



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:39 PM UTC

PDB ID : 1MFZ / pdb_00001mfz
Title : Partially refined 2.8 Å Crystal structure of GDP-mannose dehydrogenase from *P. aeruginosa*
Authors : Snook, C.F.; Tipton, P.A.; Beamer, L.J.
Deposited on : 2002-08-14
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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

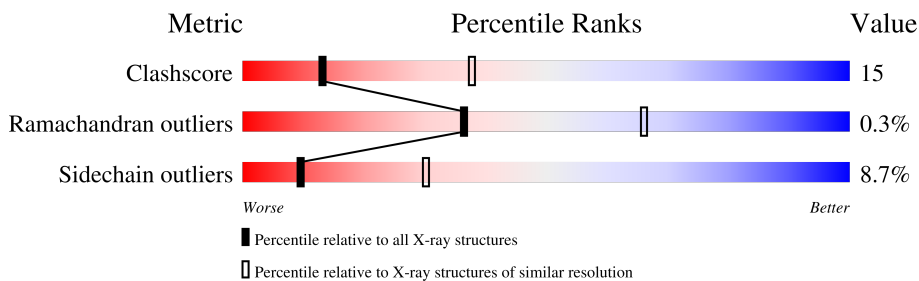
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	436	
1	B	436	
1	C	436	
1	D	436	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13283 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 GDP-mannose 6-dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	Se	0	0	0
			3271	2061	560	632	9	9			
1	B	436	Total	C	N	O	S	Se	0	0	0
			3258	2053	558	629	9	9			
1	C	436	Total	C	N	O	S	Se	0	0	0
			3233	2032	556	627	9	9			
1	D	436	Total	C	N	O	S	Se	0	0	0
			3255	2052	561	624	9	9			

There are 36 discrepancies between the modelled and reference sequences:

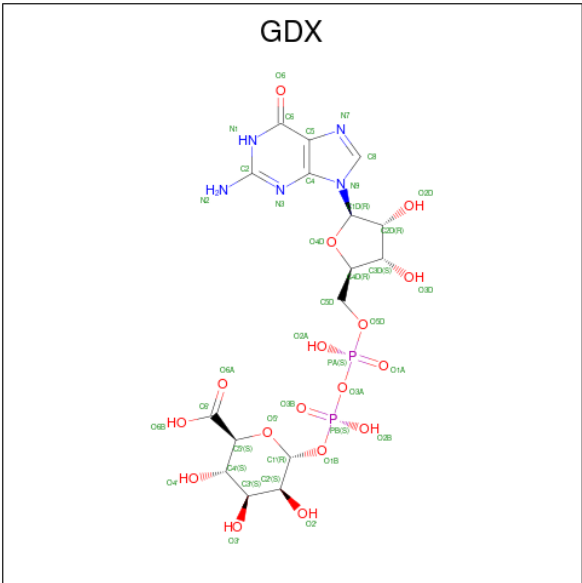
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P11759
A	173	MSE	MET	modified residue	UNP P11759
A	208	MSE	MET	modified residue	UNP P11759
A	242	MSE	MET	modified residue	UNP P11759
A	258	MSE	MET	modified residue	UNP P11759
A	289	MSE	MET	modified residue	UNP P11759
A	294	MSE	MET	modified residue	UNP P11759
A	341	MSE	MET	modified residue	UNP P11759
A	423	MSE	MET	modified residue	UNP P11759
B	1	MSE	MET	modified residue	UNP P11759
B	173	MSE	MET	modified residue	UNP P11759
B	208	MSE	MET	modified residue	UNP P11759
B	242	MSE	MET	modified residue	UNP P11759
B	258	MSE	MET	modified residue	UNP P11759
B	289	MSE	MET	modified residue	UNP P11759
B	294	MSE	MET	modified residue	UNP P11759
B	341	MSE	MET	modified residue	UNP P11759
B	423	MSE	MET	modified residue	UNP P11759
C	1	MSE	MET	modified residue	UNP P11759
C	173	MSE	MET	modified residue	UNP P11759
C	208	MSE	MET	modified residue	UNP P11759

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Chain	Residue	Modelled	Actual	Comment	Reference
C	242	MSE	MET	modified residue	UNP P11759
C	258	MSE	MET	modified residue	UNP P11759
C	289	MSE	MET	modified residue	UNP P11759
C	294	MSE	MET	modified residue	UNP P11759
C	341	MSE	MET	modified residue	UNP P11759
C	423	MSE	MET	modified residue	UNP P11759
D	1	MSE	MET	modified residue	UNP P11759
D	173	MSE	MET	modified residue	UNP P11759
D	208	MSE	MET	modified residue	UNP P11759
D	242	MSE	MET	modified residue	UNP P11759
D	258	MSE	MET	modified residue	UNP P11759
D	289	MSE	MET	modified residue	UNP P11759
D	294	MSE	MET	modified residue	UNP P11759
D	341	MSE	MET	modified residue	UNP P11759
D	423	MSE	MET	modified residue	UNP P11759

- Molecule 2 is GUANOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), P'-D-MANNOPYRANOSYL ESTER (CCD ID: GDX) (formula: C₁₆H₂₃N₅O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			40	16	5	17	2		
2	B	1	Total	C	N	O	P	0	0
			40	16	5	17	2		
2	D	1	Total	C	N	O	P	0	0
			40	16	5	17	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			40	16	5	17	2		

- Molecule 3 is water.

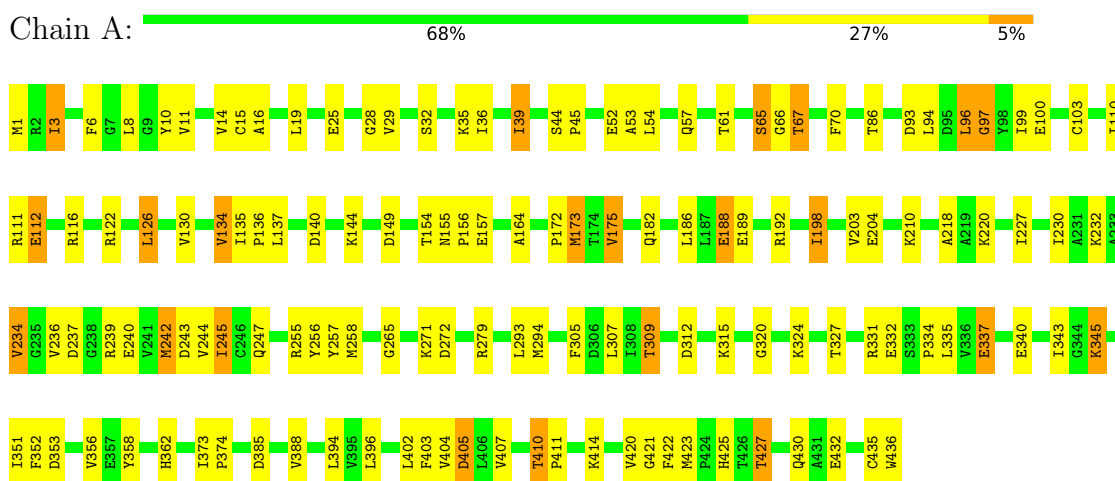
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		
3	B	31	Total	O	0	0
			31	31		
3	C	26	Total	O	0	0
			26	26		
3	D	22	Total	O	0	0
			22	22		

3 Residue-property plots [i](#)

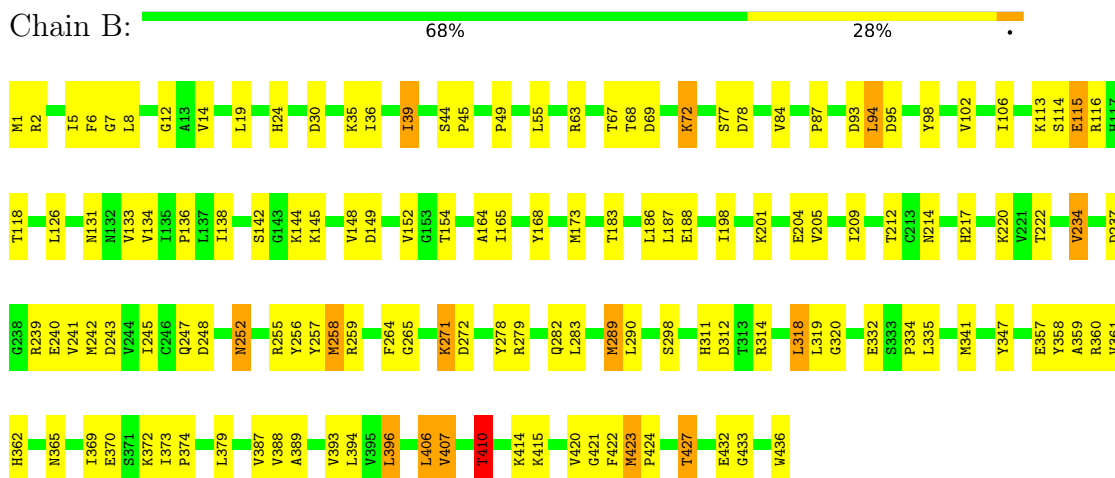
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: GDP-mannose 6-dehydrogenase

