



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:52 PM UTC

PDB ID : 2NYA / pdb_00002nya
Title : Crystal structure of the periplasmic nitrate reductase (NAP) from Escherichia coli
Authors : Jepson, B.J.N.; Richardson, D.J.; Hemmings, A.M.
Deposited on : 2006-11-20
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

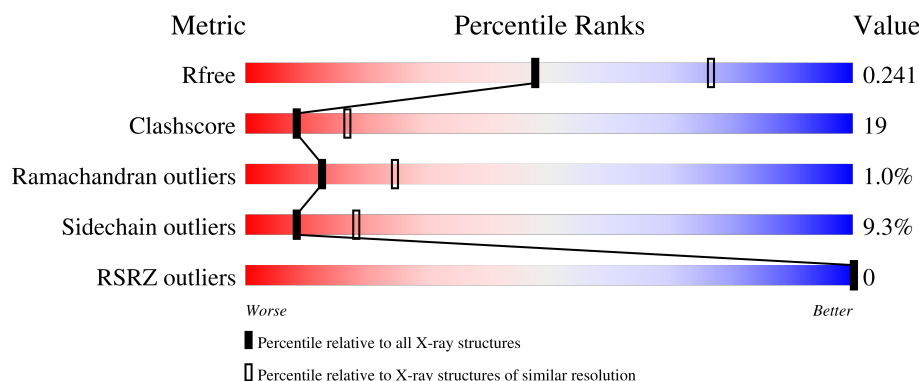
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	792	 66% 28% 6%
1	F	792	 63% 31% 6%

2 Entry composition [i](#)

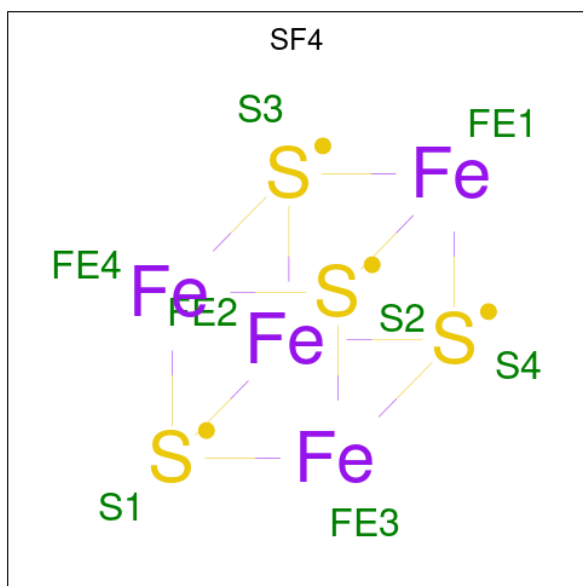
There are 5 unique types of molecules in this entry. The entry contains 13733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Periplasmic nitrate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	791	Total	C	N	O	S	0	0	0
			6301	4012	1100	1157	32			
1	F	791	Total	C	N	O	S	0	0	0
			6301	4012	1100	1157	32			

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

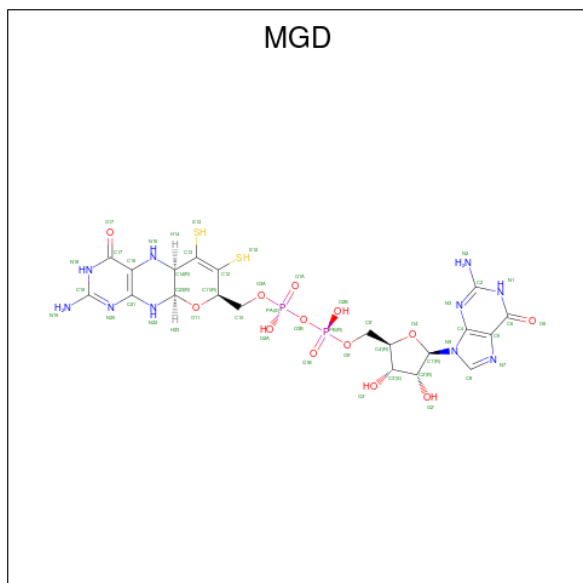


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is MOLYBDENUM(VI) ION (CCD ID: 6MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mo	0	0
			1	1		
3	F	1	Total	Mo	0	0
			1	1		

- Molecule 4 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	F	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	F	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

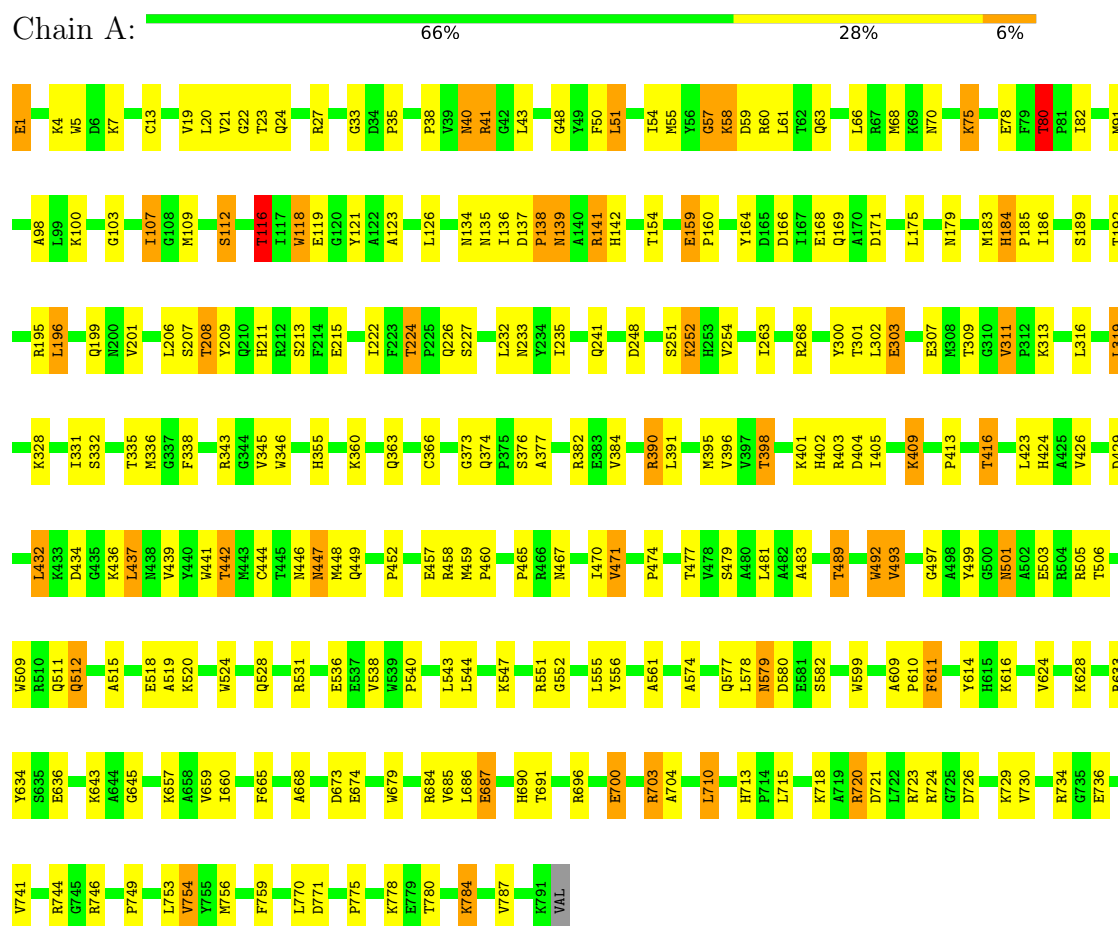
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	489	Total	O	0	0
			489	489		
5	F	436	Total	O	0	0
			436	436		

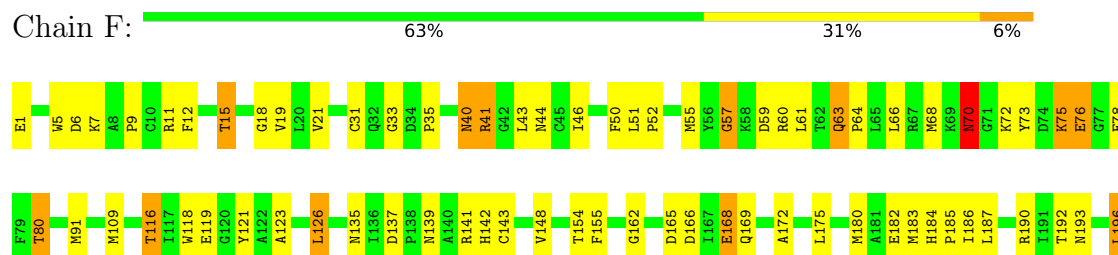
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

- Molecule 1: Periplasmic nitrate reductase



- Molecule 1: Periplasmic nitrate reductase



K197	M308	K408	A498	A598	K718
M198	T309	K409	Y499	W599	A719
Q199	G310	G311	G500	F600	R720
	V311	I412	N501	G601	D721
T202	K312	P413	A502	L722	L722
V203	D314	T416	E503	H606	R723
	Q315		R504		
L206	L316		R505	Y614	D726
S207	E317	I421	T506	G619	V730
T208	L317	G422	Q507	L620	V731
Y209	Q318	L423	F508	R621	S732
Q210	L319	H424	W509		R733
H211			R510	K628	R734
E212	I331	A427	Q511		G735
S213	S332		Q512	Q631	
F214	M336	L432	A515	Y634	T740
E215	Q337	D434			V741
L216	F338		E518	D639	N747
A217	R339	L437	A519	V642	R748
D218	Q340	T442	K520	K643	P749
	H341	M443	Q525	A644	P750
I222	T342	C444			
F223	R343	T445	Q528	G652	L753
T224		M446			V754
P225	W346	M447	R531		Y755
Q226	N353	M448	R532	V659	N756
S227	L354	Q449	F533	I660	
	H355		V538	A668	F759
V230	K360	P452	W539		
I231	C366	E456	L543	D673	L764
L232		E457	L544	E674	L768
N233		N457	R551	R684	T769
Y234	G373	I470		V685	L770
I235	Q374	V471	T554	L686	
	S376	S472	L555	E687	P775
	R382	D473	Y556	H690	E779
S251	E383	P474	A561	T691	T780
K252	V384	S479		R696	K783
H253	R390		E572	R697	K784
	L391	A483	L573		
L256	M395	D484	A574	E700	V787
I263	V396	I486	Q577	L701	K791
	V397	L487	L578	H702	VAL
R288	T398	F488	N579	R703	
	N399	T489	D580	A704	
G281	A400	A490	E581	P706	
	K401	M491	S582		
T301	H402	W492	F587	V709	L710
L302	R403	W493	Y588	F711	F711
E303	D404	E494	L589	H713	I712
R304	I405	E496			
T305	C406	G497	Y597		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.45Å 94.60Å 131.21Å 90.00° 96.34° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (50.00-2.50) 97.1 (50.00-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.181 , 0.243 0.181 , 0.241	Depositor DCC
R_{free} test set	2860 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13733	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 6MO, MGD

