



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:21 pm BST

PDB ID : 2NYA
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 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) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

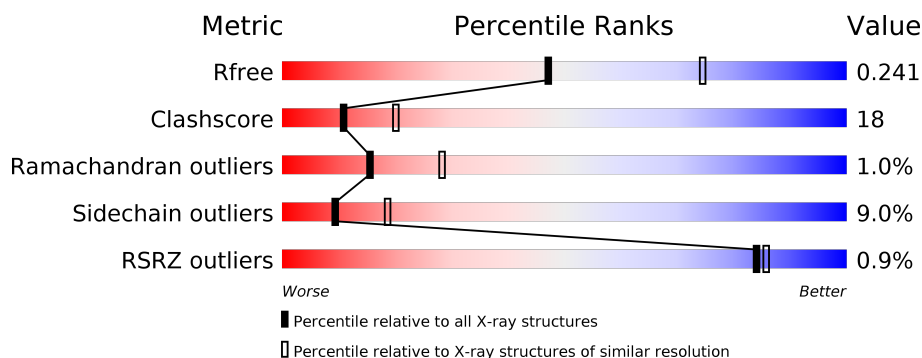
1 Overall quality at a glance ⓘ

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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 $\leq 5\%$. 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	<div> <div></div> <div>68% 27% 5%</div> </div>
1	F	792	<div> <div></div> <div>64% 30% 5%</div> </div>

2 Entry composition [i](#)

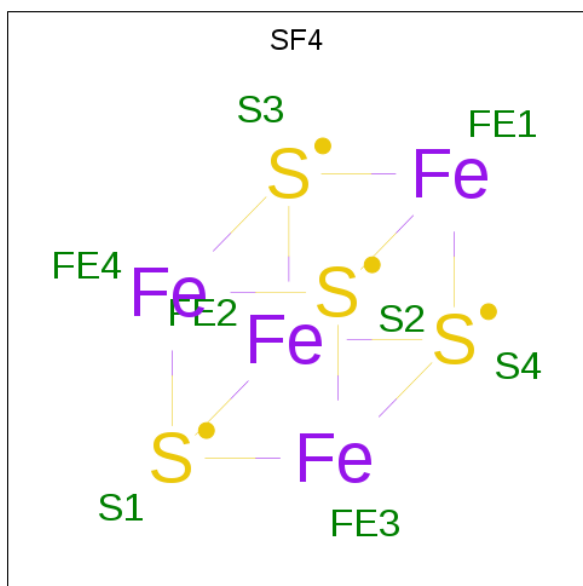
There are 5 unique types of molecules in this entry. The entry contains 13733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: SF4) (formula: Fe₄S₄).

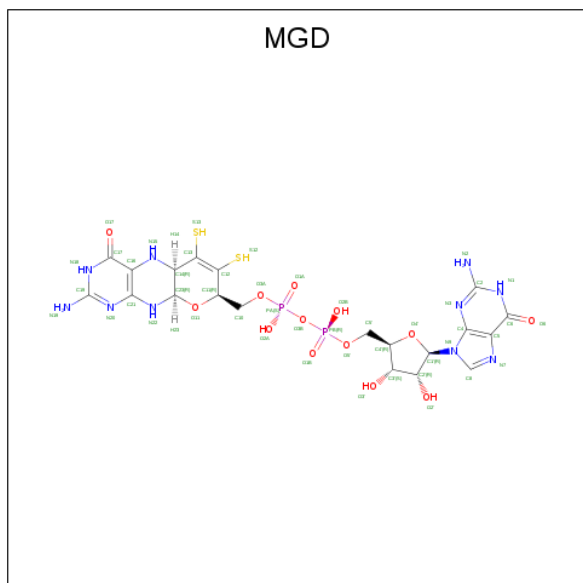


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is MOLYBDENUM(VI) ION (three-letter code: 6MO) (formula: Mo).

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

- 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 (three-letter code: 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

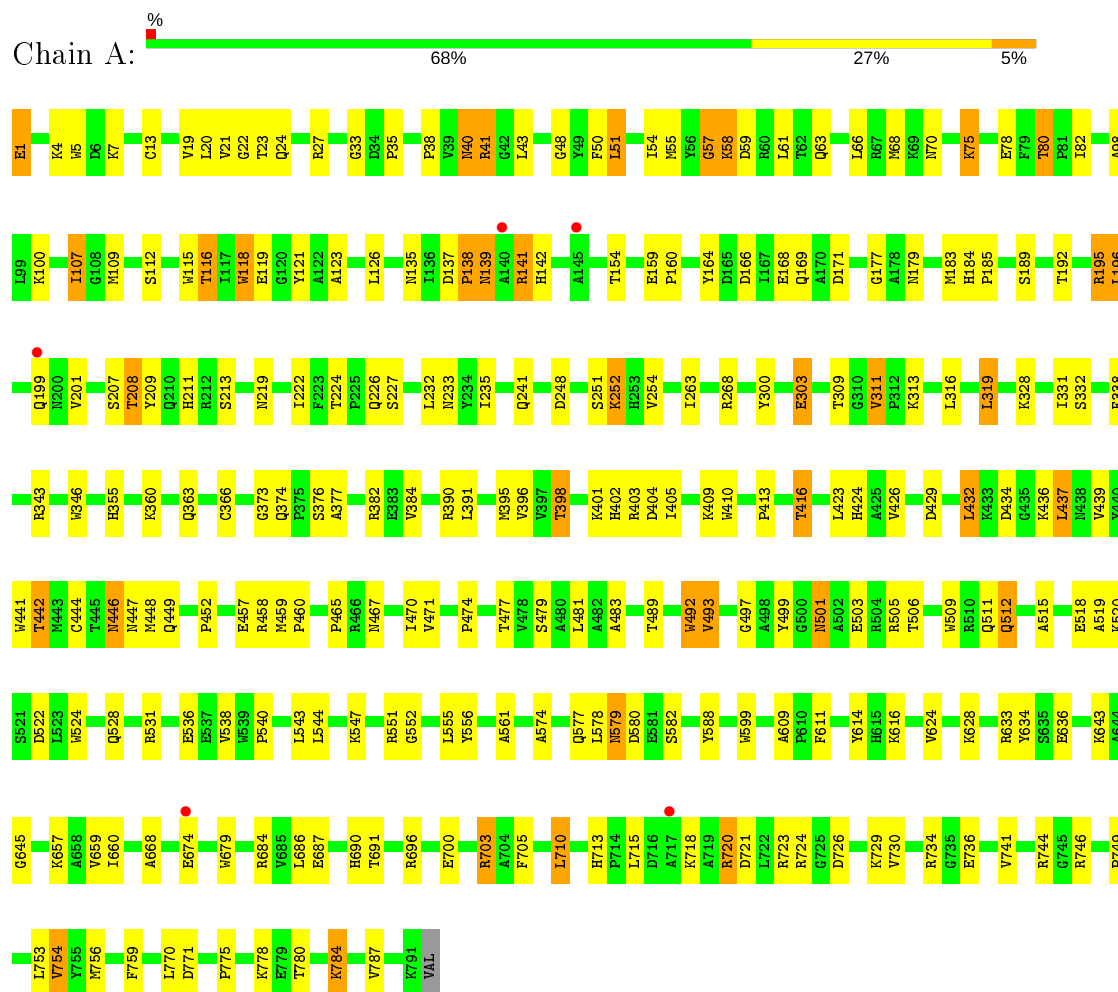
- Molecule 5 is water.

