Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:08 pm BST

PDB ID	:	1MFZ
Title	:	Partially refined 2.8 A 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 following versions of software and data (see references ⓘ) were used in the production of this report:

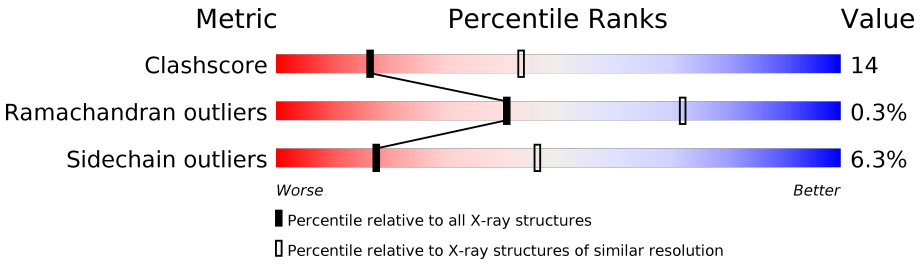
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 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	436	70% 25% 5%
1	B	436	70% 27% .
1	C	436	71% 26% .
1	D	436	67% 30% .

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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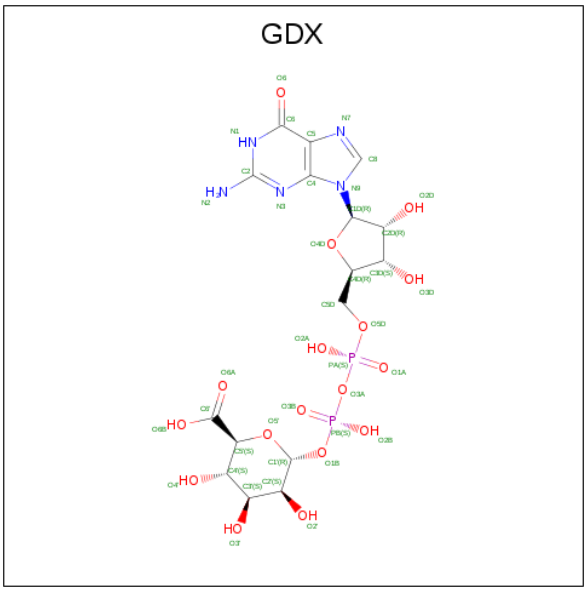
Chain	Residue	Modelled	Actual	Comment	Reference
C	242	MSE	MET	MODIFIED RESIDUE	UNP P11759
C	258	MSE	MET	MODIFIED RESIDUE	UNP P11759
C	289	MSE	MET	MODIFIED RESIDUE	UNP P11759
C	294	MSE	MET	MODIFIED RESIDUE	UNP P11759
C	341	MSE	MET	MODIFIED RESIDUE	UNP P11759
C	423	MSE	MET	MODIFIED RESIDUE	UNP P11759
D	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 (three-letter code: GDX) (formula: $C_{16}H_{23}N_5O_{17}P_2$).



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		

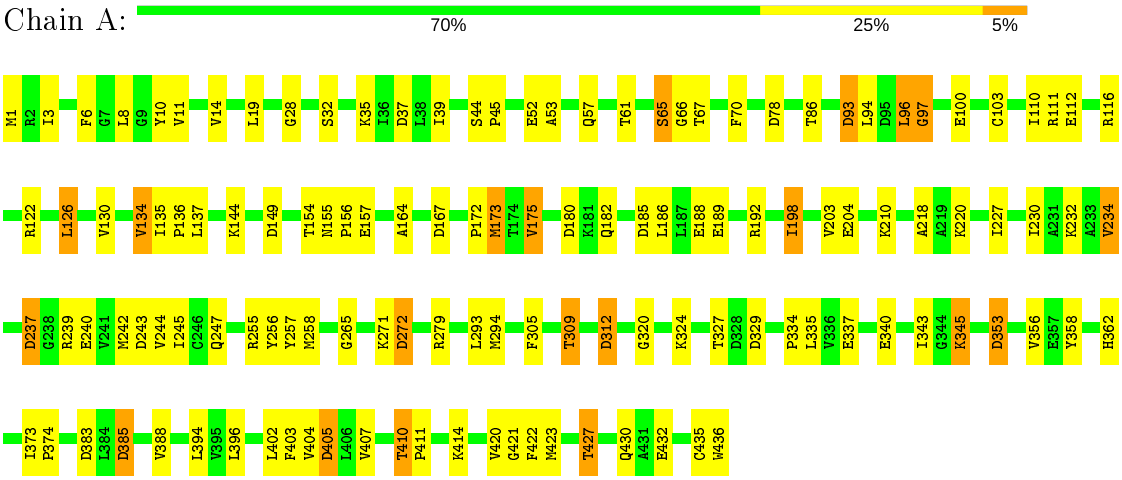
3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

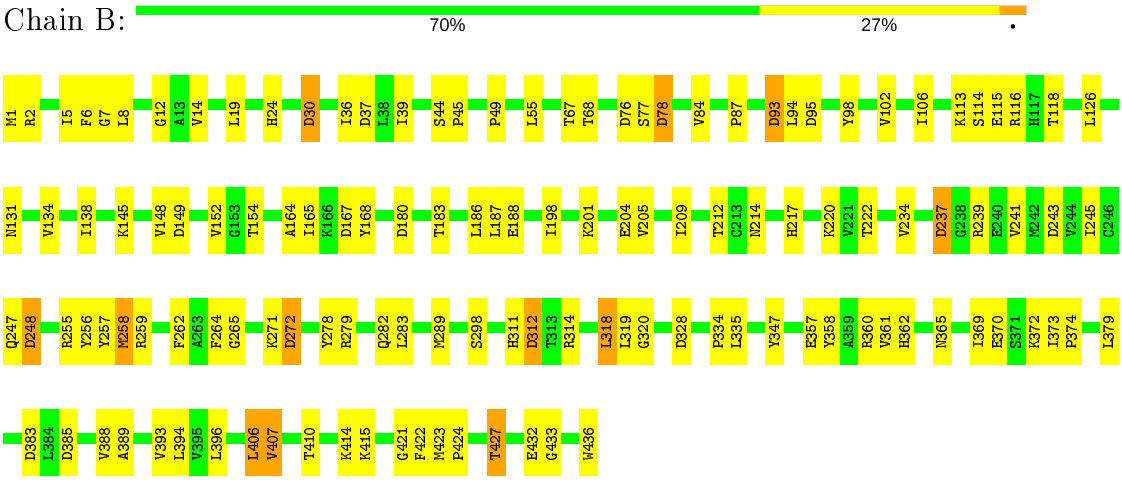
- Molecule 1: GDP-mannose 6-dehydrogenase

