Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 08:06 AM EDT

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 (i) 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 (i)) were used in the production of this report:

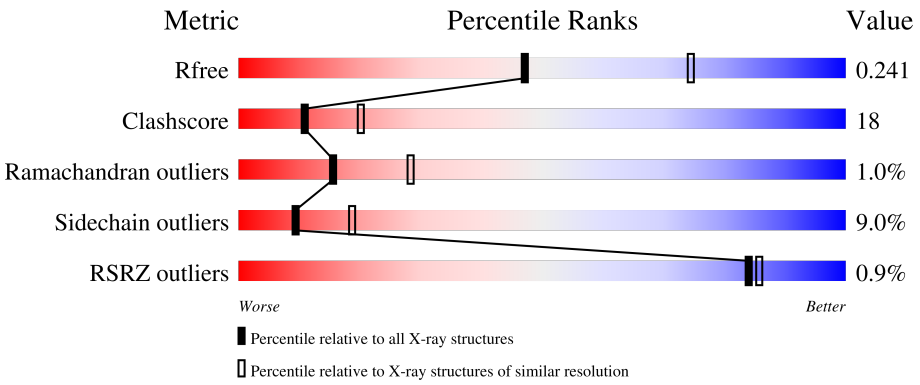
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

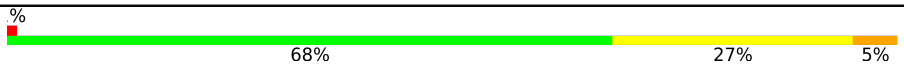
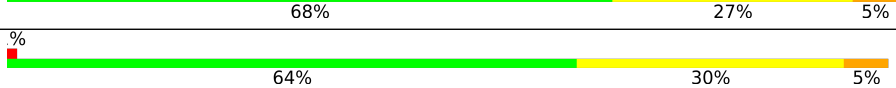
The reported resolution of this entry is 2.50 Å.

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 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 <=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	
1	F	792	

2 Entry composition (i)

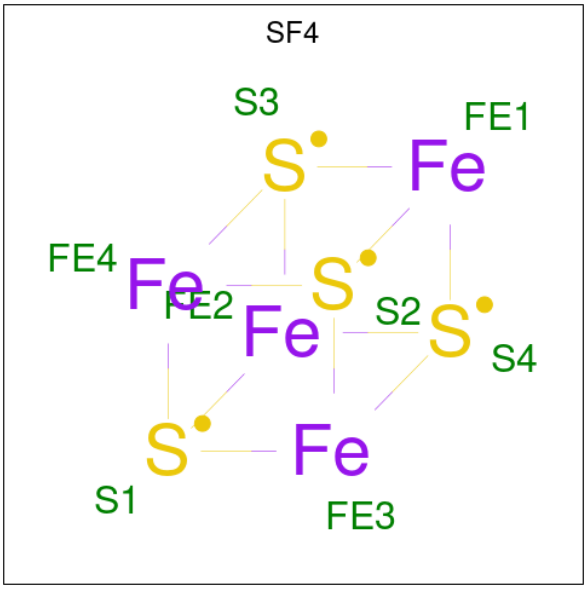
There are 5 unique types of molecules in this entry. The entry contains 13733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	791	6301	4012	1100	1157	32	0	0	0
1	F	791	6301	4012	1100	1157	32	0	0	0

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

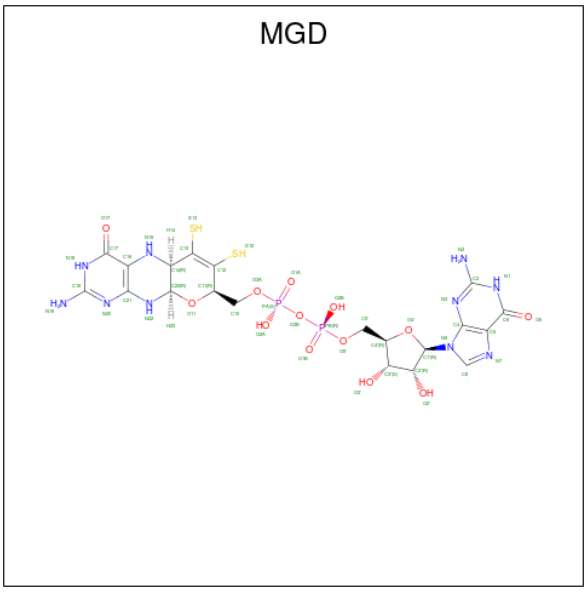


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	8	4	4	0	0
2	F	1	8	4	4	0	0

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

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

- Molecule 5 is water.