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

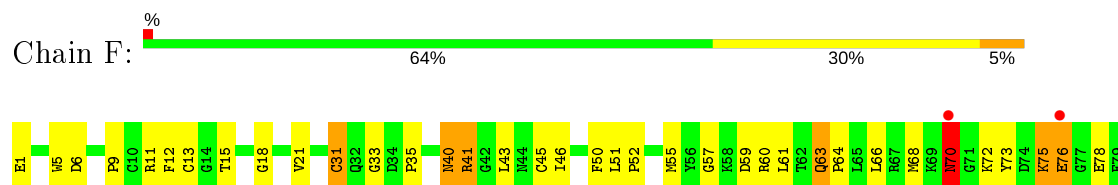
3 Residue-property plots [i](#)

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



T80	L196	K408	A502	H606	V731
E93	S197	K409	E503	Y614	S732
M109	M198	P413	R504	R733	R733
T116	Q199	T416	R505	G619	G735
I117	T202	I421	Q507	L620	I740
W118	V203	G422	F508	R621	V741
E119	L206	L423	W509	K628	N747
G120	S207	H424	R510	Q631	R748
Y121	T208	A427	Q512	D639	P749
A122	Y209	A515	A515		P750
A123	D210	A519	A519	V642	
L126	R211	K432	K520	K643	L753
N135	R212	D434	Q525	A644	V754
Y136	F214	L437	Q528	G652	M755
D137	E215	T442	R531	V659	F759
P138	G337	M443	R532	I660	L764
N139	I216	C444	F533	A668	
A140	I217	T445	V538	D673	L768
R141	D218	N446	W539	E674	T769
H142	N219	N447	L543	R684	L770
C143	I222	P452	L544	R685	P775
V148	T224	E457	R551	L686	E779
T154	F225	N467	T554	H690	T780
F155	S227	V471	Y556	R696	K783
M161	I231	D472	A561	R697	K784
G162	L232	P474	E572	E700	V787
D165	N233	S479	L573	L701	K791
D166	Y234	A483	A574	H702	VAL
I167	I235	D484	Q577	R703	
E168	I240	L485	L578	F705	
Q169	Q241	I486	D580	P706	
A172	I245	T489	E581	V709	
L175	D248	A490	S582	L710	
M179	S251	N491	F587	F711	
M180	K252	W492	Y588	I712	
M183	H253	E494	L589	H713	
H184	L256	K495	Y597	A719	
P185	R268	E496	L598	R720	
I186	G281	G497	Y598	D721	
L187	E291	A500	F600	L722	
R190	T301	G501	G601	R723	
Y191	L302	N501		D726	
T192	E303			V730	
N193	R304				
R194	T305				
R195					

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 49.69 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (50.00-2.50) 97.1 (49.69-2.50)	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 (5.03%)	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 , 44.3	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: 6MO, SF4, 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	0.72	1/6470 (0.0%)	0.80	3/8770 (0.0%)
1	F	0.68	0/6470	0.76	2/8770 (0.0%)
All	All	0.70	1/12940 (0.0%)	0.78	5/17540 (0.0%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	TRP	CB-CG	-5.06	1.41	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	GLY	O-C-N	-5.99	113.12	122.70
1	A	720	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	F	578	LEU	CA-CB-CG	5.20	127.25	115.30
1	F	319	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	720	ARG	NE-CZ-NH2	-5.18	117.71	120.30

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

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	215	0
1	F	6301	0	6155	247	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	15	0
4	F	94	0	44	17	0
5	A	489	0	0	15	0
5	F	436	0	0	29	1
All	All	13733	0	12398	458	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 18.