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	0.88	2/6470 (0.0%)	1.07	13/8770 (0.1%)
1	F	0.83	0/6470	1.03	9/8770 (0.1%)
All	All	0.86	2/12940 (0.0%)	1.05	22/17540 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	THR	CA-CB	5.12	1.63	1.53
1	A	80	THR	CA-CB	5.05	1.62	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	GLY	O-C-N	-7.37	113.12	122.70
1	F	263	ILE	N-CA-C	7.33	118.44	111.91
1	A	103	GLY	CA-C-N	7.23	127.85	119.47
1	A	103	GLY	C-N-CA	7.23	127.85	119.47
1	F	126	LEU	N-CA-C	-6.48	104.13	111.07
1	A	704	ALA	N-CA-C	-6.34	105.70	113.50
1	A	390	ARG	N-CA-C	6.24	119.71	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	GLU	CA-C-N	6.17	126.13	119.78
1	A	159	GLU	C-N-CA	6.17	126.13	119.78
1	F	390	ARG	N-CA-C	5.92	119.19	109.72
1	F	57	GLY	O-C-N	-5.86	115.09	122.70
1	A	489	THR	N-CA-C	5.81	118.37	108.90
1	F	741	VAL	N-CA-C	5.57	116.78	108.54
1	F	412	ILE	N-CA-CB	-5.50	108.03	111.83
1	A	116	THR	N-CA-C	-5.45	102.41	110.48
1	A	345	VAL	N-CA-C	-5.33	105.31	110.42
1	A	184	HIS	CA-C-N	5.27	125.33	119.32
1	A	184	HIS	C-N-CA	5.27	125.33	119.32
1	F	7	LYS	N-CA-C	5.18	117.37	110.53
1	F	652	GLY	N-CA-C	-5.14	106.19	112.77
1	A	112	SER	N-CA-C	5.12	117.51	108.75
1	F	15	THR	N-CA-C	-5.01	105.71	111.07

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	PRO	Peptide
1	F	313	LYS	Peptide
1	F	57	GLY	Peptide

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	6301	0	6155	227	0
1	F	6301	0	6155	258	0
2	A	8	0	0	0	0
2	F	8	0	0	0	0
3	A	1	0	0	0	0
3	F	1	0	0	0	0
4	A	94	0	44	14	0
4	F	94	0	44	17	0
5	A	489	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	436	0	0	29	1
All	All	13733	0	12398	481	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 19.