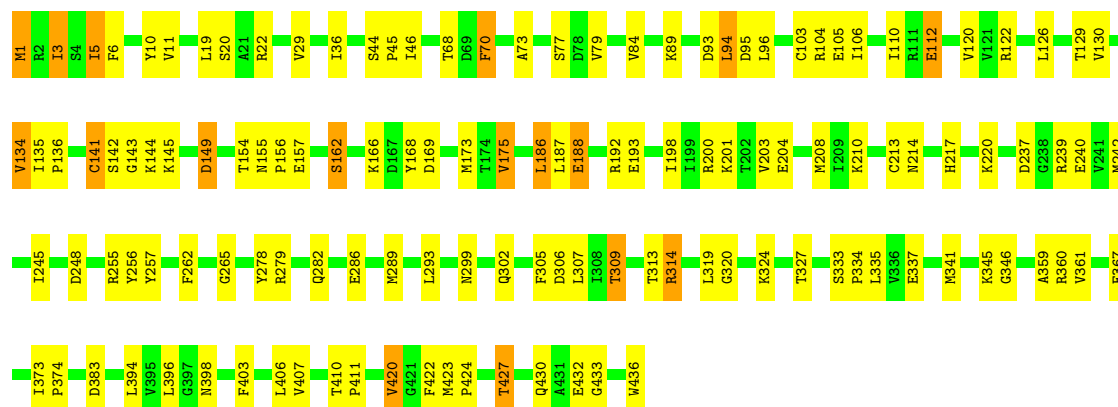


- Molecule 1: GDP-mannose 6-dehydrogenase

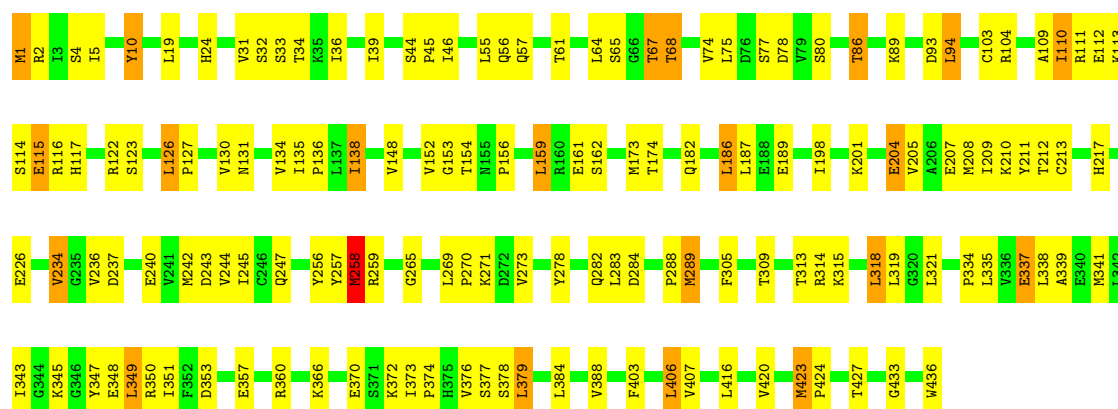


- Molecule 1: GDP-mannose 6-dehydrogenase





• Molecule 1: GDP-mannose 6-dehydrogenase



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	131.17Å 136.83Å 218.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80	Depositor
% Data completeness (in resolution range)	100.0 (40.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.204 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13283	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.71	4/3317 (0.1%)	1.00	5/4484 (0.1%)
1	B	0.65	6/3303 (0.2%)	0.99	3/4470 (0.1%)
1	C	0.63	4/3279 (0.1%)	0.99	4/4440 (0.1%)
1	D	0.64	8/3299 (0.2%)	0.98	6/4464 (0.1%)
All	All	0.66	22/13198 (0.2%)	0.99	18/17858 (0.1%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	423	MSE	SE-CE	-15.29	1.49	1.95
1	A	294	MSE	SE-CE	-10.71	1.63	1.95
1	B	258	MSE	SE-CE	-10.25	1.64	1.95
1	A	173	MSE	SE-CE	-10.20	1.64	1.95
1	C	173	MSE	SE-CE	-9.79	1.66	1.95
1	B	173	MSE	SE-CE	-9.51	1.67	1.95
1	D	423	MSE	SE-CE	-9.48	1.67	1.95
1	A	242	MSE	SE-CE	-9.13	1.68	1.95
1	B	289	MSE	SE-CE	-8.23	1.70	1.95
1	D	173	MSE	SE-CE	-7.86	1.71	1.95
1	C	208	MSE	SE-CE	-7.72	1.72	1.95
1	C	341	MSE	SE-CE	-7.61	1.72	1.95
1	D	258	MSE	SE-CE	-7.35	1.73	1.95
1	D	242	MSE	SE-CE	-7.27	1.73	1.95
1	B	341	MSE	SE-CE	-6.74	1.75	1.95
1	D	341	MSE	SE-CE	-6.49	1.75	1.95
1	C	289	MSE	SE-CE	-6.40	1.76	1.95
1	B	423	MSE	SE-CE	-5.89	1.77	1.95
1	D	1	MSE	SE-CE	-5.72	1.78	1.95
1	D	289	MSE	SE-CE	-5.58	1.78	1.95
1	D	208	MSE	SE-CE	-5.50	1.78	1.95
1	B	242	MSE	SE-CE	-5.04	1.80	1.95

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	141	CYS	N-CA-C	-7.08	105.83	114.75
1	D	89	LYS	N-CA-C	-6.21	101.33	110.52
1	A	425	HIS	N-CA-C	6.10	116.49	108.07
1	D	68	THR	N-CA-C	-5.97	106.33	113.97
1	D	112	GLU	N-CA-C	-5.76	104.91	111.14
1	A	337	GLU	N-CA-C	-5.62	104.36	111.11
1	B	410	THR	N-CA-C	5.52	116.62	109.72
1	A	315	LYS	N-CA-C	5.51	118.34	107.98
1	D	337	GLU	N-CA-C	-5.38	105.10	110.97
1	A	351	ILE	N-CA-C	5.35	116.19	108.48
1	B	240	GLU	N-CA-C	-5.32	105.48	111.28
1	B	252	ASN	N-CA-C	5.30	116.75	110.97
1	C	143	GLY	N-CA-C	-5.24	108.68	115.59
1	A	3	ILE	N-CA-C	5.14	115.30	108.11
1	D	86	THR	O-C-N	5.09	124.33	121.27
1	C	5	ILE	N-CA-C	5.07	115.34	107.28
1	C	166	LYS	N-CA-C	-5.05	105.78	111.28
1	D	349	LEU	N-CA-C	5.03	116.71	108.52

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	3271	0	3233	114	1
1	B	3258	0	3211	105	0
1	C	3233	0	3136	98	0
1	D	3255	0	3219	112	0
2	B	80	0	30	1	0
2	D	80	0	31	3	0
3	A	27	0	0	2	0
3	B	31	0	0	1	0
3	C	26	0	0	1	0
3	D	22	0	0	1	0
All	All	13283	0	12860	389	1

