



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:22 AM UTC

PDB ID : 1TP7 / pdb_00001tp7
Title : Crystal Structure of the RNA-dependent RNA Polymerase from Human Rhinovirus 16
Authors : Appleby, T.C.; Luecke, H.; Shim, J.H.; Wu, J.Z.; Cheney, I.W.; Zhong, W.; Vogeley, L.; Hong, Z.; Yao, N.
Deposited on : 2004-06-15
Resolution : 2.40 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

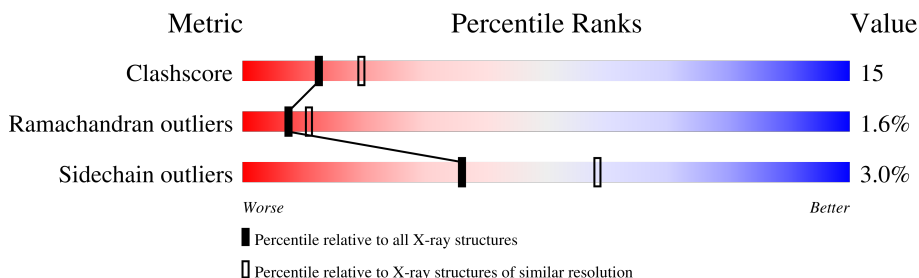
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	460	 75% 22% •
1	B	460	 70% 27% •
1	C	460	 61% 35% •
1	D	460	 55% 43% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15051 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 polypeptide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	Se	0	0	0
			3686	2383	599	687	7	10			
1	B	460	Total	C	N	O	S	Se	0	0	0
			3686	2383	599	687	7	10			
1	C	460	Total	C	N	O	S	Se	0	0	0
			3686	2383	599	687	7	10			
1	D	460	Total	C	N	O	S	Se	0	0	0
			3686	2383	599	687	7	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	MSE	MET	modified residue	UNP Q82122
A	104	MSE	MET	modified residue	UNP Q82122
A	154	MSE	MET	modified residue	UNP Q82122
A	224	MSE	MET	modified residue	UNP Q82122
A	231	MSE	MET	modified residue	UNP Q82122
A	252	MSE	MET	modified residue	UNP Q82122
A	298	MSE	MET	modified residue	UNP Q82122
A	339	MSE	MET	modified residue	UNP Q82122
A	409	MSE	MET	modified residue	UNP Q82122
A	420	MSE	MET	modified residue	UNP Q82122
B	97	MSE	MET	modified residue	UNP Q82122
B	104	MSE	MET	modified residue	UNP Q82122
B	154	MSE	MET	modified residue	UNP Q82122
B	224	MSE	MET	modified residue	UNP Q82122
B	231	MSE	MET	modified residue	UNP Q82122
B	252	MSE	MET	modified residue	UNP Q82122
B	298	MSE	MET	modified residue	UNP Q82122
B	339	MSE	MET	modified residue	UNP Q82122
B	409	MSE	MET	modified residue	UNP Q82122
B	420	MSE	MET	modified residue	UNP Q82122
C	97	MSE	MET	modified residue	UNP Q82122

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Chain	Residue	Modelled	Actual	Comment	Reference
C	104	MSE	MET	modified residue	UNP Q82122
C	154	MSE	MET	modified residue	UNP Q82122
C	224	MSE	MET	modified residue	UNP Q82122
C	231	MSE	MET	modified residue	UNP Q82122
C	252	MSE	MET	modified residue	UNP Q82122
C	298	MSE	MET	modified residue	UNP Q82122
C	339	MSE	MET	modified residue	UNP Q82122
C	409	MSE	MET	modified residue	UNP Q82122
C	420	MSE	MET	modified residue	UNP Q82122
D	97	MSE	MET	modified residue	UNP Q82122
D	104	MSE	MET	modified residue	UNP Q82122
D	154	MSE	MET	modified residue	UNP Q82122
D	224	MSE	MET	modified residue	UNP Q82122
D	231	MSE	MET	modified residue	UNP Q82122
D	252	MSE	MET	modified residue	UNP Q82122
D	298	MSE	MET	modified residue	UNP Q82122
D	339	MSE	MET	modified residue	UNP Q82122
D	409	MSE	MET	modified residue	UNP Q82122
D	420	MSE	MET	modified residue	UNP Q82122

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



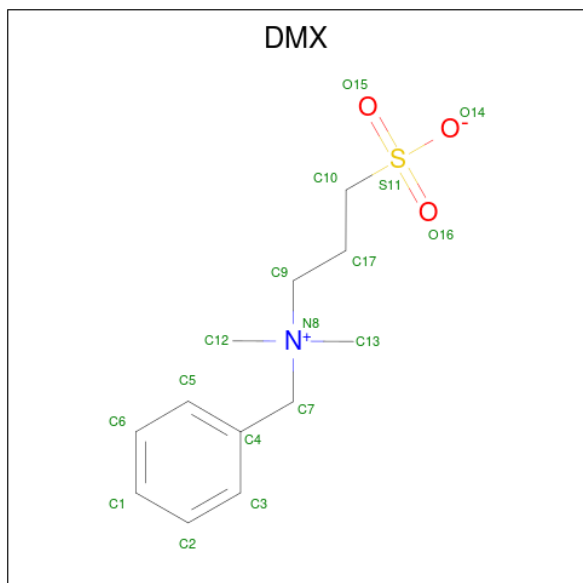
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 3-[BENZYL(DIMETHYL)AMMONIO]PROPANE-1-SULFONATE (CCD ID: DMX) (formula: $C_{12}H_{19}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			17	12	1	3	1		

- Molecule 4 is water.

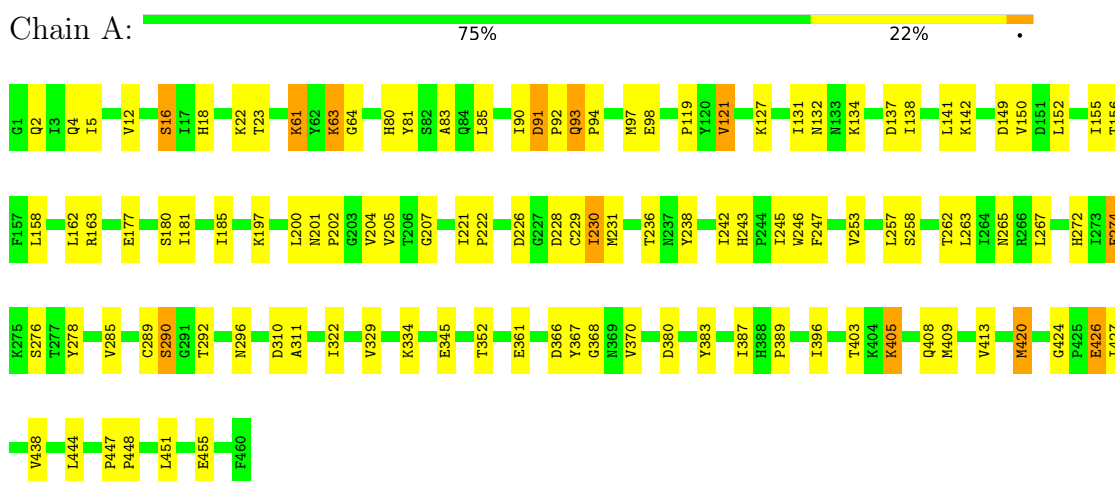
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	120	Total	O	0	0
			120	120		
4	B	97	Total	O	0	0
			97	97		
4	C	33	Total	O	0	0
			33	33		
4	D	20	Total	O	0	0
			20	20		