All (481) 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:F:783:LYS:HG3	5:F:7033:HOH:O	1.43	1.18
1:F:109:MET:CE	1:F:123:ALA:HB1	1.95	0.96
1:F:684:ARG:NH2	4:F:6001:MGD:H15	1.63	0.95
1:F:193:ASN:HB3	5:F:7024:HOH:O	1.68	0.93
1:F:668:ALA:HA	5:F:7032:HOH:O	1.67	0.93
1:A:395:MET:HE2	1:A:402:HIS:HA	1.52	0.91
1:A:684:ARG:HH12	1:A:690:HIS:CE1	1.89	0.91
1:F:50:PHE:CZ	1:F:700:GLU:HG3	2.10	0.87
1:A:227:SER:HB2	1:A:309:THR:HG22	1.56	0.87
1:A:442:THR:HG22	1:A:471:VAL:HB	1.57	0.84
1:F:684:ARG:NH1	1:F:690:HIS:CE1	2.46	0.83
1:A:40:ASN:HD22	1:A:40:ASN:H	1.27	0.83
1:A:109:MET:CE	1:A:123:ALA:HB1	2.09	0.82
1:A:68:MET:HB2	1:A:80:THR:CG2	2.10	0.82
1:F:78:GLU:O	1:F:80:THR:HG22	1.80	0.82
1:F:684:ARG:HH22	4:F:6001:MGD:H15	1.28	0.80
1:F:55:MET:HE1	1:F:493:VAL:H	1.46	0.80
1:F:721:ASP:OD1	1:F:791:LYS:NZ	2.16	0.79
1:F:456:GLU:OE1	5:F:7320:HOH:O	1.99	0.79
1:F:579:ASN:ND2	1:F:582:SER:HB2	1.96	0.79
1:A:684:ARG:NH1	1:A:690:HIS:CE1	2.49	0.79
1:F:240:ILE:HD13	1:F:245:ILE:HD11	1.66	0.77
1:A:413:PRO:O	1:A:416:THR:HG23	1.83	0.77
1:F:342:THR:OG1	5:F:7032:HOH:O	2.03	0.76
1:A:55:MET:HE3	1:A:492:TRP:HB3	1.67	0.76
1:A:68:MET:HB2	1:A:80:THR:HG23	1.67	0.76
1:F:137:ASP:OD2	1:F:141:ARG:HD2	1.87	0.75
1:F:382:ARG:O	1:F:390:ARG:NH2	2.20	0.75
1:F:109:MET:HE1	1:F:123:ALA:HB1	1.70	0.74
1:A:442:THR:CG2	1:A:471:VAL:HB	2.18	0.74
1:F:421:ILE:HG13	5:F:7028:HOH:O	1.87	0.74
1:A:78:GLU:O	1:A:80:THR:HG22	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:SER:OG	1:A:355:HIS:HE1	1.69	0.74
1:F:141:ARG:HD3	1:F:424:HIS:HB2	1.70	0.74
1:F:142:HIS:HE1	1:F:447:ASN:HD21	1.36	0.74
1:A:382:ARG:O	1:A:390:ARG:NH2	2.22	0.73
1:F:413:PRO:O	1:F:416:THR:CG2	2.37	0.73
1:A:33:GLY:O	1:A:35:PRO:HD3	1.88	0.73
1:A:263:ILE:HG13	1:A:775:PRO:HG2	1.71	0.73
1:A:720:ARG:HG2	5:A:4431:HOH:O	1.88	0.72
1:F:109:MET:HE3	1:F:123:ALA:HB1	1.69	0.72
1:A:413:PRO:HD2	1:A:416:THR:HG21	1.72	0.72
1:F:432:LEU:HD13	1:F:437:LEU:HB3	1.70	0.72
1:F:696:ARG:NH2	5:F:7432:HOH:O	2.23	0.72
1:F:456:GLU:OE2	5:F:7292:HOH:O	2.05	0.72
1:A:511:GLN:HE22	1:A:580:ASP:H	1.38	0.72
1:F:343:ARG:HD2	1:F:346:TRP:CE3	2.25	0.71
1:A:684:ARG:HH12	1:A:690:HIS:HE1	1.35	0.70
1:A:690:HIS:HD2	4:A:3001:MGD:O1B	1.74	0.70
1:F:398:THR:CG2	5:F:7221:HOH:O	2.39	0.70
1:A:40:ASN:HD22	1:A:40:ASN:N	1.89	0.70
1:A:403:ARG:HD2	5:A:4367:HOH:O	1.91	0.70
1:F:703:ARG:O	1:F:705:PHE:N	2.24	0.70
1:A:109:MET:HE1	1:A:123:ALA:HB1	1.74	0.70
1:A:112:SER:HA	1:A:139:ASN:HB2	1.74	0.70
1:F:511:GLN:HE22	1:F:580:ASP:H	1.40	0.69
1:A:55:MET:HE1	1:A:493:VAL:H	1.58	0.69
1:F:506:THR:HB	1:F:614:TYR:CE2	2.28	0.68
1:A:684:ARG:NH2	4:A:3001:MGD:H15	1.92	0.68
1:A:141:ARG:HD3	1:A:424:HIS:HB2	1.76	0.68
1:A:224:THR:HG22	1:A:227:SER:HB3	1.76	0.68
1:A:432:LEU:HD13	1:A:437:LEU:HB3	1.74	0.68
1:F:59:ASP:N	1:F:59:ASP:OD1	2.25	0.68
1:A:195:ARG:NH1	1:A:201:VAL:O	2.26	0.68
1:A:684:ARG:NH1	1:A:690:HIS:HE1	1.89	0.67
1:F:684:ARG:NH1	1:F:690:HIS:HE1	1.93	0.67
1:A:116:THR:CG2	1:A:118:TRP:CD1	2.78	0.67
1:A:50:PHE:CZ	1:A:700:GLU:HG3	2.29	0.67
1:F:55:MET:CE	1:F:492:TRP:HB3	2.25	0.67
1:A:744:ARG:HD2	5:A:4452:HOH:O	1.95	0.66
1:F:390:ARG:NH1	1:F:391:LEU:O	2.28	0.66
1:F:398:THR:HG23	5:F:7221:HOH:O	1.94	0.66
1:A:40:ASN:H	1:A:40:ASN:ND2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:VAL:HG22	1:A:512:GLN:HG2	1.76	0.66
1:F:332:SER:OG	1:F:355:HIS:HE1	1.79	0.66
1:F:50:PHE:CE2	1:F:700:GLU:HG3	2.31	0.66
1:F:116:THR:HG22	1:F:119:GLU:H	1.59	0.66
1:F:471:VAL:HG13	1:F:483:ALA:HB2	1.76	0.65
1:A:109:MET:HE3	1:A:123:ALA:HB1	1.76	0.65
1:F:303:GLU:CD	1:F:303:GLU:H	2.04	0.64
1:F:396:VAL:H	1:F:402:HIS:HD2	1.45	0.64
1:F:233:ASN:ND2	5:F:7054:HOH:O	2.30	0.64
1:F:684:ARG:HH12	1:F:690:HIS:CE1	2.15	0.64
1:F:55:MET:HE3	1:F:492:TRP:HB3	1.79	0.64
1:A:55:MET:CE	1:A:492:TRP:HB3	2.27	0.64
1:F:413:PRO:O	1:F:416:THR:HG22	1.98	0.64
1:A:254:VAL:HG11	1:A:660:ILE:HD12	1.79	0.63
1:A:66:LEU:HB2	1:A:82:ILE:HD13	1.81	0.63
1:F:166:ASP:HB3	1:F:331:ILE:HD11	1.79	0.63
1:F:501:ASN:ND2	1:F:505:ARG:H	1.96	0.63
1:F:407:GLU:OE2	5:F:7358:HOH:O	2.15	0.63
1:A:396:VAL:H	1:A:402:HIS:HD2	1.46	0.63
1:A:226:GLN:HG3	1:A:668:ALA:HB2	1.81	0.62
1:A:38:PRO:HG2	1:A:505:ARG:NH2	2.14	0.62
1:F:208:THR:HG22	1:F:209:TYR:HD2	1.62	0.62
1:A:713:HIS:HD2	1:A:715:LEU:H	1.48	0.62
1:A:227:SER:CB	1:A:309:THR:HG22	2.28	0.61
1:A:43:LEU:HD21	1:F:43:LEU:HD21	1.82	0.61
1:F:544:LEU:HD13	1:F:551:ARG:HG2	1.81	0.61
1:F:75:LYS:NZ	1:F:467:ASN:O	2.33	0.61
1:A:208:THR:HG22	1:A:209:TYR:HD2	1.66	0.61
1:F:376:SER:HB2	1:F:499:TYR:CD1	2.36	0.61
1:A:135:ASN:HD22	1:A:423:LEU:H	1.48	0.61
1:A:413:PRO:O	1:A:416:THR:CG2	2.49	0.61
1:F:702:HIS:O	1:F:706:PRO:HA	2.01	0.61
1:F:403:ARG:NH2	5:F:7134:HOH:O	2.34	0.60
1:F:135:ASN:HD22	1:F:423:LEU:H	1.48	0.60
1:F:76:GLU:HG3	5:F:7235:HOH:O	2.00	0.60
1:F:248:ASP:OD1	1:F:252:LYS:HE3	2.00	0.60
1:A:226:GLN:HG2	1:A:784:LYS:HD3	1.84	0.60
1:A:328:LYS:HE2	5:A:4456:HOH:O	2.00	0.60
1:A:374:GLN:HB2	1:A:377:ALA:HB2	1.82	0.60
1:F:40:ASN:HD22	1:F:40:ASN:N	1.99	0.60
1:F:18:GLY:H	1:F:40:ASN:ND2	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:THR:CG2	1:A:227:SER:HB3	2.31	0.60
1:A:501:ASN:C	1:A:501:ASN:HD22	2.09	0.60
1:A:116:THR:HG21	1:A:118:TRP:CD1	2.36	0.60
1:F:355:HIS:HD2	1:F:360:LYS:O	1.85	0.60
1:A:91:MET:HE3	1:A:470:ILE:HD13	1.84	0.59
1:A:730:VAL:HG21	1:A:756:MET:HE1	1.85	0.59
1:A:142:HIS:HE1	1:A:447:ASN:HD21	1.50	0.59
1:F:31:CYS:HB2	1:F:52:PRO:HG3	1.85	0.59
1:F:59:ASP:OD1	1:F:697:ARG:NH1	2.36	0.59
1:F:208:THR:HG23	1:F:753:LEU:HD11	1.85	0.59
1:A:395:MET:HE1	1:A:405:ILE:HB	1.85	0.59
1:F:505:ARG:NH2	5:F:7138:HOH:O	2.31	0.59
1:F:343:ARG:HD2	1:F:346:TRP:CZ3	2.37	0.58
1:F:235:ILE:HD11	1:F:319:LEU:HD13	1.84	0.58
1:F:211:HIS:HD2	1:F:213:SER:H	1.51	0.58
1:A:121:TYR:HA	1:A:384:VAL:HG11	1.84	0.58
1:A:166:ASP:HB3	1:A:331:ILE:HD11	1.85	0.58
1:F:684:ARG:HH11	1:F:690:HIS:CE1	2.19	0.58
1:F:446:ASN:HD21	1:F:479:SER:H	1.49	0.57
1:A:477:THR:O	1:A:481:LEU:HG	2.05	0.57
1:F:690:HIS:HD2	4:F:6001:MGD:O1B	1.88	0.57
1:A:98:ALA:HB3	1:A:107:ILE:HD11	1.86	0.57
1:A:116:THR:HG22	1:A:119:GLU:H	1.70	0.57
1:F:493:VAL:HG22	1:F:512:GLN:CG	2.35	0.57
1:A:48:GLY:HA2	1:A:51:LEU:HD22	1.85	0.57
1:A:506:THR:HB	1:A:614:TYR:CE2	2.39	0.57
1:A:135:ASN:ND2	1:A:423:LEU:H	2.02	0.57
1:F:63:GLN:HG3	1:F:64:PRO:HD2	1.87	0.57
1:A:540:PRO:HD2	1:A:543:LEU:HD12	1.87	0.57
1:A:235:ILE:HD11	1:A:319:LEU:HD13	1.87	0.56
1:F:116:THR:CG2	1:F:118:TRP:CD1	2.88	0.56
1:A:355:HIS:HD2	1:A:360:LYS:O	1.88	0.56
1:F:109:MET:HE1	1:F:123:ALA:CB	2.36	0.56
1:F:211:HIS:CD2	1:F:213:SER:HB2	2.41	0.56
1:F:309:THR:HB	1:F:311:VAL:HG13	1.87	0.56
1:A:233:ASN:ND2	5:A:4022:HOH:O	2.38	0.56
1:F:208:THR:HG23	1:F:753:LEU:CD1	2.36	0.56
1:A:58:LYS:HG3	1:A:59:ASP:OD1	2.06	0.56
1:A:211:HIS:HD2	1:A:213:SER:H	1.53	0.56
1:A:303:GLU:CD	1:A:303:GLU:H	2.14	0.56
1:A:343:ARG:HD2	1:A:346:TRP:CE3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:THR:HG22	1:F:227:SER:OG	2.06	0.56
1:F:515:ALA:HB1	1:F:519:ALA:HB3	1.88	0.56
1:A:360:LYS:HB3	1:A:366:CYS:SG	2.46	0.55
1:F:413:PRO:O	1:F:416:THR:HG23	2.06	0.55
1:F:116:THR:HB	1:F:119:GLU:OE1	2.07	0.55
1:A:1:GLU:O	1:A:24:GLN:NE2	2.37	0.55
1:A:376:SER:HB2	1:A:499:TYR:CD1	2.42	0.55
1:F:504:ARG:O	1:F:621:ARG:HA	2.06	0.55
1:F:506:THR:O	1:F:619:GLY:HA2	2.07	0.55
1:A:684:ARG:HD3	4:A:4001:MGD:C16	2.37	0.55
1:F:360:LYS:HB3	1:F:366:CYS:SG	2.48	0.54
1:A:413:PRO:HB2	1:A:416:THR:HG22	1.89	0.54
1:F:579:ASN:ND2	1:F:582:SER:H	2.04	0.54
1:F:18:GLY:H	1:F:40:ASN:HD21	1.55	0.54
1:F:501:ASN:C	1:F:501:ASN:HD22	2.16	0.54
1:F:40:ASN:HD22	1:F:40:ASN:H	1.54	0.54
1:F:253:HIS:HD2	5:F:7105:HOH:O	1.90	0.54
1:A:309:THR:OG1	1:A:311:VAL:HG13	2.08	0.54
1:F:764:LEU:HD12	5:F:7436:HOH:O	2.08	0.54
1:A:395:MET:CE	1:A:405:ILE:HD12	2.38	0.53
1:A:424:HIS:CD2	1:A:778:LYS:HG3	2.42	0.53
1:F:116:THR:HG21	1:F:118:TRP:CD1	2.43	0.53
1:F:409:LYS:HG3	1:F:599:TRP:CE3	2.43	0.53
1:F:726:ASP:O	1:F:741:VAL:HG23	2.08	0.53
1:F:731:VAL:O	1:F:787:VAL:HG22	2.08	0.53
1:A:493:VAL:HG22	1:A:512:GLN:CG	2.39	0.53
1:F:168:GLU:OE1	1:F:190:ARG:NH2	2.30	0.53
1:A:749:PRO:HB2	1:A:753:LEU:O	2.09	0.53
1:F:182:GLU:HB2	1:F:183:MET:HE2	1.90	0.53
1:F:390:ARG:HD2	1:F:395:MET:O	2.08	0.53
1:F:208:THR:HG22	1:F:209:TYR:CD2	2.43	0.53
1:F:413:PRO:HB2	1:F:543:LEU:HD22	1.91	0.53
1:F:203:VAL:N	1:F:218:ASP:OD2	2.41	0.53
1:F:690:HIS:CE1	4:F:7001:MGD:H15	2.27	0.53
1:A:55:MET:CE	1:A:493:VAL:H	2.22	0.53
1:A:335:THR:C	1:A:336:MET:HE2	2.34	0.53
1:A:501:ASN:C	1:A:501:ASN:ND2	2.66	0.53
1:F:268:ARG:NH1	1:F:457:GLU:OE1	2.42	0.53
1:A:233:ASN:HB3	1:A:300:TYR:CD2	2.44	0.53
1:A:395:MET:HE2	1:A:402:HIS:CA	2.31	0.53
1:A:98:ALA:HB3	1:A:107:ILE:CD1	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:GLN:O	1:A:531:ARG:HG2	2.09	0.52
1:A:690:HIS:CD2	4:A:3001:MGD:O1B	2.60	0.52
1:F:474:PRO:HA	5:F:7041:HOH:O	2.09	0.52
1:F:507:GLN:HA	5:F:7191:HOH:O	2.09	0.52
1:A:208:THR:HG23	1:A:753:LEU:CD1	2.40	0.52
1:A:226:GLN:CG	1:A:668:ALA:HB2	2.39	0.52
1:A:609:ALA:HB3	1:A:614:TYR:CE1	2.44	0.52
1:F:40:ASN:ND2	1:F:40:ASN:H	2.08	0.52
1:F:702:HIS:C	1:F:703:ARG:O	2.50	0.52
1:A:579:ASN:C	1:A:579:ASN:HD22	2.17	0.52
1:F:55:MET:HE1	1:F:493:VAL:N	2.21	0.52
1:A:452:PRO:HB3	1:A:780:THR:HG21	1.92	0.52
1:A:51:LEU:O	1:A:54:ILE:HG12	2.09	0.52
1:A:574:ALA:HB3	1:A:577:GLN:HB2	1.92	0.52
1:A:184:HIS:N	1:A:185:PRO:HD3	2.24	0.52
1:F:442:THR:HG22	1:F:471:VAL:HG12	1.92	0.52
1:F:70:ASN:O	1:F:72:LYS:HG2	2.10	0.52
1:F:202:THR:HA	1:F:218:ASP:OD2	2.10	0.52
1:F:531:ARG:NH1	5:F:7203:HOH:O	2.43	0.52
1:F:395:MET:HE1	1:F:405:ILE:CD1	2.40	0.52
1:A:7:LYS:O	5:A:4013:HOH:O	2.19	0.51
1:F:723:ARG:HG3	1:F:726:ASP:CG	2.35	0.51
1:A:409:LYS:HG3	1:A:599:TRP:CE3	2.45	0.51
1:A:723:ARG:O	1:A:724:ARG:C	2.53	0.51
1:F:15:THR:HG23	1:F:187:LEU:HG	1.92	0.51
1:F:337:GLY:HA2	5:F:7033:HOH:O	2.10	0.51
1:F:579:ASN:CG	1:F:582:SER:HB2	2.35	0.51
1:A:137:ASP:OD2	1:A:141:ARG:HD2	2.10	0.51
1:F:248:ASP:OD1	1:F:252:LYS:CE	2.58	0.51
1:F:493:VAL:HG22	1:F:512:GLN:HG3	1.92	0.51
1:F:501:ASN:ND2	1:F:505:ARG:HB3	2.25	0.51
1:F:690:HIS:CE1	4:F:7001:MGD:S13	3.04	0.51
1:A:633:ARG:O	1:A:634:TYR:HB2	2.10	0.51
1:F:216:LEU:O	1:F:216:LEU:HG	2.11	0.51
1:F:413:PRO:HB2	1:F:416:THR:HG22	1.92	0.51
1:F:456:GLU:OE2	1:F:734:ARG:HG2	2.10	0.51
1:A:426:VAL:O	1:A:429:ASP:HB2	2.11	0.51
1:A:224:THR:HG22	1:A:227:SER:CB	2.41	0.51
1:F:503:GLU:O	1:F:504:ARG:HB2	2.10	0.50
1:A:1:GLU:O	1:A:1:GLU:HG3	2.11	0.50
1:A:524:TRP:CE2	1:A:528:GLN:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:TYR:HA	1:F:384:VAL:HG11	1.93	0.50
1:F:222:ILE:HG21	1:F:750:PRO:HG3	1.93	0.50
1:A:442:THR:HG22	1:A:442:THR:O	2.10	0.50
1:A:390:ARG:NH1	1:A:391:LEU:O	2.44	0.50
