:HB3	2.32	0.69
1:A:327:LYS:O	1:A:331:GLN:HG3	1.93	0.69
2:D:113:LEU:HG	2:D:117:PHE:CE1	2.27	0.68
1:A:219:VAL:HG23	1:A:220:THR:H	1.59	0.68
1:C:114:THR:HG22	1:C:116:LYS:N	2.00	0.68
1:A:557:ILE:HD13	1:A:762:VAL:HG11	1.75	0.68
1:C:756:MET:O	1:C:759:LEU:HB3	1.94	0.68
1:A:574:PHE:CD2	1:A:760:GLN:HG2	2.29	0.67
1:C:111:GLU:HB2	1:C:503:ARG:HD3	1.76	0.67
1:A:564:ALA:HB2	1:A:576:LEU:HD13	1.77	0.67
2:D:85:LYS:HA	2:D:88:PHE:CD2	2.29	0.67
2:D:110:ARG:HG3	2:D:110:ARG:HH11	1.59	0.67
1:C:74:ARG:HG3	1:C:75:ASN:H	1.59	0.67
1:C:514:PHE:O	1:C:514:PHE:CD2	2.48	0.67
1:A:264:SER:O	1:A:268:ILE:HG12	1.95	0.66
1:A:132:SER:HB3	1:A:289:SER:OG	1.96	0.66
2:D:117:PHE:CA	2:D:164:ARG:HH12	2.09	0.66
2:D:85:LYS:HA	2:D:88:PHE:CE2	2.30	0.66
1:A:175:THR:HG23	1:C:196:MET:SD	2.36	0.66
1:A:298:LEU:HD12	1:A:299:ILE:N	2.10	0.65
2:D:128:VAL:HG22	2:D:185:TRP:HZ3	1.60	0.65
2:D:155:THR:HG21	2:D:166:VAL:H	1.62	0.65
1:A:702:LEU:CD2	1:A:709:PRO:HG2	2.26	0.65
1:C:492:THR:HG22	6:C:821:HOH:O	1.95	0.65
2:D:129:ILE:HB	2:D:168:VAL:HG22	1.78	0.65
2:D:100:ALA:HB3	2:D:132:ASN:O	1.97	0.65
1:C:301:ASN:ND2	1:C:306:ASP:OD1	2.30	0.65
1:C:677:GLY:HA2	1:C:679:GLN:NE2	2.12	0.65
1:A:550:ARG:O	1:A:554:ARG:HG2	1.96	0.65
1:C:682:PRO:C	1:C:684:TYR:H	2.04	0.64
1:A:436:GLU:HG2	1:A:440:GLY:HA3	1.79	0.64
1:C:589:TYR:OH	1:C:643:LEU:HB3	1.96	0.64
1:A:166:VAL:HG22	1:A:182:PHE:HB2	1.79	0.64
1:C:406:VAL:HG21	1:C:458:ILE:HD13	1.79	0.64
1:C:47:ASN:O	1:C:110:ILE:HG13	1.97	0.63
1:C:605:GLU:HG3	2:D:55:TRP:CE3	2.34	0.63
2:D:110:ARG:HD2	2:D:148:ALA:O	1.99	0.63
1:A:130:LEU:HD11	1:A:161:THR:HG23	1.79	0.63
1:C:347:ALA:HB2	1:C:353:ILE:HD13	1.81	0.63
2:D:128:VAL:HG22	2:D:185:TRP:CZ3	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:PRO:HD2	6:A:804:HOH:O	1.98	0.62
2:D:117:PHE:HA	2:D:164:ARG:NH1	2.14	0.62
1:C:616:GLU:CG	1:C:620:ASN:HB2	2.29	0.62
1:C:349:CYS:O	1:C:373:ASP:HA	1.99	0.62
2:D:132:ASN:O	2:D:133:LYS:HB2	1.99	0.62
1:C:171:LEU:CB	1:C:237:LYS:HE3	2.27	0.62
2:D:155:THR:HG23	2:D:156:GLY:N	2.12	0.62
1:C:171:LEU:HD12	1:C:171:LEU:N	2.14	0.62
2:D:101:ALA:C	2:D:103:PRO:HD3	2.25	0.61
1:C:102:PRO:HD2	1:C:105:LEU:HD12	1.82	0.61
2:B:99:ASP:OD1	2:B:133:LYS:HD2	2.00	0.61
1:C:653:ILE:HA	1:C:665:TYR:O	2.00	0.61
1:C:722:ARG:NH1	5:D:7200:GNP:HNB3	1.89	0.61
1:A:241:LEU:C	1:A:241:LEU:HD23	2.26	0.61
1:C:729:ASN:HD21	1:C:752:LEU:H	1.49	0.60
1:C:71:ILE:HD13	1:C:78:TRP:HB3	1.84	0.60
1:C:514:PHE:O	1:C:514:PHE:HD2	1.83	0.60
1:C:198:THR:HG22	1:C:222:PHE:O	2.01	0.60
1:C:324:LYS:HA	1:C:327:LYS:CE	2.31	0.60
1:C:677:GLY:HA2	1:C:679:GLN:HE22	1.65	0.60
1:A:170:ASP:HB3	1:A:178:ARG:HB2	1.82	0.60
1:C:512:LEU:HD13	1:C:516:THR:HG21	1.84	0.60
1:C:415:GLN:HE21	1:C:435:SER:HB3	1.67	0.60
1:A:234:VAL:HG12	1:A:234:VAL:O	2.00	0.59
2:D:42:MET:HE3	2:D:173:VAL:O	2.02	0.59
1:C:264:SER:O	1:C:268:ILE:HG12	2.02	0.59
2:D:43:LEU:HD22	2:D:64:ILE:HD11	1.83	0.59
1:C:569:ASP:O	1:C:571:PRO:HD3	2.01	0.59
2:B:67:ILE:CD1	2:B:190:ILE:HD11	2.32	0.59
1:C:66:ASN:HD22	1:C:68:TYR:H	1.49	0.59
1:A:164:ASN:HD22	1:A:164:ASN:H	1.48	0.59
