Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 06:29 pm BST

PDB ID	:	1TP7
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 following versions of software and data (see references ⓘ) were used in the production of this report:

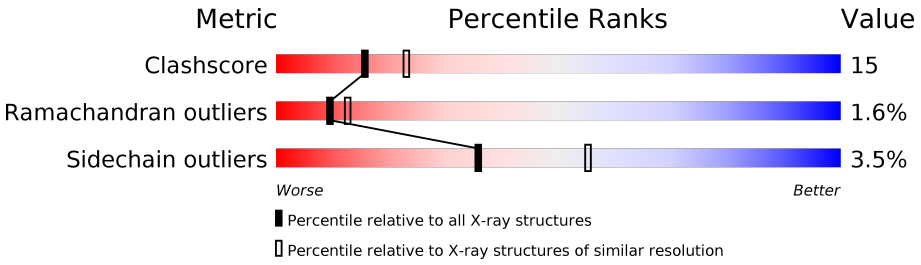
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (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 on 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	460	77% 21% .
1	B	460	71% 27% .
1	C	460	62% 35% .
1	D	460	56% 41% .

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 polyprotein.

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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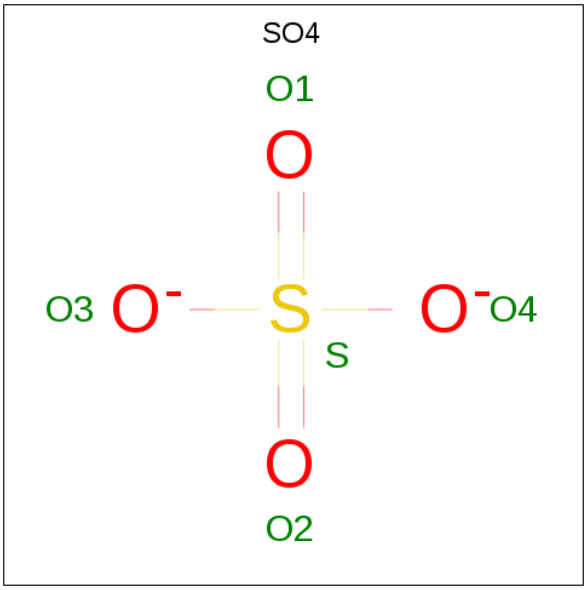
Chain	Residue	Modelled	Actual	Comment	Reference
C	104	MSE	MET	MODIFIED RESIDUE	UNP Q82122
C	154	MSE	MET	MODIFIED RESIDUE	UNP Q82122
C	224	MSE	MET	MODIFIED RESIDUE	UNP Q82122
C	231	MSE	MET	MODIFIED RESIDUE	UNP Q82122
C	252	MSE	MET	MODIFIED RESIDUE	UNP Q82122
C	298	MSE	MET	MODIFIED RESIDUE	UNP Q82122
C	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 (three-letter code: SO4) (formula: O_4S).



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

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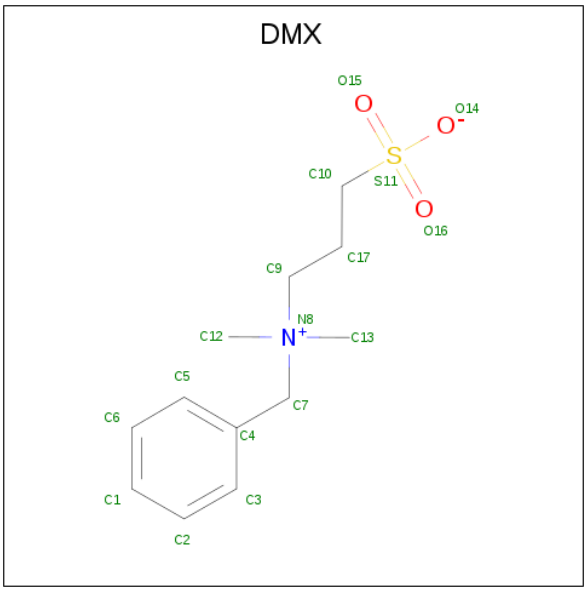
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

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



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

- Molecule 4 is water.