Chain A:



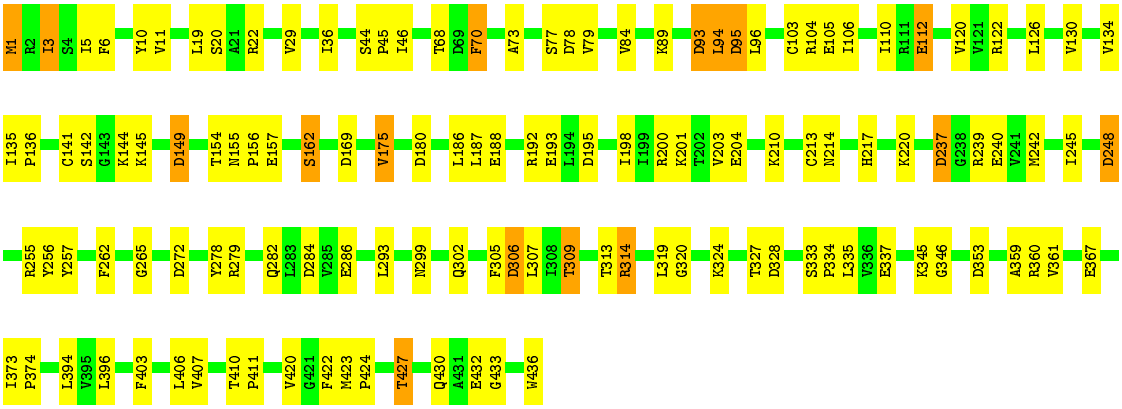
- Molecule 1: GDP-mannose 6-dehydrogenase

Chain B:



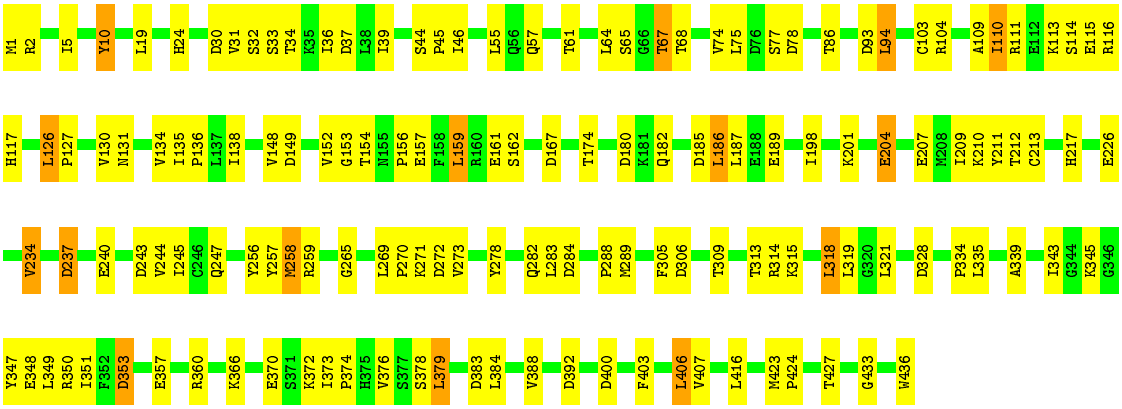
- Molecule 1: GDP-mannose 6-dehydrogenase

Chain C:



- Molecule 1: GDP-mannose 6-dehydrogenase

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	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

5.1 Standard geometry

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	0.50	3/3317 (0.1%)	0.81	14/4484 (0.3%)
1	B	0.46	1/3303 (0.0%)	0.78	14/4470 (0.3%)
1	C	0.45	0/3279	0.78	13/4440 (0.3%)
1	D	0.45	0/3299	0.77	14/4464 (0.3%)
All	All	0.47	4/13198 (0.0%)	0.78	55/17858 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	423	MSE	SE-CE	-7.78	1.49	1.95
1	A	294	MSE	SE-CE	-5.45	1.63	1.95
1	B	258	MSE	SE-CE	-5.21	1.64	1.95
1	A	173	MSE	SE-CE	-5.19	1.64	1.95

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	328	ASP	CB-CG-OD2	7.16	124.75	118.30
1	D	167	ASP	CB-CG-OD2	6.90	124.51	118.30
1	C	272	ASP	CB-CG-OD2	6.60	124.24	118.30
1	D	272	ASP	CB-CG-OD2	6.43	124.09	118.30
1	D	237	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	385	ASP	CB-CG-OD2	6.35	124.01	118.30
1	C	284	ASP	CB-CG-OD2	6.34	124.01	118.30
1	B	167	ASP	CB-CG-OD2	6.26	123.94	118.30
1	C	353	ASP	CB-CG-OD2	6.11	123.79	118.30
1	C	180	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	237	ASP	CB-CG-OD2	5.96	123.66	118.30
1	C	328	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	167	ASP	CB-CG-OD2	5.91	123.62	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	353	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	93	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	185	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	272	ASP	CB-CG-OD2	5.76	123.49	118.30
1	D	383	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	312	ASP	CB-CG-OD2	5.66	123.39	118.30
1	C	195	ASP	CB-CG-OD2	5.61	123.35	118.30
1	C	237	ASP	CB-CG-OD2	5.61	123.35	118.30
1	D	37	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	272	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	78	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	78	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	95	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	37	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	385	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	185	ASP	CB-CG-OD2	5.47	123.22	118.30
1	D	400	ASP	CB-CG-OD2	5.47	123.22	118.30
1	C	248	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	383	ASP	CB-CG-OD2	5.45	123.20	118.30
1	C	78	ASP	CB-CG-OD2	5.43	123.19	118.30
1	D	353	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	312	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	30	ASP	CB-CG-OD2	5.38	123.15	118.30
1	B	93	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	76	ASP	CB-CG-OD2	5.35	123.11	118.30
1	D	392	ASP	CB-CG-OD2	5.32	123.09	118.30
1	D	306	ASP	CB-CG-OD2	5.32	123.08	118.30
1	B	180	ASP	CB-CG-OD2	5.31	123.08	118.30
1	D	30	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	329	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	306	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	180	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	383	ASP	CB-CG-OD2	5.16	122.95	118.30
1	D	149	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	37	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	328	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	93	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	180	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	237	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	405	ASP	CB-CG-OD2	5.05	122.84	118.30
1	C	149	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	248	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3271	0	3233	107	1
1	B	3258	0	3211	99	0
1	C	3233	0	3136	93	0
1	D	3255	0	3219	109	0
2	B	80	0	30	1	0
2	D	80	0	31	2	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	369	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 14.