2:D:117:PHE:CD2	2:D:164:ARG:NH1	2.69	0.59
1:C:234:VAL:HG12	1:C:234:VAL:O	2.02	0.59
2:B:146:ARG:HH12	2:B:154:THR:CG2	2.16	0.58
2:B:155:THR:HG23	2:B:156:GLY:H	1.66	0.58
1:A:371:LEU:HD21	2:B:56:HIS:CE1	2.33	0.58
1:A:298:LEU:HD11	1:A:300:VAL:O	2.02	0.58
1:C:191:GLU:OE2	1:C:202:PRO:HG3	2.03	0.58
2:D:51:LEU:HD12	2:D:51:LEU:N	2.17	0.58
1:A:273:LEU:HB3	1:A:341:HIS:CE1	2.38	0.58
1:A:757:THR:O	1:A:761:GLN:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ASP:OD1	1:C:178:ARG:N	2.37	0.58
1:C:616:GLU:HG2	1:C:620:ASN:HB2	1.83	0.58
1:A:323:LYS:O	1:A:327:LYS:HG3	2.04	0.58
1:C:600:ASN:HB2	2:D:51:LEU:CD2	2.33	0.58
2:D:169:PHE:CD2	2:D:182:ALA:HA	2.39	0.58
1:C:46:LEU:HD12	6:C:827:HOH:O	2.03	0.58
1:C:114:THR:CG2	1:C:116:LYS:H	2.02	0.58
1:A:454:HIS:CD2	1:A:615:ARG:HG3	2.39	0.58
1:C:298:LEU:HD11	1:C:300:VAL:C	2.29	0.57
2:D:141:SER:C	2:D:143:ALA:H	2.12	0.57
1:A:722:ARG:NH1	5:B:5200:GNP:HNB3	1.99	0.57
1:A:153:PRO:HB3	1:A:232:GLU:HG3	1.86	0.57
1:C:420:HIS:CE1	1:C:615:ARG:HB2	2.40	0.57
1:C:663:LEU:C	1:C:663:LEU:HD23	2.29	0.57
2:D:155:THR:HG22	2:D:166:VAL:H	1.69	0.57
1:A:220:THR:HG23	1:A:221:PRO:CD	2.35	0.57
1:A:420:HIS:CE1	1:A:615:ARG:HB2	2.40	0.57
1:C:579:ASN:OD1	1:C:580:PHE:HD1	1.88	0.57
2:D:29:LEU:HD22	2:D:84:TRP:CD2	2.40	0.57
2:D:122:LEU:O	2:D:164:ARG:NH2	2.37	0.57
1:A:193:LEU:HA	1:A:196:MET:CE	2.35	0.57
1:C:171:LEU:HD23	1:C:237:LYS:HG2	1.87	0.57
2:B:155:THR:CG2	2:B:166:VAL:H	2.17	0.57
2:D:29:LEU:HB3	2:D:84:TRP:CZ3	2.40	0.57
1:A:161:THR:HB	1:A:169:HIS:NE2	2.19	0.56
1:C:570:ASP:OD2	1:C:573:SER:HB3	2.06	0.56
2:D:164:ARG:O	2:D:166:VAL:HG23	2.05	0.56
1:A:531:LEU:O	1:A:535:ILE:HG13	2.06	0.56
1:A:682:PRO:C	1:A:684:TYR:N	2.62	0.56
2:B:50:THR:O	2:B:50:THR:HG23	2.06	0.56
2:B:110:ARG:HH11	2:B:110:ARG:HG3	1.71	0.56
1:A:7:GLU:O	1:A:41:LYS:NZ	2.39	0.55
1:A:332:ILE:O	1:A:336:VAL:HG22	2.06	0.55
1:A:570:ASP:OD2	1:A:573:SER:HB3	2.07	0.55
1:C:386:ARG:NH2	1:C:708:LEU:CD1	2.69	0.55
1:C:682:PRO:C	1:C:684:TYR:N	2.64	0.55
1:A:176:ILE:HD11	1:C:183:ARG:HG2	1.88	0.55
1:C:161:THR:HG22	1:C:167:GLN:HB2	1.89	0.55
1:A:131:THR:OG1	1:A:260:ARG:NH1	2.39	0.55
1:A:42:GLU:OE2	1:A:397:LYS:HE2	2.07	0.55
1:A:702:LEU:HD23	1:A:709:PRO:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:714:THR:HG21	1:C:721:ALA:CA	2.34	0.55
1:A:588:TYR:O	1:A:591:ARG:HG2	2.07	0.55
1:A:682:PRO:O	1:A:684:TYR:N	2.40	0.55
2:B:155:THR:HG22	2:B:166:VAL:H	1.72	0.55
1:A:514:PHE:O	1:A:514:PHE:CD2	2.59	0.54
1:A:634:MET:HE1	1:A:687:PHE:HA	1.89	0.54
1:A:745:VAL:HG23	1:A:747:THR:HG22	1.87	0.54
1:C:451:SER:HB2	1:C:452:PRO:CD	2.38	0.54
2:D:31:LEU:O	2:D:36:LYS:NZ	2.40	0.54
1:C:330:ASN:O	1:C:334:GLN:HG3	2.07	0.54
1:C:60:HIS:HD2	1:C:428:ASP:HB2	1.73	0.54
2:D:147:SER:OG	2:D:152:LEU:HD21	2.07	0.54
2:B:32:ASP:HA	5:B:5200:GNP:O3G	2.07	0.54
2:B:38:THR:HG22	2:B:173:VAL:HG11	1.89	0.54
1:C:161:THR:HG23	1:C:167:GLN:NE2	2.23	0.54
1:C:42:GLU:HG3	1:C:452:PRO:HB3	1.89	0.54
1:C:514:PHE:CD2	1:C:514:PHE:C	2.85	0.54
2:B:43:LEU:HD13	2:B:64:ILE:HD11	1.89	0.54
1:A:651:ASN:HD22	1:A:651:ASN:N	2.00	0.54