3 Residue-property plots

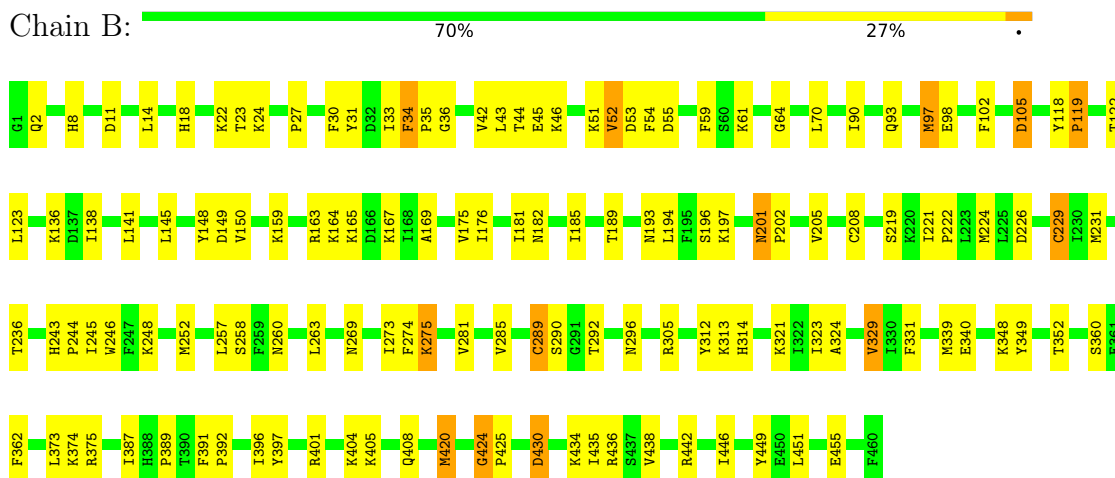
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

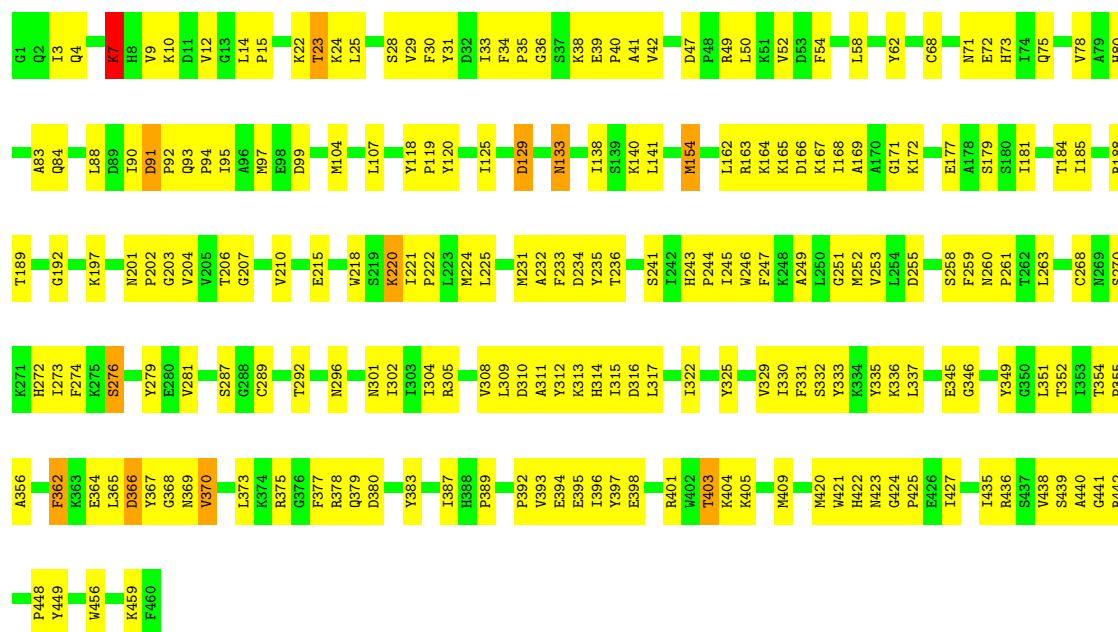


• Molecule 1: Genome polyprotein



• Molecule 1: Genome polyprotein





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.43Å 118.89Å 183.11Å 90.00° 96.06° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40	Depositor
% Data completeness (in resolution range)	95.1 (50.00-2.40)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.243 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15051	wwPDB-VP
Average B, all atoms (Å ²)	64.0	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: SO4, DMX

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	0/3767	0.93	15/5080 (0.3%)
1	B	0.47	0/3767	0.91	13/5080 (0.3%)
1	C	0.38	0/3767	0.85	8/5080 (0.2%)
1	D	0.36	0/3767	0.83	7/5080 (0.1%)
All	All	0.43	0/15068	0.88	43/20320 (0.2%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	MSE	N-CA-C	9.12	120.83	111.07
1	B	205	VAL	N-CA-C	-8.11	103.91	111.45
1	B	420	MSE	N-CA-C	7.77	120.49	111.02
1	B	329	VAL	N-CA-C	7.43	118.15	108.35
1	A	205	VAL	N-CA-C	-7.13	104.02	111.58
1	A	405	LYS	CA-C-N	6.89	127.17	119.32
1	A	405	LYS	C-N-CA	6.89	127.17	119.32
1	A	424	GLY	CA-C-N	6.82	126.33	119.24
1	A	424	GLY	C-N-CA	6.82	126.33	119.24
1	C	91	ASP	CA-C-N	6.66	126.25	119.19
1	C	91	ASP	C-N-CA	6.66	126.25	119.19
1	C	329	VAL	N-CA-C	6.53	116.42	108.06
1	B	260	ASN	CA-C-N	6.25	125.95	119.64
1	B	260	ASN	C-N-CA	6.25	125.95	119.64
1	A	93	GLN	CA-C-N	6.07	126.04	120.21
1	A	93	GLN	C-N-CA	6.07	126.04	120.21
1	D	91	ASP	CA-C-N	6.04	125.92	119.28
1	D	91	ASP	C-N-CA	6.04	125.92	119.28
1	C	227	GLY	N-CA-C	6.03	127.46	113.18
1	B	34	PHE	CA-C-N	6.00	125.91	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	PHE	C-N-CA	6.00	125.91	119.85
1	C	405	LYS	CA-C-N	5.88	125.36	119.24
1	C	405	LYS	C-N-CA	5.88	125.36	119.24
1	D	424	GLY	CA-C-N	5.76	124.96	118.97
1	D	424	GLY	C-N-CA	5.76	124.96	118.97
1	B	312	TYR	N-CA-C	5.69	118.73	109.06
1	C	221	ILE	CB-CA-C	-5.57	108.41	113.70
1	A	387	ILE	N-CA-C	5.48	115.75	107.80
1	B	201	ASN	N-CA-C	5.46	119.19	110.73
1	D	47	ASP	CA-C-N	5.33	126.51	119.84
1	D	47	ASP	C-N-CA	5.33	126.51	119.84
1	A	91	ASP	CA-C-N	5.33	124.94	119.56
1	A	91	ASP	C-N-CA	5.33	124.94	119.56
1	B	389	PRO	N-CA-C	-5.33	101.50	112.47
1	A	267	LEU	N-CA-C	-5.19	107.08	113.41
1	D	129	ASP	N-CA-C	-5.15	105.88	113.61
1	C	129	ASP	N-CA-C	-5.15	106.96	114.12
1	A	64	GLY	N-CA-C	-5.12	105.14	111.70
1	A	329	VAL	N-CA-C	5.12	116.02	108.45
1	A	389	PRO	N-CA-C	-5.08	102.00	112.47
1	B	424	GLY	CA-C-N	5.08	124.69	119.05
1	B	424	GLY	C-N-CA	5.08	124.69	119.05
1	B	194	LEU	N-CA-C	-5.05	105.68	111.14

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	3686	0	3694	74	0
1	B	3686	0	3694	91	0
1	C	3686	0	3694	132	0
1	D	3686	0	3694	160	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	17	0	19	2	0
4	A	120	0	0	1	0
4	B	97	0	0	4	0
4	C	33	0	0	1	0
4	D	20	0	0	2	0
All	All	15051	0	14795	451	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 15.