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 (389) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LYS:HB3	1:B:258:MSE:HE3	1.32	1.12
1:B:1:MSE:HE1	1:B:186:LEU:HD11	1.39	1.04
1:A:44:SER:HB3	1:A:52:GLU:OE1	1.59	1.01
1:D:427:THR:HG22	1:D:433:GLY:H	1.24	1.00
1:B:8:LEU:HD13	1:B:39:ILE:HD12	1.40	0.99
1:C:70:PHE:HD1	1:C:70:PHE:H	0.98	0.97
1:D:427:THR:HG23	1:D:436:TRP:OXT	1.68	0.94
1:C:314:ARG:NH1	1:C:346:GLY:O	2.01	0.92
1:A:427:THR:HG22	1:A:436:TRP:OXT	1.69	0.92
1:A:245:ILE:HD11	1:B:212:THR:HB	1.51	0.92
1:B:427:THR:HG22	1:B:432:GLU:HA	1.59	0.84
1:C:157:GLU:O	1:C:210:LYS:HE2	1.80	0.81
1:D:116:ARG:HG3	1:D:116:ARG:HH11	1.46	0.79
1:D:32:SER:OG	1:D:34:THR:HG22	1.82	0.79
1:C:396:LEU:HD11	1:C:407:VAL:HG22	1.64	0.79
1:D:86:THR:HB	1:D:94:LEU:CD2	2.12	0.79
1:C:427:THR:HB	1:C:432:GLU:HA	1.65	0.79
1:D:86:THR:CB	1:D:94:LEU:HD21	2.13	0.79
1:D:86:THR:HB	1:D:94:LEU:HD21	1.65	0.79
1:A:427:THR:HB	1:A:432:GLU:HA	1.65	0.78
1:B:406:LEU:O	1:B:410:THR:OG1	2.03	0.77
1:A:220:LYS:HB3	1:B:258:MSE:CE	2.14	0.76
1:A:130:VAL:HG21	1:A:154:THR:HG22	1.68	0.75
1:D:427:THR:CG2	1:D:436:TRP:OXT	2.33	0.75
1:C:1:MSE:SE	1:C:186:LEU:CD2	2.85	0.74
1:A:3:ILE:HD13	1:A:19:LEU:HD13	1.68	0.73
1:A:230:ILE:O	1:A:234:VAL:HG13	1.87	0.73
1:A:237:ASP:OD1	1:A:239:ARG:N	2.22	0.73
1:A:220:LYS:CB	1:B:258:MSE:HE3	2.16	0.72
1:C:255:ARG:NH2	1:D:243:ASP:OD1	2.16	0.72
1:A:427:THR:CG2	1:A:436:TRP:OXT	2.38	0.71
1:D:116:ARG:HG3	1:D:116:ARG:NH1	2.04	0.71
1:C:262:PHE:CE2	1:C:334:PRO:HB2	2.25	0.71
1:A:189:GLU:HG2	1:A:192:ARG:NH2	2.06	0.70
1:D:314:ARG:O	1:D:348:GLU:N	2.23	0.70
1:D:2:ARG:NH2	1:D:78:ASP:OD1	2.24	0.70
1:B:427:THR:CG2	1:B:433:GLY:H	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:GLU:OE1	1:B:370:GLU:HA	1.90	0.70
1:C:130:VAL:HA	1:C:134:VAL:HG13	1.74	0.69
1:C:70:PHE:CD1	1:C:70:PHE:N	2.50	0.69
1:A:44:SER:H	1:A:52:GLU:CD	2.01	0.69
1:C:396:LEU:HD11	1:C:407:VAL:CG2	2.21	0.69
1:D:115:GLU:H	1:D:115:GLU:CD	2.01	0.68
1:A:305:PHE:O	1:A:309:THR:HB	1.93	0.68
1:A:407:VAL:HG21	1:A:422:PHE:CB	2.24	0.67
1:A:154:THR:CG2	1:A:203:VAL:HG13	2.25	0.67
1:B:427:THR:HG23	1:B:436:TRP:OXT	1.94	0.66
1:A:53:ALA:O	1:A:57:GLN:HG3	1.95	0.66
1:C:94:LEU:H	1:C:94:LEU:CD2	2.09	0.66
1:B:427:THR:HG22	1:B:433:GLY:H	1.61	0.66
1:A:94:LEU:HD22	1:A:126:LEU:HD22	1.77	0.65
1:D:269:LEU:O	1:D:273:VAL:HG23	1.97	0.65
1:A:135:ILE:HB	1:A:136:PRO:HD3	1.77	0.65
1:C:73:ALA:O	1:C:77:SER:OG	2.13	0.65
1:B:115:GLU:H	1:B:115:GLU:CD	2.03	0.64
1:C:373:ILE:N	1:C:374:PRO:HD3	2.13	0.64
1:A:8:LEU:HD13	1:A:39:ILE:HD12	1.78	0.64
1:A:353:ASP:CG	1:A:356:VAL:HG23	2.22	0.64
1:D:130:VAL:HA	1:D:134:VAL:HB	1.80	0.64
1:C:94:LEU:H	1:C:94:LEU:HD23	1.61	0.64
1:C:135:ILE:HB	1:C:136:PRO:HD3	1.80	0.64
1:D:226:GLU:OE2	1:D:288:PRO:HD2	1.97	0.64
1:A:86:THR:O	1:B:271:LYS:HD2	1.97	0.63
1:C:130:VAL:HG21	1:C:154:THR:HG22	1.80	0.63
1:D:321:LEU:HD13	1:D:351:ILE:HG21	1.80	0.63
1:C:430:GLN:O	1:C:430:GLN:HG2	1.98	0.63
1:C:142:SER:C	1:C:144:LYS:H	2.06	0.62
1:B:241:VAL:O	1:B:245:ILE:HG12	1.99	0.62
1:B:373:ILE:N	1:B:374:PRO:HD3	2.14	0.62
1:C:293:LEU:CD2	1:D:289:MSE:CE	2.78	0.62
1:B:84:VAL:HG11	1:B:102:VAL:HG21	1.81	0.62
1:C:70:PHE:CD2	1:C:105:GLU:HG2	2.35	0.62
1:B:8:LEU:HD13	1:B:39:ILE:CD1	2.22	0.62
1:D:1:MSE:HE1	1:D:186:LEU:HD11	1.82	0.62
1:D:131:ASN:ND2	1:D:204:GLU:OE2	2.29	0.62
1:A:94:LEU:HD21	3:A:447:HOH:O	2.00	0.62
1:A:243:ASP:OD1	1:B:255:ARG:NH2	2.33	0.61
1:A:388:VAL:HG13	1:A:394:LEU:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLU:OE2	1:A:198:ILE:HD12	2.00	0.61
1:D:134:VAL:O	1:D:138:ILE:HG13	2.01	0.61
1:C:427:THR:HG22	1:C:436:TRP:O	2.01	0.60
1:C:240:GLU:HG2	1:D:201:LYS:NZ	2.17	0.60
1:C:299:ASN:HB3	3:C:456:HOH:O	2.00	0.60
1:A:234:VAL:HG23	1:A:234:VAL:O	2.01	0.60
1:A:10:TYR:HD1	1:A:10:TYR:H	1.47	0.60
1:A:35:LYS:O	1:A:39:ILE:HG13	2.02	0.59
1:A:130:VAL:HG21	1:A:154:THR:CG2	2.31	0.59
1:B:271:LYS:HE3	1:B:272:ASP:OD1	2.01	0.59
1:D:5:ILE:HD11	1:D:19:LEU:HD12	1.83	0.59
1:A:154:THR:HG23	1:A:203:VAL:HG13	1.84	0.59
1:D:427:THR:HG23	1:D:436:TRP:C	2.27	0.59
1:A:257:TYR:CE2	1:B:217:HIS:CG	2.90	0.59
1:D:86:THR:OG1	1:D:94:LEU:HD21	2.02	0.59
1:B:118:THR:CG2	1:B:183:THR:HG23	2.32	0.59
1:D:357:GLU:OE2	1:D:360:ARG:HD3	2.02	0.59
1:A:57:GLN:O	1:A:61:THR:HG23	2.02	0.58
1:D:373:ILE:N	1:D:374:PRO:HD3	2.19	0.58
1:A:403:PHE:O	1:A:407:VAL:HG23	2.03	0.58
1:C:36:ILE:CD1	1:C:68:THR:HG22	2.34	0.58
1:B:115:GLU:CD	1:B:115:GLU:N	2.61	0.58
1:B:234:VAL:HG13	1:B:234:VAL:O	2.03	0.58
1:A:309:THR:O	1:A:309:THR:CG2	2.51	0.58
1:B:256:TYR:O	1:B:257:TYR:HB2	2.02	0.58
1:A:407:VAL:HG21	1:A:422:PHE:HB2	1.85	0.58
1:D:357:GLU:O	1:D:360:ARG:HG2	2.04	0.57
1:A:232:LYS:NZ	1:B:427:THR:HG21	2.20	0.57
1:C:3:ILE:HG23	1:C:79:VAL:HB	1.87	0.57
1:B:314:ARG:HA	1:B:347:TYR:CD2	2.39	0.56
1:A:245:ILE:CD1	1:B:212:THR:HB	2.29	0.56
1:B:393:VAL:HG22	1:B:415:LYS:HB2	1.87	0.56
1:B:77:SER:O	1:B:113:LYS:NZ	2.38	0.56
1:D:115:GLU:CD	1:D:115:GLU:N	2.64	0.56
1:A:3:ILE:CD1	1:A:19:LEU:HD13	2.36	0.56
1:A:407:VAL:HG21	1:A:422:PHE:HB3	1.88	0.56
1:D:427:THR:CG2	1:D:433:GLY:H	2.08	0.56
1:B:1:MSE:N	1:B:24:HIS:HD2	2.04	0.55
1:A:189:GLU:HG2	1:A:192:ARG:HH21	1.68	0.55
1:C:319:LEU:HD12	1:C:396:LEU:HD23	1.87	0.55
1:D:234:VAL:O	1:D:234:VAL:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:VAL:O	1:C:420:VAL:HG23	2.06	0.55
1:B:131:ASN:ND2	1:B:204:GLU:OE2	2.38	0.55
1:B:134:VAL:O	1:B:138:ILE:HG13	2.07	0.55
1:D:427:THR:HG22	1:D:433:GLY:N	2.07	0.55
1:C:396:LEU:HD13	1:C:422:PHE:CD2	2.42	0.55
1:B:361:VAL:HG12	1:B:362:HIS:CE1	2.42	0.55
1:C:112:GLU:N	1:C:112:GLU:OE1	2.40	0.54
1:A:237:ASP:OD1	1:A:237:ASP:C	2.50	0.54
1:C:427:THR:HG22	1:C:436:TRP:C	2.32	0.54
1:A:8:LEU:HD13	1:A:39:ILE:CD1	2.38	0.54
1:B:222:THR:HG21	1:B:289:MSE:HE3	1.88	0.54
1:B:388:VAL:HA	1:B:394:LEU:HD21	1.90	0.54
1:B:116:ARG:HG3	1:B:116:ARG:HH11	1.72	0.54
1:C:94:LEU:HD23	1:C:94:LEU:N	2.22	0.54
1:D:126:LEU:HD13	1:D:211:TYR:CZ	2.43	0.54
1:C:145:LYS:N	1:C:149:ASP:OD2	2.35	0.53
1:A:320:GLY:O	1:A:335:LEU:HD13	2.08	0.53
1:C:22:ARG:NH2	1:C:169:ASP:OD1	2.34	0.53
1:C:396:LEU:CD1	1:C:407:VAL:CG2	2.86	0.53
1:B:372:LYS:C	1:B:374:PRO:HD3	2.34	0.53
1:A:324:LYS:O	1:A:327:THR:HG22	2.08	0.53
1:C:122:ARG:NE	1:C:155:ASN:OD1	2.40	0.53
1:A:265:GLY:HA3	1:A:334:PRO:HD3	1.89	0.53
1:D:154:THR:HG22	1:D:156:PRO:HD3	1.90	0.53
1:A:154:THR:HG21	1:A:203:VAL:HG13	1.91	0.53
1:A:358:TYR:CZ	1:A:362:HIS:HD2	2.27	0.53
1:C:201:LYS:HZ1	1:D:240:GLU:HG3	1.74	0.53
1:C:427:THR:HG22	1:C:436:TRP:OXT	2.08	0.53
1:B:116:ARG:HG3	1:B:116:ARG:NH1	2.25	0.52
1:B:234:VAL:O	1:B:234:VAL:CG1	2.57	0.52
1:A:130:VAL:HB	1:A:203:VAL:HG11	1.92	0.52
1:D:406:LEU:O	1:D:406:LEU:HD22	2.10	0.52
1:C:94:LEU:CD2	1:C:94:LEU:N	2.72	0.52
1:A:244:VAL:O	1:A:247:GLN:HB2	2.10	0.52
1:C:305:PHE:O	1:C:309:THR:HB	2.09	0.52
1:D:1:MSE:HB2	1:D:24:HIS:CD2	2.45	0.52
1:D:44:SER:OG	1:D:46:ILE:O	2.24	0.52
1:D:259:ARG:HB2	2:D:501:GDX:O6	2.09	0.52
1:B:256:TYR:HD2	1:B:257:TYR:CD2	2.28	0.52
1:C:154:THR:HG21	1:C:203:VAL:HG13	1.92	0.52
1:B:1:MSE:CE	1:B:186:LEU:HD11	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:PRO:HD2	1:B:95:ASP:HB3	1.92	0.52
1:C:293:LEU:HD21	1:D:289:MSE:CE	2.40	0.52
1:C:188:GLU:HG2	1:C:198:ILE:HG21	1.92	0.52
1:D:4:SER:HG	1:D:80:SER:HG	1.58	0.52
1:D:77:SER:O	1:D:113:LYS:NZ	2.42	0.52
1:D:189:GLU:OE1	1:D:189:GLU:HA	2.09	0.52
1:D:313:THR:C	1:D:315:LYS:H	2.17	0.51
1:B:319:LEU:HD12	1:B:396:LEU:HD13	1.93	0.51
1:C:248:ASP:OD1	1:C:248:ASP:C	2.49	0.51
1:C:320:GLY:O	1:C:335:LEU:HD13	2.09	0.51
1:D:10:TYR:C	1:D:10:TYR:CD1	2.88	0.51
1:D:174:THR:HB	1:D:198:ILE:HG12	1.93	0.51
1:C:5:ILE:HD11	1:C:19:LEU:HD12	1.92	0.51
1:C:36:ILE:HD12	1:C:68:THR:HG22	1.91	0.51
1:D:313:THR:HG23	1:D:313:THR:O	2.10	0.51
1:A:244:VAL:HG11	1:B:209:ILE:HD13	1.93	0.51
1:B:118:THR:HG21	1:B:183:THR:HG23	1.93	0.51
1:C:89:LYS:HE3	1:C:93:ASP:HB3	1.92	0.51
1:D:126:LEU:HD13	1:D:211:TYR:CE2	2.46	0.51
1:C:1:MSE:SE	1:C:186:LEU:HD22	2.61	0.51
1:D:278:TYR:OH	1:D:282:GLN:NE2	2.44	0.51
1:D:237:ASP:OD1	1:D:237:ASP:C	2.54	0.50
1:D:339:ALA:O	1:D:343:ILE:HG13	2.10	0.50
1:D:57:GLN:O	1:D:61:THR:HG23	2.11	0.50
1:A:135:ILE:CB	1:A:136:PRO:HD3	2.41	0.50
1:D:384:LEU:O	1:D:388:VAL:HG23	2.11	0.50
1:B:102:VAL:O	1:B:106:ILE:HG13	2.12	0.50
1:B:222:THR:CG2	1:B:289:MSE:HE3	2.40	0.50
1:B:318:LEU:HD13	1:B:320:GLY:O	2.12	0.50
1:B:358:TYR:CE1	1:B:362:HIS:HB2	2.47	0.50
1:C:120:VAL:HG21	1:C:187:LEU:HD21	1.92	0.50
1:C:142:SER:C	1:C:144:LYS:N	2.69	0.50
1:C:213:CYS:SG	1:D:245:ILE:HD13	2.51	0.50