All (369) 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:H	1:C:70:PHE:HD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:370:GLU:HA	1:B:370:GLU:OE1	1.90	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
1:C:130:VAL:HA	1:C:134:VAL:HG13	1.74	0.69
1:C:70:PHE:N	1:C:70:PHE:CD1	2.50	0.69
1:C:396:LEU:HD11	1:C:407:VAL:CG2	2.21	0.69
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: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:D:130:VAL:HA	1:D:134:VAL:HB	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:44:SER:H	1:A:52:GLU:CD	2.01	0.63
1:D:115:GLU:CD	1:D:115:GLU:H	2.01	0.63
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: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:131:ASN:ND2	1:D:204:GLU:OE2	2.29	0.62
1:D:1:MSE:HE1	1:D:186:LEU:HD11	1.82	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
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:299:ASN:HB3	3:C:456:HOH:O	2.00	0.60
1:C:240:GLU:HG2	1:D:201:LYS:NZ	2.17	0.60
1:A:234:VAL:O	1:A:234:VAL:HG23	2.01	0.60
1:B:115:GLU:H	1:B:115:GLU:CD	2.03	0.60
1:A:10:TYR:H	1:A:10:TYR:HD1	1.47	0.60
1:A:130:VAL:HG21	1:A:154:THR:CG2	2.31	0.59
1:A:35:LYS:O	1:A:39:ILE:HG13	2.02	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:353:ASP:CG	1:A:356:VAL:HG23	2.22	0.59
1:A:154:THR:HG23	1:A:203:VAL:HG13	1.84	0.59
1:B:256:TYR:O	1:B:257:TYR:HB2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:234:VAL:O	1:B:234:VAL:HG13	2.03	0.58
1:C:142:SER:C	1:C:144:LYS:H	2.06	0.58
1:A:309:THR:O	1:A:309:THR:CG2	2.51	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:240:GLU:HG3	1:B:201:LYS:HZ1	1.70	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: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
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:D:427:THR:HG23	1:D:436:TRP:C	2.27	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:A:324:LYS:O	1:A:327:THR:HG22	2.08	0.53
1:B:115:GLU:N	1:B:115:GLU:CD	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	1:B:116:ARG:HG3	2.25	0.52
1:B:234:VAL:CG1	1:B:234:VAL:O	2.57	0.52
1:A:130:VAL:HB	1:A:203:VAL:HG11	1.92	0.52
1:C:73:ALA:O	1:C:77:SER:OG	2.13	0.52
1:D:406:LEU:HD22	1:D:406:LEU:O	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
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:115:GLU:N	1:D:115:GLU:CD	2.64	0.52
1:D:189:GLU:OE1	1:D:189:GLU:HA	2.09	0.52
1:D:77:SER:O	1:D:113:LYS:NZ	2.42	0.52
1:B:319:LEU:HD12	1:B:396:LEU:HD13	1.93	0.51
1:C:320:GLY:O	1:C:335:LEU:HD13	2.09	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:O	1:D:313:THR:HG23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:237:ASP:C	1:A:237:ASP:OD1	2.50	0.50
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:N	1:A:10:TYR:CD1	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
1:A:144:LYS:HD3	1:A:149:ASP:HB3	1.94	0.49
1:C:427:THR:HG22	1:C:436:TRP:C	2.32	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:D:135:ILE:HB	1:D:136:PRO:HD3	1.94	0.49
1:D:305:PHE:O	1:D:309:THR:OG1	2.24	0.49
1:A:218:ALA:HB1	1:B:264:PHE:CE2	2.48	0.48
1:B:372:LYS:C	1:B:374:PRO:HD3	2.34	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:D:318:LEU:HB2	1:D:349:LEU:HD11	1.95	0.48
1:D:36:ILE:O	1:D:39:ILE:HG22	2.13	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: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:116:ARG:NH1	1:A:182:GLN:OE1	2.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ARG:CG	1:D:116:ARG:HH11	2.19	0.48
1:B:7:GLY:O	1:B:12:GLY:HA3	2.13	0.47
1:D:1:MSE:HB2	1:D:24:HIS:HD2	1.79	0.47
1:C:240:GLU:HG2	1:D:201:LYS:HZ1	1.78	0.47
1:C:104:ARG:HG2	1:C:141:CYS:SG	2.54	0.47
1:D:157:GLU:O	1:D:210:LYS:NZ	2.42	0.47
1:B:93:ASP:OD1	1:B:94:LEU:N	2.45	0.47
1:A:28:GLY:O	1:A:66:GLY:HA2	2.13	0.47
1:A:421:GLY:HA2	1:A:436:TRP:CZ2	2.50	0.47
1:A:358:TYR:O	1:A:362:HIS:HB2	2.14	0.47
1:C:319:LEU:HB3	1:C:403:PHE:CZ	2.50	0.47
1:D:313:THR:C	1:D:315:LYS:H	2.17	0.47
1:B:67:THR:OG1	1:B:68:THR:N	2.48	0.47