All (458) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:721:ASP:OD1	1:F:791:LYS:NZ	2.16	0.79
1:F:109:MET:HE1	1:F:123:ALA:HB1	1.63	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: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: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
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: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:690:HIS:HD2	4:A:3001:MGD:O1B	1.74	0.70
1:A:684:ARG:HH12	1:A:690:HIS:HE1	1.35	0.70
1:F:398:THR:CG2	5:F:7221:HOH:O	2.39	0.70
1:A:395:MET:HE2	1:A:402:HIS:HA	1.73	0.70
1:A:403:ARG:HD2	5:A:4367:HOH:O	1.91	0.70
1:A:40:ASN:N	1:A:40:ASN:HD22	1.89	0.70
1:F:703:ARG:O	1:F:705:PHE:N	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:109:MET:HE3	1:A:123:ALA:HB1	1.73	0.68
1:A:224:THR:HG22	1:A:227:SER:HB3	1.76	0.68
1:A:141:ARG:HD3	1:A:424:HIS:HB2	1.76	0.68
1:A:432:LEU:HD13	1:A:437:LEU:HB3	1.74	0.68
1:F:59:ASP:OD1	1:F:59:ASP:N	2.25	0.68
1:A:195:ARG:NH1	1:A:201:VAL:O	2.26	0.68
1:F:109:MET:HE3	1:F:123:ALA:HB1	1.76	0.67
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:109:MET:HE1	1:A:123:ALA:HB1	1.77	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:ND2	1:A:40:ASN:H	1.94	0.66
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:55:MET:CE	1:A:492:TRP:HB3	2.27	0.65
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: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:109:MET:HE1	1:F:123:ALA:CB	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:413:PRO:O	1:A:416:THR:CG2	2.49	0.61
1:A:135:ASN:HD22	1:A:423:LEU:H	1.48	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:248:ASP:OD1	1:F:252:LYS:HE3	2.00	0.60
1:F:76:GLU:HG3	5:F:7235:HOH:O	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:N	1:F:40:ASN:HD22	1.99	0.60
1:F:303:GLU:H	1:F:303:GLU:CD	2.04	0.60
1:F:18:GLY:H	1:F:40:ASN:ND2	1.99	0.60
1:A:224:THR:CG2	1:A:227:SER:HB3	2.31	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: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: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:730:VAL:HG21	1:F:756:MET:HE1	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:343:ARG:HD2	1:A:346:TRP:CE3	2.41	0.56
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:A:501:ASN:C	1:A:501:ASN:HD22	2.09	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:40:ASN:ND2	1:A:40:ASN:N	2.54	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:A:395:MET:CE	1:A:402:HIS:HA	2.36	0.54
1:F:55:MET:HE1	1:F:493:VAL:H	1.73	0.54
1:F:253:HIS:HD2	5:F:7105:HOH:O	1.90	0.54
1:F:40:ASN:HD22	1:F:40:ASN:H	1.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:VAL:HG22	1:A:512:GLN:CG	2.39	0.53
1:A:55:MET:HE3	1:A:492:TRP:HB3	1.91	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: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:A:395:MET:HE1	1:A:405:ILE:CD1	2.38	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:F:268:ARG:NH1	1:F:457:GLU:OE1	2.42	0.53
1:F:55:MET:HE3	1:F:492:TRP:HB3	1.91	0.53
1:A:233:ASN:HB3	1:A:300:TYR:CD2	2.44	0.53
1:A:395:MET:HE1	1:A:405:ILE:HD12	1.91	0.53
1:A:528:GLN:O	1:A:531:ARG:HG2	2.09	0.52
1:A:98:ALA:HB3	1:A:107:ILE:CD1	2.38	0.52
1:F:55:MET:CE	1:F:493:VAL:H	2.21	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: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:A:208:THR:HG23	1:A:753:LEU:CD1	2.40	0.52
1:F:40:ASN:ND2	1:F:40:ASN:H	2.08	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: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:70:ASN:O	1:F:72:LYS:HG2	2.10	0.52
1:A:7:LYS:O	5:A:4013:HOH:O	2.19	0.51
1:A:409:LYS:HG3	1:A:599:TRP:CE3	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLU:H	1:A:303:GLU:CD	2.14	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:HG	1:F:216:LEU:O	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:395:MET:HE2	1:F:405:ILE:HD12	1.93	0.51
1:F:503:GLU:O	1:F:504:ARG:HB2	2.10	0.50
1:A:68:MET:HE1	1:A:82:ILE:HG22	1.94	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
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:O	1:A:442:THR:HG22	2.10	0.50
1:A:390:ARG:NH1	1:A:391:LEU:O	2.44	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:ND2	1:F:40:ASN:N	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:474:PRO:HD2	4:A:3001:MGD:H1'	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: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:F:501:ASN:C	1:F:501:ASN:HD22	2.16	0.49
1:A:556:TYR:CE2	1:A:561:ALA:HB2	2.47	0.49
1:F:227:SER:HB2	1:F:309:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:HIS:CE1	1:F:447:ASN:HD21	2.25	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: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: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:A:684:ARG:NE	4:A:4001:MGD:H102	2.29	0.48
1:A:501:ASN:ND2	1:A:501:ASN:C	2.66	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: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:F:702:HIS:C	1:F:703:ARG:O	2.50	0.47
1:A:171:ASP:O	1:A:201:VAL:HA	2.13	0.47
1:A:579:ASN:C	1:A:579:ASN:HD22	2.17	0.47
1:A:628:LYS:HD2	5:A:4426:HOH:O	2.14	0.47
1:F:172:ALA:HA	1:F:202:THR:O	2.15	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: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:448:MET:HE1	1:A:458:ARG:HG2	1.97	0.47
1:A:471:VAL:HG13	1:A:483:ALA:HB2	1.95	0.47
1:A:730:VAL:HG21	1:A:756:MET:HE1	1.96	0.47
1:F:684:ARG:NE	4:F:7001:MGD:H102	2.30	0.47
1:A:75:LYS:HG3	1:A:465:PRO:HA	1.96	0.47
1:F:709:VAL:HG12	1:F:740:ILE:HB	1.97	0.47
1:A:268:ARG:NH2	1:A:434:ASP:OD1	2.48	0.47
1:A:59:ASP:OD1	1:A:59:ASP:N	2.42	0.47
1:F:493:VAL:HG22	1:F:512:GLN:HG2	1.97	0.47
1:F:723:ARG:HG3	1:F:726:ASP:CG	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:GLU:OE2	1:A:746:ARG:NH1	2.44	0.47
1:A:723:ARG:O	1:A:724:ARG:C	2.53	0.47
1:F:396:VAL:CG2	1:F:398:THR:HG22	2.44	0.47
1:F:579:ASN:CG	1:F:582:SER:HB2	2.35	0.47
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: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
1:F:442:THR:CG2	1:F:471:VAL:HB	2.46	0.46
1:F:442:THR:HG22	1:F:471:VAL:HB	1.97	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:497:GLY:HA3	1:A:509:TRP:CZ2	2.51	0.45
1:F:155:PHE:O	1:F:652:GLY:HA3	2.16	0.45
1:A:20:LEU:HD12	1:F:196:LEU:HG	1.98	0.45
1:F:33:GLY:O	1:F:35:PRO:HD3	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:336:MET:HG3	1:F:340:GLN:NE2	2.31	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: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: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: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:75:LYS:NZ	1:A:467:ASN:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:20:LEU:CD1	1:F:196:LEU:HG	2.48	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
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:F:68:MET:HB2	1:F:80:THR:HG21	1.99	0.44
1:A:139:ASN:HB3	1:A:374:GLN:HE22	1.83	0.44
1:A:41:ARG:CG	1:A:41:ARG:O	2.66	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:226:GLN:CD	5:F:7032:HOH:O	2.56	0.44
1:F:485:LEU:HG	1:F:487:LEU:HD21	2.00	0.44
1:F:121:TYR:CE2	1:F:597:TYR:HB2	2.52	0.44
1:F:759:PHE:CD2	1:F:759:PHE:C	2.91	0.44
1:A:107:ILE:HG13	1:A:439:VAL:HB	2.01	0.43
1:A:55:MET:HE3	1:A:493:VAL:H	1.82	0.43
1:F:301:THR:HB	1:F:303:GLU:OE1	2.18	0.43
1:F:148:VAL:HG22	1:F:382:ARG:HE	1.83	0.43
1:F:46:ILE:HD12	1:F:46:ILE:HA	1.91	0.43
1:F:784:LYS:HB2	1:F:784:LYS:HE3	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:231:ILE:HG13	1:F:309:THR:HG21	2.00	0.43
1:F:183:MET:SD	1:F:684:ARG:HB2	2.59	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:353:ASN:CG	1:F:660:ILE:HG23	2.40	0.43
1:F:501:ASN:ND2	1:F:501:ASN:C	2.73	0.43
1:A:544:LEU:HD13	1:A:551:ARG:HG2	2.01	0.42
1:F:684:ARG:HH22	4:F:6001:MGD:C13	2.32	0.42
1:F:281:GLY:HA2	1:F:775:PRO:HB2	2.00	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:A:199:GLN:H	1:A:199:GLN:HG2	1.62	0.42
1:A:710:LEU:HD12	1:A:756:MET:HE1	2.02	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: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:268:ARG:HH22	1:F:434:ASP:CG	2.22	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:A:636:GLU:CD	1:A:645:GLY:H	2.22	0.41
1:F:446:ASN:HD22	1:F:479:SER:HB2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLU:HA	1:A:160:PRO:HD3	1.90	0.41
1:A:41:ARG:CB	5:A:4458:HOH:O	2.68	0.41
1:A:442:THR:CG2	5:A:4114:HOH:O	2.68	0.41
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: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: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:207:SER:OG	1:A:209:TYR:O	2.35	0.41
1:A:684:ARG:HH22	4:A:3001:MGD:H15	1.67	0.41
1:A:121:TYR:CA	1:A:384:VAL:HG11	2.51	0.41
1:A:505:ARG:NH2	5:A:4116:HOH:O	2.36	0.41
1:F:711:PHE:CD1	1:F:747:ASN:HB2	2.56	0.41
1:A:177:GLY:O	4:A:4001:MGD:O3'	2.32	0.41
1:A:436:LYS:HB3	1:A:436:LYS:HE2	1.95	0.41
1:A:142:HIS:CE1	1:A:447:ASN:HD21	2.34	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:121:TYR:HH	1:A:410:TRP:HE1	1.68	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:207:SER:O	1:A:222:ILE:HA	2.21	0.40
1:F:314:ASP:HB3	1:F:315:GLN:H	1.57	0.40
1:F:41:ARG:O	1:F:41:ARG:CG	2.69	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:A:55:MET:HE2	1:A:492:TRP:HB3	1.99	0.40
1:F:710:LEU:HG	1:F:754:VAL:CG2	2.51	0.40
1:F:442:THR:HG22	1:F:471:VAL:CG1	2.51	0.40
1:F:59:ASP:O	1:F:60:ARG:C	2.59	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%)	19	35
1	F	789/792 (100%)	725 (92%)	55 (7%)	9 (1%)	14	26
All	All	1578/1584 (100%)	1461 (93%)	102 (6%)	15 (1%)	15	28

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%)	600 (91%)	61 (9%)	9	18
1	F	661/663 (100%)	603 (91%)	58 (9%)	10	19
All	All	1322/1326 (100%)	1203 (91%)	119 (9%)	9	19

All (119) 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	179	ASN
1	A	189	SER
1	A	195	ARG
1	A	196	LEU
1	A	208	THR
1	A	219	ASN
1	A	241	GLN
1	A	251	SER
1	A	252	LYS
1	A	303	GLU
1	A	311	VAL