1:A:100:GLU:HG2	1:A:137:LEU:CD1	2.42	0.50
1:A:52:GLU:O	1:A:53:ALA:C	2.55	0.49
1:D:305:PHE:CZ	1:D:309:THR:HG21	2.46	0.49
1:C:373:ILE:N	1:C:374:PRO:CD	2.75	0.49
1:A:10:TYR:CD1	1:A:10:TYR:N	2.80	0.49
1:A:388:VAL:O	1:A:414:LYS:NZ	2.40	0.49
1:B:370:GLU:O	1:B:374:PRO:HG3	2.11	0.49
1:B:389:ALA:O	1:B:414:LYS:NZ	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LEU:O	1:A:97:GLY:C	2.56	0.49
1:A:144:LYS:HD3	1:A:149:ASP:HB3	1.94	0.49
1:A:293:LEU:CD2	1:B:289:MSE:HE3	2.42	0.49
1:D:110:ILE:HG21	1:D:117:HIS:HB3	1.95	0.49
1:A:240:GLU:HG3	1:B:201:LYS:HZ1	1.78	0.49
1:D:135:ILE:HB	1:D:136:PRO:HD3	1.94	0.49
1:A:218:ALA:HB1	1:B:264:PHE:CE2	2.48	0.48
1:A:396:LEU:HD22	1:A:403:PHE:HB3	1.96	0.48
1:D:376:VAL:O	1:D:379:LEU:HB2	2.12	0.48
1:A:116:ARG:HH12	1:A:182:GLN:CD	2.21	0.48
1:D:36:ILE:O	1:D:39:ILE:HG22	2.13	0.48
1:D:318:LEU:HB2	1:D:349:LEU:HD11	1.95	0.48
1:C:20:SER:C	1:C:22:ARG:H	2.22	0.48
1:D:370:GLU:O	1:D:374:PRO:HG3	2.13	0.48
1:A:14:VAL:HG21	1:A:164:ALA:CB	2.44	0.48
1:B:205:VAL:O	1:B:209:ILE:HG13	2.13	0.48
1:B:49:PRO:O	1:B:165:ILE:HD12	2.13	0.48
1:C:44:SER:OG	1:C:46:ILE:O	2.27	0.48
1:B:14:VAL:HG21	1:B:164:ALA:HB1	1.94	0.48
1:B:365:ASN:O	1:B:369:ILE:HG13	2.13	0.48
1:D:244:VAL:HA	1:D:247:GLN:HE21	1.77	0.48
1:A:6:PHE:CE2	1:A:70:PHE:CD2	3.02	0.48
1:A:6:PHE:HE2	1:A:70:PHE:CD2	2.32	0.48
1:A:116:ARG:NH1	1:A:182:GLN:OE1	2.46	0.48
1:B:5:ILE:HD11	1:B:19:LEU:HD12	1.96	0.48
1:D:319:LEU:HB3	1:D:403:PHE:CZ	2.49	0.48
1:A:373:ILE:N	1:A:374:PRO:HD3	2.29	0.48
1:D:116:ARG:HH11	1:D:116:ARG:CG	2.19	0.48
1:B:7:GLY:O	1:B:12:GLY:HA3	2.13	0.47
1:C:240:GLU:HG2	1:D:201:LYS:HZ1	1.78	0.47
1:D:1:MSE:HB2	1:D:24:HIS:HD2	1.79	0.47
1:B:311:HIS:O	1:B:312:ASP:C	2.56	0.47
1:C:104:ARG:HG2	1:C:141:CYS:SG	2.54	0.47
1:B:168:TYR:CD1	1:B:168:TYR:C	2.92	0.47
1:B:93:ASP:OD1	1:B:94:LEU:N	2.45	0.47
1:D:109:ALA:C	1:D:111:ARG:H	2.22	0.47
1:A:28:GLY:O	1:A:66:GLY:HA2	2.13	0.47
1:A:358:TYR:O	1:A:362:HIS:HB2	2.14	0.47
1:A:421:GLY:HA2	1:A:436:TRP:CZ2	2.50	0.47
1:D:103:CYS:O	1:D:104:ARG:C	2.58	0.47
1:C:319:LEU:HB3	1:C:403:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:VAL:HG13	1:D:117:HIS:NE2	2.30	0.46
1:C:394:LEU:HD13	1:C:406:LEU:HD21	1.96	0.46
1:A:373:ILE:O	1:A:373:ILE:HG13	2.15	0.46
1:B:358:TYR:CD1	1:B:358:TYR:C	2.94	0.46
1:D:67:THR:OG1	1:D:68:THR:N	2.47	0.46
1:A:272:ASP:OD2	1:B:214:ASN:ND2	2.41	0.46
1:C:156:PRO:HD2	1:C:175:VAL:HG22	1.97	0.46
1:B:67:THR:OG1	1:B:68:THR:N	2.48	0.46
1:B:248:ASP:OD1	1:B:248:ASP:C	2.58	0.46
1:B:421:GLY:HA2	1:B:436:TRP:CZ2	2.50	0.46
1:B:394:LEU:HD13	1:B:406:LEU:HD11	1.97	0.46
1:C:95:ASP:C	1:C:95:ASP:OD1	2.59	0.46
1:D:372:LYS:C	1:D:374:PRO:HD3	2.41	0.46
1:A:28:GLY:N	1:A:65:SER:O	2.39	0.46
1:A:309:THR:O	1:A:309:THR:HG23	2.16	0.46
1:C:220:LYS:HE2	1:D:258:MSE:HG2	1.97	0.46
1:D:44:SER:HA	1:D:45:PRO:HD3	1.81	0.46
1:B:259:ARG:CZ	3:B:532:HOH:O	2.64	0.45
1:D:209:ILE:HG22	1:D:210:LYS:N	2.31	0.45
1:D:350:ARG:HG3	3:D:506:HOH:O	2.15	0.45
1:C:265:GLY:HA3	1:C:334:PRO:HD3	1.99	0.45
1:D:265:GLY:HA3	1:D:334:PRO:HD3	1.97	0.45
1:A:173:MSE:HB3	1:A:173:MSE:HE2	1.72	0.45
1:B:357:GLU:OE1	1:B:360:ARG:HD3	2.17	0.45
1:D:349:LEU:O	1:D:379:LEU:HG	2.16	0.45
1:A:110:ILE:O	1:A:111:ARG:C	2.59	0.45
1:B:44:SER:HA	1:B:45:PRO:HD3	1.82	0.45
1:C:106:ILE:O	1:C:110:ILE:HG13	2.16	0.45
1:A:173:MSE:HE1	1:B:247:GLN:C	2.42	0.45
1:B:427:THR:HG22	1:B:432:GLU:CA	2.41	0.45
1:C:433:GLY:HA3	1:C:436:TRP:CE2	2.52	0.45
1:B:2:ARG:NH2	1:B:78:ASP:OD1	2.45	0.45
1:B:145:LYS:N	1:B:149:ASP:OD2	2.41	0.45
1:B:279:ARG:NH1	1:B:282:GLN:OE1	2.50	0.45
1:C:20:SER:C	1:C:22:ARG:N	2.75	0.45
1:A:103:CYS:SG	1:A:134:VAL:HB	2.56	0.45
1:A:396:LEU:HD13	1:A:422:PHE:CD2	2.52	0.45
1:A:435:CYS:HB2	1:A:436:TRP:CE3	2.52	0.45
1:D:110:ILE:H	1:D:110:ILE:HG12	1.49	0.45
1:A:352:PHE:CD1	1:A:352:PHE:C	2.95	0.44
1:D:1:MSE:CE	1:D:186:LEU:HD11	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LYS:HZ3	1:B:427:THR:HG21	1.81	0.44
1:B:69:ASP:CG	1:B:72:LYS:HB2	2.42	0.44
1:C:44:SER:HA	1:C:45:PRO:HD3	1.86	0.44
1:C:242:MSE:HE2	1:D:258:MSE:HE2	1.98	0.44
1:D:127:PRO:HA	1:D:207:GLU:OE1	2.17	0.44
1:C:6:PHE:HA	1:C:29:VAL:HB	1.99	0.44
1:C:257:TYR:CE2	1:D:217:HIS:CG	3.05	0.44
1:D:161:GLU:O	1:D:162:SER:CB	2.66	0.44
1:C:302:GLN:NE2	1:C:306:ASP:OD1	2.48	0.44
1:B:427:THR:HG22	1:B:433:GLY:N	2.31	0.44
1:D:257:TYR:OH	2:D:501:GDX:O1A	2.25	0.44
1:A:15:CYS:O	1:A:16:ALA:C	2.61	0.43
1:A:36:ILE:HD13	1:A:67:THR:C	2.43	0.43
1:A:404:VAL:O	1:A:407:VAL:N	2.51	0.43
1:B:359:ALA:C	1:B:361:VAL:H	2.25	0.43
1:C:423:MSE:HA	1:C:424:PRO:HD3	1.83	0.43
1:B:407:VAL:HG11	1:B:422:PHE:HB3	1.99	0.43
1:C:257:TYR:OH	2:D:502:GDX:O1A	2.29	0.43
1:D:213:CYS:O	1:D:217:HIS:CD2	2.71	0.43
1:A:122:ARG:HG2	1:A:155:ASN:O	2.19	0.43
1:A:156:PRO:HG2	1:A:175:VAL:CG2	2.48	0.43
1:C:188:GLU:O	1:C:192:ARG:HB2	2.18	0.43
1:C:213:CYS:SG	1:D:245:ILE:CD1	3.06	0.43
1:D:159:LEU:H	1:D:159:LEU:HG	1.68	0.43
1:A:116:ARG:HH12	1:A:182:GLN:CB	2.32	0.43
1:A:110:ILE:C	1:A:112:GLU:N	2.75	0.43
1:D:152:VAL:HG12	1:D:153:GLY:N	2.34	0.43
1:D:186:LEU:HD22	1:D:186:LEU:HA	1.63	0.43
1:B:98:TYR:O	1:B:102:VAL:HG23	2.19	0.43
1:B:142:SER:C	1:B:144:LYS:H	2.24	0.43
1:B:148:VAL:HG23	1:B:149:ASP:N	2.33	0.43
1:A:358:TYR:CE2	1:A:362:HIS:HD2	2.36	0.43
1:C:245:ILE:HD11	1:D:212:THR:HB	1.99	0.43
1:C:359:ALA:O	1:C:361:VAL:N	2.52	0.43
1:D:374:PRO:O	1:D:378:SER:HB3	2.19	0.43
1:B:289:MSE:O	1:B:290:LEU:C	2.62	0.42
1:B:1:MSE:H3	1:B:24:HIS:HD2	1.67	0.42
1:A:172:PRO:HB3	1:B:248:ASP:OD1	2.19	0.42
1:C:10:TYR:HA	1:C:46:ILE:HD13	2.01	0.42
1:A:293:LEU:CD2	1:B:289:MSE:CE	2.98	0.42
1:B:114:SER:HB3	1:B:115:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:ASN:C	1:C:398:ASN:OD1	2.62	0.42
1:D:258:MSE:CE	1:D:258:MSE:HA	2.49	0.42
1:A:331:ARG:O	1:A:332:GLU:C	2.62	0.42
1:C:217:HIS:CG	1:D:257:TYR:CE2	3.08	0.42
1:C:309:THR:O	1:C:309:THR:CG2	2.67	0.42
1:D:314:ARG:HA	1:D:347:TYR:CD2	2.55	0.42
1:A:256:TYR:O	1:A:257:TYR:HB2	2.20	0.42
1:C:237:ASP:OD1	1:C:239:ARG:HB2	2.19	0.42
1:A:44:SER:HA	1:A:45:PRO:HD3	1.78	0.42
1:C:70:PHE:CD2	1:C:105:GLU:CG	3.01	0.42
1:B:265:GLY:HA3	1:B:334:PRO:HD3	2.02	0.42
1:C:293:LEU:CD2	1:D:289:MSE:HE3	2.47	0.42
1:A:388:VAL:HG13	1:A:394:LEU:CD1	2.49	0.42
1:C:333:SER:HA	1:C:334:PRO:HD3	1.88	0.42
1:A:157:GLU:H	1:A:157:GLU:HG3	1.70	0.41
1:A:258:MSE:HG2	1:B:220:LYS:HE2	2.02	0.41
1:B:423:MSE:HA	1:B:424:PRO:HD3	1.86	0.41
1:D:256:TYR:O	1:D:257:TYR:HB2	2.19	0.41
1:A:343:ILE:HG23	3:A:450:HOH:O	2.21	0.41
1:A:404:VAL:O	1:A:405:ASP:C	2.62	0.41
1:D:305:PHE:CZ	1:D:345:LYS:HG3	2.55	0.41
1:D:366:LYS:HB3	1:D:366:LYS:HE2	1.76	0.41
1:D:377:SER:C	1:D:379:LEU:H	2.26	0.41
1:A:93:ASP:HB2	1:B:278:TYR:CE2	2.55	0.41
1:A:156:PRO:HD2	1:A:175:VAL:O	2.20	0.41
1:B:188:GLU:HG3	1:B:198:ILE:CD1	2.50	0.41
1:C:383:ASP:C	1:C:383:ASP:OD1	2.63	0.41
1:D:258:MSE:HA	1:D:258:MSE:HE3	2.02	0.41
1:D:305:PHE:HZ	1:D:345:LYS:HG3	1.84	0.41
1:A:210:LYS:NZ	2:B:503:GDX:O6A	2.42	0.41
1:C:240:GLU:HG2	1:D:201:LYS:HZ2	1.84	0.41
1:C:256:TYR:O	1:C:257:TYR:HB2	2.21	0.41
1:D:423:MSE:HA	1:D:424:PRO:HD3	1.85	0.41
1:A:182:GLN:H	1:A:182:GLN:HG3	1.47	0.41
1:D:56:GLN:O	1:D:57:GLN:C	2.63	0.41
1:C:134:VAL:CG2	1:C:135:ILE:N	2.82	0.41
1:C:200:ARG:O	1:C:201:LYS:HD3	2.20	0.41
1:D:1:MSE:N	1:D:24:HIS:HD2	2.19	0.41
1:D:122:ARG:O	1:D:123:SER:C	2.64	0.41
1:D:64:LEU:HG	1:D:65:SER:N	2.35	0.41
1:A:156:PRO:HB3	1:A:210:LYS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ILE:HG21	1:A:242:MSE:SE	2.70	0.41
1:A:430:GLN:O	1:A:430:GLN:HG2	2.19	0.41
1:C:103:CYS:SG	1:C:134:VAL:HB	2.61	0.41
1:C:122:ARG:HG2	1:C:155:ASN:O	2.20	0.41
1:D:337:GLU:O	1:D:338:LEU:C	2.64	0.41
1:A:255:ARG:NH2	1:B:243:ASP:OD1	2.52	0.41
1:B:237:ASP:OD1	1:B:239:ARG:HB2	2.21	0.41
1:C:134:VAL:HG22	1:C:135:ILE:N	2.35	0.41
1:C:210:LYS:NZ	1:C:214:ASN:ND2	2.69	0.41
1:C:410:THR:HA	1:C:411:PRO:HD3	1.93	0.40
1:D:93:ASP:OD1	1:D:94:LEU:N	2.53	0.40
1:D:182:GLN:O	1:D:186:LEU:HB2	2.21	0.40
1:A:220:LYS:NZ	1:B:252:ASN:O	2.50	0.40
1:A:227:ILE:HG13	1:B:212:THR:HG23	2.03	0.40
1:B:6:PHE:CD2	1:B:102:VAL:HG13	2.55	0.40
1:A:410:THR:HA	1:A:411:PRO:HD3	1.76	0.40
1:B:373:ILE:N	1:B:374:PRO:CD	2.82	0.40
1:C:168:TYR:C	1:C:168:TYR:CD1	2.99	0.40
1:C:278:TYR:CE2	1:D:93:ASP:HB2	2.56	0.40
1:A:293:LEU:HD21	1:B:289:MSE:CE	2.51	0.40
1:B:30:ASP:HB3	1:B:36:ILE:HD11	2.04	0.40
1:B:133:VAL:C	1:B:136:PRO:HD2	2.47	0.40
1:C:324:LYS:O	1:C:327:THR:HG22	2.22	0.40
1:D:269:LEU:CB	1:D:270:PRO:HD3	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:GLU:OE1	1:A:345:LYS:NZ[4_566]	2.17	0.03