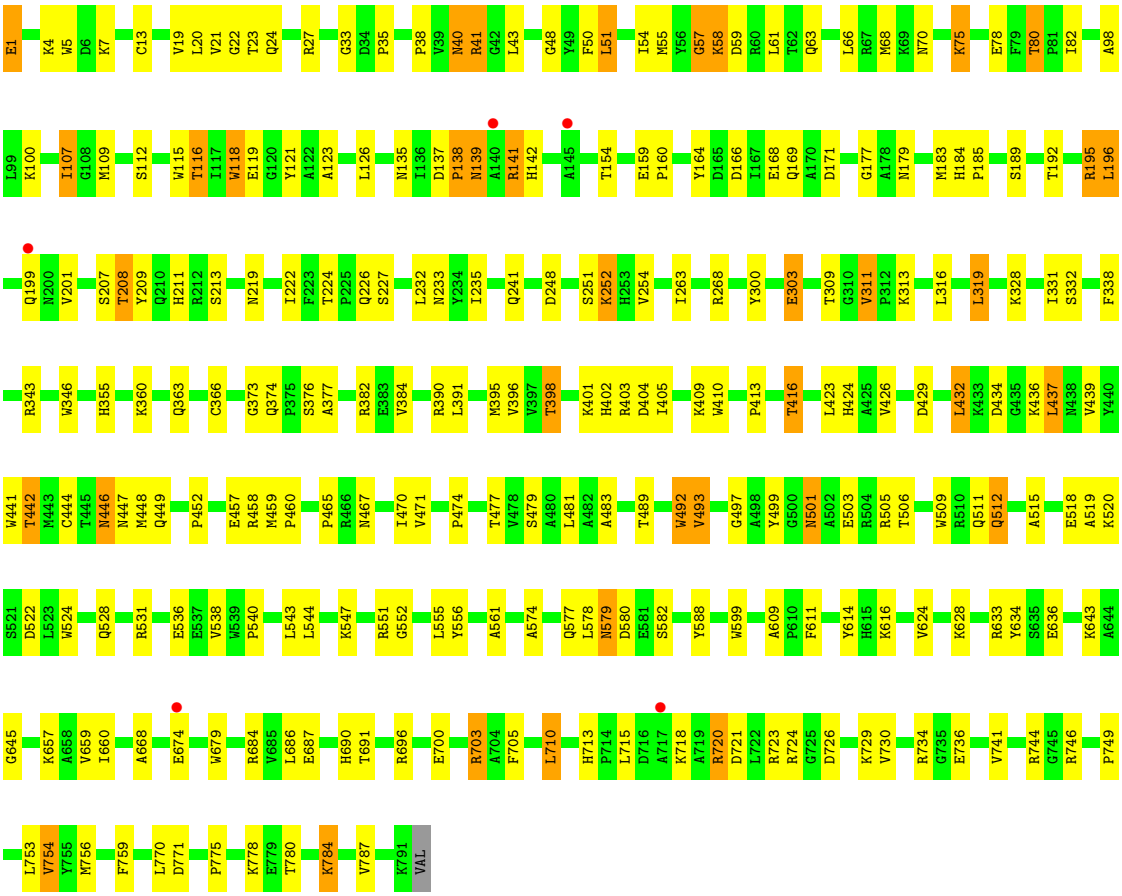
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	489	489	489	0	0
			Total	O		
5	F	436	436	436	0	0

3 Residue-property plots (i)

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

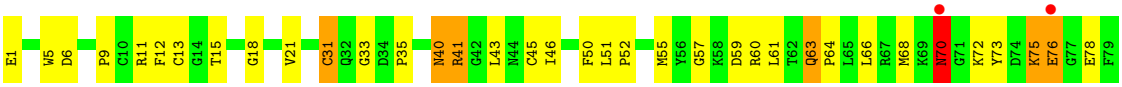
• Molecule 1: Periplasmic nitrate reductase