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

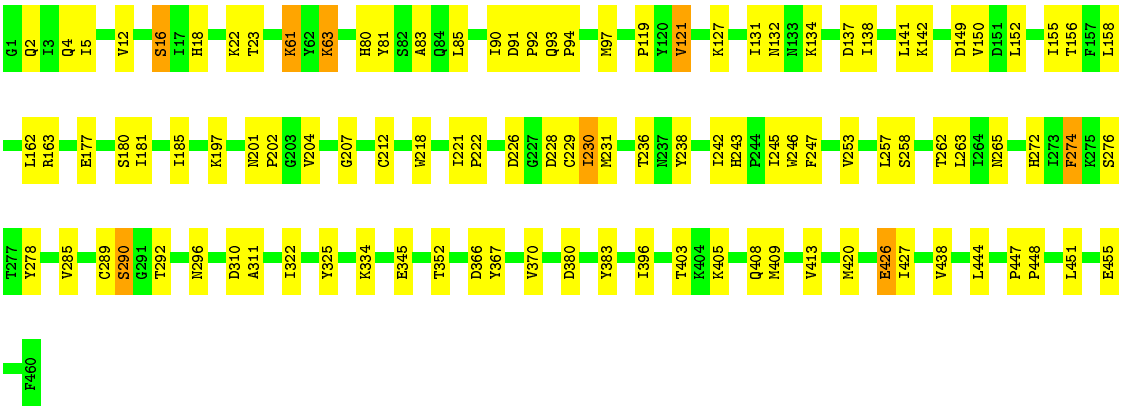
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

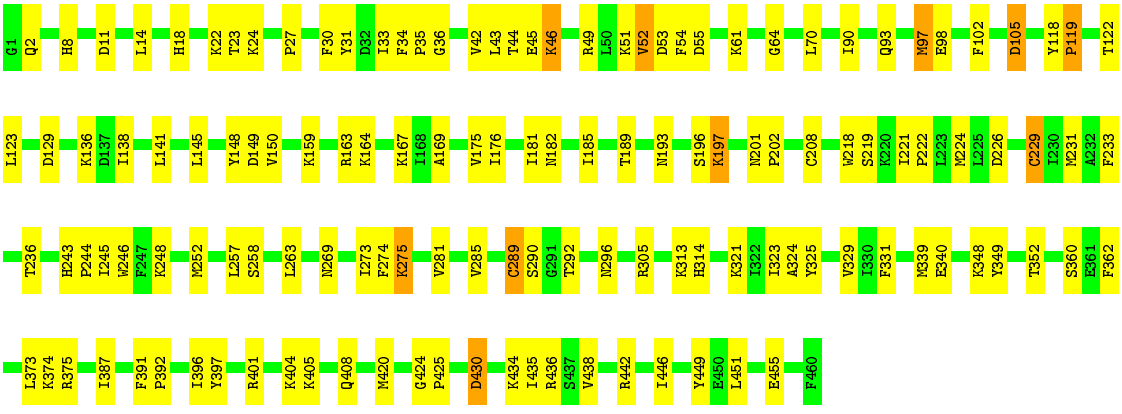
- Molecule 1: Genome polyprotein

Chain A:



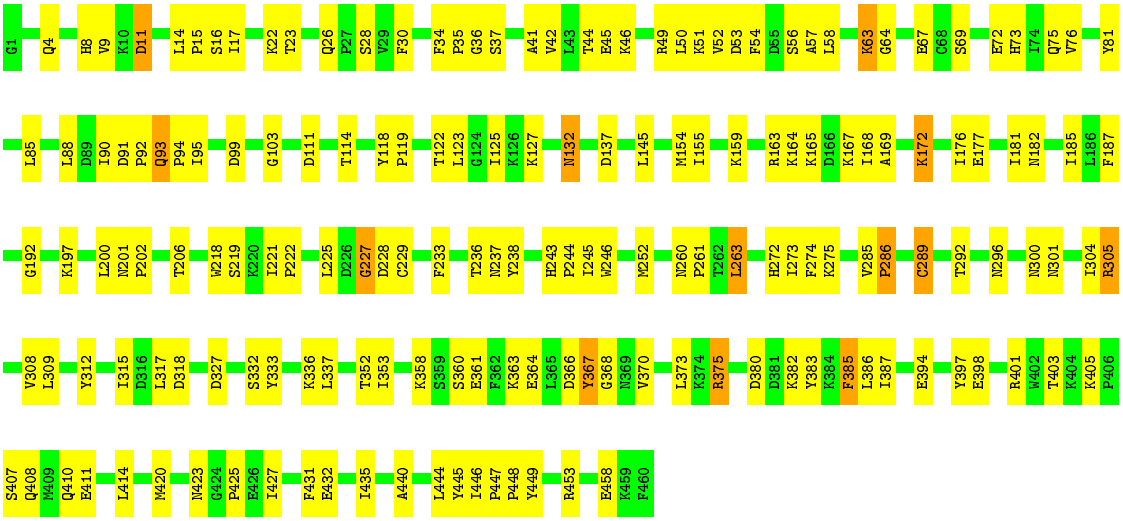
- Molecule 1: Genome polyprotein

Chain B:



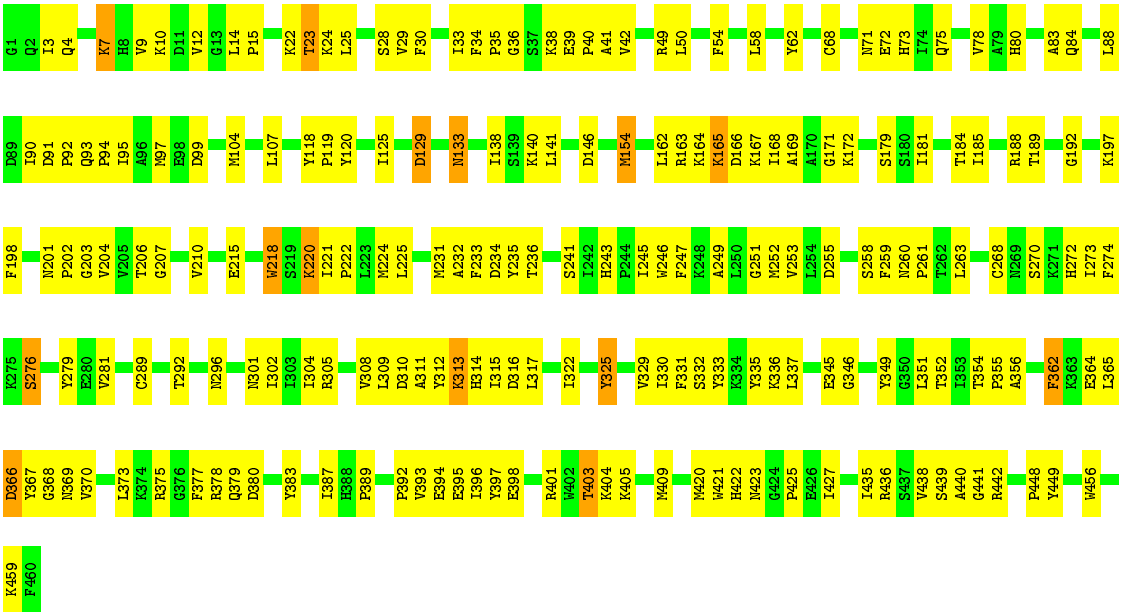
- Molecule 1: Genome polyprotein

Chain C:



- Molecule 1: Genome polyprotein

Chain D:



4 Data and refinement statistics (i)

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: DMX, 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	0.40	0/3767	0.59	0/5080
1	B	0.40	0/3767	0.59	0/5080
1	C	0.31	0/3767	0.52	1/5080 (0.0%)
1	D	0.29	0/3767	0.49	0/5080
All	All	0.35	0/15068	0.55	1/20320 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	227	GLY	N-CA-C	5.75	127.46	113.10