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	434/436 (100%)	400 (92%)	32 (7%)	2 (0%)	24	55
1	B	434/436 (100%)	405 (93%)	29 (7%)	0	100	100
1	C	434/436 (100%)	395 (91%)	36 (8%)	3 (1%)	18	47
1	D	434/436 (100%)	405 (93%)	28 (6%)	1 (0%)	43	72
All	All	1736/1744 (100%)	1605 (92%)	125 (7%)	6 (0%)	36	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	360	ARG
1	A	97	GLY
1	C	162	SER
1	C	367	GLU
1	D	353	ASP
1	A	112	GLU

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	352/361 (98%)	317 (90%)	35 (10%)	7	24
1	B	349/361 (97%)	323 (93%)	26 (7%)	13	37
1	C	340/361 (94%)	311 (92%)	29 (8%)	10	31
1	D	347/361 (96%)	316 (91%)	31 (9%)	9	29
All	All	1388/1444 (96%)	1267 (91%)	121 (9%)	9	30

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	11	VAL
1	A	25	GLU

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Mol	Chain	Res	Type
1	A	29	VAL
1	A	32	SER
1	A	39	ILE
1	A	54	LEU
1	A	65	SER
1	A	67	THR
1	A	96	LEU
1	A	99	ILE
1	A	126	LEU
1	A	134	VAL
1	A	140	ASP
1	A	175	VAL
1	A	186	LEU
1	A	188	GLU
1	A	198	ILE
1	A	204	GLU
1	A	234	VAL
1	A	236	VAL
1	A	245	ILE
1	A	271	LYS
1	A	279	ARG
1	A	307	LEU
1	A	309	THR
1	A	312	ASP
1	A	337	GLU
1	A	345	LYS
1	A	385	ASP
1	A	402	LEU
1	A	405	ASP
1	A	410	THR
1	A	420	VAL
1	A	427	THR
1	B	35	LYS
1	B	39	ILE
1	B	55	LEU
1	B	63	ARG
1	B	72	LYS
1	B	94	LEU
1	B	115	GLU
1	B	126	LEU
1	B	152	VAL
1	B	154	THR