2:D:31:LEU:CD2	2:D:108:GLU:HG2	2.38	0.54
2:D:169:PHE:CE2	2:D:182:ALA:HA	2.43	0.54
1:C:386:ARG:NH1	1:C:705:ARG:O	2.41	0.53
1:C:298:LEU:O	6:C:825:HOH:O	2.18	0.53
2:D:88:PHE:O	2:D:91:VAL:HG23	2.07	0.53
2:D:171:CYS:HB3	2:D:178:GLY:C	2.33	0.53
1:A:116:LYS:HB3	1:A:500:ASN:HD22	1.74	0.53
1:A:544:ASP:O	1:A:548:VAL:HG23	2.09	0.53
1:A:161:THR:HG22	1:A:167:GLN:CD	2.34	0.53
1:C:231:LEU:O	1:C:235:GLU:HB2	2.09	0.53
2:D:83:LEU:O	2:D:86:ASP:HB2	2.08	0.53
1:A:324:LYS:HA	1:A:327:LYS:CE	2.38	0.53
1:C:293:THR:HG22	1:C:300:VAL:O	2.09	0.53
1:C:132:SER:HB3	1:C:289:SER:OG	2.09	0.53
1:C:602:SER:OG	1:C:605:GLU:HB2	2.09	0.53
1:C:722:ARG:C	1:C:724:LEU:H	2.16	0.53
2:D:29:LEU:HD22	2:D:84:TRP:CE3	2.43	0.53
2:B:99:ASP:CG	2:B:133:LYS:HD2	2.34	0.52
1:A:616:GLU:CG	1:A:620:ASN:HB2	2.40	0.52
2:B:128:VAL:CG2	2:B:186:LEU:HD13	2.40	0.52
2:B:40:LEU:HD22	2:B:73:ASP:HB2	1.91	0.52
1:C:358:MET:HB3	1:C:361:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:57:PRO:HG2	2:D:87:TYR:HE2	1.75	0.52
2:D:95:VAL:O	2:D:97:LEU:HD12	2.10	0.52
1:C:166:VAL:HG21	1:C:268:ILE:HG13	1.92	0.52
1:A:111:GLU:HB2	1:A:503:ARG:HD3	1.92	0.52
1:C:13:ARG:HG3	1:C:527:ALA:HB2	1.91	0.52
1:C:161:THR:HG23	1:C:167:GLN:HE21	1.73	0.52
1:C:279:ASN:HA	1:C:339:ASN:O	2.10	0.52
1:C:605:GLU:HG3	2:D:55:TRP:CZ3	2.44	0.52
1:C:651:ASN:HD22	1:C:651:ASN:N	1.92	0.52
2:D:48:LEU:HG	2:D:49:ALA:N	2.25	0.52
2:D:25:LYS:O	2:D:92:ASN:HB2	2.11	0.51
1:C:147:SER:HB3	1:C:384:TYR:CE2	2.45	0.51
1:C:185:ASP:HA	1:C:295:ALA:O	2.11	0.51
2:D:66:ASN:N	2:D:66:ASN:HD22	2.08	0.51
1:C:130:LEU:HD21	1:C:245:LEU:HG	1.92	0.51
1:C:415:GLN:HE21	1:C:435:SER:CB	2.23	0.51
1:C:616:GLU:HG3	1:C:620:ASN:HB2	1.93	0.51
1:A:616:GLU:HG2	1:A:620:ASN:HB2	1.92	0.51
1:A:629:LEU:HD22	1:A:643:LEU:HD12	1.93	0.51
1:C:167:GLN:HB3	1:C:179:CYS:SG	2.49	0.51
1:C:323:LYS:O	1:C:327:LYS:HG3	2.11	0.51
2:B:85:LYS:HA	2:B:88:PHE:CD2	2.44	0.51
1:C:602:SER:O	1:C:603:PRO:C	2.51	0.51
1:C:353:ILE:HD11	1:C:355:MET:HE3	1.93	0.51
1:C:678:TYR:O	1:C:684:TYR:HB3	2.10	0.51
1:A:615:ARG:NH1	6:A:814:HOH:O	2.41	0.51
1:A:721:ALA:O	1:A:725:LEU:HG	2.11	0.51
1:C:241:LEU:HD23	1:C:241:LEU:C	2.35	0.51
1:A:634:MET:CE	1:A:687:PHE:HA	2.41	0.51
1:A:651:ASN:H	1:A:651:ASN:ND2	2.05	0.51
1:C:618:THR:O	1:C:622:LEU:HG	2.11	0.51
2:D:31:LEU:HD11	2:D:109:ALA:HB2	1.92	0.51
2:D:134:ILE:C	2:D:136:ALA:H	2.19	0.51
1:A:23:ARG:HG3	1:A:462:ILE:O	2.10	0.50
1:A:68:TYR:O	1:A:81:PRO:HG3	2.11	0.50
1:C:72:ASP:OD1	1:C:74:ARG:HG3	2.11	0.50
1:C:566:TYR:CD1	1:C:764:VAL:HG12	2.46	0.50
2:D:69:PHE:O	2:D:71:THR:HG23	2.10	0.50
1:A:55:VAL:HG12	1:A:56:CYS:O	2.11	0.50
2:B:187:SER:O	2:B:190:ILE:HG13	2.11	0.50
1:A:129:ASP:OD2	1:A:260:ARG:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:677:GLY:O	1:C:679:GLN:N	2.45	0.50
2:D:141:SER:C	2:D:143:ALA:N	2.67	0.50
2:D:155:THR:HG21	2:D:165:PRO:HA	1.94	0.50
1:C:19:PHE:HB2	1:C:511:LEU:HD23	1.93	0.50
1:C:658:THR:O	1:C:659:PHE:HB3	2.11	0.50
1:C:661:PHE:HB2	1:C:710:ARG:O	2.12	0.50
1:C:136:ASN:OD1	1:C:375:PHE:HD1	1.95	0.50