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Mol	Chain	Res	Type
1	A	313	LYS
1	A	319	LEU
1	A	398	THR
1	A	401	LYS
1	A	404	ASP
1	A	416	THR
1	A	432	LEU
1	A	437	LEU
1	A	442	THR
1	A	446	ASN
1	A	493	VAL
1	A	501	ASN
1	A	512	GLN
1	A	518	GLU
1	A	522	ASP
1	A	578	LEU
1	A	579	ASN
1	A	588	TYR
1	A	616	LYS
1	A	643	LYS
1	A	674	GLU
1	A	686	LEU
1	A	703	ARG
1	A	705	PHE
1	A	710	LEU
1	A	718	LYS
1	A	721	ASP
1	A	754	VAL
1	A	784	LYS
1	A	787	VAL
1	F	1	GLU
1	F	13	CYS
1	F	31	CYS
1	F	40	ASN
1	F	41	ARG
1	F	45	CYS
1	F	51	LEU
1	F	61	LEU
1	F	63	GLN
1	F	70	ASN
1	F	75	LYS
1	F	76	GLU

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Mol	Chain	Res	Type
1	F	80	THR
1	F	93	GLU
1	F	116	THR
1	F	118	TRP
1	F	126	LEU
1	F	161	MET
1	F	168	GLU
1	F	169	GLN
1	F	179	ASN
1	F	195	ARG
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	219	ASN
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	376	SER
1	F	398	THR
1	F	401	LYS
1	F	404	ASP
1	F	416	THR
1	F	432	LEU
1	F	437	LEU
1	F	442	THR
1	F	446	ASN
1	F	471	VAL
1	F	493	VAL
1	F	501	ASN
1	F	505	ARG
1	F	578	LEU
1	F	579	ASN
1	F	588	TYR
1	F	643	LYS
1	F	685	VAL
1	F	686	LEU

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Mol	Chain	Res	Type
1	F	703	ARG
1	F	705	PHE
1	F	720	ARG
1	F	787	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	135	ASN
1	A	139	ASN
1	A	142	HIS
1	A	179	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	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
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	253	HIS

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Mol	Chain	Res	Type
1	F	355	HIS
1	F	402	HIS
1	F	411	ASN
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	606	HIS
1	F	690	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	F	7001	3	41,52,52	1.54	3 (7%)	43,81,81	2.25	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SF4	A	2001	1	0,12,12	0.00	-	-		
2	SF4	F	5001	1	0,12,12	0.00	-	-		
4	MGD	A	3001	3	41,52,52	1.50	6 (14%)	43,81,81	2.57	17 (39%)
4	MGD	A	4001	3	41,52,52	1.40	4 (9%)	43,81,81	2.36	14 (32%)
4	MGD	F	6001	3	41,52,52	1.55	6 (14%)	43,81,81	2.58	18 (41%)

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	F	7001	3	-	6/18/66/66	0/6/6/6
2	SF4	A	2001	1	-	-	0/6/5/5
2	SF4	F	5001	1	-	-	0/6/5/5
4	MGD	A	3001	3	-	6/18/66/66	0/6/6/6
4	MGD	A	4001	3	-	6/18/66/66	0/6/6/6
4	MGD	F	6001	3	-	4/18/66/66	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	7001	MGD	C17-C16	6.24	1.50	1.41
4	A	3001	MGD	C17-C16	5.63	1.49	1.41
4	A	4001	MGD	C17-C16	5.21	1.48	1.41
4	F	6001	MGD	C17-C16	4.91	1.48	1.41
4	A	3001	MGD	C6-C5	4.57	1.49	1.41
4	A	4001	MGD	C6-C5	4.14	1.48	1.41
4	F	6001	MGD	C6-C5	4.00	1.48	1.41
4	F	7001	MGD	C6-C5	3.58	1.47	1.41
4	A	4001	MGD	C16-C21	3.57	1.48	1.41
4	F	7001	MGD	C16-C21	3.57	1.48	1.41
4	F	6001	MGD	C16-C21	3.05	1.47	1.41
4	A	3001	MGD	C16-C21	2.80	1.46	1.41
4	F	6001	MGD	O4'-C1'	2.65	1.44	1.41
4	A	3001	MGD	C5-C4	2.50	1.47	1.40
4	A	4001	MGD	C5-C4	2.34	1.47	1.40
4	F	6001	MGD	C6-N1	2.29	1.37	1.33
4	A	3001	MGD	O4'-C1'	2.24	1.44	1.41
4	A	3001	MGD	C2'-C1'	-2.11	1.50	1.53
4	F	6001	MGD	C2'-C1'	-2.03	1.50	1.53

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4001	MGD	C17-C16-N15	6.89	124.91	119.12
4	A	3001	MGD	C17-C16-N15	6.20	124.33	119.12
4	F	7001	MGD	C2-N3-C4	5.76	121.93	115.36
4	F	6001	MGD	O11-C23-C14	-5.40	105.36	108.96
4	F	7001	MGD	C17-C16-N15	5.30	123.57	119.12
4	A	4001	MGD	C2-N3-C4	5.20	121.30	115.36
4	F	7001	MGD	C6-C5-C4	-5.09	115.94	120.80
4	A	3001	MGD	C6-N1-C2	4.93	123.76	115.93
4	F	6001	MGD	C17-C16-N15	4.83	123.17	119.12
4	A	3001	MGD	C5-C6-N1	-4.79	116.88	123.43
4	F	7001	MGD	N3-C2-N1	-4.73	120.91	127.22
4	F	6001	MGD	O11-C23-N22	-4.72	103.72	108.57
4	A	3001	MGD	C2-N3-C4	4.71	120.73	115.36
4	F	6001	MGD	C5-C6-N1	-4.65	117.08	123.43
4	A	4001	MGD	C17-N18-C19	4.61	123.25	115.93
4	A	4001	MGD	C6-C5-C4	-4.51	116.49	120.80
4	F	6001	MGD	C2-N3-C4	4.47	120.46	115.36
4	A	3001	MGD	C6-C5-C4	-4.45	116.55	120.80
4	F	6001	MGD	C1'-N9-C4	-4.20	119.27	126.64
4	F	6001	MGD	C6-C5-C4	-4.14	116.84	120.80
4	F	6001	MGD	C6-N1-C2	4.14	122.50	115.93
4	A	4001	MGD	C6-N1-C2	4.09	122.43	115.93
4	F	7001	MGD	C6-N1-C2	3.96	122.22	115.93
4	F	6001	MGD	C17-C16-C21	3.92	118.05	114.57
4	A	3001	MGD	C1'-N9-C4	-3.87	119.85	126.64
4	A	3001	MGD	N3-C2-N1	-3.81	122.14	127.22
4	F	6001	MGD	N3-C2-N1	-3.80	122.15	127.22
4	A	3001	MGD	C4-C5-N7	-3.79	105.45	109.40
4	A	4001	MGD	C5-C6-N1	-3.75	118.31	123.43
4	A	3001	MGD	C19-N20-C21	3.74	122.92	114.54
4	F	7001	MGD	C19-N20-C21	3.55	122.49	114.54
4	A	4001	MGD	N3-C2-N1	-3.54	122.50	127.22
4	A	3001	MGD	C17-C16-C21	3.48	117.66	114.57
4	F	6001	MGD	N2-C2-N1	3.42	122.57	117.25
4	A	3001	MGD	O4'-C1'-C2'	-3.37	102.00	106.93
4	F	6001	MGD	C17-N18-C19	3.28	121.14	115.93
4	F	6001	MGD	C4-C5-N7	-3.14	106.13	109.40
4	F	7001	MGD	C17-N18-C19	3.10	120.85	115.93
4	A	3001	MGD	C17-N18-C19	3.07	120.81	115.93
4	A	3001	MGD	C16-C21-N22	3.02	120.90	118.13
4	F	7001	MGD	C17-C16-C21	3.00	117.23	114.57
4	A	4001	MGD	C19-N20-C21	2.98	121.22	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3001	MGD	PA-O3B-PB	-2.91	122.85	132.83
4	A	4001	MGD	C21-N22-C23	-2.89	118.01	123.67
4	F	6001	MGD	C19-N20-C21	2.87	120.96	114.54
4	A	4001	MGD	N19-C19-N20	2.84	121.67	117.25
4	A	4001	MGD	C4-C5-N7	-2.78	106.50	109.40
4	F	7001	MGD	C5-C6-N1	-2.77	119.64	123.43
4	F	6001	MGD	O4'-C1'-C2'	-2.77	102.88	106.93
4	F	7001	MGD	O4'-C1'-C2'	-2.77	102.88	106.93
4	F	7001	MGD	O11-C23-N22	-2.54	105.96	108.57
4	A	3001	MGD	N19-C19-N18	2.50	121.15	117.25
4	A	4001	MGD	N18-C19-N20	-2.27	121.86	125.42
4	F	6001	MGD	PA-O3B-PB	-2.20	125.27	132.83
4	A	4001	MGD	O3'-C3'-C2'	-2.16	104.85	111.82
4	F	6001	MGD	N19-C19-N18	2.12	120.55	117.25
4	F	6001	MGD	O2A-PA-O1A	2.09	122.56	112.24
4	A	4001	MGD	O4'-C1'-C2'	-2.08	103.89	106.93
4	A	3001	MGD	O4'-C4'-C5'	2.06	116.14	109.37
4	A	3001	MGD	N2-C2-N1	2.04	120.42	117.25