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Mol	Chain	Res	Type
1	B	187	LEU
1	B	234	VAL
1	B	271	LYS
1	B	283	LEU
1	B	298	SER
1	B	318	LEU
1	B	332	GLU
1	B	335	LEU
1	B	379	LEU
1	B	387	VAL
1	B	396	LEU
1	B	406	LEU
1	B	407	VAL
1	B	410	THR
1	B	420	VAL
1	B	427	THR
1	C	1	MSE
1	C	3	ILE
1	C	11	VAL
1	C	70	PHE
1	C	84	VAL
1	C	94	LEU
1	C	96	LEU
1	C	112	GLU
1	C	126	LEU
1	C	129	THR
1	C	134	VAL
1	C	149	ASP
1	C	162	SER
1	C	175	VAL
1	C	186	LEU
1	C	188	GLU
1	C	193	GLU
1	C	204	GLU
1	C	279	ARG
1	C	282	GLN
1	C	286	GLU
1	C	307	LEU
1	C	309	THR
1	C	313	THR
1	C	314	ARG
1	C	337	GLU

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Mol	Chain	Res	Type
1	C	345	LYS
1	C	420	VAL
1	C	427	THR
1	D	10	TYR
1	D	31	VAL
1	D	33	SER
1	D	55	LEU
1	D	67	THR
1	D	75	LEU
1	D	94	LEU
1	D	110	ILE
1	D	114	SER
1	D	115	GLU
1	D	126	LEU
1	D	138	ILE
1	D	148	VAL
1	D	159	LEU
1	D	186	LEU
1	D	187	LEU
1	D	204	GLU
1	D	205	VAL
1	D	234	VAL
1	D	236	VAL
1	D	258	MSE
1	D	271	LYS
1	D	283	LEU
1	D	284	ASP
1	D	318	LEU
1	D	335	LEU
1	D	379	LEU
1	D	406	LEU
1	D	407	VAL
1	D	416	LEU
1	D	420	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	362	HIS
1	B	24	HIS
1	B	155	ASN
1	B	182	GLN

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Mol	Chain	Res	Type
1	B	362	HIS
1	C	302	GLN
1	C	430	GLN
1	D	24	HIS
1	D	155	ASN
1	D	247	GLN
1	D	249	HIS
1	D	282	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GDX	B	504	-	42,43,43	4.36	18 (42%)	63,67,67	2.08	18 (28%)
2	GDX	D	501	-	42,43,43	4.27	17 (40%)	63,67,67	2.15	18 (28%)
2	GDX	D	502	-	42,43,43	4.36	19 (45%)	63,67,67	2.24	18 (28%)
2	GDX	B	503	-	42,43,43	4.29	17 (40%)	63,67,67	2.15	19 (30%)

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
2	GDX	B	504	-	-	2/25/61/61	0/4/4/4
2	GDX	D	501	-	-	7/25/61/61	0/4/4/4
2	GDX	D	502	-	-	0/25/61/61	0/4/4/4
2	GDX	B	503	-	-	2/25/61/61	0/4/4/4

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	504	GDX	C4'-C5'	-12.07	1.33	1.53
2	D	502	GDX	C4'-C5'	-11.79	1.33	1.53
2	B	503	GDX	C4'-C5'	-11.02	1.35	1.53
2	D	501	GDX	C4'-C5'	-11.02	1.35	1.53
2	D	502	GDX	C5'-C6'	-9.09	1.34	1.53
2	B	504	GDX	C5'-C6'	-9.09	1.34	1.53
2	D	501	GDX	C5'-C6'	-8.81	1.34	1.53
2	D	502	GDX	O2'-C2'	-8.28	1.22	1.43
2	B	503	GDX	C5'-C6'	-8.28	1.35	1.53
2	B	503	GDX	O2D-C2D	-7.95	1.23	1.43
2	D	502	GDX	O4'-C4'	-7.93	1.23	1.43
2	B	504	GDX	O4'-C4'	-7.92	1.23	1.43
2	D	501	GDX	O4'-C4'	-7.84	1.23	1.43
2	B	503	GDX	O3'-C3'	-7.82	1.23	1.43
2	B	504	GDX	O2D-C2D	-7.79	1.23	1.43
2	B	503	GDX	O2'-C2'	-7.78	1.23	1.43
2	D	501	GDX	O2'-C2'	-7.77	1.23	1.43
2	D	501	GDX	C3D-C4D	-7.72	1.33	1.53
2	D	502	GDX	O3'-C3'	-7.72	1.23	1.43
2	B	503	GDX	C3D-C4D	-7.71	1.33	1.53
2	B	503	GDX	O4'-C4'	-7.70	1.23	1.43
2	D	502	GDX	O2D-C2D	-7.70	1.23	1.43
2	B	504	GDX	O2'-C2'	-7.69	1.23	1.43
2	D	501	GDX	O2D-C2D	-7.58	1.24	1.43
2	B	504	GDX	O3'-C3'	-7.48	1.24	1.43
2	B	504	GDX	C3D-C4D	-7.46	1.34	1.53
2	D	501	GDX	O3'-C3'	-7.39	1.24	1.43
2	D	502	GDX	C3D-C4D	-7.21	1.34	1.53
2	B	504	GDX	C4'-C3'	-6.85	1.34	1.52
2	D	502	GDX	C3D-C2D	-6.65	1.35	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	GDX	C3'-C2'	-6.58	1.35	1.52
2	B	503	GDX	C4'-C3'	-6.54	1.35	1.52
2	D	501	GDX	C2D-C1D	-6.52	1.33	1.53
2	B	503	GDX	C3D-C2D	-6.39	1.36	1.53
2	B	503	GDX	C2D-C1D	-6.39	1.33	1.53
2	B	503	GDX	C3'-C2'	-6.38	1.35	1.52
2	B	504	GDX	C1'-C2'	-6.37	1.33	1.52
2	D	502	GDX	C2D-C1D	-6.37	1.33	1.53
2	D	501	GDX	C4'-C3'	-6.36	1.35	1.52
2	D	502	GDX	C4'-C3'	-6.35	1.35	1.52
2	D	501	GDX	C3D-C2D	-6.34	1.36	1.53
2	B	503	GDX	C1'-C2'	-6.30	1.34	1.52
2	B	504	GDX	C3'-C2'	-6.30	1.36	1.52
2	D	502	GDX	C3'-C2'	-6.18	1.36	1.52
2	B	504	GDX	C3D-C2D	-6.15	1.36	1.53
2	D	502	GDX	C1'-C2'	-6.12	1.34	1.52
2	B	504	GDX	C2D-C1D	-6.05	1.34	1.53
2	D	501	GDX	C1'-C2'	-6.03	1.34	1.52
2	D	502	GDX	C1D-N9	-4.43	1.35	1.47
2	D	501	GDX	C1D-N9	-4.36	1.35	1.47
2	B	503	GDX	C1D-N9	-4.22	1.35	1.47
2	B	504	GDX	C1D-N9	-4.11	1.35	1.47
2	B	503	GDX	C5-C4	3.09	1.47	1.38
2	D	501	GDX	C5-C4	3.04	1.47	1.38
2	B	504	GDX	C6-N1	-2.92	1.33	1.38
2	D	502	GDX	C6-N1	-2.87	1.33	1.38
2	B	504	GDX	C5-N7	-2.82	1.33	1.39
2	D	502	GDX	C5-C4	2.61	1.45	1.38
2	B	503	GDX	C6-N1	-2.60	1.34	1.38
2	B	504	GDX	C5-C4	2.58	1.45	1.38
2	D	501	GDX	C5-N7	-2.45	1.34	1.39
2	D	501	GDX	O6B-C6'	-2.43	1.22	1.30
2	D	502	GDX	O6B-C6'	-2.41	1.23	1.30
2	D	502	GDX	C4-N9	-2.34	1.32	1.38
2	B	504	GDX	O6B-C6'	-2.29	1.23	1.30
2	B	503	GDX	C5-N7	-2.26	1.34	1.39
2	B	504	GDX	C8-N9	-2.24	1.32	1.37
2	D	502	GDX	C5-N7	-2.21	1.34	1.39
2	D	502	GDX	C8-N9	-2.16	1.32	1.37
2	D	501	GDX	C4-N9	-2.16	1.32	1.38
2	B	503	GDX	O6B-C6'	-2.10	1.23	1.30