1:C:682:PRO:O	1:C:683:GLN:HG2	2.12	0.50
2:D:115:ALA:O	2:D:119:ILE:HG12	2.12	0.50
2:D:132:ASN:HA	2:D:171:CYS:O	2.12	0.50
2:B:73:ASP:C	2:B:74:LEU:HD23	2.37	0.49
2:D:32:ASP:O	2:D:33:ASN:HB3	2.12	0.49
2:D:43:LEU:HD22	2:D:64:ILE:CD1	2.42	0.49
2:D:99:ASP:CG	2:D:102:ASP:HB2	2.36	0.49
1:C:712:ILE:HG22	1:C:713:ASP:N	2.27	0.49
2:D:78:ILE:HG23	2:D:79:GLN:N	2.27	0.49
1:A:66:ASN:HB2	1:A:67:PRO:CD	2.43	0.49
1:C:170:ASP:C	1:C:171:LEU:HD12	2.37	0.49
1:C:564:ALA:HB2	1:C:576:LEU:HD13	1.94	0.49
2:D:129:ILE:HG22	2:D:130:LEU:N	2.27	0.49
1:A:171:LEU:HD12	1:A:171:LEU:N	2.27	0.49
1:C:220:THR:HG22	1:C:222:PHE:H	1.75	0.49
1:C:714:THR:HB	1:C:720:GLN:HB2	1.92	0.49
1:C:399:ALA:HB3	1:C:450:LEU:HD13	1.93	0.49
1:C:423:ALA:HB2	1:C:439:ILE:CG2	2.43	0.49
1:C:520:ALA:HB2	1:C:563:TYR:HE2	1.76	0.49
1:C:583:TYR:HB3	1:C:584:PRO:HD3	1.94	0.49
1:A:634:MET:HE1	1:A:687:PHE:HD1	1.76	0.49
1:C:317:ASP:OD1	1:C:317:ASP:O	2.30	0.49
2:D:26:LEU:O	2:D:27:LEU:HD23	2.13	0.49
2:D:50:THR:HG23	2:D:50:THR:O	2.12	0.49
1:A:432:ILE:HD13	1:A:442:THR:HA	1.94	0.49
1:A:637:ASP:O	1:A:638:PRO:C	2.55	0.49
1:C:402:GLY:HA2	1:C:492:THR:O	2.12	0.49
1:C:637:ASP:O	1:C:638:PRO:C	2.56	0.49
1:A:238:LEU:HD22	1:A:242:LEU:HD11	1.95	0.49
1:C:171:LEU:HB3	1:C:237:LYS:CE	2.38	0.49
1:C:644:ASP:OD2	1:C:729:ASN:HB3	2.13	0.49
2:D:31:LEU:HD22	2:D:108:GLU:HG2	1.95	0.49
1:A:173:SER:OG	1:A:174:GLU:N	2.43	0.48
1:A:354:GLY:O	1:A:358:MET:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LYS:HE2	1:A:363:ASP:OD2	2.12	0.48
1:A:512:LEU:HD13	1:A:516:THR:HG21	1.93	0.48
2:B:26:LEU:HB2	2:B:71:THR:HG22	1.94	0.48
1:C:253:PRO:O	1:C:256:HIS:HB2	2.13	0.48
2:D:73:ASP:C	2:D:74:LEU:HD23	2.38	0.48
1:A:327:LYS:NZ	6:A:828:HOH:O	2.46	0.48
1:A:455:SER:O	1:A:534:ARG:NH2	2.47	0.48
2:B:128:VAL:HG22	2:B:185:TRP:CZ3	2.48	0.48
1:C:309:ARG:NH2	1:C:357:GLU:OE1	2.38	0.48
1:A:74:ARG:HG3	1:A:75:ASN:N	2.24	0.48
1:A:278:LYS:HG2	1:A:279:ASN:ND2	2.29	0.48
1:C:10:ASN:O	1:C:12:VAL:HG23	2.13	0.48
1:A:238:LEU:HD22	1:A:242:LEU:CD1	2.44	0.48
1:A:409:SER:HB2	1:A:411:ASP:OD2	2.14	0.48
1:C:533:ALA:O	1:C:537:VAL:HG23	2.13	0.48
1:C:744:ILE:HG22	1:C:745:VAL:N	2.28	0.48
1:C:20:PRO:HG2	1:C:29:ASN:ND2	2.29	0.48
1:C:656:LEU:HD22	1:C:724:LEU:HD13	1.94	0.48
1:A:464:ASN:HB2	6:A:852:HOH:O	2.14	0.48
1:A:645:SER:HA	1:A:728:LEU:HD13	1.95	0.48
1:C:520:ALA:HB2	1:C:563:TYR:CE2	2.49	0.48
2:D:176:ARG:HA	2:D:179:TYR:CE2	2.49	0.48
1:A:130:LEU:CD1	1:A:161:THR:HG23	2.43	0.48
1:C:166:VAL:CG2	1:C:182:PHE:HB2	2.42	0.48
1:C:552:LEU:HD21	1:C:590:LEU:HD23	1.96	0.48
2:B:128:VAL:HG22	2:B:185:TRP:HZ3	1.79	0.47
1:C:200:GLN:O	1:C:201:LYS:O	2.32	0.47
2:D:171:CYS:HB2	2:D:177:ASN:O	2.13	0.47
1:C:19:PHE:CD1	1:C:19:PHE:N	2.80	0.47
1:C:200:GLN:O	1:C:201:LYS:C	2.56	0.47
1:C:574:PHE:CD2	1:C:760:GLN:HG2	2.49	0.47
2:D:40:LEU:HD22	2:D:73:ASP:CB	2.44	0.47
2:B:41:HIS:CE1	2:B:45:ASN:HD22	2.33	0.47
2:B:142:GLU:O	2:B:146:ARG:HB2	2.14	0.47
1:C:155:ALA:O	1:C:230:PRO:HA	2.14	0.47
1:C:195:GLU:O	1:C:199:GLY:HA2	2.13	0.47
2:D:154:THR:HB	2:D:166:VAL:O	2.15	0.47
1:A:92:GLN:C	1:A:93:TYR:HD1	2.21	0.47