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	7001	MGD	C5'-O5'-PB-O2B
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	F	6001	MGD	C5'-O5'-PB-O2B
4	F	6001	MGD	C5'-O5'-PB-O3B
4	A	4001	MGD	C3'-C4'-C5'-O5'
4	F	6001	MGD	PA-O3B-PB-O5'
4	F	7001	MGD	C5'-O5'-PB-O3B
4	A	3001	MGD	C10-O3A-PA-O3B
4	A	4001	MGD	C5'-O5'-PB-O3B
4	F	7001	MGD	PB-O3B-PA-O1A
4	F	7001	MGD	C5'-O5'-PB-O1B
4	A	4001	MGD	O4'-C4'-C5'-O5'
4	A	3001	MGD	O4'-C4'-C5'-O5'
4	F	6001	MGD	O4'-C4'-C5'-O5'
4	A	4001	MGD	PB-O3B-PA-O1A

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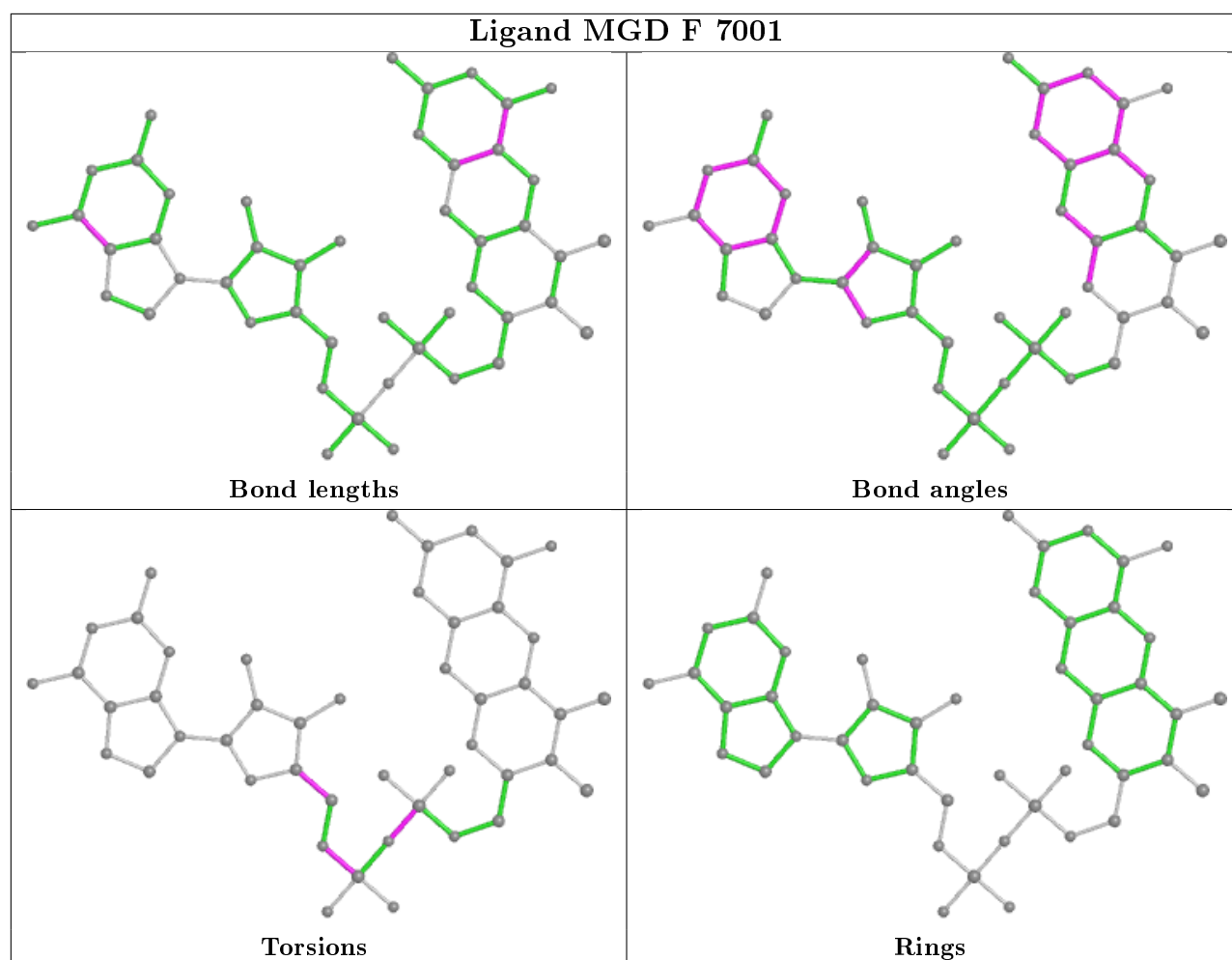
Mol	Chain	Res	Type	Atoms
4	F	7001	MGD	C3'-C4'-C5'-O5'
4	F	7001	MGD	PB-O3B-PA-O2A
4	A	3001	MGD	C10-O3A-PA-O1A

There are no ring outliers.