1:F:55:MET:CE	1:F:493:VAL:H	2.21	0.50
1:F:116:THR:HG21	5:F:7352:HOH:O	2.12	0.50
1:F:313:LYS:O	1:F:317:GLU:HG3	2.11	0.50
1:A:449:GLN:NE2	5:A:4004:HOH:O	2.44	0.50
1:F:40:ASN:N	1:F:40:ASN:ND2	2.58	0.50
1:F:424:HIS:CE1	1:F:427:ALA:HB2	2.47	0.50
1:F:491:MET:O	1:F:494:GLU:HB2	2.12	0.50
1:A:609:ALA:HB2	1:A:624:VAL:HG11	1.94	0.50
1:A:691:THR:O	1:A:696:ARG:NH1	2.45	0.50
1:A:734:ARG:NH1	1:A:770:LEU:HD13	2.27	0.50
1:F:373:GLY:HA3	4:F:7001:MGD:C12	2.40	0.50
1:F:353:ASN:OD1	1:F:660:ILE:HG23	2.12	0.49
1:A:332:SER:OG	1:A:355:HIS:CE1	2.58	0.49
1:F:396:VAL:HG23	1:F:398:THR:HG22	1.93	0.49
1:A:4:LYS:O	1:A:22:GLY:HA2	2.12	0.49
1:A:409:LYS:HG3	1:A:599:TRP:CZ3	2.47	0.49
1:A:474:PRO:HD2	4:A:3001:MGD:H1'	1.93	0.49
1:F:373:GLY:HA3	4:F:7001:MGD:C13	2.42	0.49
1:F:497:GLY:HA3	1:F:509:TRP:CE2	2.47	0.49
1:A:441:TRP:HA	1:A:470:ILE:HB	1.94	0.49
1:A:684:ARG:HH11	4:A:4001:MGD:H15	1.61	0.49
1:F:533:PHE:O	1:F:554:THR:HA	2.13	0.49
1:A:556:TYR:CE2	1:A:561:ALA:HB2	2.47	0.49
1:F:142:HIS:CE1	1:F:447:ASN:HD21	2.25	0.49
1:F:227:SER:HB2	1:F:309:THR:HG22	1.94	0.49
1:A:248:ASP:O	1:A:252:LYS:HG3	2.13	0.49
1:F:142:HIS:HD2	5:F:7063:HOH:O	1.95	0.49
1:F:628:LYS:HB2	5:F:7398:HOH:O	2.12	0.49
1:A:373:GLY:HA3	4:A:4001:MGD:C12	2.43	0.48
1:F:226:GLN:CD	5:F:7032:HOH:O	2.56	0.48
1:F:166:ASP:CB	1:F:331:ILE:HD11	2.42	0.48
1:F:211:HIS:HB3	1:F:747:ASN:OD1	2.13	0.48
1:A:373:GLY:HA3	4:A:4001:MGD:C13	2.43	0.48
1:A:448:MET:HE1	1:A:458:ARG:HG2	1.95	0.48
1:A:448:MET:CE	1:A:458:ARG:HG2	2.43	0.48
1:A:497:GLY:HA3	1:A:509:TRP:CE2	2.48	0.48
1:F:759:PHE:C	1:F:759:PHE:CD2	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:ARG:NE	4:A:4001:MGD:H102	2.29	0.48
1:F:309:THR:CB	1:F:311:VAL:HG13	2.44	0.48
1:A:226:GLN:HE21	1:A:784:LYS:HD2	1.79	0.48
1:F:224:THR:HG21	1:F:308:MET:O	2.14	0.48
1:F:395:MET:HE1	1:F:405:ILE:HD12	1.95	0.48
1:F:207:SER:O	1:F:222:ILE:HA	2.14	0.48
1:F:442:THR:HG22	1:F:471:VAL:CB	2.43	0.48
1:A:116:THR:HG21	5:A:4362:HOH:O	2.14	0.48
1:F:413:PRO:HD2	1:F:416:THR:HG21	1.96	0.48
1:A:684:ARG:NH2	4:A:3001:MGD:S13	2.87	0.47
1:F:685:VAL:HG21	1:F:705:PHE:CE2	2.49	0.47
1:A:171:ASP:O	1:A:201:VAL:HA	2.13	0.47
1:A:628:LYS:HD2	5:A:4426:HOH:O	2.14	0.47
1:F:501:ASN:ND2	1:F:501:ASN:C	2.73	0.47
1:F:172:ALA:HA	1:F:202:THR:O	2.15	0.47
1:F:353:ASN:CG	1:F:660:ILE:HG23	2.40	0.47
1:A:268:ARG:NH1	1:A:457:GLU:OE1	2.47	0.47
1:F:68:MET:HB2	1:F:80:THR:CG2	2.44	0.47
1:F:684:ARG:HD3	4:F:7001:MGD:C16	2.43	0.47
1:F:730:VAL:HG21	1:F:756:MET:HE1	1.96	0.47
1:F:232:LEU:HD11	1:F:338:PHE:CZ	2.48	0.47
1:A:710:LEU:HD12	1:A:756:MET:CE	2.45	0.47
1:A:75:LYS:HG3	1:A:465:PRO:HA	1.96	0.47
1:A:471:VAL:HG13	1:A:483:ALA:HB2	1.95	0.47
1:F:684:ARG:NE	4:F:7001:MGD:H102	2.30	0.47
1:F:709:VAL:HG12	1:F:740:ILE:HB	1.97	0.47
1:A:59:ASP:OD1	1:A:59:ASP:N	2.42	0.47
1:A:268:ARG:NH2	1:A:434:ASP:OD1	2.48	0.47
1:F:493:VAL:HG22	1:F:512:GLN:HG2	1.97	0.47
1:A:687:GLU:OE2	1:A:746:ARG:NH1	2.44	0.47
1:F:396:VAL:CG2	1:F:398:THR:HG22	2.44	0.47
1:A:68:MET:HE3	1:A:80:THR:HG23	1.97	0.47
1:F:268:ARG:HH22	1:F:434:ASP:CG	2.22	0.46
1:A:729:LYS:HE3	1:A:736:GLU:OE1	2.15	0.46
1:F:5:TRP:HA	1:F:21:VAL:O	2.15	0.46
1:A:636:GLU:CD	1:A:645:GLY:H	2.22	0.46
1:A:40:ASN:N	1:A:40:ASN:ND2	2.54	0.46
1:A:68:MET:HE2	1:A:82:ILE:CG2	2.44	0.46
1:F:673:ASP:OD1	1:F:733:ARG:NH1	2.48	0.46
1:A:633:ARG:O	1:A:634:TYR:CB	2.64	0.46
1:F:135:ASN:ND2	1:F:423:LEU:H	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:442:THR:HG22	1:F:471:VAL:HB	1.97	0.46
1:F:442:THR:CG2	1:F:471:VAL:HB	2.46	0.46
1:A:311:VAL:HG22	1:A:316:LEU:HG	1.98	0.46
1:F:184:HIS:N	1:F:185:PRO:HD3	2.31	0.46
1:F:710:LEU:HD23	1:F:712:ILE:HB	1.97	0.46
1:A:226:GLN:HG3	1:A:668:ALA:H	1.80	0.46
1:F:684:ARG:NH2	4:F:6001:MGD:S13	2.88	0.46
1:F:12:PHE:O	1:F:375:PRO:HD3	2.16	0.45
1:F:175:LEU:HD13	1:F:180:MET:HG3	1.97	0.45
1:A:363:GLN:OE1	1:A:363:GLN:HA	2.14	0.45
1:A:343:ARG:HD2	1:A:346:TRP:CZ3	2.51	0.45
1:F:253:HIS:HE1	5:F:7061:HOH:O	2.00	0.45
1:A:20:LEU:HD12	1:F:196:LEU:HG	1.98	0.45
1:A:497:GLY:HA3	1:A:509:TRP:CZ2	2.51	0.45
1:F:33:GLY:O	1:F:35:PRO:HD3	2.16	0.45
1:F:155:PHE:O	1:F:652:GLY:HA3	2.16	0.45
1:F:268:ARG:NH2	1:F:434:ASP:OD1	2.50	0.45
1:A:235:ILE:HD11	1:A:319:LEU:CD1	2.45	0.45
1:F:11:ARG:HH21	4:F:6001:MGD:C8	2.30	0.45
1:F:256:LEU:HD23	1:F:660:ILE:HB	1.99	0.45
1:F:336:MET:HG3	1:F:340:GLN:NE2	2.31	0.45
1:A:336:MET:HE2	1:A:336:MET:HA	1.98	0.45
1:F:59:ASP:O	1:F:60:ARG:C	2.59	0.45
1:F:226:GLN:HE21	1:F:784:LYS:NZ	2.13	0.45
1:A:536:GLU:OE2	1:A:552:GLY:N	2.50	0.45
1:F:474:PRO:HD2	4:F:6001:MGD:H1'	1.98	0.45
1:A:710:LEU:HD11	1:A:754:VAL:HG21	1.98	0.45
1:F:192:THR:HG23	1:F:216:LEU:HD13	1.98	0.45
1:A:756:MET:HE3	1:A:756:MET:HB2	1.74	0.44
1:F:162:GLY:O	1:F:504:ARG:NH2	2.49	0.44
1:A:511:GLN:NE2	1:A:579:ASN:HA	2.31	0.44
1:F:493:VAL:CG2	1:F:512:GLN:HG3	2.47	0.44
1:A:75:LYS:NZ	1:A:467:ASN:O	2.48	0.44
1:A:252:LYS:O	1:A:657:LYS:HE2	2.17	0.44
1:A:355:HIS:CD2	1:A:360:LYS:O	2.70	0.44
1:A:20:LEU:CD1	1:F:196:LEU:HG	2.48	0.44
1:A:446:ASN:HD21	1:A:479:SER:H	1.66	0.44
1:A:501:ASN:ND2	1:A:505:ARG:H	2.16	0.44
1:F:395:MET:CE	1:F:405:ILE:HD12	2.48	0.44
1:A:409:LYS:HE2	1:A:599:TRP:CD2	2.52	0.44
1:A:696:ARG:HD3	1:A:759:PHE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:MET:HB2	1:F:80:THR:HG21	1.99	0.44
1:F:302:LEU:HG	1:F:313:LYS:HG2	1.99	0.44
1:F:452:PRO:HB3	1:F:780:THR:HG21	2.00	0.44
1:F:735:GLY:O	1:F:768:LEU:HD23	2.18	0.44
1:A:139:ASN:HB3	1:A:374:GLN:HE22	1.83	0.44
1:A:489:THR:HA	1:A:520:LYS:O	2.18	0.44
1:A:734:ARG:CZ	1:A:770:LEU:HB2	2.48	0.44
1:F:165:ASP:OD1	1:F:631:GLN:NE2	2.50	0.44
1:F:718:LYS:C	1:F:720:ARG:H	2.26	0.44
1:F:485:LEU:HG	1:F:487:LEU:HD21	2.00	0.44
1:A:41:ARG:CG	1:A:41:ARG:O	2.66	0.44
1:A:395:MET:CE	1:A:402:HIS:HA	2.36	0.44
1:F:121:TYR:CE2	1:F:597:TYR:HB2	2.52	0.44
1:A:107:ILE:HG13	1:A:439:VAL:HB	2.01	0.43
1:F:148:VAL:HG22	1:F:382:ARG:HE	1.83	0.43
1:F:301:THR:HB	1:F:303:GLU:OE1	2.18	0.43
1:A:729:LYS:HE3	1:A:736:GLU:CD	2.44	0.43
1:F:46:ILE:HD12	1:F:46:ILE:HA	1.91	0.43
1:F:784:LYS:HE3	1:F:784:LYS:HB2	1.79	0.43
1:A:51:LEU:HG	1:A:492:TRP:CH2	2.53	0.43
1:A:538:VAL:HG21	1:A:555:LEU:HD21	1.99	0.43
1:F:183:MET:SD	1:F:684:ARG:HB2	2.59	0.43
1:F:231:ILE:HG13	1:F:309:THR:HG21	2.00	0.43
1:A:5:TRP:HA	1:A:21:VAL:O	2.19	0.43
1:A:703:ARG:HH12	1:F:704:ALA:CA	2.31	0.43
1:F:66:LEU:HD21	1:F:73:TYR:HB2	2.01	0.43
1:A:142:HIS:HD2	5:A:4031:HOH:O	2.01	0.43
1:A:208:THR:HG23	1:A:753:LEU:HD13	2.00	0.43
1:A:673:ASP:C	1:A:673:ASP:OD2	2.61	0.43
1:F:690:HIS:HE1	4:F:7001:MGD:S13	2.41	0.43
1:A:154:THR:HG23	1:A:659:VAL:O	2.18	0.43
1:A:301:THR:O	1:A:302:LEU:C	2.62	0.43
1:F:235:ILE:HD11	1:F:319:LEU:CD1	2.47	0.43
1:F:749:PRO:HD2	5:F:7231:HOH:O	2.18	0.43
1:A:139:ASN:ND2	1:A:374:GLN:OE1	2.52	0.43
1:A:192:THR:O	1:A:196:LEU:HB2	2.19	0.43
1:A:442:THR:HG23	5:A:4114:HOH:O	2.19	0.43
1:A:734:ARG:HH11	1:A:770:LEU:HD13	1.83	0.43
1:F:538:VAL:HG23	1:F:539:TRP:CD1	2.53	0.43
1:F:116:THR:HB	1:F:119:GLU:CD	2.44	0.43
1:A:544:LEU:HD13	1:A:551:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:GLY:HA2	1:F:775:PRO:HB2	2.00	0.42
1:F:684:ARG:HH22	4:F:6001:MGD:C13	2.32	0.42
1:F:556:TYR:CE2	1:F:561:ALA:HB2	2.54	0.42
1:F:579:ASN:HD22	1:F:582:SER:H	1.66	0.42
1:F:41:ARG:HG2	1:F:41:ARG:O	2.19	0.42
1:F:673:ASP:HB2	1:F:674:GLU:OE1	2.19	0.42
1:F:756:MET:HE3	1:F:756:MET:HB2	1.71	0.42
1:A:59:ASP:O	1:A:60:ARG:C	2.62	0.42
1:A:199:GLN:H	1:A:199:GLN:HG2	1.62	0.42
1:F:192:THR:CG2	1:F:196:LEU:HD22	2.50	0.42
1:F:472:SER:OG	1:F:525:GLN:NE2	2.47	0.42
1:F:574:ALA:HB3	1:F:577:GLN:HB2	2.01	0.42
1:F:684:ARG:HD3	4:F:7001:MGD:N15	2.35	0.42
1:F:495:LYS:HA	1:F:511:GLN:HG3	2.02	0.42
1:F:528:GLN:O	1:F:531:ARG:HG2	2.19	0.42
1:A:459:MET:HB3	1:A:460:PRO:HD3	2.02	0.42
1:F:139:ASN:ND2	4:F:6001:MGD:O2A	2.48	0.42
1:F:183:MET:C	1:F:185:PRO:HD3	2.45	0.42
1:F:634:TYR:C	1:F:642:VAL:HG21	2.44	0.42
1:A:398:THR:HG23	5:A:4204:HOH:O	2.19	0.42
1:A:515:ALA:HB1	1:A:519:ALA:HB3	2.02	0.42
1:A:679:TRP:CZ3	1:A:784:LYS:HG2	2.55	0.42
1:F:355:HIS:CD2	1:F:360:LYS:O	2.68	0.42
1:F:489:THR:HA	1:F:520:LYS:O	2.19	0.42
1:F:572:GLU:HB3	5:F:7290:HOH:O	2.19	0.42
1:F:710:LEU:CD2	1:F:712:ILE:HB	2.50	0.42
1:A:444:CYS:HA	4:A:3001:MGD:N3	2.34	0.42
1:F:446:ASN:HD22	1:F:479:SER:CB	2.33	0.42
1:F:601:GLY:HA3	1:F:606:HIS:HB2	2.01	0.42
1:A:726:ASP:O	1:A:741:VAL:HG23	2.19	0.42
1:F:713:HIS:HA	5:F:7101:HOH:O	2.18	0.42
1:A:208:THR:HG23	1:A:753:LEU:HD11	2.00	0.42
1:F:639:ASP:HB3	1:F:642:VAL:HG23	2.00	0.42
1:A:226:GLN:HG3	1:A:668:ALA:N	2.35	0.41
1:F:154:THR:HG23	1:F:659:VAL:O	2.20	0.41
1:F:210:GLN:HB3	1:F:748:ARG:HB2	2.02	0.41
1:F:399:ASN:OD1	1:F:399:ASN:C	2.62	0.41
1:F:446:ASN:HD22	1:F:479:SER:HB2	1.85	0.41
1:A:41:ARG:CB	5:A:4458:HOH:O	2.68	0.41
1:A:159:GLU:HA	1:A:160:PRO:HD3	1.90	0.41
1:A:442:THR:CG2	5:A:4114:HOH:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LEU:HD11	1:A:338:PHE:CZ	2.56	0.41
1:F:6:ASP:HB3	1:F:512:GLN:HE22	1.84	0.41
1:A:579:ASN:ND2	1:A:582:SER:H	2.18	0.41
1:A:690:HIS:CE1	4:A:4001:MGD:H15	2.38	0.41
1:A:710:LEU:HB2	1:A:756:MET:HE2	2.02	0.41
1:F:446:ASN:ND2	1:F:479:SER:H	2.17	0.41
1:F:734:ARG:CZ	1:F:770:LEU:HB2	2.50	0.41
1:F:68:MET:HE3	1:F:80:THR:HG23	2.03	0.41
1:F:234:TYR:HB2	1:F:305:THR:OG1	2.21	0.41
1:F:723:ARG:CG	1:F:726:ASP:OD2	2.68	0.41
1:A:55:MET:HE1	1:A:493:VAL:N	2.32	0.41
1:A:121:TYR:CA	1:A:384:VAL:HG11	2.51	0.41
1:A:207:SER:OG	1:A:209:TYR:O	2.35	0.41
1:A:505:ARG:NH2	5:A:4116:HOH:O	2.36	0.41
1:A:684:ARG:HH22	4:A:3001:MGD:H15	1.67	0.41
1:F:91:MET:HE3	1:F:470:ILE:HD13	2.02	0.41
1:F:449:GLN:CD	1:F:691:THR:HB	2.45	0.41
1:F:711:PHE:CD1	1:F:747:ASN:HB2	2.56	0.41
1:A:142:HIS:CE1	1:A:447:ASN:HD21	2.34	0.41
1:A:436:LYS:HE2	1:A:436:LYS:HB3	1.95	0.41
1:F:143:CYS:CA	1:F:779:GLU:OE2	2.69	0.41
1:F:587:PHE:O	1:F:589:LEU:N	2.54	0.41
1:A:23:THR:HA	1:A:27:ARG:O	2.21	0.41
1:A:336:MET:HE2	1:A:336:MET:N	2.35	0.41
1:A:413:PRO:CD	1:A:416:THR:HG21	2.47	0.41
1:A:413:PRO:HA	1:A:547:LYS:HD2	2.03	0.41
1:F:9:PRO:HD2	1:F:509:TRP:CE3	2.55	0.41
1:A:179:ASN:C	1:A:179:ASN:HD22	2.29	0.40
1:A:207:SER:O	1:A:222:ILE:HA	2.21	0.40
1:A:665:PHE:CD2	1:A:665:PHE:C	3.00	0.40
1:F:314:ASP:HB3	1:F:315:GLN:H	1.57	0.40
1:A:137:ASP:OD2	1:A:141:ARG:CD	2.69	0.40
1:A:164:TYR:CE1	1:A:503:GLU:HG2	2.56	0.40
1:F:710:LEU:HG	1:F:754:VAL:CG2	2.51	0.40
1:A:134:ASN:C	1:A:136:ILE:H	2.29	0.40
1:F:442:THR:HG22	1:F:471:VAL:CG1	2.51	0.40
1:A:610:PRO:O	1:A:611:PHE:C	2.64	0.40
1:F:444:CYS:HA	4:F:6001:MGD:N3	2.35	0.40
1:A:183:MET:HG3	4:A:4001:MGD:O3B	2.21	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)
5:F:7379:HOH:O	5:F:7409:HOH:O[2_655]	1.98	0.22