All (451) 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:312:TYR:HB2	1:C:315:ILE:HD11	1.48	0.95
1:B:159:LYS:HD3	1:B:176:ILE:HD11	1.49	0.94
1:C:308:VAL:HG12	1:C:315:ILE:HD13	1.54	0.88
1:B:22:LYS:HZ1	1:B:23:THR:HG22	1.40	0.85
1:D:154:MSE:HB3	1:D:179:SER:HA	1.58	0.83
1:D:23:THR:HG22	1:D:24:LYS:H	1.42	0.83
1:D:95:ILE:HG21	1:D:104:MSE:HE1	1.61	0.82
1:C:14:LEU:HD13	1:C:273:ILE:HD11	1.61	0.81
1:D:312:TYR:HB2	1:D:315:ILE:HD11	1.63	0.81
1:B:22:LYS:NZ	1:B:23:THR:HG22	1.97	0.80
1:A:405:LYS:HD3	1:A:408:GLN:HG3	1.64	0.79
1:A:228:ASP:HB2	1:A:334:LYS:O	1.82	0.79
1:C:127:LYS:HG2	1:C:181:ILE:HD11	1.64	0.79
1:D:75:GLN:HE22	1:D:252:MSE:HE1	1.47	0.79
1:B:52:VAL:HG12	1:B:53:ASP:H	1.48	0.78
1:C:219:SER:HA	1:C:387:ILE:HD13	1.66	0.78
1:D:308:VAL:HG12	1:D:315:ILE:HD13	1.66	0.76
1:C:425:PRO:HG3	1:C:449:TYR:CZ	2.21	0.76
1:D:133:ASN:N	1:D:133:ASN:HD22	1.85	0.75
1:C:22:LYS:HZ2	1:C:23:THR:H	1.33	0.74
1:D:97:MSE:HE3	1:D:185:ILE:HG21	1.70	0.74
1:A:131:ILE:HD11	1:A:141:LEU:HD22	1.68	0.73
1:D:436:ARG:HG3	1:D:436:ARG:HH11	1.54	0.72
1:B:149:ASP:CG	1:B:150:VAL:H	1.98	0.72
1:A:97:MSE:HE2	1:A:138:ILE:HD12	1.69	0.72
1:D:270:SER:HB2	1:D:281:VAL:HB	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:LYS:HD2	1:C:176:ILE:HD11	1.73	0.71
1:C:301:ASN:HB3	1:C:305:ARG:HH21	1.55	0.71
1:D:259:PHE:O	1:D:261:PRO:HD3	1.92	0.70
1:B:36:GLY:HA3	1:B:401:ARG:HH11	1.58	0.68
1:C:8:HIS:HB2	1:C:11:ASP:OD1	1.93	0.68
1:B:396:ILE:HG21	1:B:420:MSE:HE2	1.75	0.68
1:B:181:ILE:O	1:B:185:ILE:HG12	1.94	0.67
1:B:2:GLN:HB2	1:B:64:GLY:HA2	1.76	0.67
1:B:14:LEU:HD13	1:B:273:ILE:HD11	1.75	0.67
1:D:167:LYS:HG2	1:D:172:LYS:HD2	1.76	0.67
1:D:438:VAL:HG13	1:D:441:GLY:H	1.60	0.67
1:A:22:LYS:HD2	1:A:23:THR:H	1.58	0.67
1:C:75:GLN:OE1	1:C:252:MSE:HE1	1.96	0.65
1:D:355:PRO:HG3	1:D:362:PHE:CD1	2.32	0.65
1:D:378:ARG:H	1:D:387:ILE:HG23	1.60	0.65
1:A:83:ALA:HB2	1:D:448:PRO:HG3	1.80	0.64
1:B:61:LYS:NZ	1:B:175:VAL:HG13	2.14	0.63
1:D:425:PRO:HD3	4:D:474:HOH:O	1.98	0.63
1:C:154:MSE:HE2	1:C:177:GLU:HB3	1.81	0.63
1:C:9:VAL:HG22	1:C:14:LEU:O	1.99	0.63
1:D:184:THR:O	1:D:188:ARG:HG3	1.99	0.63
1:D:36:GLY:HA3	1:D:401:ARG:CZ	2.29	0.63
1:C:411:GLU:HA	1:C:414:LEU:HD12	1.81	0.62
1:D:204:VAL:HG22	1:D:224:MSE:HE2	1.79	0.62
1:C:90:ILE:HG12	1:C:197:LYS:HG2	1.80	0.62
1:D:14:LEU:HD13	1:D:273:ILE:HD11	1.81	0.62
1:D:133:ASN:HD22	1:D:133:ASN:H	1.46	0.62
1:A:396:ILE:HG21	1:A:420:MSE:HE2	1.81	0.62
1:C:373:LEU:O	1:C:375:ARG:HD2	1.99	0.62
1:D:309:LEU:HD11	1:D:317:LEU:HD11	1.81	0.62
1:D:305:ARG:NH2	1:D:322:ILE:HD12	2.15	0.62
1:D:88:LEU:HD11	1:D:206:THR:HG22	1.82	0.61
1:B:236:THR:HB	1:B:352:THR:HB	1.81	0.61
1:C:301:ASN:HB3	1:C:305:ARG:NH2	2.16	0.61
1:D:225:LEU:HB3	1:D:332:SER:HB2	1.82	0.61
1:D:218:TRP:HH2	1:D:373:LEU:HD12	1.64	0.61
1:C:236:THR:HB	1:C:352:THR:HB	1.83	0.61
1:D:30:PHE:HA	1:D:33:ILE:HD12	1.83	0.61
1:A:426:GLU:CD	1:A:426:GLU:H	2.09	0.60
1:C:44:THR:HG22	1:C:45:GLU:H	1.67	0.60
1:C:52:VAL:HG12	1:C:53:ASP:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:PRO:HA	1:C:367:TYR:OH	2.01	0.59
1:C:410:GLN:HE21	1:C:414:LEU:HD11	1.68	0.59
1:B:18:HIS:HE1	1:B:122:THR:HG22	1.68	0.59
1:C:22:LYS:NZ	1:C:23:THR:H	2.00	0.59
1:D:154:MSE:HE2	1:D:179:SER:HB3	1.84	0.59
1:D:255:ASP:HB2	1:D:261:PRO:HG2	1.84	0.59
1:C:44:THR:HG21	1:C:46:LYS:NZ	2.17	0.58
1:B:42:VAL:O	1:B:43:LEU:HD23	2.02	0.58
1:C:22:LYS:HA	1:C:22:LYS:HZ3	1.68	0.58
1:D:41:ALA:HB2	1:D:163:ARG:HG3	1.85	0.58
1:D:133:ASN:H	1:D:133:ASN:ND2	2.01	0.58
1:A:229:CYS:SG	1:A:231:MSE:HE2	2.44	0.58
1:D:333:TYR:CD2	1:D:337:LEU:HD11	2.38	0.58
1:C:308:VAL:HG12	1:C:315:ILE:CD1	2.31	0.57
1:B:45:GLU:HA	1:B:54:PHE:HB2	1.86	0.57
1:D:322:ILE:HG23	1:D:331:PHE:HB3	1.86	0.57
1:C:36:GLY:HA2	1:C:398:GLU:HG2	1.87	0.57
1:D:164:LYS:O	1:D:168:ILE:HG12	2.04	0.57
1:D:296:ASN:N	1:D:296:ASN:HD22	2.02	0.57
1:B:451:LEU:O	1:B:455:GLU:HG3	2.04	0.57
1:D:90:ILE:O	1:D:92:PRO:HD3	2.04	0.57
1:D:203:GLY:HA3	1:D:224:MSE:HE1	1.86	0.57
1:B:339:MSE:HE2	4:B:501:HOH:O	2.04	0.57
1:C:22:LYS:NZ	1:C:23:THR:HG22	2.19	0.57
1:C:54:PHE:O	1:C:58:LEU:HB2	2.05	0.57
1:A:222:PRO:HB3	3:A:500:DMX:H133	1.85	0.57
1:D:305:ARG:HH21	1:D:322:ILE:HD12	1.70	0.57
1:B:219:SER:HA	1:B:387:ILE:HD12	1.87	0.56
1:C:380:ASP:HB3	1:C:383:TYR:O	2.05	0.56
1:D:133:ASN:N	1:D:133:ASN:ND2	2.52	0.56
1:B:8:HIS:HB2	1:B:11:ASP:OD2	2.06	0.56
1:C:8:HIS:HB2	1:C:11:ASP:CG	2.30	0.56
1:B:27:PRO:HB3	1:B:31:TYR:CD1	2.41	0.56
1:C:387:ILE:HD12	1:C:387:ILE:N	2.21	0.56
1:D:28:SER:C	1:D:30:PHE:H	2.14	0.56
1:D:210:VAL:HA	1:D:325:TYR:CE1	2.41	0.55
1:B:269:ASN:HA	1:B:281:VAL:O	2.05	0.55
1:C:111:ASP:OD2	1:C:114:THR:HG23	2.07	0.55
1:B:119:PRO:O	1:B:123:LEU:HD12	2.07	0.55
1:C:69:SER:HA	1:C:245:ILE:HG21	1.89	0.55
1:D:301:ASN:O	1:D:305:ARG:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:HIS:HA	1:D:448:PRO:HG2	1.87	0.55
1:B:430:ASP:OD1	1:B:434:LYS:HE3	2.07	0.55
1:D:71:ASN:OD1	1:D:73:HIS:HB2	2.06	0.55
1:A:221:ILE:HB	1:A:222:PRO:HD3	1.89	0.55