1:C:248:ASP:C	1:C:248:ASP:OD1	2.49	0.47
1:D:10:TYR:CD1	1:D:10:TYR:C	2.88	0.47
1:D:67:THR:OG1	1:D:68:THR:N	2.47	0.46
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: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: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:D:237:ASP:OD1	1:D:237:ASP:C	2.54	0.46
1:A:309:THR:O	1:A:309:THR:HG23	2.16	0.46
1:A:28:GLY:N	1:A:65:SER:O	2.39	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:C:142:SER:C	1:C:144:LYS:N	2.69	0.45
1:D:349:LEU:O	1:D:379:LEU:HG	2.16	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLU:O	1:A:53:ALA:C	2.55	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:B:2:ARG:NH2	1:B:78:ASP:OD1	2.45	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:D:1:MSE:CE	1:D:186:LEU:HD11	2.46	0.44
1:A:232:LYS:HZ3	1:B:427:THR:HG21	1.81	0.44
1:A:96:LEU:O	1:A:97:GLY:C	2.56	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:257:TYR:CE2	1:D:217:HIS:CG	3.05	0.44
1:C:6:PHE:HA	1:C:29:VAL:HB	1.99	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:A:116:ARG:HH12	1:A:182:GLN:CD	2.21	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:B:311:HIS:O	1:B:312:ASP:C	2.56	0.43
1:C:20:SER:C	1:C:22:ARG:H	2.22	0.43
1:A:404:VAL:O	1:A:407:VAL:N	2.51	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: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:HG	1:D:159:LEU:H	1.68	0.43
1:A:116:ARG:HH12	1:A:182:GLN:CB	2.32	0.43
1:D:152:VAL:HG12	1:D:153:GLY:N	2.34	0.43
1:D:186:LEU:HA	1:D:186:LEU:HD22	1.63	0.43
1:B:148:VAL:HG23	1:B:149:ASP:N	2.33	0.43
1:B:98:TYR:O	1:B:102:VAL:HG23	2.19	0.43
1:A:358:TYR:CE2	1:A:362:HIS:HD2	2.36	0.43
1:C:359:ALA:O	1:C:361:VAL:N	2.52	0.43
1:C:245:ILE:HD11	1:D:212:THR:HB	1.99	0.43
1:D:374:PRO:O	1:D:378:SER:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:TYR:CD1	1:B:168:TYR:C	2.92	0.42
1:D:109:ALA:C	1:D:111:ARG:H	2.22	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:B:114:SER:HB3	1:B:115:GLU:OE2	2.19	0.42
1:A:293:LEU:CD2	1:B:289:MSE:CE	2.98	0.42
1:D:258:MSE:CE	1:D:258:MSE:HA	2.49	0.42
1:C:309:THR:O	1:C:309:THR:CG2	2.67	0.42
1:D:103:CYS:O	1:D:104:ARG:C	2.58	0.42
1:C:217:HIS:CG	1:D:257:TYR:CE2	3.08	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:D:256:TYR:O	1:D:257:TYR: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:HG3	1:A:157:GLU:H	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:A:343:ILE:HG23	3:A:450:HOH:O	2.21	0.41
1:B:358:TYR:CD1	1:B:358:TYR:C	2.94	0.41
1:D:305:PHE:CZ	1:D:345:LYS:HG3	2.55	0.41
1:D:366:LYS:HE2	1:D:366:LYS:HB3	1.76	0.41
1:A:156:PRO:HD2	1:A:175:VAL:O	2.20	0.41
1:A:93:ASP:HB2	1:B:278:TYR:CE2	2.55	0.41
1:B:188:GLU:HG3	1:B:198:ILE:CD1	2.50	0.41
1:D:258:MSE:HE3	1:D:258:MSE:HA	2.02	0.41
1:D:305:PHE:HZ	1:D:345:LYS:HG3	1.84	0.41
1:B:248:ASP:C	1:B:248:ASP:OD1	2.58	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:B:1:MSE:H3	1:B:24:HIS:HD2	1.69	0.41
1:C:95:ASP:C	1:C:95:ASP:OD1	2.59	0.41
1:D:372:LYS:C	1:D:374:PRO:HD3	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:64:LEU:HG	1:D:65:SER:N	2.35	0.41
1:A:227:ILE:HG21	1:A:242:MSE:SE	2.70	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:A:156:PRO:HB3	1:A:210:LYS:HB2	2.03	0.41
1:A:430:GLN:O	1:A:430:GLN:HG2	2.19	0.41
1:B:237:ASP:OD1	1:B:239:ARG:HB2	2.21	0.41
1:A:255:ARG:NH2	1:B:243:ASP:OD1	2.52	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:182:GLN:O	1:D:186:LEU:HB2	2.21	0.40
1:D:93:ASP:OD1	1:D:94:LEU:N	2.53	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:110:ILE:O	1:A:111:ARG:C	2.59	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:A:173:MSE:HE1	1:B:247:GLN:C	2.42	0.40
1:C:20:SER:C	1:C:22:ARG:N	2.75	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: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%)	29	61
1	B	434/436 (100%)	405 (93%)	29 (7%)	0	100	100
1	C	434/436 (100%)	395 (91%)	36 (8%)	3 (1%)	22	53
1	D	434/436 (100%)	405 (93%)	28 (6%)	1 (0%)	47	78
All	All	1736/1744 (100%)	1605 (92%)	125 (7%)	6 (0%)	41	72