1:C:440:GLY:O	1:C:441:ALA:HB3	2.13	0.47
1:A:195:GLU:O	1:A:199:GLY:HA2	2.15	0.47
1:A:534:ARG:NH1	6:A:808:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ILE:HG21	1:A:238:LEU:HD11	1.96	0.47
1:A:161:THR:HG22	1:A:167:GLN:HB2	1.95	0.47
1:C:408:THR:HB	1:C:412:LEU:HB3	1.97	0.47
1:C:646:ILE:HG22	1:C:646:ILE:O	2.14	0.47
2:D:99:ASP:C	2:D:101:ALA:H	2.23	0.47
2:D:103:PRO:HA	2:D:106:PHE:CE2	2.49	0.47
1:A:650:PRO:O	1:A:669:GLN:HB3	2.14	0.47
1:C:396:LEU:HB3	1:C:398:MET:HG2	1.97	0.47
1:C:456:TYR:CD1	1:C:456:TYR:N	2.82	0.47
2:D:99:ASP:HB3	2:D:102:ASP:HB3	1.96	0.47
1:A:15:THR:HG22	1:A:528:ALA:HA	1.97	0.47
1:A:255:GLY:HA2	1:A:304:LEU:HD12	1.95	0.47
1:A:653:ILE:HG13	1:A:670:ILE:HD13	1.97	0.47
1:A:200:GLN:O	1:A:201:LYS:C	2.57	0.47
1:C:590:LEU:O	1:C:596:LEU:HD12	2.15	0.47
2:D:110:ARG:NH1	2:D:149:LEU:O	2.48	0.47
1:A:330:ASN:O	1:A:334:GLN:HG3	2.15	0.46
1:C:409:SER:OG	1:C:486:TYR:HB2	2.15	0.46
1:C:712:ILE:HD13	1:C:723:PHE:CD1	2.50	0.46
1:A:703:VAL:HG12	1:A:704:ASP:CG	2.40	0.46
1:C:25:ASP:O	1:C:29:ASN:ND2	2.47	0.46
1:C:682:PRO:O	1:C:684:TYR:N	2.48	0.46
2:D:129:ILE:HG22	2:D:130:LEU:H	1.80	0.46
2:D:169:PHE:HZ	2:D:185:TRP:HB2	1.80	0.46
1:C:281:PRO:HB3	1:C:400:PHE:HB3	1.97	0.46
1:C:679:GLN:HG3	1:C:687:PHE:CD2	2.50	0.46
1:A:13:ARG:HG3	1:A:527:ALA:HB2	1.97	0.46
1:A:592:ARG:HD3	6:A:866:HOH:O	2.15	0.46
1:A:722:ARG:HD3	5:B:5200:GNP:H5'1	1.96	0.46
1:A:324:LYS:HA	1:A:327:LYS:HE3	1.96	0.46
1:C:600:ASN:CB	2:D:51:LEU:HD23	2.40	0.46
1:C:677:GLY:C	1:C:679:GLN:H	2.22	0.46
1:A:74:ARG:C	1:A:76:SER:H	2.23	0.46
1:A:298:LEU:HD12	1:A:299:ILE:H	1.80	0.46
1:A:351:ASP:HB3	6:A:871:HOH:O	2.15	0.46
2:B:32:ASP:O	2:B:33:ASN:HB3	2.15	0.46
1:C:229:LEU:CD1	1:C:234:VAL:HG21	2.46	0.46
1:C:536:ALA:O	1:C:539:LYS:HB2	2.15	0.46
2:D:169:PHE:HZ	2:D:185:TRP:CB	2.28	0.46
1:A:51:TYR:HD1	1:A:52:ASN:O	1.99	0.46
1:C:53:PRO:HG2	1:C:502:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:616:GLU:HG3	1:C:617:ASP:H	1.81	0.46
1:C:631:SER:OG	1:C:652:THR:HB	2.16	0.46
2:B:29:LEU:C	2:B:36:LYS:HD3	2.41	0.46
2:D:181:GLU:O	2:D:184:GLN:HB3	2.16	0.46
1:A:747:THR:HB	2:B:50:THR:HG22	1.98	0.46
2:B:88:PHE:N	2:B:89:PRO:CD	2.79	0.46
1:C:298:LEU:HD11	1:C:300:VAL:O	2.15	0.46
1:A:293:THR:HA	1:A:298:LEU:HD13	1.98	0.45
2:D:103:PRO:HA	2:D:106:PHE:CZ	2.51	0.45
1:A:377:THR:O	1:A:381:LYS:HG3	2.16	0.45
2:B:146:ARG:HH12	2:B:154:THR:HG23	1.80	0.45
1:C:145:ILE:HG23	1:C:239:ASN:OD1	2.15	0.45
1:C:399:ALA:HB3	1:C:450:LEU:CD1	2.47	0.45
1:C:729:ASN:HA	1:C:730:PRO:HD3	1.69	0.45
1:C:758:HIS:CE1	1:C:762:VAL:HG21	2.51	0.45
1:C:182:PHE:HZ	1:C:197:LEU:HD21	1.82	0.45
1:C:634:MET:SD	1:C:686:ASP:CB	3.04	0.45
2:D:175:MET:O	2:D:176:ARG:C	2.59	0.45
2:B:67:ILE:HD13	2:B:190:ILE:HD11	1.97	0.45
1:C:662:ILE:HG21	1:C:698:ALA:HB1	1.98	0.45
1:C:171:LEU:CA	1:C:237:LYS:HE3	2.46	0.45
2:D:84:TRP:H	2:D:84:TRP:CD1	2.35	0.45
1:A:616:GLU:HG2	1:A:620:ASN:CB	2.45	0.45
2:D:181:GLU:CD	2:D:181:GLU:H	2.24	0.45
2:B:179:TYR:O	2:B:182:ALA:HB3	2.17	0.45
1:C:666:HIS:HB2	1:C:715:GLU:HG2	1.98	0.45