1:D:436:ARG:HG3	1:D:436:ARG:NH1	2.16	0.55
1:D:95:ILE:HG12	1:D:189:THR:HA	1.89	0.55
1:C:22:LYS:HZ2	1:C:23:THR:N	2.03	0.54
1:D:404:LYS:O	1:D:405:LYS:HD2	2.07	0.54
1:D:23:THR:HG22	1:D:25:LEU:H	1.71	0.54
1:D:233:PHE:HA	1:D:356:ALA:HB2	1.89	0.54
1:C:233:PHE:CD1	1:C:353:ILE:HG23	2.42	0.54
1:D:233:PHE:HZ	1:D:304:ILE:HD11	1.73	0.54
1:C:304:ILE:O	1:C:308:VAL:HG23	2.07	0.54
1:D:80:HIS:O	1:D:83:ALA:HB3	2.08	0.54
1:D:312:TYR:C	1:D:313:LYS:HD2	2.33	0.54
1:D:243:HIS:CE1	1:D:245:ILE:HG23	2.43	0.54
1:A:207:GLY:HA2	1:A:322:ILE:O	2.07	0.53
1:B:425:PRO:HG3	1:B:449:TYR:CZ	2.42	0.53
1:A:2:GLN:HG3	1:A:4:GLN:HE21	1.72	0.53
1:D:220:LYS:O	1:D:224:MSE:HG3	2.08	0.53
1:C:420:MSE:HG2	1:C:431:PHE:CD2	2.43	0.53
1:B:119:PRO:HG3	1:B:148:TYR:CD2	2.43	0.53
1:B:22:LYS:HZ2	1:B:23:THR:H	1.54	0.53
1:B:61:LYS:HZ1	1:B:175:VAL:HG13	1.73	0.53
1:B:289:CYS:H	1:B:292:THR:HG21	1.74	0.53
1:D:12:VAL:HG23	1:D:14:LEU:H	1.74	0.53
1:C:72:GLU:O	1:C:76:VAL:HG23	2.09	0.53
1:A:405:LYS:HG3	1:A:408:GLN:HB2	1.91	0.53
1:C:382:LYS:HD2	1:C:383:TYR:CD1	2.44	0.53
1:A:2:GLN:HG3	1:A:4:GLN:NE2	2.23	0.52
1:D:80:HIS:ND1	1:D:317:LEU:HB3	2.24	0.52
1:A:380:ASP:HB3	1:A:383:TYR:O	2.10	0.52
1:B:90:ILE:HG12	1:B:197:LYS:HG2	1.91	0.52
1:C:49:ARG:HD2	1:C:168:ILE:HD12	1.89	0.52
1:A:22:LYS:HD2	1:A:23:THR:N	2.25	0.52
1:C:42:VAL:HG11	1:C:50:LEU:HD21	1.92	0.52
1:C:63:LYS:HG3	1:C:64:GLY:H	1.73	0.52
1:C:81:TYR:CZ	1:C:85:LEU:HD11	2.44	0.52
1:C:305:ARG:HG2	1:C:317:LEU:HD22	1.90	0.52
1:D:456:TRP:O	1:D:459:LYS:HB2	2.09	0.52
1:B:145:LEU:O	1:B:149:ASP:N	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:THR:HG22	1:D:24:LYS:N	2.17	0.52
1:D:442:ARG:HH11	1:D:442:ARG:HG2	1.74	0.52
1:A:177:GLU:HG2	1:A:272:HIS:CE1	2.45	0.52
1:D:80:HIS:CE1	1:D:317:LEU:HB3	2.45	0.52
1:D:129:ASP:O	1:D:140:LYS:HD2	2.09	0.52
1:B:36:GLY:HA3	1:B:401:ARG:NH1	2.25	0.52
1:B:224:MSE:HE2	4:B:488:HOH:O	2.09	0.52
1:B:257:LEU:O	1:B:258:SER:HB2	2.10	0.52
1:C:17:ILE:HG21	1:C:155:ILE:HG23	1.92	0.52
1:D:185:ILE:O	1:D:189:THR:HG23	2.10	0.52
1:C:308:VAL:CG1	1:C:315:ILE:HD13	2.34	0.52
1:D:393:VAL:HG23	1:D:394:GLU:OE2	2.10	0.52
1:B:201:ASN:N	1:B:202:PRO:HD3	2.24	0.51
1:C:145:LEU:HA	1:C:182:ASN:ND2	2.25	0.51
1:D:15:PRO:HD2	1:D:118:TYR:HE1	1.74	0.51
1:A:257:LEU:O	1:A:258:SER:HB2	2.10	0.51
1:B:70:LEU:HD11	1:B:248:LYS:HD2	1.92	0.51
1:C:366:ASP:C	1:C:368:GLY:H	2.18	0.51
1:B:98:GLU:H	1:B:98:GLU:CD	2.18	0.51
1:D:181:ILE:O	1:D:185:ILE:HG12	2.10	0.51
1:D:329:VAL:HG22	1:D:330:ILE:N	2.25	0.51
1:D:234:ASP:OD1	1:D:356:ALA:HA	2.11	0.51
1:C:181:ILE:HG22	1:C:185:ILE:HG12	1.93	0.51
1:B:24:LYS:O	1:B:404:LYS:HA	2.10	0.51
1:D:346:GLY:HA2	1:D:349:TYR:HD1	1.75	0.51
1:C:440:ALA:O	1:C:444:LEU:HG	2.10	0.51
1:D:221:ILE:HB	1:D:222:PRO:HD3	1.93	0.51
1:D:375:ARG:HG3	1:D:375:ARG:HH11	1.76	0.51
1:A:149:ASP:CG	1:A:150:VAL:H	2.17	0.51
1:C:360:SER:O	1:C:361:GLU:HG3	2.11	0.51
1:D:442:ARG:HG2	1:D:442:ARG:NH1	2.26	0.51
1:A:426:GLU:CD	1:A:426:GLU:N	2.68	0.51
1:B:436:ARG:O	1:B:442:ARG:HD3	2.11	0.50
1:C:44:THR:HG21	1:C:46:LYS:HZ2	1.74	0.50
1:D:251:GLY:O	1:D:261:PRO:HB3	2.10	0.50
1:B:52:VAL:HG12	1:B:53:ASP:N	2.24	0.50
1:C:132:ASN:C	1:C:132:ASN:HD22	2.19	0.50
1:C:397:TYR:O	1:C:401:ARG:HG3	2.11	0.50
1:D:54:PHE:O	1:D:58:LEU:HB2	2.10	0.50
1:A:367:TYR:HA	1:A:370:VAL:HG12	1.93	0.50
1:D:249:ALA:O	1:D:253:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:GLN:O	1:C:403:THR:HG22	2.11	0.50
1:A:311:ALA:HB2	1:A:345:GLU:HG3	1.93	0.50
1:B:163:ARG:NH1	1:B:167:LYS:HD3	2.26	0.50
1:C:312:TYR:HB2	1:C:315:ILE:CD1	2.32	0.50
1:B:51:LYS:HD3	1:B:169:ALA:HB1	1.94	0.50
1:D:49:ARG:O	1:D:169:ALA:HA	2.12	0.50
1:D:78:VAL:HG13	1:D:253:VAL:HG22	1.93	0.50
1:A:201:ASN:N	1:A:202:PRO:HD3	2.27	0.49
1:A:63:LYS:HD2	1:A:63:LYS:O	2.12	0.49
1:D:380:ASP:HB3	1:D:383:TYR:O	2.12	0.49
1:A:426:GLU:OE2	1:A:427:ILE:HG13	2.12	0.49
1:D:425:PRO:HG3	1:D:449:TYR:CZ	2.48	0.49
1:C:383:TYR:HB3	1:C:385:PHE:CE2	2.48	0.49
1:D:308:VAL:CG1	1:D:315:ILE:HD13	2.41	0.49
1:B:438:VAL:HG22	4:B:526:HOH:O	2.12	0.49
1:A:262:THR:O	1:A:265:ASN:HB2	2.13	0.49
1:C:301:ASN:CB	1:C:305:ARG:HH21	2.24	0.49
1:D:201:ASN:N	1:D:202:PRO:HD3	2.28	0.49
1:B:340:GLU:HG2	1:B:362:PHE:CD1	2.48	0.49
1:D:30:PHE:CE2	1:D:435:ILE:HG23	2.48	0.49
1:D:138:ILE:O	1:D:141:LEU:HB3	2.13	0.49
1:D:375:ARG:HD3	1:D:389:PRO:HB3	1.93	0.49
1:A:236:THR:HB	1:A:352:THR:HB	1.95	0.48
1:A:156:THR:HB	1:A:274:PHE:HA	1.94	0.48
1:A:230:ILE:HD12	1:A:367:TYR:CZ	2.48	0.48
1:B:119:PRO:HG3	1:B:148:TYR:CE2	2.48	0.48
1:C:44:THR:HG22	1:C:45:GLU:N	2.29	0.48
1:D:309:LEU:HA	1:D:315:ILE:HD12	1.96	0.48
1:C:228:ASP:HB3	1:C:333:TYR:O	2.13	0.48
1:B:289:CYS:H	1:B:292:THR:CG2	2.26	0.48
1:C:22:LYS:NZ	1:C:22:LYS:HA	2.28	0.48
1:D:9:VAL:HG22	1:D:276:SER:O	2.13	0.48
1:A:253:VAL:O	1:A:257:LEU:HG	2.14	0.48
1:C:177:GLU:HG2	1:C:272:HIS:CE1	2.49	0.48
1:C:85:LEU:O	1:C:88:LEU:HB2	2.14	0.48
1:C:123:LEU:C	1:C:125:ILE:H	2.22	0.48
1:B:149:ASP:CG	1:B:150:VAL:N	2.68	0.48
1:C:245:ILE:HG13	1:C:246:TRP:N	2.28	0.48
1:A:245:ILE:HG13	1:A:246:TRP:N	2.28	0.47