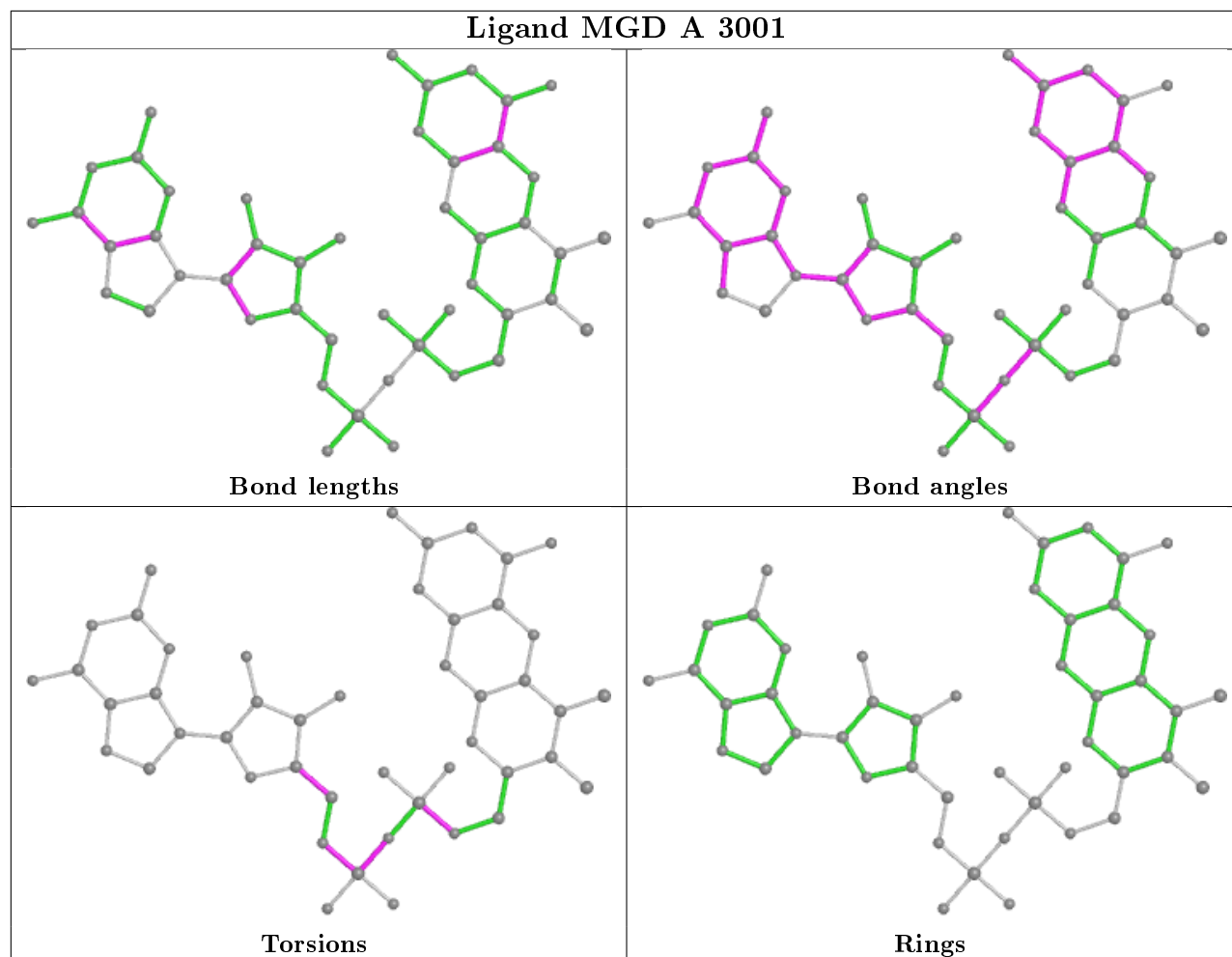
4 monomers are involved in 32 short contacts:

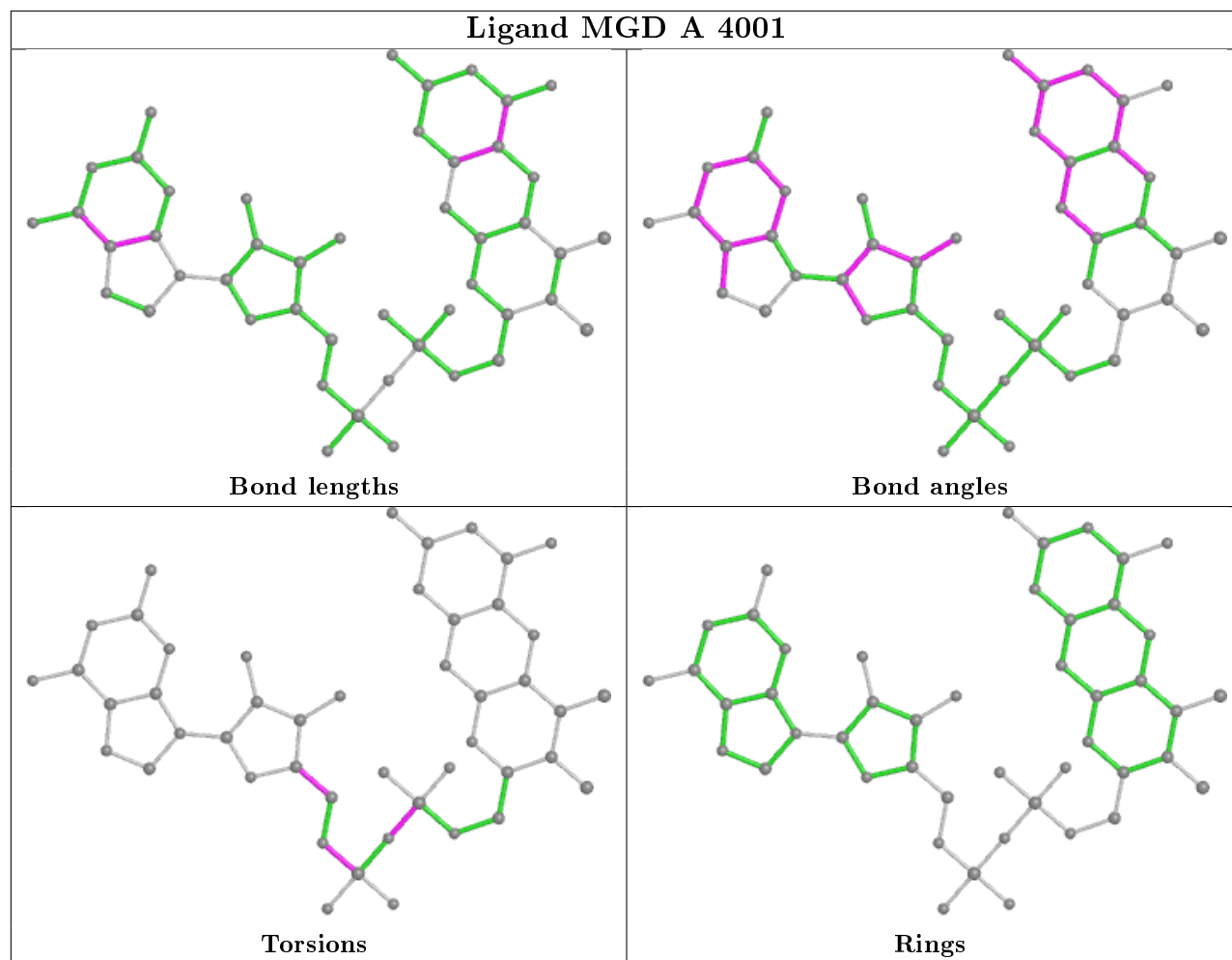
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	7001	MGD	8	0
4	A	3001	MGD	7	0
4	A	4001	MGD	8	0
4	F	6001	MGD	9	0