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 (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	352/361 (98%)	327 (93%)	25 (7%)	14	39
1	B	349/361 (97%)	335 (96%)	14 (4%)	31	65
1	C	340/361 (94%)	317 (93%)	23 (7%)	16	42
1	D	347/361 (96%)	321 (92%)	26 (8%)	13	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1388/1444 (96%)	1300 (94%)	88 (6%)	18 46

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	11	VAL
1	A	32	SER
1	A	65	SER
1	A	67	THR
1	A	96	LEU
1	A	126	LEU
1	A	134	VAL
1	A	175	VAL
1	A	186	LEU
1	A	198	ILE
1	A	204	GLU
1	A	234	VAL
1	A	271	LYS
1	A	279	ARG
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	55	LEU
1	B	126	LEU
1	B	152	VAL
1	B	154	THR
1	B	187	LEU
1	B	262	PHE
1	B	283	LEU
1	B	298	SER
1	B	318	LEU
1	B	335	LEU
1	B	379	LEU
1	B	406	LEU

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Mol	Chain	Res	Type
1	B	407	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	162	SER
1	C	175	VAL
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
1	C	345	LYS
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	126	LEU
1	D	148	VAL
1	D	159	LEU
1	D	186	LEU
1	D	187	LEU
1	D	204	GLU
1	D	234	VAL
1	D	258	MSE

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Mol	Chain	Res	Type
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	362	HIS
1	B	24	HIS
1	D	24	HIS
1	D	247	GLN
1	D	282	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

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	D	501	-	33,43,43	4.86	14 (42%)	45,67,67	2.15	10 (22%)
2	GDX	B	504	-	33,43,43	4.82	13 (39%)	45,67,67	2.16	13 (28%)
2	GDX	B	503	-	33,43,43	4.88	14 (42%)	45,67,67	2.20	13 (28%)
2	GDX	D	502	-	33,43,43	4.89	12 (36%)	45,67,67	2.35	13 (28%)

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	D	501	-	-	6/17/61/61	0/4/4/4
2	GDX	B	504	-	-	3/17/61/61	0/4/4/4
2	GDX	B	503	-	-	2/17/61/61	0/4/4/4
2	GDX	D	502	-	-	1/17/61/61	0/4/4/4

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	GDX	C2D-C1D	-13.69	1.33	1.53
2	B	503	GDX	C2D-C1D	-13.41	1.33	1.53
2	D	502	GDX	C2D-C1D	-13.37	1.33	1.53
2	B	504	GDX	C2D-C1D	-12.72	1.34	1.53
2	B	504	GDX	C4'-C5'	-9.13	1.33	1.53
2	D	502	GDX	C4'-C5'	-8.93	1.33	1.53
2	D	502	GDX	O2'-C2'	-8.71	1.22	1.43
2	B	503	GDX	O2D-C2D	-8.36	1.23	1.43
2	D	501	GDX	C4'-C5'	-8.35	1.35	1.53
2	B	503	GDX	C4'-C5'	-8.35	1.35	1.53
2	D	502	GDX	O4'-C4'	-8.35	1.23	1.43
2	B	504	GDX	O4'-C4'	-8.33	1.23	1.43
2	D	501	GDX	O4'-C4'	-8.25	1.23	1.43
2	B	503	GDX	O3'-C3'	-8.23	1.23	1.43
2	B	504	GDX	O2D-C2D	-8.20	1.23	1.43
2	B	503	GDX	O2'-C2'	-8.19	1.23	1.43
2	D	501	GDX	O2'-C2'	-8.18	1.23	1.43
2	D	502	GDX	O3'-C3'	-8.12	1.23	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	503	GDX	O4'-C4'	-8.10	1.23	1.43
2	D	502	GDX	O2D-C2D	-8.10	1.23	1.43
2	B	504	GDX	O2'-C2'	-8.10	1.23	1.43
2	D	501	GDX	O2D-C2D	-7.98	1.24	1.43
2	B	504	GDX	O3'-C3'	-7.88	1.24	1.43
2	D	501	GDX	O3'-C3'	-7.77	1.24	1.43
2	D	501	GDX	C3D-C4D	-7.66	1.33	1.53
2	B	503	GDX	C3D-C4D	-7.65	1.33	1.53
2	B	504	GDX	C3D-C4D	-7.40	1.34	1.53
2	D	502	GDX	C3D-C4D	-7.15	1.34	1.53
2	B	504	GDX	C4'-C3'	-6.97	1.34	1.52
2	D	501	GDX	C3'-C2'	-6.70	1.35	1.52
2	B	503	GDX	C4'-C3'	-6.67	1.35	1.52
2	D	502	GDX	C3D-C2D	-6.58	1.35	1.53
2	B	503	GDX	C3'-C2'	-6.50	1.35	1.52
2	D	501	GDX	C4'-C3'	-6.48	1.35	1.52
2	B	504	GDX	C1'-C2'	-6.47	1.33	1.52
2	D	502	GDX	C4'-C3'	-6.47	1.35	1.52
2	B	504	GDX	C3'-C2'	-6.42	1.36	1.52
2	B	503	GDX	C1'-C2'	-6.41	1.34	1.52
2	B	503	GDX	C3D-C2D	-6.32	1.36	1.53
2	D	502	GDX	C3'-C2'	-6.29	1.36	1.52
2	D	501	GDX	C3D-C2D	-6.27	1.36	1.53
2	D	502	GDX	C1'-C2'	-6.22	1.34	1.52
2	D	501	GDX	C1'-C2'	-6.13	1.34	1.52
2	B	504	GDX	C3D-C2D	-6.08	1.36	1.53
2	D	502	GDX	C6-C5	3.87	1.48	1.41
2	B	503	GDX	C6-C5	3.59	1.47	1.41
2	D	501	GDX	C6-C5	3.49	1.47	1.41
2	B	504	GDX	C6-C5	2.71	1.46	1.41
2	D	501	GDX	O4D-C1D	2.49	1.44	1.41
2	B	503	GDX	C5-C4	2.38	1.47	1.40
2	B	503	GDX	O4D-C1D	2.36	1.44	1.41
2	D	501	GDX	C5-C4	2.33	1.47	1.40
2	B	504	GDX	O4D-C1D	2.31	1.44	1.41