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	GDX	N9-C4-N3	6.26	138.46	125.95
2	B	503	GDX	O4D-C1D-N9	6.00	121.95	108.36
2	B	503	GDX	N9-C4-N3	5.90	137.75	125.95
2	D	501	GDX	O4D-C1D-N9	5.82	121.54	108.36
2	B	504	GDX	C5-C4-N3	-5.81	119.14	128.39
2	D	502	GDX	N9-C4-N3	5.80	137.54	125.95
2	B	503	GDX	C5-C4-N3	-5.74	119.26	128.39
2	B	504	GDX	N9-C4-N3	5.72	137.39	125.95
2	D	502	GDX	C5-C4-N3	-5.61	119.46	128.39
2	D	502	GDX	O4D-C1D-N9	5.54	120.91	108.36
2	D	502	GDX	C2-N3-C4	5.40	121.59	112.30
2	D	501	GDX	C5-C4-N3	-5.31	119.95	128.39
2	B	504	GDX	C2-N3-C4	5.22	121.28	112.30
2	B	504	GDX	O4D-C1D-N9	5.16	120.05	108.36
2	B	503	GDX	C2-N3-C4	5.16	121.19	112.30
2	D	501	GDX	C2-N3-C4	5.10	121.09	112.30
2	D	501	GDX	C8-N9-C4	4.64	114.72	106.03
2	D	502	GDX	C8-N9-C4	4.57	114.60	106.03
2	B	503	GDX	C3D-C2D-C1D	4.34	109.66	101.46
2	D	502	GDX	C3D-C2D-C1D	4.08	109.18	101.46
2	B	503	GDX	C8-N9-C4	4.07	113.65	106.03
2	B	504	GDX	C3D-C2D-C1D	4.05	109.13	101.46
2	D	501	GDX	C3D-C2D-C1D	4.04	109.11	101.46
2	B	504	GDX	C8-N9-C4	4.00	113.53	106.03
2	D	502	GDX	N9-C8-N7	-3.95	106.07	113.40
2	D	502	GDX	O5'-C1'-O1B	-3.77	106.44	111.36
2	D	501	GDX	O5'-C1'-O1B	-3.76	106.44	111.36
2	B	504	GDX	N9-C8-N7	-3.76	106.43	113.40
2	D	501	GDX	N9-C8-N7	-3.49	106.93	113.40
2	D	501	GDX	C2D-C3D-C4D	3.45	109.27	102.61
2	B	503	GDX	N9-C8-N7	-3.44	107.02	113.40
2	D	502	GDX	C2D-C3D-C4D	3.43	109.23	102.61
2	D	502	GDX	C1'-O5'-C5'	-3.36	106.72	112.23
2	B	503	GDX	C2D-C3D-C4D	3.33	109.04	102.61
2	D	502	GDX	C6-C5-N7	3.32	136.32	130.29
2	B	503	GDX	C6-C5-N7	3.18	136.07	130.29
2	B	504	GDX	C2D-C3D-C4D	3.17	108.73	102.61
2	B	504	GDX	C8-N7-C5	2.93	109.48	104.26
2	B	504	GDX	C6-C5-N7	2.85	135.47	130.29
2	D	502	GDX	O2A-PA-O3A	-2.84	99.61	107.27
2	D	502	GDX	C8-N7-C5	2.81	109.27	104.26
2	B	504	GDX	C2D-C1D-N9	2.73	120.84	113.25
2	D	502	GDX	O2A-PA-O1A	2.70	125.02	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	503	GDX	PB-O1B-C1'	-2.70	110.23	121.21
2	D	501	GDX	O6-C6-C5	-2.65	119.54	126.53
2	B	503	GDX	O5'-C1'-O1B	-2.61	107.95	111.36
2	D	501	GDX	C1D-N9-C8	-2.61	119.32	126.73
2	B	504	GDX	O5'-C1'-O1B	-2.60	107.96	111.36
2	B	503	GDX	C8-N7-C5	2.59	108.88	104.26
2	D	501	GDX	O6B-C6'-O6A	-2.55	118.29	124.08
2	B	503	GDX	O1B-C1'-C2'	2.50	112.95	108.38
2	B	503	GDX	O6B-C6'-C5'	2.45	122.48	113.64
2	B	504	GDX	O6B-C6'-C5'	2.40	122.29	113.64
2	D	501	GDX	C6-C5-N7	2.33	134.54	130.29
2	B	503	GDX	C4D-O4D-C1D	-2.33	104.33	109.47
2	D	502	GDX	O2B-PB-O3A	-2.29	101.08	107.27
2	D	501	GDX	C8-N7-C5	2.29	108.33	104.26
2	D	501	GDX	C5-C4-N9	-2.28	101.58	105.66
2	D	502	GDX	C4-C5-N7	-2.27	107.08	110.67
2	D	502	GDX	C1D-N9-C8	-2.26	120.31	126.73
2	D	501	GDX	O6B-C6'-C5'	2.25	121.78	113.64
2	B	504	GDX	C4-C5-N7	-2.24	107.12	110.67
2	B	503	GDX	C1D-N9-C8	-2.23	120.39	126.73
2	B	503	GDX	O6B-C6'-O6A	-2.23	119.02	124.08
2	B	504	GDX	O2A-PA-O1A	2.21	122.71	112.44
2	D	501	GDX	PB-O1B-C1'	-2.20	112.26	121.21
2	B	504	GDX	PB-O1B-C1'	-2.18	112.35	121.21
2	D	502	GDX	C4D-O4D-C1D	-2.17	104.67	109.47
2	B	503	GDX	O6-C6-C5	-2.12	120.93	126.53
2	D	501	GDX	C4D-O4D-C1D	-2.11	104.80	109.47
2	B	503	GDX	C4-C5-N7	-2.05	107.42	110.67
2	B	504	GDX	C4D-O4D-C1D	-2.04	104.96	109.47
2	B	504	GDX	O6-C6-C5	-2.00	121.25	126.53

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	503	GDX	C1'-O1B-PB-O3A
2	B	504	GDX	C5D-O5D-PA-O1A
2	D	501	GDX	C5D-O5D-PA-O1A
2	D	501	GDX	C5D-O5D-PA-O3A
2	D	501	GDX	C1'-O1B-PB-O3A
2	D	501	GDX	O4D-C4D-C5D-O5D
2	D	501	GDX	C3D-C4D-C5D-O5D

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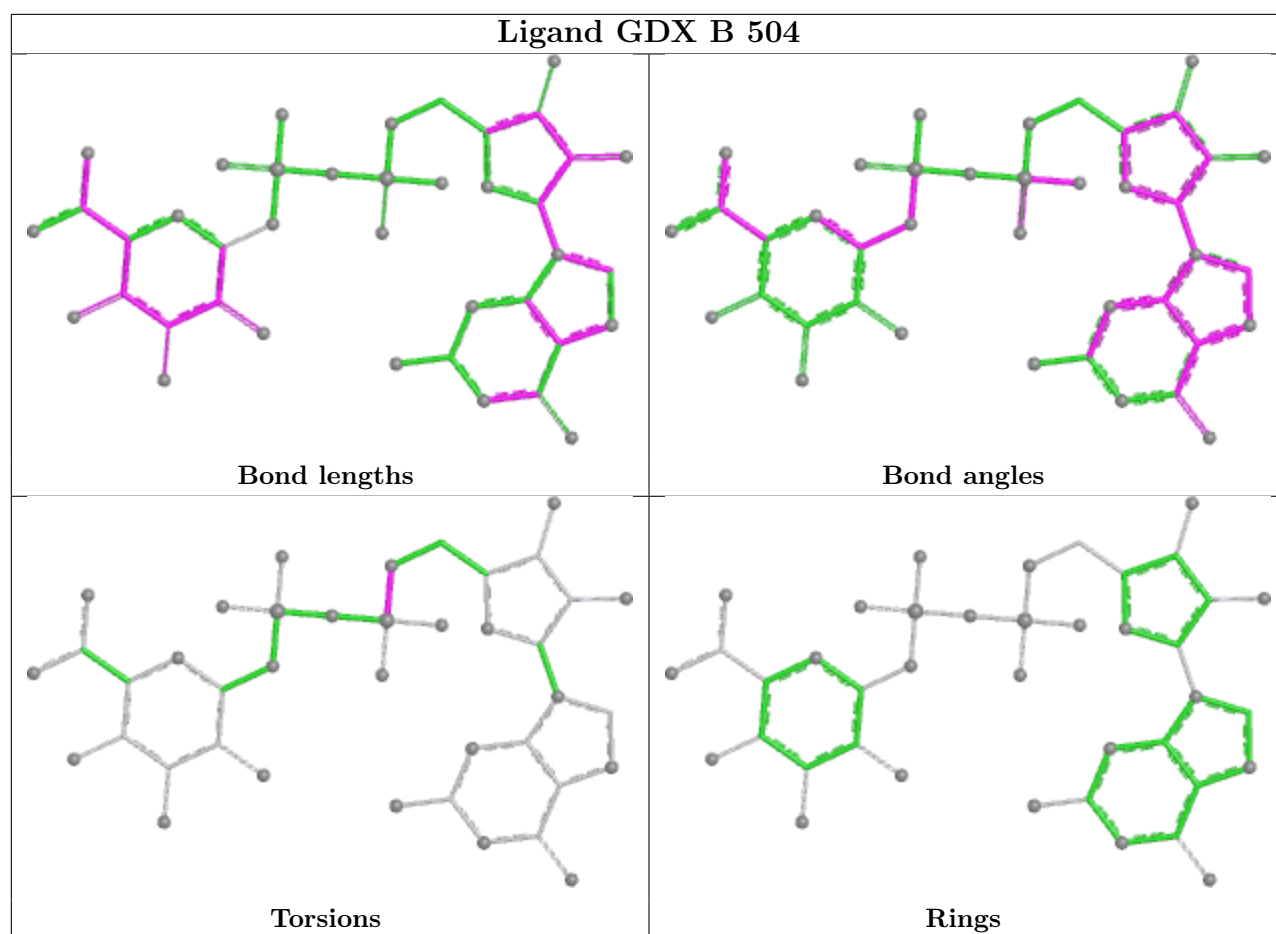
Mol	Chain	Res	Type	Atoms
2	B	503	GDX	C1'-O1B-PB-O3B
2	B	504	GDX	C5D-O5D-PA-O3A
2	D	501	GDX	C5D-O5D-PA-O2A
2	D	501	GDX	C1'-O1B-PB-O3B