1:A:526:GLU:HB3	1:A:622:LEU:HD11	1.98	0.45
1:A:589:TYR:O	1:A:592:ARG:HG3	2.17	0.45
1:C:161:THR:CG2	1:C:167:GLN:NE2	2.79	0.45
1:C:171:LEU:N	1:C:171:LEU:CD1	2.79	0.45
1:C:714:THR:OG1	1:C:715:GLU:N	2.49	0.45
1:A:66:ASN:ND2	1:A:68:TYR:H	2.15	0.45
1:A:176:ILE:O	1:A:177:ASP:HB2	2.17	0.45
1:C:386:ARG:NH2	1:C:708:LEU:HD12	2.31	0.45
1:C:603:PRO:O	1:C:604:ASP:C	2.60	0.45
2:B:146:ARG:NH1	2:B:154:THR:HG23	2.32	0.45
1:C:90:PRO:HG2	1:C:93:TYR:CD1	2.52	0.45
1:C:41:LYS:O	1:C:503:ARG:NH2	2.49	0.44
1:C:677:GLY:C	1:C:679:GLN:N	2.76	0.44
2:D:66:ASN:N	2:D:66:ASN:ND2	2.63	0.44
1:A:566:TYR:HB2	1:A:764:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ARG:HG3	1:C:75:ASN:N	2.29	0.44
1:C:587:THR:O	1:C:591:ARG:HD2	2.17	0.44
2:D:31:LEU:CD1	2:D:109:ALA:HB2	2.47	0.44
1:C:134:THR:HG22	1:C:138:ASP:OD2	2.18	0.44
1:C:342:THR:OG1	1:C:449:SER:HB2	2.17	0.44
1:C:14:PHE:CD2	1:C:35:CYS:HB3	2.52	0.44
2:D:171:CYS:SG	2:D:179:TYR:HB3	2.58	0.44
1:A:663:LEU:C	1:A:663:LEU:HD23	2.42	0.44
2:B:83:LEU:O	2:B:86:ASP:HB2	2.16	0.44
2:D:100:ALA:HB2	2:D:131:GLY:C	2.42	0.44
1:A:114:THR:HG22	1:A:115:ASN:N	2.33	0.44
1:C:589:TYR:CE2	1:C:643:LEU:HD23	2.52	0.44
1:C:623:ILE:HG22	1:C:659:PHE:HB2	1.99	0.44
1:C:66:ASN:HB2	1:C:67:PRO:CD	2.47	0.44
1:C:643:LEU:HG	1:C:727:LYS:O	2.17	0.44
1:C:714:THR:OG1	1:C:721:ALA:HB2	2.17	0.44
1:C:455:SER:O	1:C:534:ARG:NH2	2.51	0.44
1:C:557:ILE:O	1:C:559:LEU:N	2.51	0.44
1:C:722:ARG:C	1:C:724:LEU:N	2.76	0.44
1:A:88:HIS:O	1:A:89:LEU:C	2.60	0.44
1:A:139:SER:OG	1:A:376:SER:HA	2.18	0.44
1:A:583:TYR:HB3	1:A:584:PRO:HD3	1.99	0.44
2:B:129:ILE:HG21	2:B:149:LEU:CD1	2.48	0.44
1:C:69:CYS:SG	1:C:81:PRO:HD3	2.58	0.44
1:C:193:LEU:HA	1:C:196:MET:HE3	2.00	0.44
1:C:697:GLU:O	1:C:701:LEU:HG	2.18	0.44
1:C:747:THR:HB	2:D:50:THR:HG22	2.00	0.44
2:D:110:ARG:HG3	2:D:110:ARG:NH1	2.30	0.44
1:A:567:ASN:O	1:A:568:LYS:C	2.61	0.43
2:B:33:ASN:H	5:B:5200:GNP:HNB3	1.65	0.43
1:C:164:ASN:H	1:C:164:ASN:ND2	2.08	0.43
1:A:663:LEU:HD23	1:A:664:ILE:N	2.33	0.43
1:C:148:LEU:O	1:C:231:LEU:HD21	2.18	0.43
1:A:12:VAL:HG22	1:A:37:TYR:CD1	2.53	0.43
1:C:641:VAL:O	1:C:642:LEU:C	2.61	0.43
2:B:48:LEU:HA	6:B:5201:HOH:O	2.18	0.43
1:C:29:ASN:O	1:C:31:VAL:N	2.51	0.43
1:A:177:ASP:OD1	1:A:178:ARG:N	2.52	0.43
1:A:366:GLY:HA2	1:A:420:HIS:HB3	2.01	0.43
1:C:724:LEU:HD11	1:C:728:LEU:HD21	2.01	0.43
2:D:140:VAL:HG13	2:D:144:GLU:CD	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ASN:H	1:A:164:ASN:ND2	2.17	0.43
1:A:605:GLU:HG2	1:A:609:TYR:CE1	2.53	0.43
1:C:347:ALA:CB	1:C:353:ILE:HD13	2.47	0.43
2:B:67:ILE:HD11	2:B:190:ILE:HD11	2.00	0.43
1:C:649:LYS:HB2	1:C:652:THR:OG1	2.18	0.43
2:B:105:ARG:HD2	2:B:108:GLU:OE1	2.19	0.43
1:C:355:MET:H	1:C:604:ASP:CG	2.27	0.43
2:B:164:ARG:HA	2:B:165:PRO:HD3	1.84	0.42
1:C:13:ARG:NE	1:C:524:ASP:OD2	2.49	0.42
2:D:134:ILE:C	2:D:136:ALA:N	2.77	0.42
1:A:66:ASN:HD22	1:A:68:TYR:H	1.65	0.42
1:A:451:SER:HB2	1:A:452:PRO:CD	2.49	0.42
2:B:29:LEU:O	2:B:96:PHE:HA	2.18	0.42
1:C:19:PHE:HA	1:C:20:PRO:HD3	1.84	0.42
1:C:415:GLN:NE2	1:C:435:SER:HB3	2.32	0.42