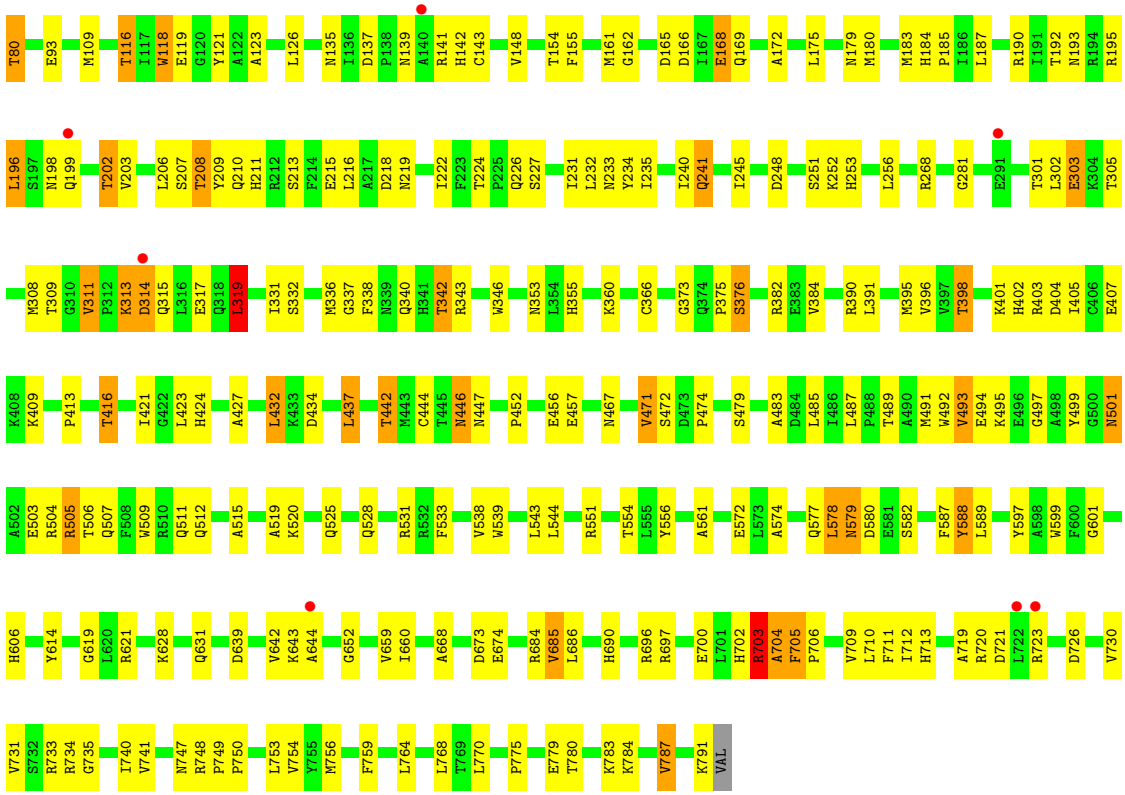
Chain A:



• Molecule 1: Periplasmic nitrate reductase

Chain F:




T80 E93 M109 T116 I117 W118 E119 G120 Y121 A122 A123 L126 N135 I136 D137 P138 N139 A140 R141 H142 C143 V148 T154 F155 M161 G162 D165 D166 I167 E168 Q169 A172 L175 N179 M180 M183 H184 P185 I186 L187 R190 I191 T192 N193 R194 R195
L196 S197 N198 Q199 T202 V203 L206 S207 T208 Y209 Q210 H211 R212 S213 F214 E215 L216 A217 D218 N219 I222 F223 T224 P225 Q226 S227 I231 L232 N233 Y234 I235 I240 Q241 I245 D248 S251 K252 H253 L256 R268 G281 E291 T301 L302 E303 K304 T305
M308 T309 G310 V311 P312 K313 D314 Q315 L316 E317 Q318 L319 I331 S332 M336 G337 F338 M339 Q340 H341 T342 R343 W346 N353 L354 H355 K360 C366 G373 Q374 P375 S376 R382 E383 V384 R390 L391 M396 V396 V397 T398 K401 H402 R403 D404 I405 C406 E407
K408 K409 P413 T416 I421 G422 L423 H424 A427 L432 K433 D434 L437 T442 M443 C444 T445 N446 N447 P452 E456 E457 N467 V471 S472 D473 P474 S479 A483 D484 L485 I486 L487 P488 T489 A490 M491 W492 V493 E494 K495 E496 G497 A498 Y499 G500 N501
A502 E503 R504 R505 T506 Q507 F508 W509 R510 Q511 Q512 A515 A519 K520 Q525 Q528 R531 R532 F533 V538 W539 L543 L544 R551 T554 L555 Y556 A561 E572 L573 A574 Q577 L578 N579 D580 E581 S582 F587 Y588 L589 Y597 A598 W599 F600 G601
H606 Y614 G619 L620 R621 K628 Q631 D639 V642 K643 A644 G652 V659 I660 A668 D673 E674 R684 V685 L686 H690 R696 R697 E700 L701 H702 R703 A704 F705 P706 V709 L710 F711 I712 H713 A719 R720 D721 L722 R723 D726 V730
V731 S732 R733 R734 G735 I740 V741 N747 R748 P749 P750 L753 V754 Y755 W756 F759 L764 L768 T769 L770 P775 E779 T780 K783 K784 V787 K791 VAL

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.72	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(^{o})	Ideal(^{o})
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 (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	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: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: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: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: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: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:H	1:A:40:ASN:ND2	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: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
1:F:303:GLU:CD	1:F:303:GLU:H	2.04	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:N	1:A:40:ASN:ND2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:MET:HE3	1:A:492:TRP:HB3	1.91	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: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:55:MET:HE3	1:F:492:TRP:HB3	1.91	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:HE1	1:A:405:ILE:HD12	1.91	0.53
1:A:98:ALA:HB3	1:A:107:ILE:CD1	2.38	0.52
1:A:528:GLN:O	1:A:531:ARG:HG2	2.09	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: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: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: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:CD	1:A:303:GLU:H	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: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: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: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: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: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:142:HIS:CE1	1:F:447:ASN:HD21	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C	1:A:501:ASN:ND2	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:75:LYS:HG3	1:A:465:PRO:HA	1.96	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: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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:41:ARG:CG	1:A:41:ARG:O	2.66	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: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: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: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: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: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: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: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:446:ASN:HD22	1:F:479:SER:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:177:GLY:O	4:A:4001:MGD:O3'	2.32	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: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:41:ARG:O	1:F:41:ARG:CG	2.69	0.40
1:F:314:ASP:HB3	1:F:315:GLN:H	1.57	0.40
1:A:55:MET:HE2	1:A:492:TRP:HB3	1.99	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: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

Sometimes 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 monosaccharides 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	$\#\|Z\| > 2$
2	SF4	F	5001	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	MGD	A	3001	3	41,52,52	1.30	5 (12%)	40,81,81	1.79	10 (25%)
2	SF4	A	2001	1	0,12,12	-	-	-		
4	MGD	F	7001	3	41,52,52	1.51	6 (14%)	40,81,81	1.68	9 (22%)
4	MGD	F	6001	3	41,52,52	1.35	5 (12%)	40,81,81	2.10	15 (37%)
4	MGD	A	4001	3	41,52,52	1.44	4 (9%)	40,81,81	1.50	7 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	F	5001	1	-	-	0/6/5/5
4	MGD	A	3001	3	-	6/18/66/66	0/6/6/6
2	SF4	A	2001	1	-	-	0/6/5/5
4	MGD	F	7001	3	-	6/18/66/66	0/6/6/6
4	MGD	F	6001	3	-	4/18/66/66	0/6/6/6
4	MGD	A	4001	3	-	6/18/66/66	0/6/6/6