1:D:311:ALA:HA	1:D:345:GLU:OE2	2.14	0.47
1:B:373:LEU:O	1:B:374:LYS:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:ASP:HB3	1:D:104:MSE:HB3	1.96	0.47
1:D:218:TRP:CH2	1:D:373:LEU:HD12	2.45	0.47
1:B:274:PHE:CG	1:B:275:LYS:N	2.82	0.47
1:C:164:LYS:HB2	1:C:167:LYS:HG2	1.96	0.47
1:C:309:LEU:HA	1:C:315:ILE:HD12	1.96	0.47
1:D:241:SER:HB3	1:D:351:LEU:HD23	1.96	0.47
1:C:99:ASP:O	1:C:103:GLY:HA2	2.13	0.47
1:A:247:PHE:HZ	1:A:285:VAL:HG22	1.80	0.47
1:C:360:SER:C	1:C:361:GLU:HG3	2.40	0.47
1:D:243:HIS:ND1	1:D:245:ILE:HG12	2.30	0.47
1:D:404:LYS:C	1:D:405:LYS:HD2	2.39	0.47
1:D:423:ASN:HB2	1:D:427:ILE:HG21	1.97	0.47
1:C:132:ASN:HB3	1:C:137:ASP:HB3	1.96	0.47
1:C:229:CYS:HB2	1:C:336:LYS:HA	1.96	0.47
1:C:243:HIS:CG	1:C:244:PRO:HD2	2.50	0.47
1:D:118:TYR:CZ	1:D:119:PRO:HB3	2.50	0.47
1:D:272:HIS:HB2	1:D:279:TYR:CZ	2.50	0.47
1:A:90:ILE:HG12	1:A:197:LYS:HG2	1.97	0.47
1:C:73:HIS:CD2	1:C:309:LEU:HB3	2.50	0.47
1:B:97:MSE:HE2	1:B:185:ILE:CG2	2.45	0.47
1:C:168:ILE:HG13	1:C:169:ALA:N	2.30	0.47
1:C:30:PHE:CE2	1:C:435:ILE:HG23	2.50	0.46
1:B:340:GLU:HG3	1:B:362:PHE:HB2	1.98	0.46
1:A:285:VAL:HG11	1:A:296:ASN:HD21	1.80	0.46
1:D:42:VAL:HG11	1:D:50:LEU:CD1	2.45	0.46
1:D:377:PHE:CD2	1:D:387:ILE:HG21	2.51	0.46
1:A:403:THR:HG21	1:A:409:MSE:HE1	1.98	0.46
1:C:95:ILE:HD13	1:C:192:GLY:HA3	1.98	0.46
1:A:16:SER:HG	1:A:276:SER:HG	1.64	0.46
1:A:61:LYS:NZ	1:A:61:LYS:HB3	2.31	0.46
1:B:197:LYS:HA	1:B:197:LYS:HD3	1.70	0.46
1:B:323:ILE:O	1:B:329:VAL:HG23	2.16	0.46
1:D:245:ILE:HG13	1:D:246:TRP:N	2.30	0.46
1:D:392:PRO:HB2	1:D:395:GLU:HG2	1.96	0.46
1:B:243:HIS:ND1	1:B:244:PRO:HD2	2.31	0.46
1:C:22:LYS:HZ2	1:C:23:THR:HG22	1.80	0.46
1:C:407:SER:CB	1:D:316:ASP:HB2	2.46	0.46
1:A:81:TYR:CE2	1:A:85:LEU:HD11	2.50	0.46
1:A:152:LEU:HD12	1:A:180:SER:OG	2.16	0.46
1:B:118:TYR:CE2	1:B:119:PRO:HB3	2.51	0.45
1:D:38:LYS:HG3	1:D:398:GLU:CD	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:MSE:HE3	1:D:185:ILE:CG2	2.44	0.45
1:B:45:GLU:OE1	1:B:275:LYS:HE3	2.17	0.45
1:B:145:LEU:HA	1:B:182:ASN:ND2	2.32	0.45
1:C:165:LYS:C	1:C:167:LYS:H	2.24	0.45
1:C:200:LEU:C	1:C:202:PRO:HD3	2.42	0.45
1:D:68:CYS:SG	1:D:245:ILE:HD13	2.57	0.45
1:B:221:ILE:HB	1:B:222:PRO:HD3	1.98	0.45
1:D:28:SER:C	1:D:30:PHE:N	2.75	0.45
1:D:236:THR:HB	1:D:352:THR:HB	1.98	0.45
1:B:164:LYS:HD2	1:B:167:LYS:HE3	1.98	0.45
1:C:382:LYS:HD2	1:C:383:TYR:CE1	2.51	0.45
1:D:120:TYR:HB3	1:D:125:ILE:HB	1.99	0.45
1:A:127:LYS:HG2	1:A:181:ILE:HD12	1.98	0.45
1:B:405:LYS:HD3	1:B:408:GLN:NE2	2.32	0.45
1:C:431:PHE:O	1:C:435:ILE:HG13	2.17	0.45
1:B:229:CYS:SG	1:B:231:MSE:HE2	2.57	0.45
1:D:232:ALA:HB2	1:D:330:ILE:HG22	1.99	0.45
1:D:438:VAL:C	1:D:440:ALA:H	2.23	0.45
1:B:30:PHE:HA	1:B:33:ILE:HG12	1.99	0.45
1:D:207:GLY:HA2	1:D:322:ILE:O	2.17	0.45
1:D:420:MSE:O	1:D:422:HIS:N	2.50	0.45
1:B:163:ARG:CZ	1:B:167:LYS:HD3	2.46	0.45
1:C:221:ILE:HB	1:C:222:PRO:HD3	1.99	0.45
1:C:385:PHE:N	1:C:385:PHE:CD2	2.84	0.45
1:A:12:VAL:HG12	1:A:12:VAL:O	2.16	0.45
1:B:46:LYS:HD2	1:B:46:LYS:O	2.16	0.45
1:A:97:MSE:CE	1:A:138:ILE:HD12	2.44	0.44
1:B:105:ASP:O	1:B:196:SER:OG	2.32	0.44
1:C:449:TYR:CE2	1:C:453:ARG:HD2	2.52	0.44
1:D:379:GLN:HA	1:D:387:ILE:HD13	2.00	0.44
1:D:253:VAL:HG21	1:D:302:ILE:HD11	2.00	0.44
1:A:403:THR:CB	1:A:409:MSE:HE1	2.47	0.44
1:B:102:PHE:CZ	1:B:136:LYS:HA	2.53	0.44
1:C:57:ALA:HB1	1:C:172:LYS:CE	2.48	0.44
1:A:98:GLU:CD	1:A:98:GLU:H	2.26	0.44
1:A:121:VAL:HG11	1:A:155:ILE:HD13	1.98	0.44
1:A:247:PHE:CZ	1:A:285:VAL:HG22	2.53	0.44
1:D:215:GLU:OE1	1:D:459:LYS:HE3	2.17	0.44
1:A:158:LEU:HA	1:A:158:LEU:HD23	1.83	0.44
1:A:181:ILE:O	1:A:185:ILE:HG12	2.16	0.44
1:B:226:ASP:HB3	4:B:563:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:TYR:CZ	1:A:242:ILE:HD11	2.52	0.44
1:A:413:VAL:HG21	1:A:444:LEU:HD13	1.99	0.44
1:A:447:PRO:HA	1:A:448:PRO:HD3	1.85	0.44
1:B:321:LYS:O	1:B:331:PHE:HB2	2.18	0.44
1:D:366:ASP:O	1:D:368:GLY:N	2.46	0.44
1:A:5:ILE:HD11	1:A:278:TYR:CE2	2.53	0.43
1:C:86:ALA:C	1:C:88:LEU:H	2.26	0.43
1:D:3:ILE:HD11	1:D:62:TYR:CD1	2.53	0.43
1:D:39:GLU:HB2	1:D:40:PRO:HD2	1.99	0.43
1:C:201:ASN:N	1:C:202:PRO:HD3	2.32	0.43
1:D:22:LYS:HA	1:D:22:LYS:HD2	1.62	0.43
1:C:367:TYR:HA	1:C:370:VAL:HG12	2.01	0.43
1:A:91:ASP:HA	1:A:92:PRO:HD3	1.86	0.43
1:A:162:LEU:O	1:A:163:ARG:HD2	2.18	0.43
1:C:98:GLU:CD	1:C:98:GLU:H	2.26	0.43
1:D:107:LEU:HG	1:D:188:ARG:NH2	2.33	0.43
1:D:356:ALA:HB3	1:D:365:LEU:HD11	2.00	0.43
1:B:59:PHE:C	1:B:61:LYS:H	2.26	0.43
1:B:285:VAL:HG11	1:B:296:ASN:OD1	2.19	0.43
1:D:95:ILE:HD13	1:D:192:GLY:HA3	2.00	0.43
1:A:132:ASN:OD1	1:A:134:LYS:HB3	2.19	0.43
1:A:204:VAL:HG22	4:A:508:HOH:O	2.18	0.43
1:B:201:ASN:N	1:B:202:PRO:CD	2.82	0.43
1:C:285:VAL:HG21	1:C:296:ASN:OD1	2.19	0.43
1:C:408:GLN:HG2	1:D:314:HIS:HB3	2.00	0.43
1:D:84:GLN:NE2	1:D:305:ARG:HH12	2.17	0.43
1:D:289:CYS:HB3	1:D:292:THR:HG21	2.01	0.43
1:C:405:LYS:HB2	1:C:408:GLN:OE1	2.18	0.43
1:C:414:LEU:HD13	1:D:72:GLU:OE1	2.18	0.43
1:D:42:VAL:HG11	1:D:50:LEU:HD11	2.01	0.43