1:C:582:LEU:O	1:C:583:TYR:C	2.62	0.42
2:D:151:LEU:O	2:D:154:THR:HG23	2.18	0.42
1:A:507:VAL:HB	6:A:877:HOH:O	2.19	0.42
1:A:537:VAL:O	1:A:540:ALA:HB3	2.19	0.42
1:C:585:GLN:O	1:C:588:TYR:HB3	2.19	0.42
2:D:179:TYR:O	2:D:182:ALA:HB3	2.19	0.42
1:C:557:ILE:O	1:C:558:LYS:C	2.62	0.42
1:C:589:TYR:HB3	1:C:625:ILE:O	2.19	0.42
2:B:146:ARG:NH1	2:B:154:THR:CG2	2.83	0.42
1:C:451:SER:HB2	1:C:452:PRO:HD2	2.00	0.42
1:C:598:VAL:HA	1:C:601:ASN:ND2	2.17	0.42
2:D:42:MET:O	2:D:46:ASP:HA	2.20	0.42
2:D:128:VAL:HG21	2:D:186:LEU:HB2	2.01	0.42
1:A:248:ASP:OD1	1:A:248:ASP:C	2.61	0.42
1:A:298:LEU:HD11	1:A:300:VAL:C	2.45	0.42
1:C:229:LEU:HD12	1:C:234:VAL:HG21	2.02	0.42
2:D:32:ASP:O	2:D:33:ASN:CB	2.67	0.42
2:D:179:TYR:CD1	2:D:180:LEU:N	2.87	0.42
1:A:74:ARG:C	1:A:76:SER:N	2.78	0.42
1:A:263:GLY:HA3	1:A:296:PRO:O	2.19	0.42
1:A:551:TRP:CE3	1:A:552:LEU:HD13	2.55	0.42
1:A:600:ASN:CG	1:A:600:ASN:O	2.62	0.42
1:C:640:PRO:C	1:C:641:VAL:HG13	2.45	0.42
1:A:551:TRP:O	1:A:555:THR:HG23	2.19	0.42
1:C:291:PRO:HD3	1:C:352:GLN:O	2.19	0.42
1:C:644:ASP:OD1	1:C:731:SER:OG	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:142:GLU:HB2	2:D:170:MET:CG	2.50	0.42
1:A:157:ILE:HG13	1:A:231:LEU:HD13	2.02	0.42
1:A:193:LEU:HD11	1:A:268:ILE:HG23	2.01	0.42
1:C:234:VAL:O	1:C:238:LEU:HB2	2.20	0.42
1:C:613:PHE:C	1:C:615:ARG:H	2.27	0.42
1:A:363:ASP:O	1:A:420:HIS:HA	2.19	0.41
1:A:399:ALA:HB3	1:A:450:LEU:CD1	2.50	0.41
1:A:420:HIS:CD2	1:A:420:HIS:N	2.85	0.41
1:C:66:ASN:ND2	1:C:68:TYR:H	2.15	0.41
1:C:123:ILE:HG12	1:C:156:LEU:HB2	2.01	0.41
1:C:722:ARG:HD3	2:D:33:ASN:OD1	2.20	0.41
1:A:48:VAL:O	1:A:50:PRO:HD3	2.19	0.41
1:A:459:PHE:CE2	1:A:535:ILE:HD11	2.55	0.41
1:C:80:CYS:HA	1:C:81:PRO:HD3	1.88	0.41
1:C:136:ASN:OD1	1:C:375:PHE:CD1	2.73	0.41
1:C:616:GLU:HG2	1:C:620:ASN:CB	2.48	0.41
1:C:654:LEU:HB2	1:C:665:TYR:HB3	2.02	0.41
1:C:111:GLU:HB2	1:C:503:ARG:CD	2.49	0.41
1:C:557:ILE:C	1:C:559:LEU:N	2.77	0.41
2:D:110:ARG:NH1	2:D:149:LEU:C	2.79	0.41
2:D:140:VAL:HG11	2:D:144:GLU:HB2	1.97	0.41
1:A:72:ASP:OD1	1:A:74:ARG:HG3	2.20	0.41
1:A:415:GLN:HE21	1:A:435:SER:HB3	1.86	0.41
1:C:222:PHE:O	1:C:226:ARG:NH1	2.53	0.41
1:C:311:HIS:CD2	1:C:598:VAL:HB	2.56	0.41
1:C:551:TRP:O	1:C:555:THR:HG23	2.21	0.41
2:D:88:PHE:N	2:D:89:PRO:CD	2.83	0.41
1:A:639:GLN:HA	1:A:640:PRO:HD3	1.93	0.41
1:A:697:GLU:O	1:A:701:LEU:HG	2.20	0.41
2:D:110:ARG:O	2:D:113:LEU:N	2.53	0.41
1:A:41:LYS:HD3	1:A:43:TYR:CE2	2.55	0.41
1:A:114:THR:HB	1:A:500:ASN:O	2.21	0.41
1:A:234:VAL:O	1:A:235:GLU:C	2.62	0.41
2:B:88:PHE:O	2:B:91:VAL:HG23	2.21	0.41
2:D:141:SER:O	2:D:143:ALA:N	2.53	0.41
1:A:198:THR:HA	1:A:222:PHE:O	2.20	0.41
1:C:417:LEU:C	1:C:417:LEU:HD23	2.45	0.41
1:C:234:VAL:HG12	1:C:238:LEU:HB2	2.03	0.41
2:D:57:PRO:HG3	2:D:74:LEU:HB3	2.02	0.41
2:D:142:GLU:O	2:D:146:ARG:HD2	2.21	0.41
1:A:66:ASN:HB2	1:A:67:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ASN:HD21	1:A:68:TYR:HB2	1.86	0.41
1:A:291:PRO:HA	1:A:353:ILE:O	2.20	0.41
1:A:729:ASN:HA	1:A:730:PRO:HD3	1.77	0.41
2:B:140:VAL:HG12	2:B:141:SER:O	2.20	0.41