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	502	GDX	O3A-PB-O1B	6.33	115.25	102.48
2	B	503	GDX	C3D-C2D-C1D	5.77	109.66	100.98
2	D	502	GDX	C2-N3-C4	5.46	121.59	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	502	GDX	C3D-C2D-C1D	5.45	109.18	100.98
2	B	504	GDX	C3D-C2D-C1D	5.41	109.13	100.98
2	D	501	GDX	C3D-C2D-C1D	5.40	109.11	100.98
2	B	504	GDX	C2-N3-C4	5.19	121.28	115.36
2	B	503	GDX	C2-N3-C4	5.10	121.19	115.36
2	D	501	GDX	C2-N3-C4	5.02	121.09	115.36
2	B	504	GDX	O3A-PB-O1B	4.98	112.54	102.48
2	B	504	GDX	C5-C6-N1	-4.95	116.66	123.43
2	B	503	GDX	O3A-PB-O1B	4.84	112.25	102.48
2	B	504	GDX	C6-N1-C2	4.67	123.35	115.93
2	D	501	GDX	C5-C6-N1	-4.57	117.19	123.43
2	B	503	GDX	C6-C5-C4	-4.50	116.50	120.80
2	D	502	GDX	C5-C6-N1	-4.45	117.34	123.43
2	D	502	GDX	C6-C5-C4	-4.40	116.60	120.80
2	D	501	GDX	C6-N1-C2	4.35	122.83	115.93
2	D	502	GDX	C6-N1-C2	4.31	122.78	115.93
2	D	501	GDX	N3-C2-N1	-3.99	121.90	127.22
2	B	503	GDX	C6-N1-C2	3.96	122.22	115.93
2	D	501	GDX	C6-C5-C4	-3.93	117.05	120.80
2	B	503	GDX	C5-C6-N1	-3.84	118.18	123.43
2	B	504	GDX	N3-C2-N1	-3.80	122.16	127.22
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	D	502	GDX	N3-C2-N1	-3.76	122.21	127.22
2	D	501	GDX	PB-O3A-PA	-3.74	120.01	132.83
2	B	504	GDX	C6-C5-C4	-3.55	117.41	120.80
2	B	503	GDX	N3-C2-N1	-3.43	122.65	127.22
2	B	503	GDX	PB-O3A-PA	-3.43	121.07	132.83
2	D	501	GDX	O3A-PB-O1B	3.42	109.39	102.48
2	D	502	GDX	C1'-O5'-C5'	-3.41	106.72	112.24
2	D	501	GDX	C2D-C3D-C4D	3.41	109.27	102.64
2	D	502	GDX	C2D-C3D-C4D	3.39	109.23	102.64
2	B	503	GDX	C2D-C3D-C4D	3.29	109.04	102.64
2	B	504	GDX	C2D-C3D-C4D	3.13	108.73	102.64
2	B	504	GDX	PB-O3A-PA	-2.66	123.70	132.83
2	B	503	GDX	O5'-C1'-O1B	-2.61	107.95	111.36
2	B	504	GDX	O5'-C1'-O1B	-2.60	107.96	111.36
2	D	502	GDX	O2A-PA-O1A	2.59	125.02	112.24
2	B	503	GDX	O1B-C1'-C2'	2.50	112.95	108.38
2	B	503	GDX	PB-O1B-C1'	-2.46	110.23	119.74
2	B	503	GDX	C1D-N9-C4	-2.30	122.61	126.64
2	D	502	GDX	C4-C5-N7	-2.23	107.08	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	504	GDX	C4-C5-N7	-2.19	107.12	109.40
2	D	502	GDX	PB-O3A-PA	-2.17	125.37	132.83
2	B	504	GDX	O2A-PA-O1A	2.12	122.71	112.24
2	B	504	GDX	O2'-C2'-C3'	2.00	114.98	110.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	GDX	C5D-O5D-PA-O1A
2	B	504	GDX	C5D-O5D-PA-O1A
2	D	501	GDX	C1'-O1B-PB-O3A
2	B	504	GDX	C1'-O1B-PB-O3A
2	B	503	GDX	C1'-O1B-PB-O3A
2	D	501	GDX	O4D-C4D-C5D-O5D
2	D	502	GDX	C1'-O1B-PB-O3A
2	D	501	GDX	C5D-O5D-PA-O3A
2	B	504	GDX	C5D-O5D-PA-O3A
2	D	501	GDX	C3D-C4D-C5D-O5D
2	D	501	GDX	C5D-O5D-PA-O2A
2	B	503	GDX	C5D-O5D-PA-O3A

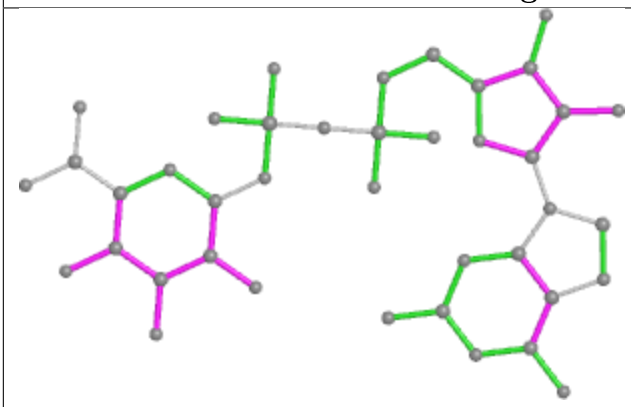
There are no ring outliers.

2 monomers are involved in 3 short contacts:

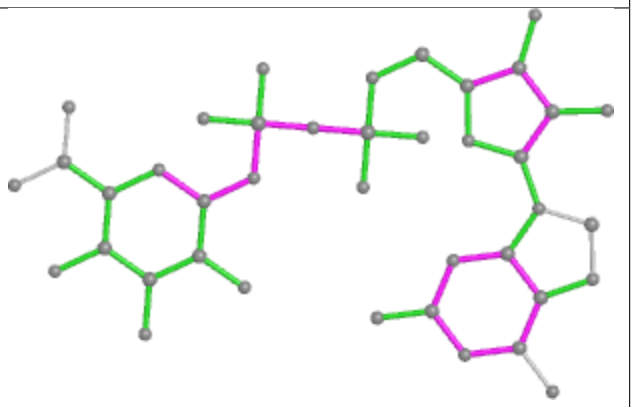
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	GDX	2	0
2	B	503	GDX	1	0

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 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.