1:A:289:CYS:SG	1:A:290:SER:N	2.92	0.43
1:B:30:PHE:HA	1:B:33:ILE:CG1	2.49	0.43
1:B:34:PHE:HA	1:B:35:PRO:HD3	1.86	0.43
1:B:97:MSE:HE2	1:B:185:ILE:HG21	1.99	0.43
1:C:447:PRO:HA	1:C:448:PRO:HD3	1.89	0.43
1:D:36:GLY:HA3	1:D:401:ARG:NE	2.33	0.43
1:D:247:PHE:CD2	1:D:268:CYS:HB2	2.54	0.43
1:B:44:THR:OG1	1:B:46:LYS:HG3	2.19	0.43
1:B:118:TYR:CD1	1:B:119:PRO:HA	2.53	0.43
1:C:51:LYS:HB2	1:C:169:ALA:O	2.19	0.43
1:C:145:LEU:HA	1:C:182:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:PHE:CZ	1:C:263:LEU:HD22	2.54	0.43
1:C:423:ASN:HB3	1:C:427:ILE:HD12	2.00	0.43
1:D:154:MSE:HB3	1:D:179:SER:CA	2.40	0.43
1:D:366:ASP:C	1:D:368:GLY:H	2.26	0.43
1:A:230:ILE:HG23	1:A:230:ILE:O	2.19	0.42
1:C:336:LYS:HG2	1:C:337:LEU:N	2.34	0.42
1:C:432:GLU:HG3	1:C:446:ILE:CD1	2.49	0.42
1:D:7:LYS:HD3	1:D:12:VAL:HG12	2.01	0.42
1:D:10:LYS:HE3	1:D:10:LYS:HB2	1.84	0.42
1:D:330:ILE:O	1:D:330:ILE:HG13	2.17	0.42
1:A:366:ASP:C	1:A:368:GLY:N	2.77	0.42
1:B:248:LYS:O	1:B:252:MSE:HG3	2.18	0.42
1:C:15:PRO:HD2	1:C:118:TYR:HE1	1.83	0.42
1:C:37:SER:O	1:C:165:LYS:HE3	2.19	0.42
1:C:91:ASP:HA	1:C:92:PRO:HD3	1.86	0.42
1:D:397:TYR:O	1:D:401:ARG:HG3	2.19	0.42
1:C:236:THR:O	1:C:237:ASN:HB3	2.20	0.42
1:C:289:CYS:HB3	1:C:292:THR:CG2	2.48	0.42
1:C:88:LEU:HD11	1:C:206:THR:HG22	2.02	0.42
1:C:119:PRO:HG2	1:C:123:LEU:HD12	2.01	0.42
1:D:260:ASN:ND2	1:D:263:LEU:HB2	2.33	0.42
1:A:289:CYS:HB3	1:A:292:THR:CG2	2.50	0.42
1:C:285:VAL:HA	1:C:286:PRO:HD3	1.92	0.42
1:D:165:LYS:HG3	1:D:166:ASP:H	1.84	0.42
1:D:241:SER:HB3	1:D:351:LEU:HA	2.01	0.42
1:D:91:ASP:OD1	1:D:93:GLN:HB2	2.18	0.42
1:D:92:PRO:HG2	1:D:258:SER:HB2	2.00	0.42
1:B:435:ILE:HG21	1:B:446:ILE:HD11	2.02	0.42
1:D:164:LYS:HB3	1:D:164:LYS:HE2	1.83	0.42
1:B:245:ILE:HG13	1:B:246:TRP:N	2.35	0.42
1:B:391:PHE:HA	1:B:392:PRO:HD3	1.95	0.42
1:C:260:ASN:HA	1:C:261:PRO:HD3	1.83	0.42
1:C:410:GLN:HE21	1:C:414:LEU:CD1	2.31	0.42
1:D:335:TYR:O	1:D:337:LEU:HG	2.20	0.42
1:D:370:VAL:O	1:D:370:VAL:HG13	2.20	0.42
1:C:41:ALA:HB2	1:C:163:ARG:HG3	2.02	0.41
1:D:420:MSE:C	1:D:422:HIS:N	2.79	0.41
1:A:200:LEU:C	1:A:202:PRO:HD3	2.45	0.41
1:B:93:GLN:O	1:B:193:ASN:ND2	2.54	0.41
1:D:403:THR:HB	1:D:409:MSE:HE1	2.01	0.41
1:B:243:HIS:CG	1:B:244:PRO:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:LYS:HE2	1:B:349:TYR:CE1	2.56	0.41
1:B:138:ILE:O	1:B:141:LEU:HB3	2.21	0.41
1:B:222:PRO:HG2	1:B:387:ILE:CD1	2.50	0.41
1:C:14:LEU:HD22	1:C:273:ILE:HD11	2.02	0.41
1:C:427:ILE:H	1:C:427:ILE:HG13	1.70	0.41
1:A:97:MSE:HE1	1:A:142:LYS:HG2	2.02	0.41
1:A:451:LEU:O	1:A:455:GLU:HG3	2.21	0.41
1:B:424:GLY:HA2	1:B:425:PRO:HD3	1.85	0.41
1:A:5:ILE:HD11	1:A:278:TYR:HE2	1.86	0.41
1:A:366:ASP:HB2	3:A:500:DMX:O16	2.21	0.41
1:D:12:VAL:HG23	1:D:14:LEU:HG	2.02	0.41
1:C:225:LEU:HB3	1:C:332:SER:HB3	2.03	0.41
1:D:107:LEU:HG	1:D:188:ARG:HH21	1.85	0.41
1:D:335:TYR:O	1:D:337:LEU:N	2.54	0.41
1:B:42:VAL:C	1:B:43:LEU:HD23	2.45	0.41
1:B:165:LYS:C	1:B:167:LYS:H	2.29	0.41
1:C:34:PHE:HA	1:C:35:PRO:HD3	1.83	0.41
1:C:385:PHE:O	1:C:386:LEU:HD23	2.20	0.41
1:C:445:TYR:CE2	1:C:447:PRO:HG3	2.55	0.41
1:D:31:TYR:C	1:D:33:ILE:H	2.28	0.41
1:A:243:HIS:CE1	1:A:245:ILE:HG23	2.56	0.41
1:B:185:ILE:O	1:B:189:THR:HG23	2.21	0.41
1:C:16:SER:O	1:C:122:THR:HG21	2.21	0.41
1:C:93:GLN:HG2	1:C:94:PRO:N	2.34	0.41
1:C:164:LYS:O	1:C:167:LYS:HB2	2.20	0.41
1:C:221:ILE:N	1:C:222:PRO:CD	2.84	0.41
1:C:336:LYS:HE3	1:C:364:GLU:HG2	2.03	0.41
1:C:432:GLU:HG3	1:C:446:ILE:HD12	2.03	0.41
1:D:9:VAL:HG23	1:D:10:LYS:N	2.36	0.41
1:A:177:GLU:HG2	1:A:272:HIS:ND1	2.36	0.41
1:D:233:PHE:HE1	1:D:235:TYR:CE1	2.38	0.41
1:D:329:VAL:CG2	1:D:330:ILE:N	2.84	0.41
1:D:378:ARG:NH2	4:D:474:HOH:O	2.54	0.41
1:A:132:ASN:HB3	1:A:137:ASP:HB3	2.03	0.40
1:A:366:ASP:C	1:A:368:GLY:H	2.28	0.40
1:C:238:TYR:CD2	1:C:327:ASP:HB3	2.57	0.40
1:C:366:ASP:C	1:C:368:GLY:N	2.79	0.40
1:A:93:GLN:HA	1:A:94:PRO:HD3	1.81	0.40
1:C:274:PHE:CG	1:C:275:LYS:N	2.88	0.40
1:C:363:LYS:NZ	4:C:474:HOH:O	2.52	0.40
1:C:407:SER:HB3	1:D:316:ASP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:LEU:HD13	1:D:162:LEU:CD2	2.51	0.40
1:D:34:PHE:HA	1:D:35:PRO:HD3	1.95	0.40
1:D:50:LEU:HD21	1:D:171:GLY:CA	2.51	0.40
1:D:221:ILE:N	1:D:222:PRO:CD	2.85	0.40
1:D:396:ILE:HG21	1:D:420:MSE:HE2	2.03	0.40
1:A:22:LYS:HE3	1:A:23:THR:HG22	2.03	0.40
1:B:208:CYS:HA	1:B:324:ALA:O	2.21	0.40
1:B:313:LYS:O	1:B:314:HIS:HB2	2.21	0.40
1:B:397:TYR:O	1:B:401:ARG:HG3	2.21	0.40
1:D:88:LEU:HB3	1:D:197:LYS:HE2	2.02	0.40
1:D:93:GLN:HA	1:D:94:PRO:HD3	1.90	0.40
1:C:53:ASP:HB3	1:C:56:SER:OG	2.21	0.40
1:A:310:ASP:HB3	1:A:345:GLU:OE1	2.21	0.40
1:C:442:ARG:C	1:C:444:LEU:H	2.29	0.40
1:D:287:SER:C	1:D:289:CYS:H	2.29	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	458/460 (100%)	426 (93%)	29 (6%)	3 (1%)	18	28
1	B	458/460 (100%)	417 (91%)	34 (7%)	7 (2%)	8	12
1	C	458/460 (100%)	399 (87%)	50 (11%)	9 (2%)	6	7
1	D	458/460 (100%)	388 (85%)	60 (13%)	10 (2%)	5	6
All	All	1832/1840 (100%)	1630 (89%)	173 (9%)	29 (2%)	7	11