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	789/792 (100%)	736 (93%)	47 (6%)	6 (1%)	16	31
1	F	789/792 (100%)	725 (92%)	55 (7%)	9 (1%)	11	22
All	All	1578/1584 (100%)	1461 (93%)	102 (6%)	15 (1%)	12	24

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	F	70	ASN
1	F	215	GLU
1	F	314	ASP
1	F	241	GLN
1	F	703	ARG
1	F	719	ALA
1	A	492	TRP
1	F	644	ALA
1	A	57	GLY
1	A	771	ASP
1	A	611	PHE
1	F	588	TYR
1	F	704	ALA
1	A	138	PRO

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	661/663 (100%)	595 (90%)	66 (10%)	7	15
1	F	661/663 (100%)	604 (91%)	57 (9%)	10	21
All	All	1322/1326 (100%)	1199 (91%)	123 (9%)	8	18

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	13	CYS
1	A	19	VAL
1	A	40	ASN
1	A	41	ARG
1	A	51	LEU
1	A	58	LYS
1	A	61	LEU
1	A	63	GLN
1	A	70	ASN
1	A	75	LYS
1	A	80	THR
1	A	100	LYS
1	A	107	ILE
1	A	116	THR
1	A	118	TRP
1	A	126	LEU
1	A	141	ARG
1	A	168	GLU
1	A	169	GLN
1	A	175	LEU
1	A	186	ILE
1	A	189	SER
1	A	196	LEU
1	A	206	LEU
1	A	208	THR
1	A	215	GLU
1	A	241	GLN
1	A	251	SER
1	A	252	LYS
1	A	303	GLU

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Mol	Chain	Res	Type
1	A	307	GLU
1	A	311	VAL
1	A	313	LYS
1	A	319	LEU
1	A	398	THR
1	A	401	LYS
1	A	404	ASP
1	A	409	LYS
1	A	416	THR
1	A	432	LEU
1	A	437	LEU
1	A	442	THR
1	A	447	ASN
1	A	471	VAL
1	A	493	VAL
1	A	501	ASN
1	A	512	GLN
1	A	518	GLU
1	A	578	LEU
1	A	579	ASN
1	A	616	LYS
1	A	643	LYS
1	A	674	GLU
1	A	685	VAL
1	A	686	LEU
1	A	687	GLU
1	A	700	GLU
1	A	703	ARG
1	A	710	LEU
1	A	718	LYS
1	A	720	ARG
1	A	721	ASP
1	A	754	VAL
1	A	784	LYS
1	A	787	VAL
1	F	1	GLU
1	F	19	VAL
1	F	40	ASN
1	F	41	ARG
1	F	44	ASN
1	F	51	LEU
1	F	61	LEU