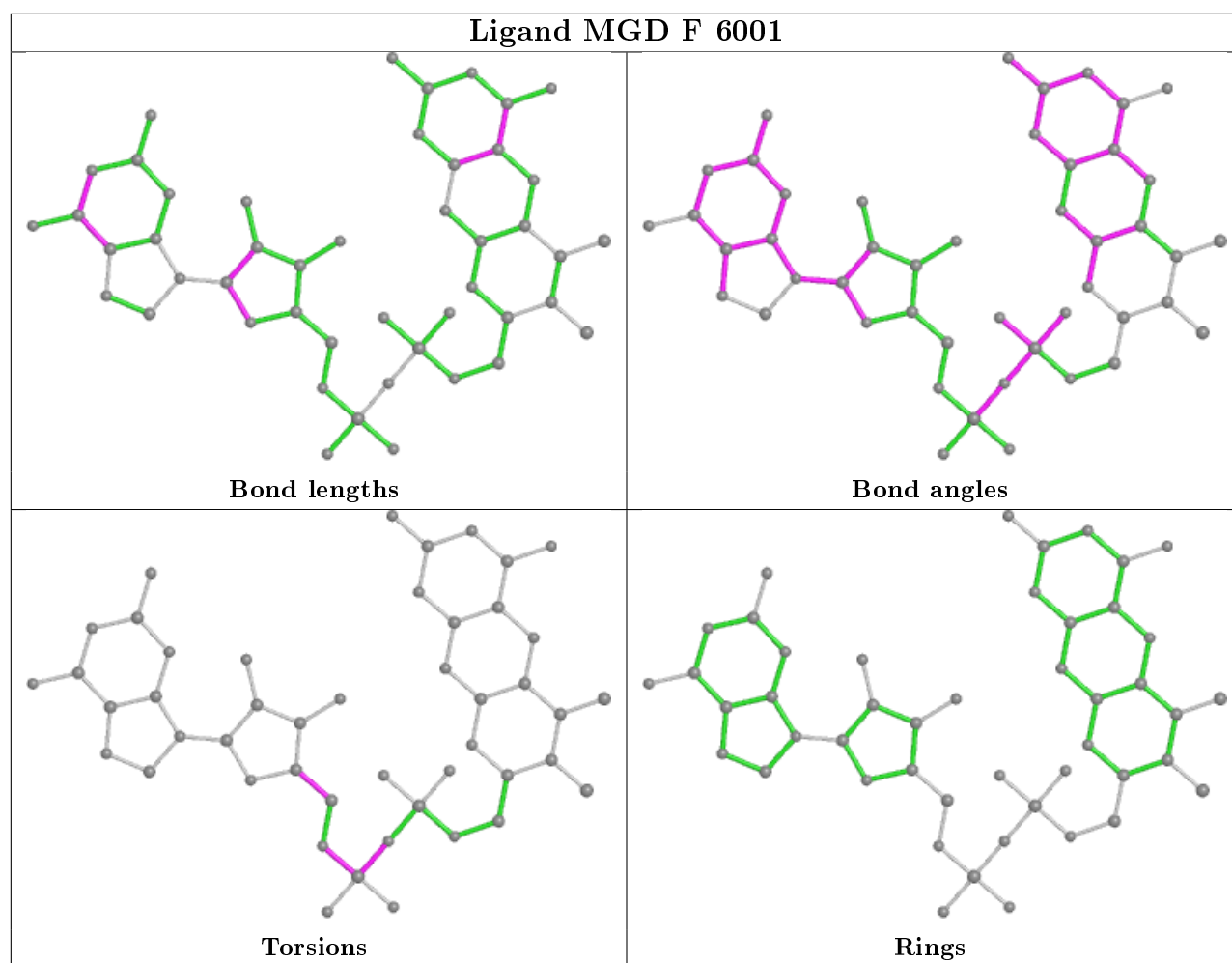
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand MGD A 3001







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%)	-0.19	5 (0%) 89 90	13, 24, 37, 46	0
1	F	791/792 (99%)	0.00	9 (1%) 80 82	17, 30, 45, 55	0
All	All	1582/1584 (99%)	-0.09	14 (0%) 84 86	13, 27, 42, 55	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	723	ARG	3.7
1	F	140	ALA	3.6
1	A	717	ALA	3.1
1	F	76	GLU	2.7
1	F	644	ALA	2.6
1	F	70	ASN	2.4
1	F	199	GLN	2.4
1	F	314	ASP	2.4
1	A	674	GLU	2.3
1	F	722	LEU	2.3
1	A	145	ALA	2.2
1	A	199	GLN	2.2
1	F	291	GLU	2.1
1	A	140	ALA	2.0

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](#)

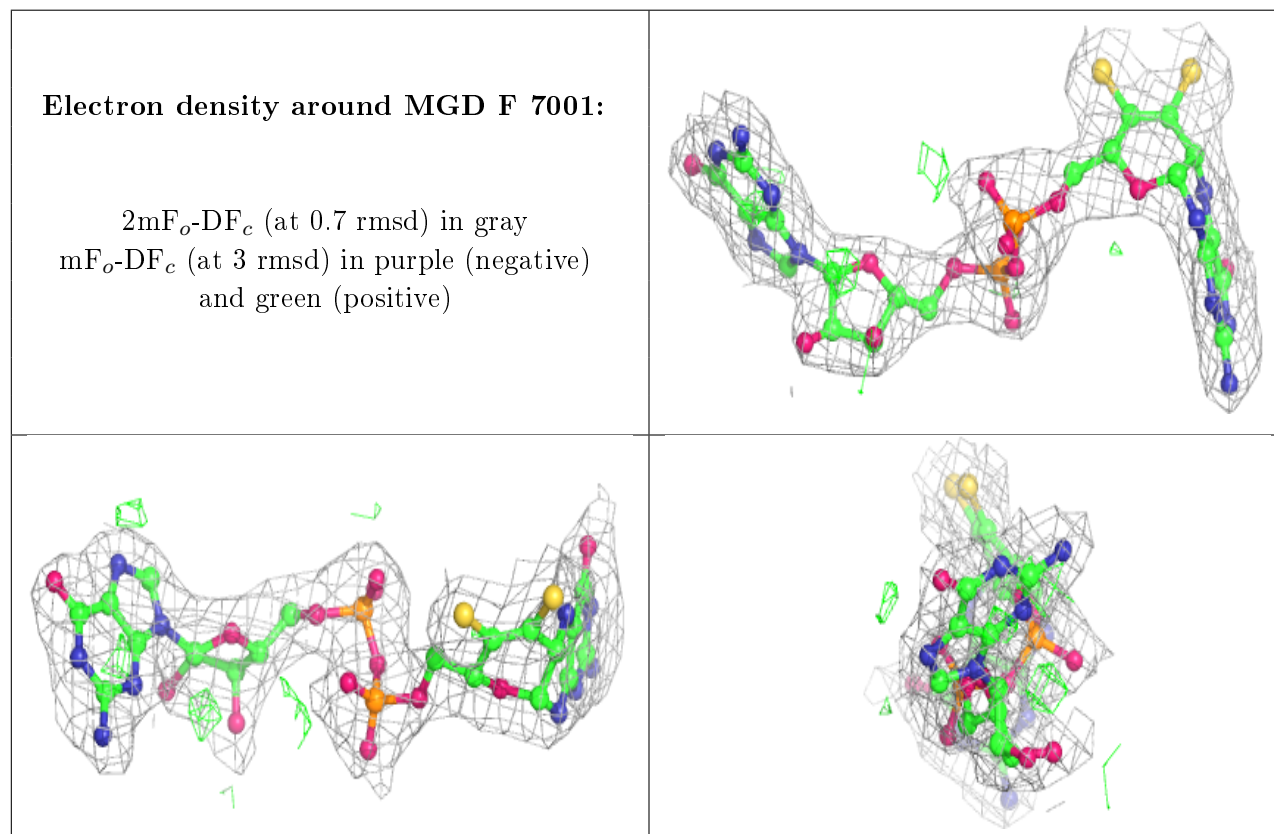
There are no carbohydrates in this entry.

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.