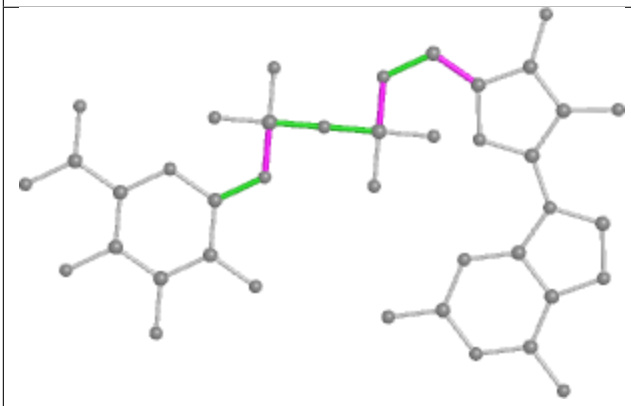
Ligand GDX D 501



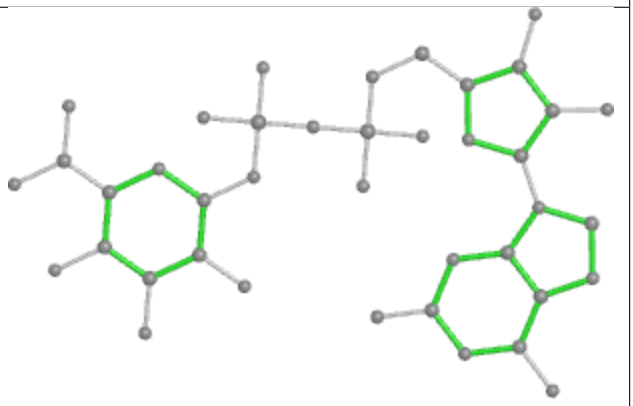
Bond lengths



Bond angles

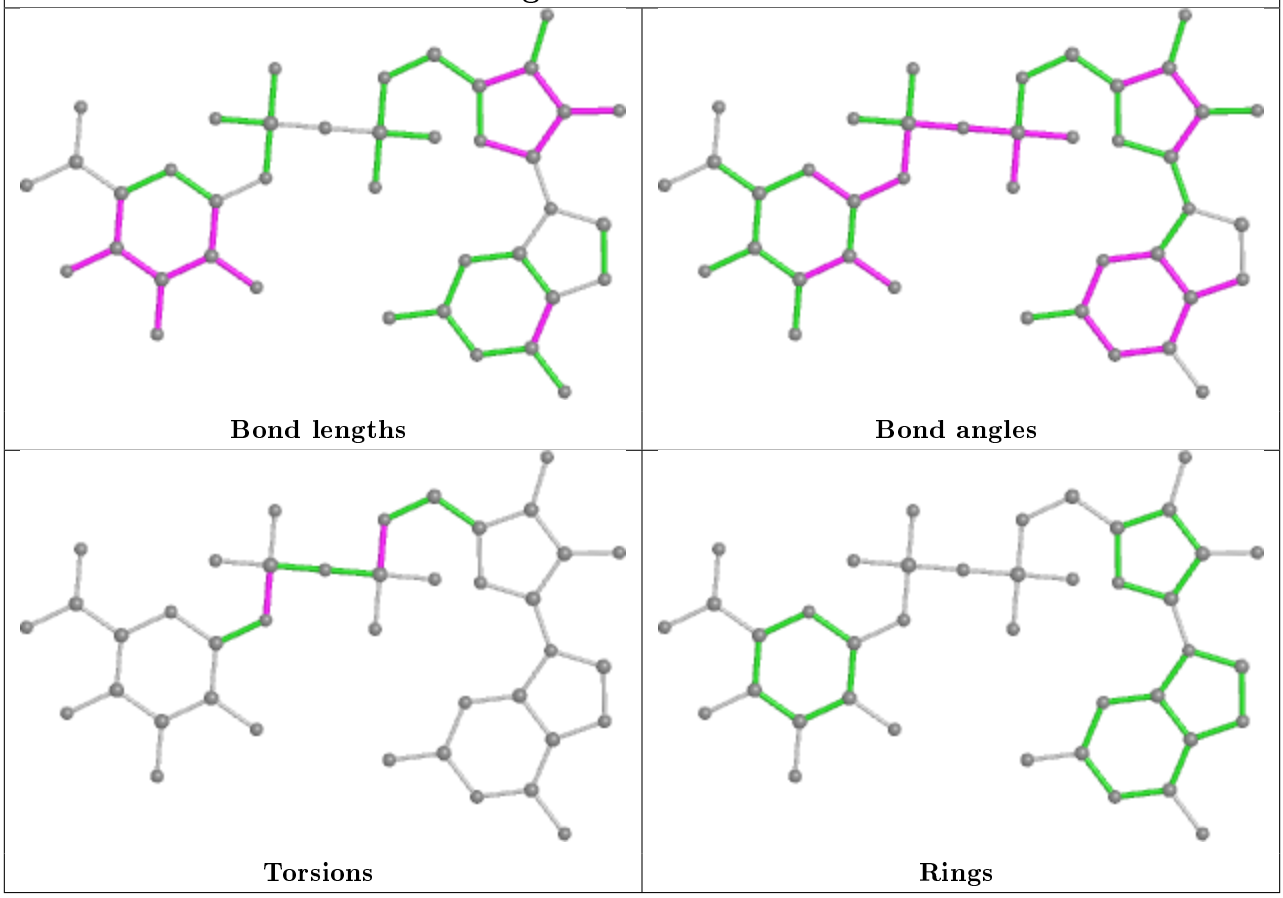


Torsions