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	70	0
1	B	3686	0	3694	88	0
1	C	3686	0	3694	129	0
1	D	3686	0	3694	155	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	436	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 (436) 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: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:B:22:LYS:HZ1	1:B:23:THR:HG22	1.43	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	1.34	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: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
1:C:159:LYS:HD2	1:C:176:ILE:HD11	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:149:ASP:CG	1:B:150:VAL:H	1.98	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:28:SER:HG	1:C:30:PHE:HD1	1.43	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:133:ASN:H	1:D:133:ASN:HD22	1.46	0.62
1:D:14:LEU:HD13	1:D:273:ILE:HD11	1.81	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:C:22:LYS:HA	1:C:22:LYS:HZ3	1.65	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:C:44:THR:HG22	1:C:45:GLU:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:VAL:HG12	1:C:53:ASP:H	1.67	0.59
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:D:41:ALA:HB2	1:D:163:ARG:HG3	1.85	0.58
1:D:133:ASN:ND2	1:D:133:ASN:H	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:203:GLY:HA3	1:D:224:MSE:HE1	1.86	0.57
1:D:90:ILE:O	1:D:92:PRO:HD3	2.04	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:B:27:PRO:HB3	1:B:31:TYR:CD1	2.41	0.56
1:C:387:ILE:N	1:C:387:ILE:HD12	2.21	0.56
1:A:426:GLU:H	1:A:426:GLU:CD	2.09	0.55
1:B:61:LYS:HZ2	1:B:175:VAL:HG13	1.70	0.55
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:B:430:ASP:OD1	1:B:434:LYS:HE3	2.07	0.55
1:A:80:HIS:HA	1:D:448:PRO:HG2	1.87	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:B:22:LYS:HZ2	1:B:23:THR:H	1.52	0.55
1:D:95:ILE:HG12	1:D:189:THR:HA	1.89	0.55
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: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:C:22:LYS:HZ2	1:C:23:THR:N	2.05	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:305:ARG:HG2	1:C:317:LEU:HD22	1.90	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:HG2	1:A:272:HIS:CE1	2.45	0.52
1:D:129:ASP:O	1:D:140:LYS:HD2	2.09	0.52
1:D:80:HIS:CE1	1:D:317:LEU:HB3	2.45	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:B:36:GLY:HA3	1:B:401:ARG:NH1	2.25	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:8:HIS:HB2	1:C:11:ASP:CG	2.30	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: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:C:44:THR:HG21	1:C:46:LYS:HZ3	1.76	0.51
1:D:28:SER:C	1:D:30:PHE:H	2.14	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: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:B:436:ARG:O	1:B:442:ARG:HD3	2.11	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:16:SER:HG	1:A:276:SER:HG	1.60	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:312:TYR:C	1:D:313:LYS:HD2	2.33	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:245:ILE:HG13	1:C:246:TRP:N	2.28	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:138:ILE:O	1:D:141:LEU:HB3	2.13	0.49
1:D:30:PHE:CE2	1:D:435:ILE:HG23	2.48	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: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:A:245:ILE:HG13	1:A:246:TRP:N	2.28	0.47
1:C:22:LYS:HZ2	1:C:23:THR:HG22	1.78	0.47
1:C:22:LYS:HA	1:C:22:LYS:NZ	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:243:HIS:ND1	1:D:245:ILE:HG12	2.30	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:366:ASP:C	1:C:368:GLY:H	2.18	0.47
1:B:98:GLU:H	1:B:98:GLU:CD	2.18	0.46
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:377:PHE:CD2	1:D:387:ILE:HG21	2.51	0.46
1:D:42:VAL:HG11	1:D:50:LEU:CD1	2.45	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:61:LYS:NZ	1:A:61:LYS:HB3	2.31	0.46
1:B:197:LYS:HD3	1:B:197:LYS:HA	1.70	0.46
1:A:12:VAL:O	1:A:12:VAL:HG12	2.16	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:132:ASN:HD22	1:C:132:ASN:C	2.19	0.46