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Mol	Chain	Res	Type
1	F	63	GLN
1	F	70	ASN
1	F	75	LYS
1	F	76	GLU
1	F	80	THR
1	F	116	THR
1	F	126	LEU
1	F	168	GLU
1	F	169	GLN
1	F	186	ILE
1	F	196	LEU
1	F	198	ASN
1	F	199	GLN
1	F	202	THR
1	F	206	LEU
1	F	208	THR
1	F	230	VAL
1	F	240	ILE
1	F	241	GLN
1	F	251	SER
1	F	303	GLU
1	F	311	VAL
1	F	319	LEU
1	F	342	THR
1	F	398	THR
1	F	401	LYS
1	F	404	ASP
1	F	409	LYS
1	F	416	THR
1	F	432	LEU
1	F	437	LEU
1	F	442	THR
1	F	447	ASN
1	F	471	VAL
1	F	493	VAL
1	F	501	ASN
1	F	512	GLN
1	F	518	GLU
1	F	578	LEU
1	F	579	ASN
1	F	643	LYS
1	F	684	ARG

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Mol	Chain	Res	Type
1	F	685	VAL
1	F	686	LEU
1	F	687	GLU
1	F	700	GLU
1	F	703	ARG
1	F	720	ARG
1	F	740	ILE
1	F	787	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	135	ASN
1	A	142	HIS
1	A	169	GLN
1	A	179	ASN
1	A	198	ASN
1	A	211	HIS
1	A	219	ASN
1	A	226	GLN
1	A	233	ASN
1	A	237	ASN
1	A	253	HIS
1	A	255	ASN
1	A	315	GLN
1	A	318	GLN
1	A	355	HIS
1	A	402	HIS
1	A	411	ASN
1	A	446	ASN
1	A	447	ASN
1	A	449	GLN
1	A	501	ASN
1	A	511	GLN
1	A	579	ASN
1	A	606	HIS
1	A	690	HIS
1	A	713	HIS
1	F	40	ASN
1	F	135	ASN
1	F	142	HIS

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Mol	Chain	Res	Type
1	F	179	ASN
1	F	200	ASN
1	F	211	HIS
1	F	219	ASN
1	F	226	GLN
1	F	233	ASN
1	F	237	ASN
1	F	241	GLN
1	F	253	HIS
1	F	255	ASN
1	F	321	GLN
1	F	340	GLN
1	F	355	HIS
1	F	402	HIS
1	F	411	ASN
1	F	424	HIS
1	F	446	ASN
1	F	447	ASN
1	F	449	GLN
1	F	501	ASN
1	F	511	GLN
1	F	512	GLN
1	F	525	GLN
1	F	579	ASN
1	F	604	HIS
1	F	606	HIS
1	F	690	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MGD	A	4001	3	47,52,52	1.46	7 (14%)	58,81,81	1.97	13 (22%)
4	MGD	F	7001	3	47,52,52	1.47	7 (14%)	58,81,81	2.22	16 (27%)
2	SF4	F	5001	1	0,12,12	-	-	-	-	-
2	SF4	A	2001	1	0,12,12	-	-	-	-	-
4	MGD	A	3001	3	47,52,52	1.33	4 (8%)	58,81,81	2.16	18 (31%)
4	MGD	F	6001	3	47,52,52	1.45	8 (17%)	58,81,81	2.26	21 (36%)

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
4	MGD	A	4001	3	-	7/22/66/66	0/6/6/6
4	MGD	F	7001	3	-	6/22/66/66	0/6/6/6
2	SF4	F	5001	1	-	-	0/6/5/5
2	SF4	A	2001	1	-	-	0/6/5/5
4	MGD	A	3001	3	-	6/22/66/66	0/6/6/6
4	MGD	F	6001	3	-	4/22/66/66	0/6/6/6

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4001	MGD	C16-C21	5.58	1.48	1.38
4	F	7001	MGD	C16-C21	5.58	1.48	1.38
4	F	6001	MGD	C16-C21	5.01	1.47	1.38
4	A	3001	MGD	C16-C21	4.72	1.46	1.38
4	A	4001	MGD	C17-N18	-3.40	1.32	1.38
4	A	3001	MGD	C5-C4	3.20	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4001	MGD	C6-N1	-3.08	1.33	1.38
4	A	4001	MGD	C5-C4	3.05	1.47	1.38
4	F	6001	MGD	PA-O3B	2.80	1.62	1.59
4	F	7001	MGD	C16-C17	2.71	1.50	1.41
4	A	3001	MGD	C17-N18	-2.68	1.33	1.38
4	F	6001	MGD	C5-C4	2.67	1.46	1.38
4	F	6001	MGD	C5-N7	-2.61	1.33	1.39
4	F	7001	MGD	C21-N22	2.59	1.38	1.35
4	F	7001	MGD	C6-N1	-2.55	1.34	1.38
4	F	7001	MGD	C5-C4	2.53	1.45	1.38
4	F	7001	MGD	C17-N18	-2.52	1.34	1.38
4	A	3001	MGD	C16-C17	2.43	1.49	1.41
4	F	6001	MGD	PB-O3B	2.39	1.62	1.59
4	A	4001	MGD	C5-N7	-2.29	1.34	1.39
4	A	4001	MGD	C16-C17	2.24	1.48	1.41
4	F	6001	MGD	C17-N18	-2.19	1.34	1.38
4	A	4001	MGD	C4-N9	-2.13	1.32	1.38
4	F	6001	MGD	C16-C17	2.11	1.48	1.41
4	F	7001	MGD	C19-N20	2.06	1.38	1.33
4	F	6001	MGD	C4-N9	-2.02	1.32	1.38

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	7001	MGD	C23-C14-N15	7.73	115.46	107.87
4	A	4001	MGD	C5-C4-N3	-5.92	118.97	128.39
4	F	7001	MGD	C5-C4-N3	-5.68	119.35	128.39
4	F	7001	MGD	C2-N3-C4	5.59	121.93	112.30
4	A	3001	MGD	C19-N20-C21	5.42	122.92	113.36
4	F	6001	MGD	O11-C23-C14	-5.40	105.36	108.96
4	F	6001	MGD	O11-C23-N22	-5.39	103.72	108.61
4	A	3001	MGD	C5-C4-N3	-5.33	119.91	128.39
4	A	4001	MGD	C2-N3-C4	5.22	121.30	112.30
4	F	7001	MGD	C19-N20-C21	5.17	122.49	113.36
4	A	3001	MGD	C2-N3-C4	4.90	120.73	112.30
4	F	6001	MGD	C2-N3-C4	4.74	120.46	112.30
4	F	6001	MGD	C5-C4-N3	-4.70	120.91	128.39
4	F	7001	MGD	N9-C4-N3	4.56	135.06	125.95
4	A	4001	MGD	C19-N20-C21	4.45	121.22	113.36
4	F	6001	MGD	C19-N20-C21	4.31	120.96	113.36
4	A	3001	MGD	C6-C5-N7	4.23	137.99	130.29
4	A	3001	MGD	C23-C14-N15	4.01	111.81	107.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3001	MGD	O4'-C1'-N9	-3.94	99.44	108.36
4	A	4001	MGD	N9-C4-N3	3.89	133.73	125.95
4	A	4001	MGD	C23-C14-N15	3.88	111.67	107.87
4	A	3001	MGD	N9-C4-N3	3.74	133.43	125.95
4	F	6001	MGD	C6-C5-N7	3.70	137.02	130.29
4	A	4001	MGD	C6-C5-N7	3.69	137.01	130.29
4	F	6001	MGD	C23-C14-N15	3.56	111.36	107.87
4	F	6001	MGD	O17-C17-C16	-3.48	118.86	127.26
4	A	3001	MGD	C4-C5-N7	-3.29	105.45	110.67
4	A	4001	MGD	C17-C16-N15	3.17	124.91	116.27
4	F	7001	MGD	O6-C6-C5	-3.03	118.54	126.53
4	A	4001	MGD	O2A-PA-O3B	3.00	115.38	107.27
4	F	6001	MGD	O4'-C1'-N9	-2.97	101.63	108.36
4	F	6001	MGD	N9-C4-N3	2.96	131.87	125.95
4	A	3001	MGD	C17-C16-N15	2.96	124.33	116.27
4	F	7001	MGD	O11-C23-N22	-2.91	105.96	108.61
4	F	7001	MGD	C6-C5-N7	2.88	135.53	130.29
4	F	6001	MGD	C4-C5-N7	-2.87	106.13	110.67
4	F	7001	MGD	C16-C17-N18	2.84	119.93	112.13
4	F	6001	MGD	N2-C2-N1	2.75	122.57	116.76
4	A	4001	MGD	O4'-C1'-N9	2.72	114.53	108.36
4	F	6001	MGD	O6-C6-C5	-2.70	119.41	126.53
4	F	7001	MGD	C17-C16-N15	2.68	123.57	116.27
4	A	4001	MGD	C4-C5-N7	-2.63	106.50	110.67
4	A	3001	MGD	O17-C17-C16	-2.61	120.96	127.26
4	F	7001	MGD	O2A-PA-O3B	2.61	114.32	107.27
4	F	7001	MGD	O17-C17-C16	-2.60	120.98	127.26
4	A	4001	MGD	C16-C17-N18	2.57	119.19	112.13
4	F	6001	MGD	C17-C16-N15	2.53	123.17	116.27
4	A	3001	MGD	C8-N7-C5	2.52	108.75	104.26
4	F	7001	MGD	C5-C6-N1	2.51	119.64	113.25
4	F	7001	MGD	O4'-C1'-N9	2.49	114.01	108.36
4	F	6001	MGD	C1'-N9-C4	-2.44	119.27	126.49
4	A	3001	MGD	C16-C17-N18	2.43	118.80	112.13
4	A	3001	MGD	C19-N18-C17	-2.37	120.81	125.11
4	F	6001	MGD	O3B-PA-O1A	-2.35	103.63	110.70
4	F	7001	MGD	C19-N18-C17	-2.35	120.85	125.11
4	F	6001	MGD	C16-C17-N18	2.33	118.52	112.13
4	F	7001	MGD	O3B-PA-O1A	-2.27	103.88	110.70
4	F	6001	MGD	N2-C2-N3	-2.26	115.26	119.67
4	A	3001	MGD	C1'-N9-C4	-2.25	119.85	126.49
4	F	6001	MGD	C8-N7-C5	2.19	108.17	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	6001	MGD	C19-N18-C17	-2.19	121.14	125.11
4	F	6001	MGD	O2A-PA-O1A	2.17	122.56	112.44
4	A	4001	MGD	O3'-C3'-C2'	-2.17	104.85	111.82
4	A	4001	MGD	O3B-PA-O1A	-2.17	104.18	110.70
4	A	3001	MGD	O4'-C1'-C2'	-2.16	102.00	106.62
4	A	3001	MGD	O4'-C4'-C5'	2.12	116.14	109.33
4	A	3001	MGD	N19-C19-N18	2.08	121.15	116.76
4	A	3001	MGD	N9-C8-N7	-2.07	109.56	113.40

There are no chirality outliers.