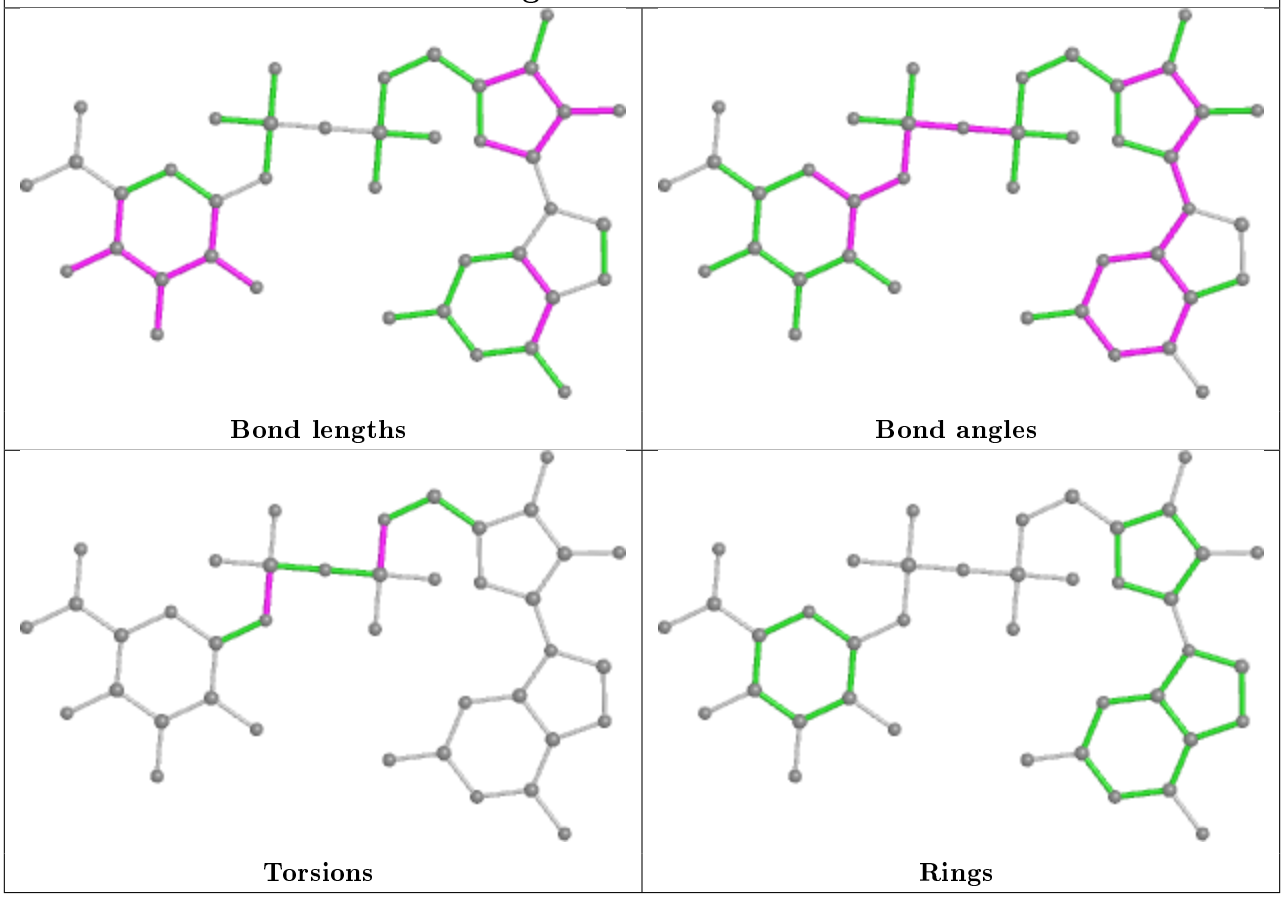


Rings

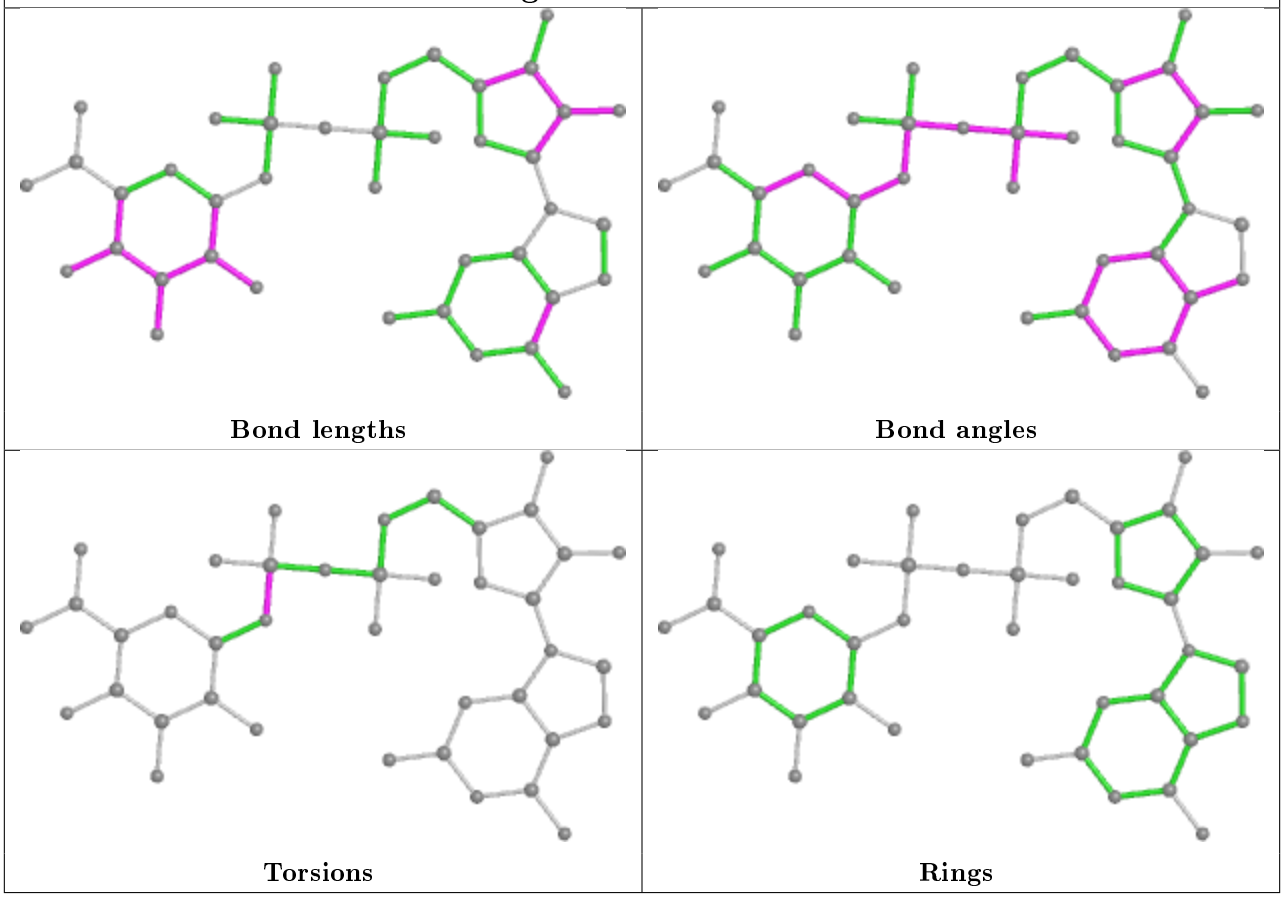
Ligand GDX B 504



Ligand GDX B 503



Ligand GDX D 502



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.