1:C:407:SER:CB	1:D:316:ASP:HB2	2.46	0.46
1:A:152:LEU:HD12	1:A:180:SER:OG	2.16	0.46
1:A:81:TYR:CE2	1:A:85:LEU:HD11	2.50	0.46
1:B:118:TYR:CE2	1:B:119:PRO:HB3	2.51	0.45
1:D:97:MSE:HE3	1:D:185:ILE:CG2	2.44	0.45
1:A:149:ASP:CG	1:A:150:VAL:H	2.17	0.45
1:B:145:LEU:HA	1:B:182:ASN:ND2	2.32	0.45
1:B:45:GLU:OE1	1:B:275:LYS:HE3	2.17	0.45
1:D:68:CYS:SG	1:D:245:ILE:HD13	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ILE:HB	1:B:222:PRO:HD3	1.98	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:A:426:GLU:CD	1:A:426:GLU:N	2.68	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: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:CD2	1:C:385:PHE:N	2.84	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: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
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:B:149:ASP:CG	1:B:150:VAL:N	2.68	0.44
1:A:5:ILE:HD11	1:A:278:TYR:CE2	2.53	0.43
1:D:39:GLU:HB2	1:D:40:PRO:HD2	1.99	0.43
1:D:3:ILE:HD11	1:D:62:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ASN:N	1:C:202:PRO:HD3	2.32	0.43
1:D:22:LYS:HD2	1:D:22:LYS:HA	1.62	0.43
1:C:367:TYR:HA	1:C:370:VAL:HG12	2.01	0.43
1:A:162:LEU:O	1:A:163:ARG:HD2	2.18	0.43
1:A:91:ASP:HA	1:A:92:PRO:HD3	1.86	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: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:289:CYS:HB3	1:D:292:THR:HG21	2.01	0.43
1:D:84:GLN:NE2	1:D:305:ARG:HH12	2.17	0.43
1:C:123:LEU:C	1:C:125:ILE:H	2.22	0.43
1:C:405:LYS:HB2	1:C:408:GLN:OE1	2.18	0.43
1:D:42:VAL:HG11	1:D:50:LEU:HD11	2.01	0.43
1:C:414:LEU:HD13	1:D:72:GLU:OE1	2.18	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:247:PHE:CD2	1:D:268:CYS:HB2	2.54	0.43
1:D:36:GLY:HA3	1:D:401:ARG:NE	2.33	0.43
1:B:118:TYR:CD1	1:B:119:PRO:HA	2.53	0.43
1:B:44:THR:OG1	1:B:46:LYS:HG3	2.19	0.43
1:C:145:LEU:HA	1:C:182:ASN:HD21	1.83	0.43
1:C:51:LYS:HB2	1:C:169:ALA:O	2.19	0.43
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:A:230:ILE:O	1:A:230:ILE:HG23	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:10:LYS:HE3	1:D:10:LYS:HB2	1.84	0.42
1:D:330:ILE:HG13	1:D:330:ILE:O	2.17	0.42
1:D:7:LYS:HD3	1:D:12:VAL:HG12	2.01	0.42
1:B:248:LYS:O	1:B:252:MSE:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:119:PRO:HG2	1:C:123:LEU:HD12	2.01	0.42
1:C:88:LEU:HD11	1:C:206:THR:HG22	2.02	0.42
1:D:260:ASN:ND2	1:D:263:LEU:HB2	2.33	0.42
1:D:404:LYS:C	1:D:405:LYS:HD2	2.39	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:C:360:SER:C	1:C:361:GLU:HG3	2.40	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: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
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:366:ASP:HB2	3:A:500:DMX:O16	2.21	0.41
1:A:5:ILE:HD11	1:A:278:TYR:HE2	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:164:LYS:O	1:C:167:LYS:HB2	2.20	0.41
1:C:165:LYS:C	1:C:167:LYS:H	2.24	0.41
1:C:16:SER:O	1:C:122:THR:HG21	2.21	0.41
1:C:221:ILE:N	1:C:222:PRO:CD	2.84	0.41
1:C:93:GLN:HG2	1:C:94:PRO:N	2.34	0.41
1:D:38:LYS:HG3	1:D:398:GLU:CD	2.41	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:200:LEU:C	1:C:202:PRO:HD3	2.42	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:C:238:TYR:CD2	1:C:327:ASP:HB3	2.57	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
1:D:221:ILE:N	1:D:222:PRO:CD	2.85	0.40
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:396:ILE:HG21	1:D:420:MSE:HE2	2.03	0.40
1:D:50:LEU:HD21	1:D:171:GLY:CA	2.51	0.40
1:A:22:LYS:HE3	1:A:23:THR:HG22	2.03	0.40
1:B:313:LYS:O	1:B:314:HIS:HB2	2.21	0.40
1:B:208:CYS:HA	1:B:324:ALA:O	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:D:438:VAL:C	1:D:440:ALA:H	2.23	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	458/460 (100%)	426 (93%)	29 (6%)	3 (1%)	22	32
1	B	458/460 (100%)	417 (91%)	34 (7%)	7 (2%)	10	14
1	C	458/460 (100%)	399 (87%)	50 (11%)	9 (2%)	7	9
1	D	458/460 (100%)	388 (85%)	60 (13%)	10 (2%)	6	7
All	All	1832/1840 (100%)	1630 (89%)	173 (9%)	29 (2%)	9	13