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	4	GLN
1	C	63	LYS
1	C	227	GLY
1	D	274	PHE
1	A	290	SER
1	B	275	LYS
1	D	367	TYR
1	B	55	ASP
1	B	290	SER
1	D	23	THR
1	D	276	SER
1	D	421	TRP
1	B	360	SER
1	C	11	ASP
1	C	172	LYS
1	C	289	CYS
1	C	367	TYR
1	D	4	GLN
1	D	220	LYS
1	D	336	LYS
1	A	274	PHE
1	B	105	ASP
1	C	358	LYS
1	B	229	CYS
1	D	7	LYS
1	B	52	VAL
1	A	230	ILE
1	C	286	PRO
1	D	29	VAL

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	410/400 (102%)	399 (97%)	11 (3%)	39	62
1	B	410/400 (102%)	403 (98%)	7 (2%)	53	74
1	C	410/400 (102%)	395 (96%)	15 (4%)	30	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	410/400 (102%)	394 (96%)	16 (4%)	28	48
All	All	1640/1600 (102%)	1591 (97%)	49 (3%)	36	58

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	18	HIS
1	A	61	LYS
1	A	63	LYS
1	A	119	PRO
1	A	121	VAL
1	A	226	ASP
1	A	263	LEU
1	A	361	GLU
1	A	426	GLU
1	A	438	VAL
1	B	97	MSE
1	B	119	PRO
1	B	263	LEU
1	B	289	CYS
1	B	305	ARG
1	B	375	ARG
1	B	430	ASP
1	C	18	HIS
1	C	22	LYS
1	C	52	VAL
1	C	67	GLU
1	C	93	GLN
1	C	218	TRP
1	C	248	LYS
1	C	263	LEU
1	C	305	ARG
1	C	318	ASP
1	C	344	LYS
1	C	382	LYS
1	C	385	PHE
1	C	394	GLU
1	C	458	GLU
1	D	7	LYS
1	D	52	VAL
1	D	133	ASN