1:C:627:PRO:HD2	1:C:643:LEU:CD2	2.50	0.41
1:C:667:GLY:O	1:C:668:GLU:C	2.64	0.41
2:D:77:HIS:NE2	2:D:80:ALA:HB2	2.36	0.41
1:A:417:LEU:C	1:A:417:LEU:HD23	2.46	0.41
1:C:41:LYS:HD3	1:C:43:TYR:CE2	2.56	0.41
1:C:634:MET:O	1:C:635:GLU:HB3	2.21	0.41
2:D:169:PHE:CZ	2:D:185:TRP:HB2	2.56	0.41
2:D:181:GLU:HA	2:D:184:GLN:HB2	2.02	0.41
1:A:23:ARG:CG	1:A:462:ILE:O	2.68	0.40
1:A:514:PHE:CD2	1:A:514:PHE:C	2.98	0.40
1:A:666:HIS:HB2	1:A:715:GLU:HG2	2.03	0.40
1:A:679:GLN:HG2	1:A:691:LEU:HD12	2.02	0.40
1:A:681:ASP:O	1:A:684:TYR:HB2	2.21	0.40
1:C:245:LEU:HD12	1:C:245:LEU:HA	1.97	0.40
2:D:74:LEU:HD23	2:D:74:LEU:N	2.36	0.40
1:A:83:CYS:O	1:A:84:ASN:HB2	2.21	0.40
1:A:332:ILE:HB	1:A:361:LEU:HD21	2.04	0.40
1:A:413:LYS:HD3	1:A:413:LYS:HA	1.82	0.40
1:C:304:LEU:HD13	2:D:86:ASP:HA	2.03	0.40
1:A:574:PHE:C	1:A:575:ARG:HG3	2.46	0.40
1:A:599:PHE:CE2	2:B:41:HIS:HD2	2.40	0.40
1:A:651:ASN:C	1:A:670:ILE:HD11	2.46	0.40
1:C:578:PRO:C	1:C:580:PHE:H	2.29	0.40
1:C:599:PHE:HD2	2:D:51:LEU:HD21	1.87	0.40
2:D:32:ASP:O	2:D:105:ARG:NH2	2.55	0.40
1:A:764:VAL:O	1:A:765:SER:C	2.65	0.40
2:B:180:LEU:HD23	2:B:180:LEU:HA	1.83	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	672/768 (88%)	619 (92%)	46 (7%)	7 (1%)	12	24
1	C	708/768 (92%)	623 (88%)	72 (10%)	13 (2%)	6	12
2	B	160/190 (84%)	150 (94%)	9 (6%)	1 (1%)	21	38
2	D	154/190 (81%)	124 (80%)	27 (18%)	3 (2%)	6	11
All	All	1694/1916 (88%)	1516 (90%)	154 (9%)	24 (1%)	9	17

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	542	THR
1	C	635	GLU
2	D	155	THR
2	B	155	THR
1	C	201	LYS
1	C	514	PHE
1	C	678	TYR
2	D	100	ALA
1	A	683	GLN
1	C	247	PRO
1	C	558	LYS
1	C	680	ASP
1	A	514	PHE
1	C	119	THR
1	C	322	TYR
1	C	683	GLN
2	D	123	LYS
1	A	680	ASP
1	C	542	THR
1	A	703	VAL
1	A	59	PRO
1	A	201	LYS
1	C	30	VAL
1	C	545	GLY

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are 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	$\# Z > 2$
5	GNP	B	5200	4	34,34,34	1.59	3 (8%)	47,54,54	0.79	1 (2%)
5	GNP	D	7200	4	34,34,34	1.67	4 (11%)	47,54,54	0.79	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GNP	B	5200	4	-	4/18/38/38	0/3/3/3
5	GNP	D	7200	4	-	2/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	7200	GNP	PA-O3A	5.48	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	5200	GNP	PG-O2G	-5.12	1.43	1.56
5	B	5200	GNP	PB-O2B	-4.64	1.44	1.56
5	D	7200	GNP	PG-O2G	-4.32	1.45	1.56
5	D	7200	GNP	PB-O2B	-3.84	1.46	1.56
5	B	5200	GNP	PA-O3A	3.49	1.63	1.59
5	D	7200	GNP	PB-O3A	2.21	1.61	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	5200	GNP	O2G-PG-O1G	-2.09	108.20	113.45

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	5200	GNP	PG-N3B-PB-O1B
5	B	5200	GNP	PG-N3B-PB-O3A
5	D	7200	GNP	PG-N3B-PB-O1B
5	B	5200	GNP	PA-O3A-PB-O2B
5	B	5200	GNP	PA-O3A-PB-O1B
5	D	7200	GNP	PG-N3B-PB-O3A

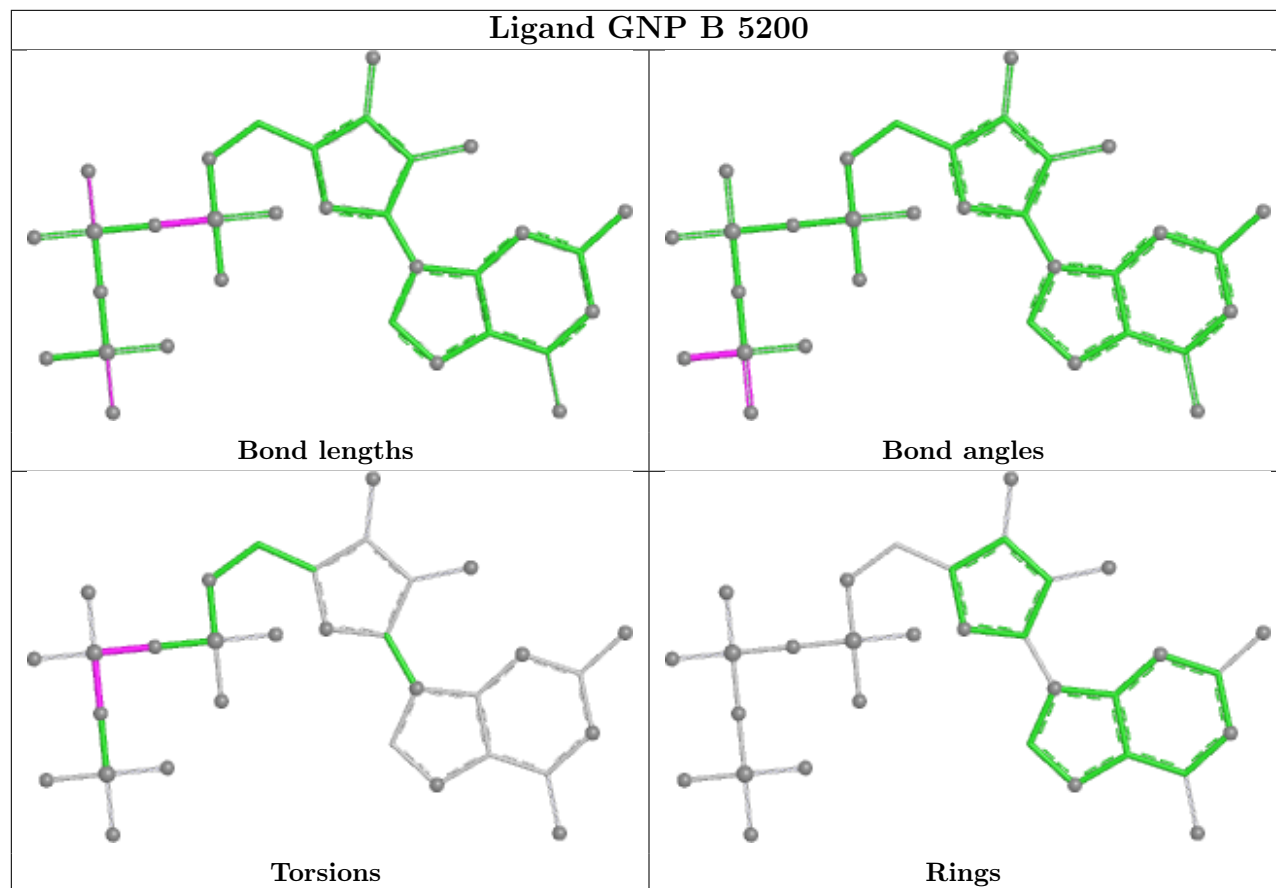
There are no ring outliers.

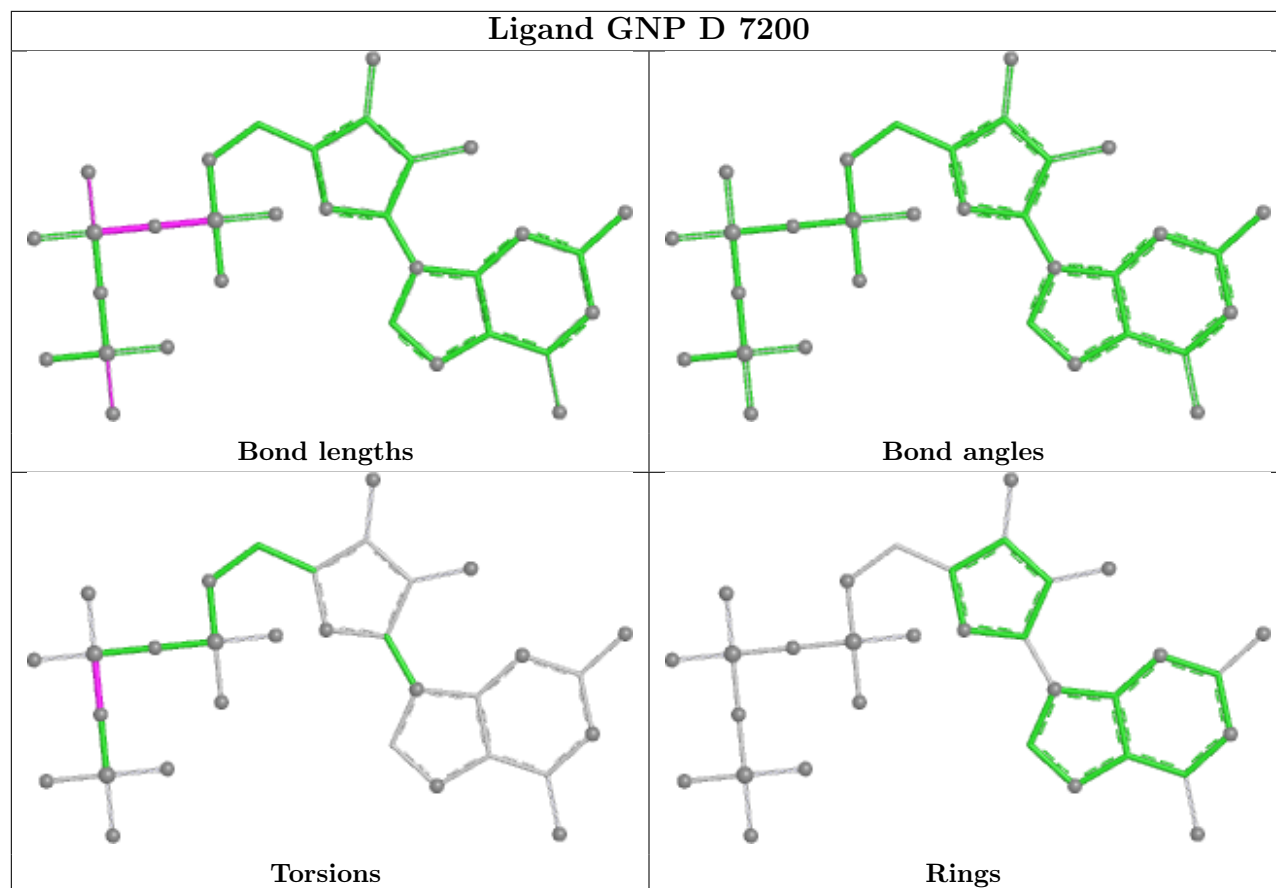
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5200	GNP	5	0
5	D	7200	GNP	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.