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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/400 (102%)	397 (97%)	13 (3%)	39	59
1	B	410/400 (102%)	396 (97%)	14 (3%)	37	56
1	C	410/400 (102%)	398 (97%)	12 (3%)	42	62
1	D	410/400 (102%)	392 (96%)	18 (4%)	28	45
All	All	1640/1600 (102%)	1583 (96%)	57 (4%)	36	55

All (57) 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	212	CYS
1	A	218	TRP
1	A	226	ASP
1	A	263	LEU
1	A	325	TYR
1	A	426	GLU

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Mol	Chain	Res	Type
1	A	438	VAL
1	B	46	LYS
1	B	49	ARG
1	B	97	MSE
1	B	119	PRO
1	B	129	ASP
1	B	197	LYS
1	B	218	TRP
1	B	233	PHE
1	B	263	LEU
1	B	289	CYS
1	B	305	ARG
1	B	325	TYR
1	B	375	ARG
1	B	430	ASP
1	C	67	GLU
1	C	93	GLN
1	C	132	ASN
1	C	218	TRP
1	C	263	LEU
1	C	300	ASN
1	C	305	ARG
1	C	318	ASP
1	C	375	ARG
1	C	385	PHE
1	C	394	GLU
1	C	458	GLU
1	D	129	ASP
1	D	133	ASN
1	D	146	ASP
1	D	154	MSE
1	D	165	LYS
1	D	198	PHE
1	D	218	TRP
1	D	231	MSE
1	D	310	ASP
1	D	313	LYS
1	D	325	TYR
1	D	354	THR
1	D	362	PHE
1	D	364	GLU
1	D	366	ASP