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Mol	Chain	Res	Type
1	D	154	MSE
1	D	177	GLU
1	D	231	MSE
1	D	244	PRO
1	D	310	ASP
1	D	354	THR
1	D	362	PHE
1	D	364	GLU
1	D	366	ASP
1	D	369	ASN
1	D	370	VAL
1	D	403	THR
1	D	439	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	4	GLN
1	A	26	GLN
1	A	193	ASN
1	A	296	ASN
1	A	314	HIS
1	A	408	GLN
1	B	2	GLN
1	B	65	ASN
1	B	201	ASN
1	B	265	ASN
1	B	269	ASN
1	B	314	HIS
1	B	379	GLN
1	B	408	GLN
1	B	423	ASN
1	B	454	HIS
1	C	80	HIS
1	C	84	GLN
1	C	113	ASN
1	C	132	ASN
1	C	193	ASN
1	C	269	ASN
1	C	347	GLN
1	C	408	GLN

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Mol	Chain	Res	Type
1	C	410	GLN
1	D	75	GLN
1	D	84	GLN
1	D	133	ASN
1	D	199	HIS
1	D	256	ASN
1	D	265	ASN
1	D	296	ASN
1	D	379	GLN
1	D	408	GLN
1	D	418	HIS

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 ⓘ

5 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	$\# Z > 2$
3	DMX	A	500	-	17,17,17	3.72	8 (47%)	24,24,24	1.50	4 (16%)
2	SO4	D	473	-	4,4,4	0.74	0	6,6,6	0.13	0
2	SO4	A	470	-	4,4,4	0.54	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	471	-	4,4,4	0.48	0	6,6,6	0.06	0
2	SO4	C	472	-	4,4,4	0.76	0	6,6,6	0.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMX	A	500	-	-	6/13/13/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	DMX	O15-S11	9.24	1.71	1.45
3	A	500	DMX	O16-S11	9.22	1.71	1.45
3	A	500	DMX	C10-S11	3.71	1.82	1.77
3	A	500	DMX	O14-S11	3.45	1.60	1.47
3	A	500	DMX	C7-C4	3.05	1.58	1.51
3	A	500	DMX	C5-C4	2.34	1.43	1.38
3	A	500	DMX	C9-N8	2.08	1.56	1.52
3	A	500	DMX	C6-C5	2.06	1.42	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	DMX	C4-C7-N8	4.21	126.37	114.66
3	A	500	DMX	C17-C9-N8	2.76	120.97	115.35
3	A	500	DMX	O15-S11-C10	2.24	110.12	106.73
3	A	500	DMX	O16-S11-C10	2.20	110.05	106.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

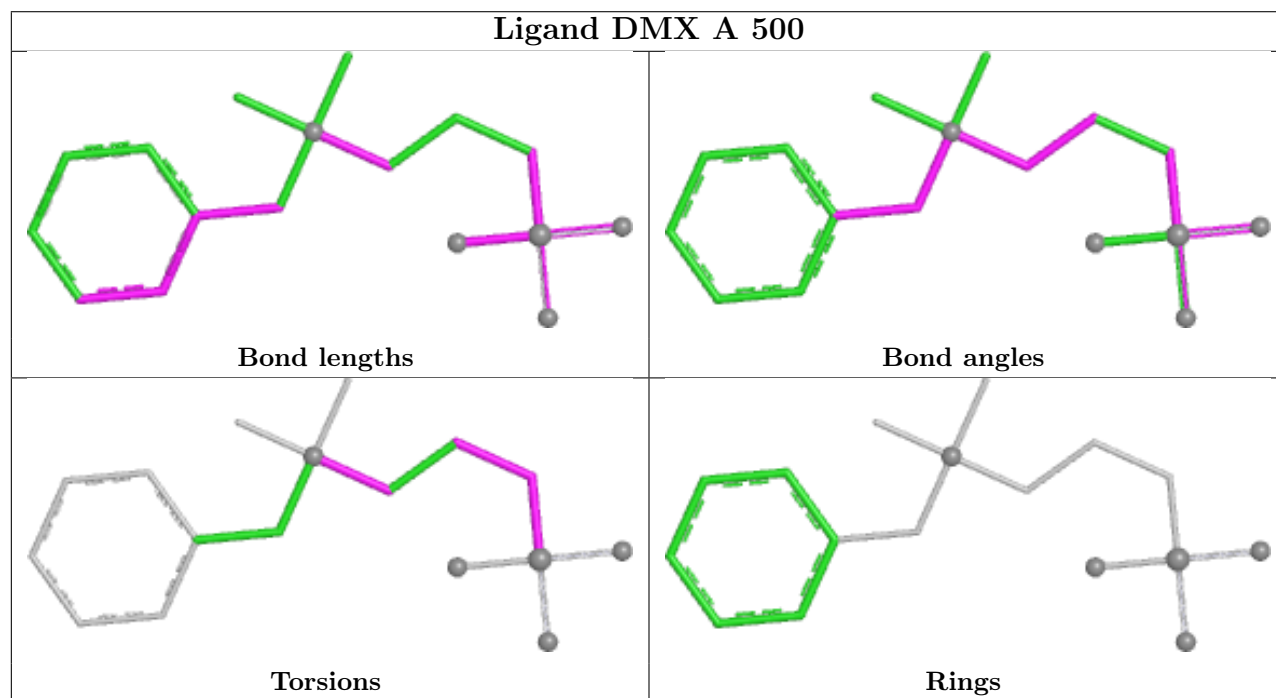
Mol	Chain	Res	Type	Atoms
3	A	500	DMX	C17-C9-N8-C12
3	A	500	DMX	C17-C9-N8-C7
3	A	500	DMX	C17-C10-S11-O14
3	A	500	DMX	C17-C10-S11-O15
3	A	500	DMX	C17-C9-N8-C13
3	A	500	DMX	S11-C10-C17-C9

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	DMX	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.