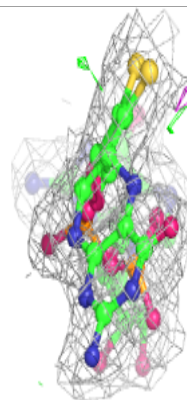
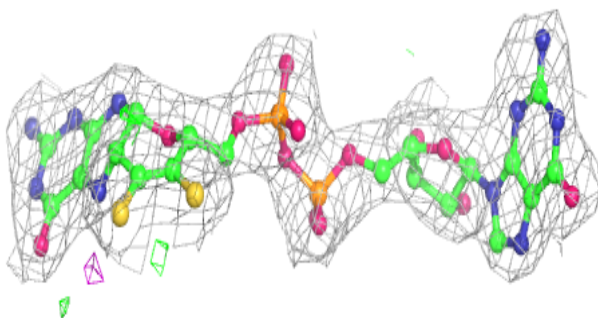
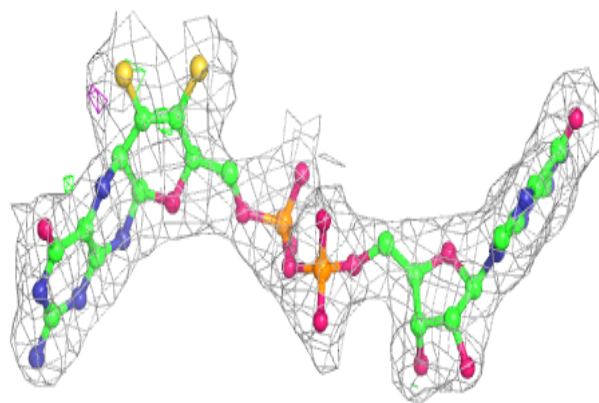
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MGD	F	7001	47/47	0.97	0.15	18,22,27,31	0
2	SF4	F	5001	8/8	0.97	0.06	25,26,29,30	0
4	MGD	A	3001	47/47	0.98	0.15	11,16,17,20	0
4	MGD	A	4001	47/47	0.98	0.17	13,21,26,30	0
4	MGD	F	6001	47/47	0.98	0.15	15,19,21,22	0
2	SF4	A	2001	8/8	0.99	0.06	24,26,28,28	0
3	6MO	F	5002	1/1	1.00	0.10	24,24,24,24	0
3	6MO	A	2002	1/1	1.00	0.12	20,20,20,20	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.

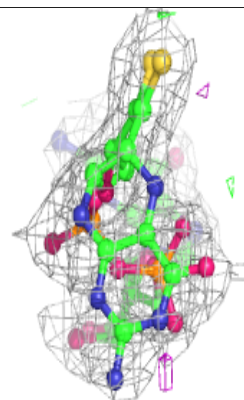
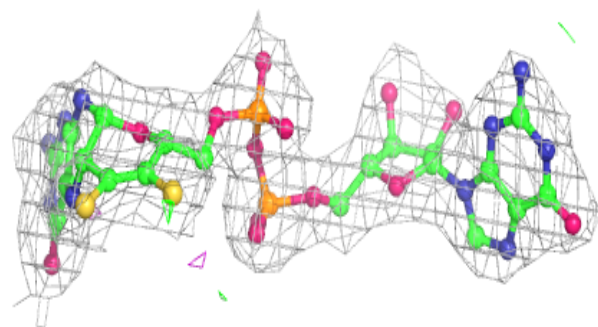
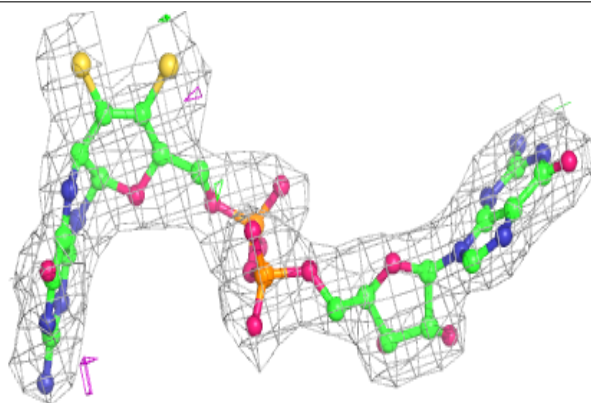


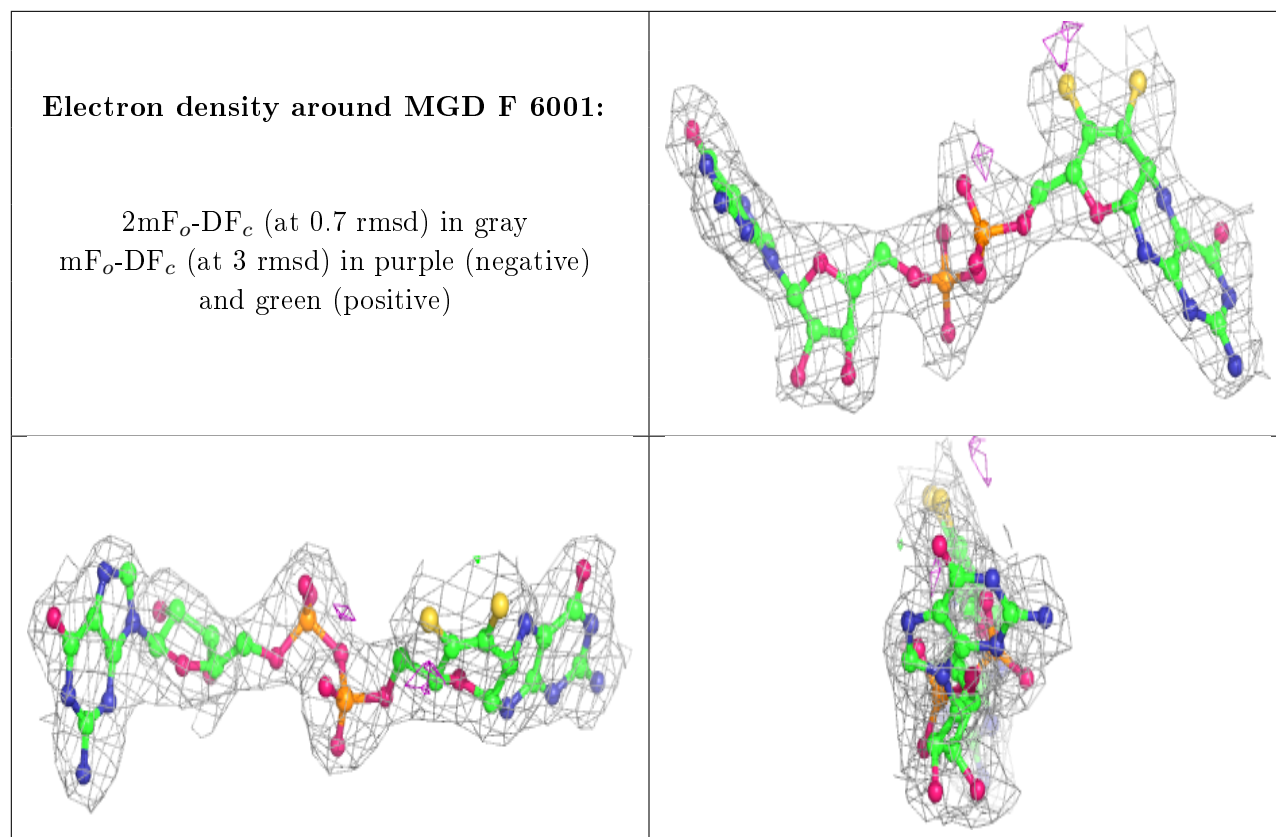
Electron density around MGD A 3001:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.