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Mol	Chain	Res	Type
1	D	369	ASN
1	D	403	THR
1	D	439	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	26	GLN
1	A	314	HIS
1	B	2	GLN
1	B	93	GLN
1	B	265	ASN
1	B	379	GLN
1	B	408	GLN
1	C	113	ASN
1	C	132	ASN
1	C	193	ASN
1	C	265	ASN
1	C	410	GLN
1	D	75	GLN
1	D	84	GLN
1	D	133	ASN
1	D	193	ASN
1	D	256	ASN
1	D	265	ASN
1	D	296	ASN
1	D	408	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	SO4	B	471	-	4,4,4	0.39	0	6,6,6	0.06	0
3	DMX	A	500	-	17,17,17	3.58	7 (41%)	23,24,24	1.68	5 (21%)
2	SO4	A	470	-	4,4,4	0.45	0	6,6,6	0.16	0
2	SO4	D	473	-	4,4,4	0.67	0	6,6,6	0.10	0
2	SO4	C	472	-	4,4,4	0.69	0	6,6,6	0.07	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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	DMX	O15-S11	8.86	1.71	1.45
3	A	500	DMX	O16-S11	8.84	1.71	1.45
3	A	500	DMX	C10-S11	3.72	1.82	1.77
3	A	500	DMX	O14-S11	3.55	1.60	1.47
3	A	500	DMX	C7-C4	3.04	1.58	1.51
3	A	500	DMX	C9-N8	2.34	1.56	1.52
3	A	500	DMX	C5-C4	2.18	1.43	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	500	DMX	C4-C7-N8	5.01	126.37	114.86
3	A	500	DMX	O15-S11-C10	2.66	110.12	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	500	DMX	C17-C9-N8	2.64	120.97	115.38
3	A	500	DMX	O16-S11-C10	2.60	110.05	106.92
3	A	500	DMX	O14-S11-C10	2.38	109.62	105.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	DMX	C17-C9-N8-C7
3	A	500	DMX	C17-C9-N8-C12
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

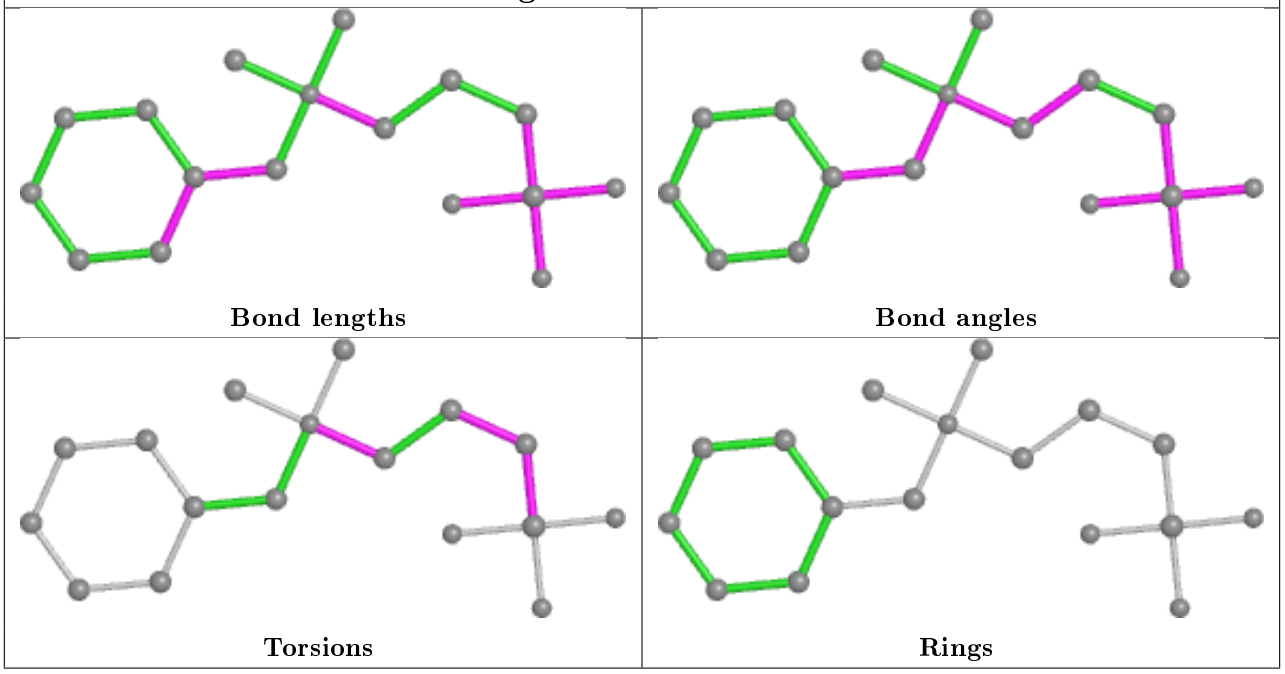
There are no ring outliers.

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 then 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.

Ligand DMX A 500



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.