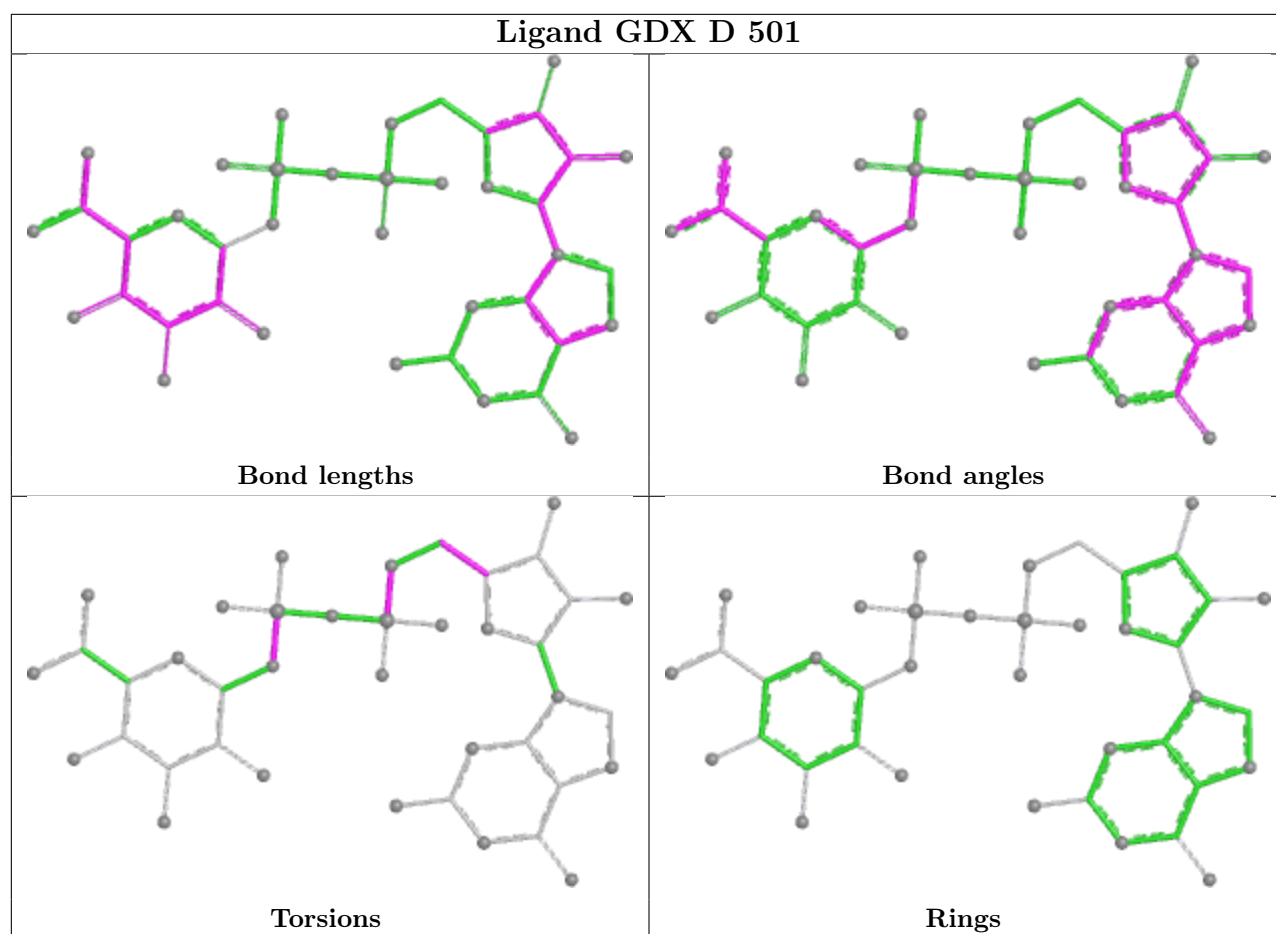
There are no ring outliers.

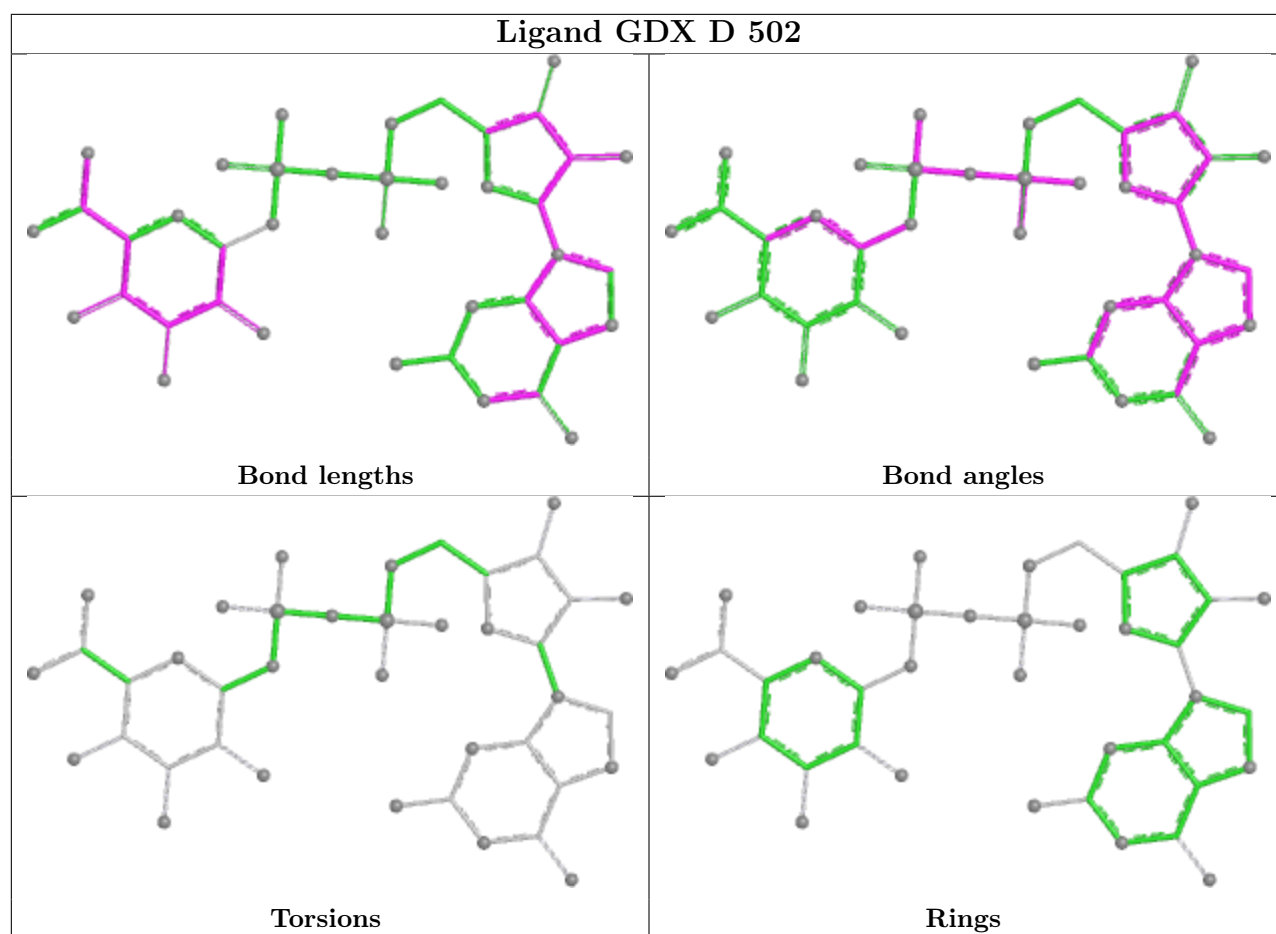
3 monomers are involved in 4 short contacts:

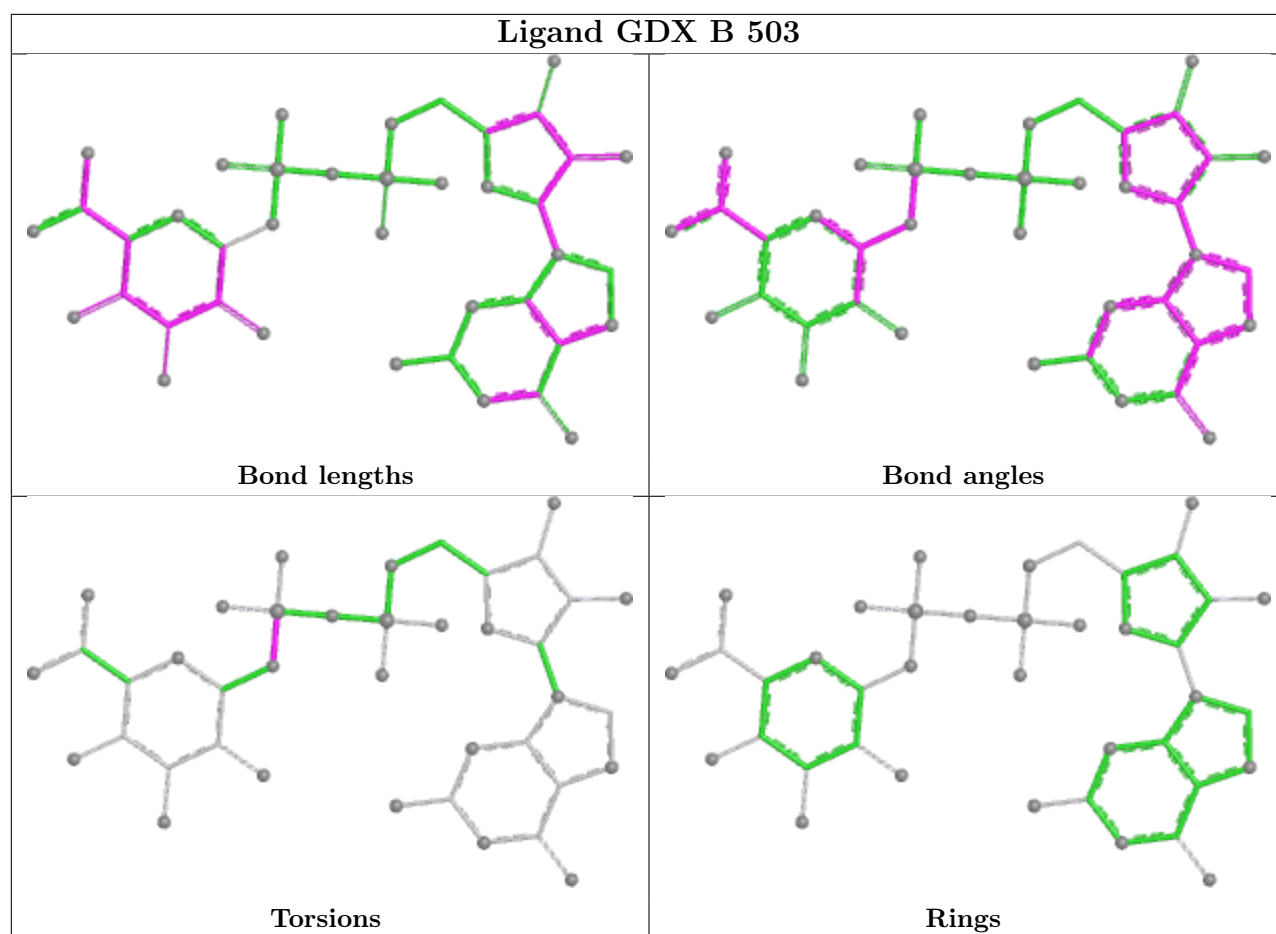
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	GDX	2	0
2	D	502	GDX	1	0
2	B	503	GDX	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.