All (23) torsion outliers are listed below:

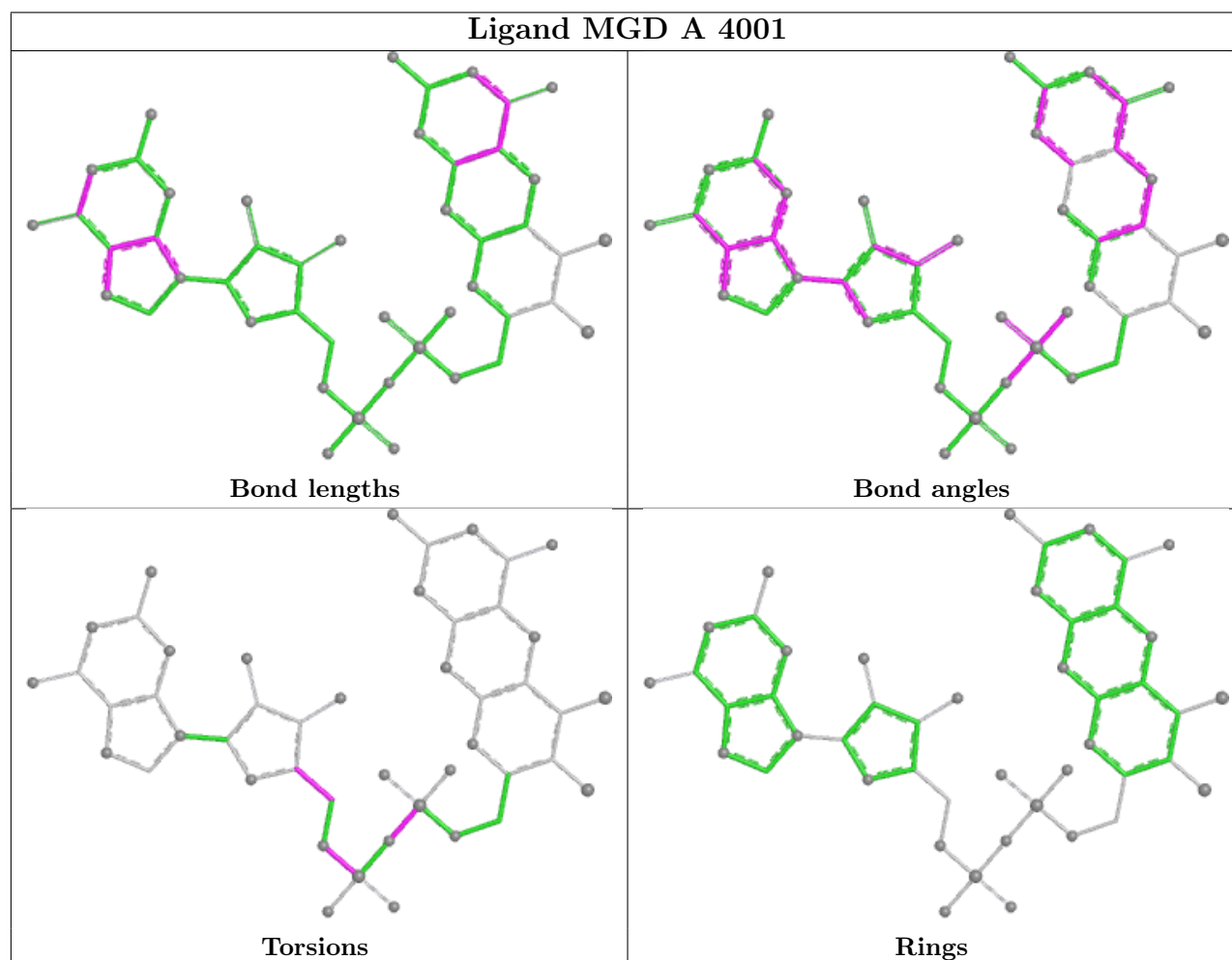
Mol	Chain	Res	Type	Atoms
4	A	3001	MGD	PA-O3B-PB-O5'
4	A	3001	MGD	C5'-O5'-PB-O2B
4	A	3001	MGD	C5'-O5'-PB-O3B
4	A	4001	MGD	C5'-O5'-PB-O1B
4	A	4001	MGD	C5'-O5'-PB-O2B
4	A	4001	MGD	C5'-O5'-PB-O3B
4	F	6001	MGD	C5'-O5'-PB-O2B
4	F	6001	MGD	C5'-O5'-PB-O3B
4	F	7001	MGD	C5'-O5'-PB-O2B
4	A	4001	MGD	C3'-C4'-C5'-O5'
4	F	6001	MGD	PA-O3B-PB-O5'
4	F	7001	MGD	PB-O3B-PA-O1A
4	F	7001	MGD	C5'-O5'-PB-O1B
4	F	7001	MGD	C5'-O5'-PB-O3B
4	A	4001	MGD	O4'-C4'-C5'-O5'
4	A	4001	MGD	PB-O3B-PA-O1A
4	A	3001	MGD	C2'-C1'-N9-C4
4	F	7001	MGD	C3'-C4'-C5'-O5'
4	A	3001	MGD	O4'-C4'-C5'-O5'
4	F	7001	MGD	PB-O3B-PA-O2A
4	A	3001	MGD	C2'-C1'-N9-C8
4	F	6001	MGD	O4'-C4'-C5'-O5'
4	A	4001	MGD	PB-O3B-PA-O2A

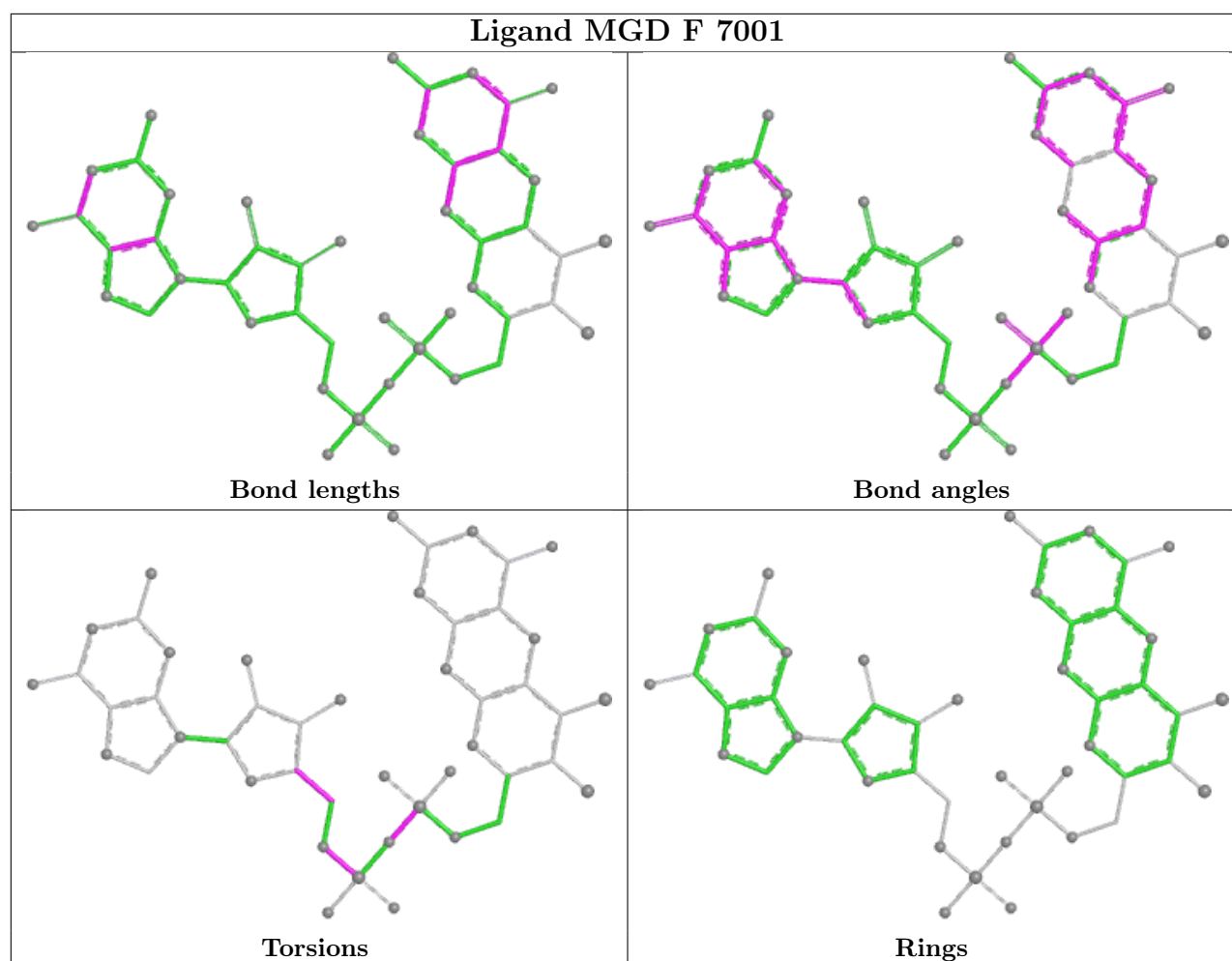
There are no ring outliers.

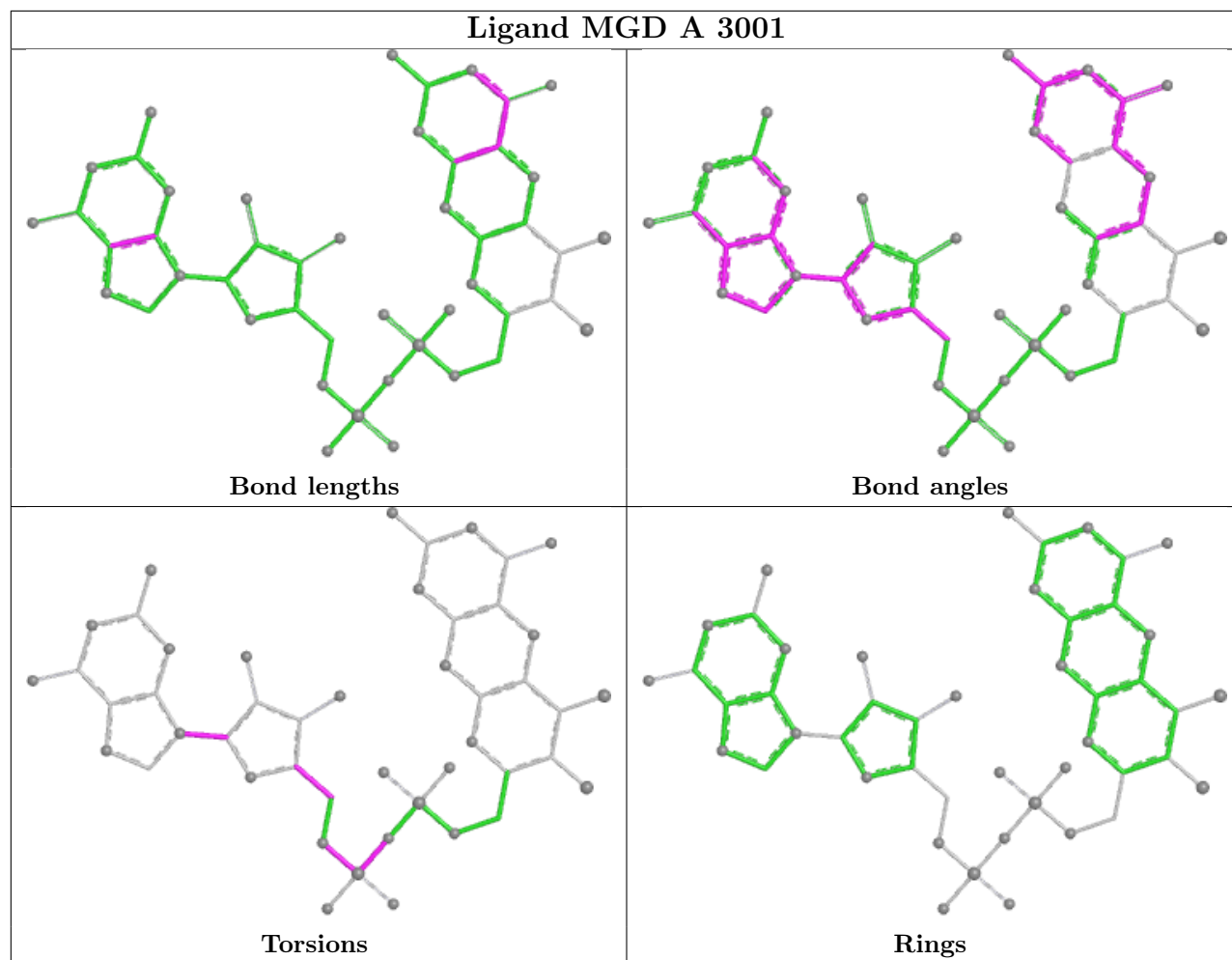
4 monomers are involved in 31 short contacts:

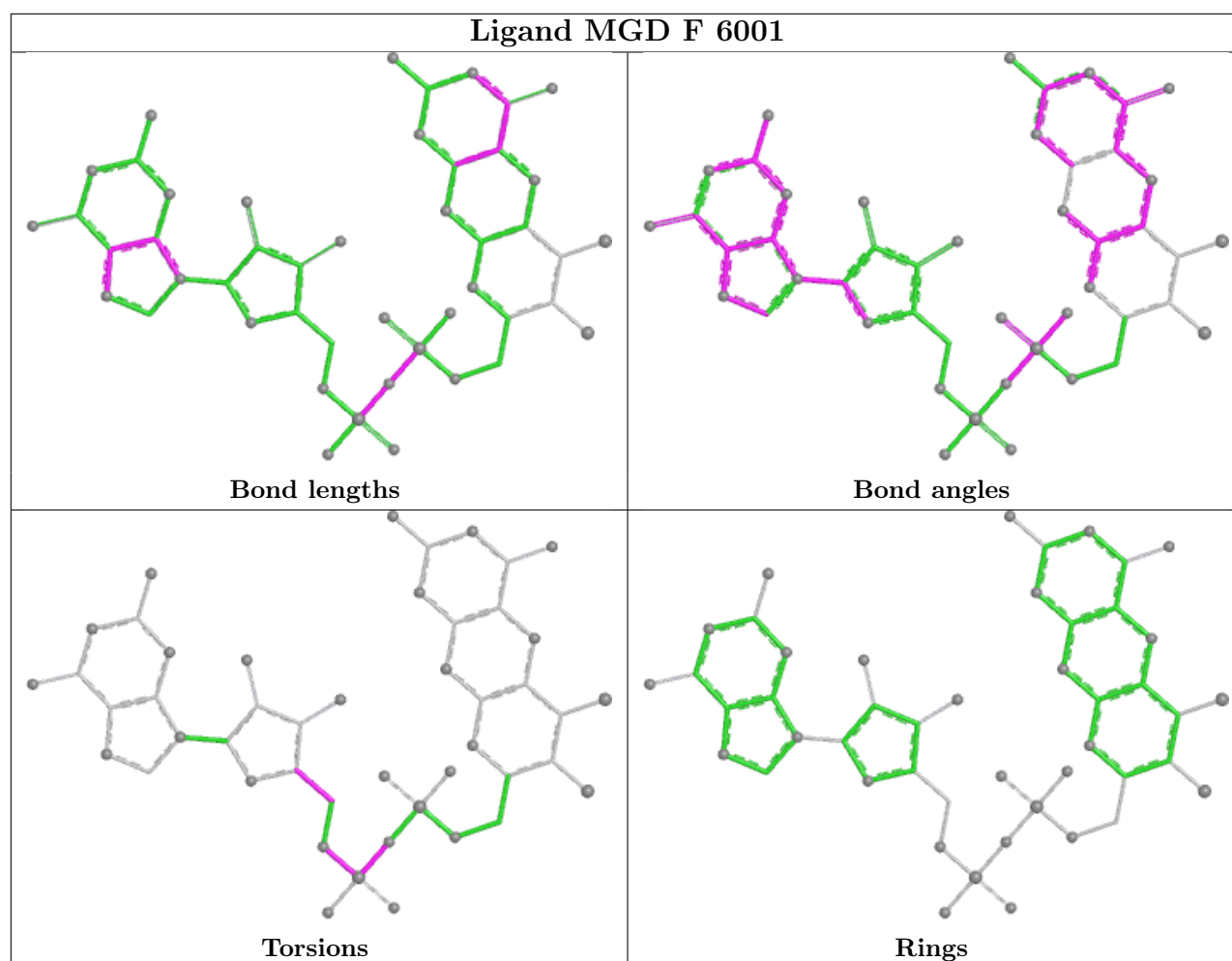
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4001	MGD	7	0
4	F	7001	MGD	8	0
4	A	3001	MGD	7	0
4	F	6001	MGD	9	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	791/792 (99%)	-0.47	0 100 100	13, 24, 37, 46	0
1	F	791/792 (99%)	-0.30	0 100 100	17, 30, 45, 55	0
All	All	1582/1584 (99%)	-0.38	0 100 100	13, 27, 42, 55	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MGD	F	7001	47/47	0.97	0.06	18,22,27,31	0
4	MGD	A	3001	47/47	0.98	0.05	11,16,17,20	0
4	MGD	A	4001	47/47	0.98	0.06	13,21,26,30	0
4	MGD	F	6001	47/47	0.98	0.05	15,19,21,22	0
2	SF4	F	5001	8/8	0.98	0.03	25,26,29,30	0
2	SF4	A	2001	8/8	0.99	0.03	24,26,28,28	0
3	6MO	A	2002	1/1	0.99	0.03	20,20,20,20	0

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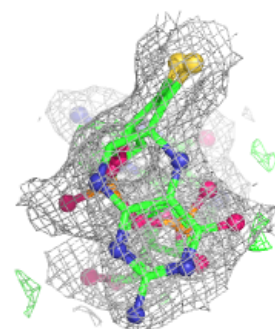
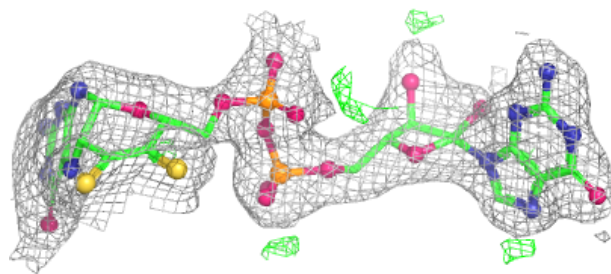
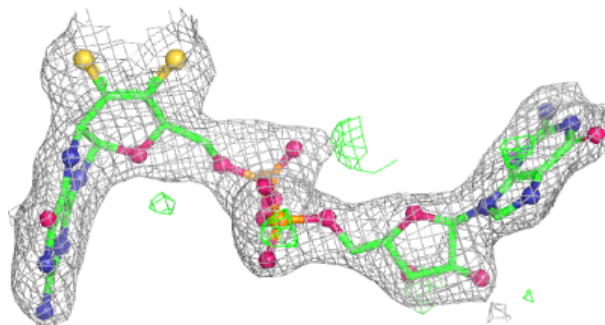
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	6MO	F	5002	1/1	1.00	0.02	24,24,24,24	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

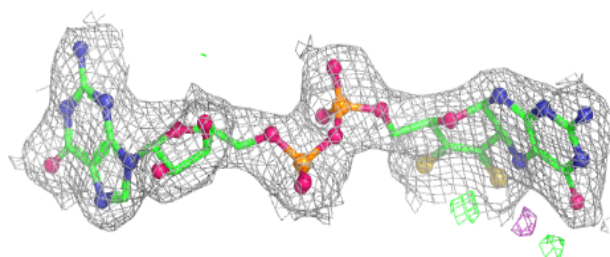
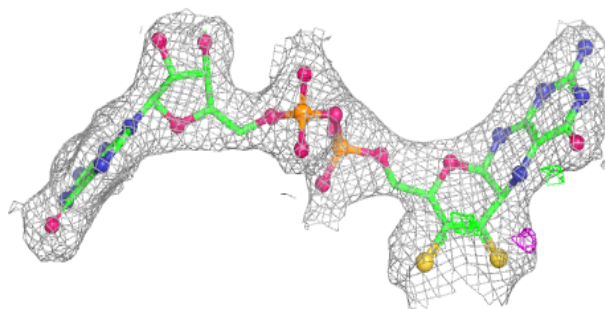
Electron density around MGD F 7001:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

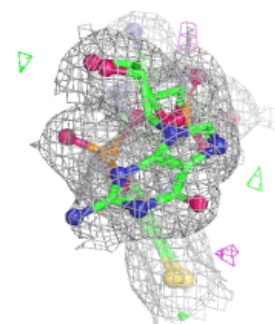
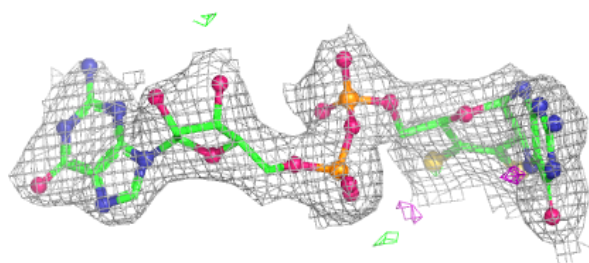


Electron density around MGD A 3001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

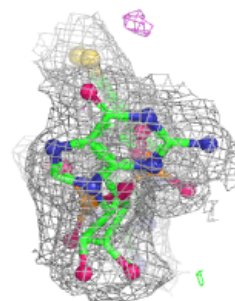
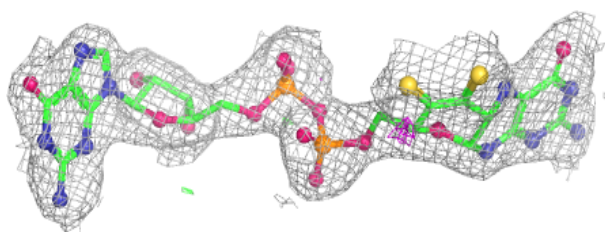
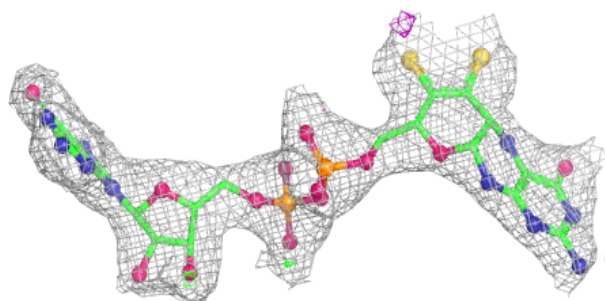
**Electron density around MGD A 4001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MGD F 6001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.