All (20) 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	-3.42	1.32	1.38
4	A	4001	MGD	C6-N1	-3.21	1.33	1.37
4	F	7001	MGD	C16-C17	2.97	1.50	1.42
4	A	3001	MGD	C17-N18	-2.69	1.33	1.38
4	A	3001	MGD	C16-C17	2.65	1.49	1.42
4	F	6001	MGD	O4'-C1'	2.65	1.44	1.41
4	F	7001	MGD	C6-N1	-2.54	1.34	1.37
4	F	7001	MGD	C17-N18	-2.54	1.34	1.38
4	F	7001	MGD	C21-N22	2.50	1.38	1.35
4	A	4001	MGD	C16-C17	2.43	1.48	1.42
4	F	6001	MGD	C16-C17	2.27	1.48	1.42
4	A	3001	MGD	O4'-C1'	2.24	1.44	1.41
4	F	6001	MGD	C17-N18	-2.20	1.34	1.38
4	A	3001	MGD	C2'-C1'	-2.11	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	7001	MGD	C19-N20	2.09	1.38	1.33
4	F	6001	MGD	C2'-C1'	-2.03	1.50	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	6001	MGD	O11-C23-C14	-5.40	105.36	108.96
4	A	3001	MGD	C19-N20-C21	5.26	122.92	113.43
4	F	7001	MGD	C19-N20-C21	5.02	122.49	113.43
4	F	6001	MGD	O11-C23-N22	-4.72	103.72	108.57
4	A	4001	MGD	C19-N20-C21	4.32	121.22	113.43
4	F	6001	MGD	C19-N20-C21	4.17	120.96	113.43
4	F	6001	MGD	O17-C17-C16	-3.65	118.86	127.24
4	A	3001	MGD	O4'-C1'-C2'	-3.37	102.00	106.93
4	F	7001	MGD	C5-C6-N1	3.22	119.64	113.95
4	A	4001	MGD	C17-C16-N15	3.04	124.91	116.76
4	A	3001	MGD	C8-N7-C5	3.02	108.75	102.99
4	F	7001	MGD	O6-C6-C5	-2.99	118.54	124.37
4	A	3001	MGD	PA-O3B-PB	-2.91	122.85	132.83
4	A	3001	MGD	C17-C16-N15	2.82	124.33	116.76
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	6001	MGD	N2-C2-N1	2.75	122.57	116.71
4	A	3001	MGD	O17-C17-C16	-2.74	120.96	127.24
4	F	7001	MGD	O17-C17-C16	-2.73	120.98	127.24
4	F	6001	MGD	C8-N7-C5	2.72	108.17	102.99
4	F	7001	MGD	C16-C17-N18	2.56	119.93	112.31
4	F	6001	MGD	O6-C6-C5	-2.54	119.41	124.37
4	F	7001	MGD	C17-C16-N15	2.54	123.57	116.76
4	F	7001	MGD	O11-C23-N22	-2.54	105.96	108.57
4	A	4001	MGD	C5-C6-N1	2.47	118.31	113.95
4	F	6001	MGD	O6-C6-N1	2.43	123.51	120.65
4	F	6001	MGD	C17-C16-N15	2.39	123.17	116.76
4	A	3001	MGD	C19-N18-C17	-2.35	120.81	125.10
4	F	7001	MGD	C19-N18-C17	-2.33	120.85	125.10
4	A	4001	MGD	C16-C17-N18	2.31	119.19	112.31
4	F	6001	MGD	N2-C2-N3	-2.30	115.26	119.74
4	F	6001	MGD	PA-O3B-PB	-2.20	125.27	132.83
4	A	3001	MGD	C16-C17-N18	2.18	118.80	112.31
4	F	6001	MGD	C19-N18-C17	-2.17	121.14	125.10
4	A	4001	MGD	C8-N7-C5	2.16	107.10	102.99
4	A	4001	MGD	O3'-C3'-C2'	-2.16	104.85	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	6001	MGD	O2A-PA-O1A	2.09	122.56	112.24
4	F	6001	MGD	C16-C17-N18	2.09	118.52	112.31
4	A	3001	MGD	N19-C19-N18	2.08	121.15	116.71
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

There are no chirality outliers.

All (22) 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	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	A	3001	MGD	C10-O3A-PA-O3B
4	A	4001	MGD	C5'-O5'-PB-O3B
4	F	7001	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
4	F	7001	MGD	C3'-C4'-C5'-O5'
4	F	7001	MGD	PB-O3B-PA-O2A
4	A	3001	MGD	C10-O3A-PA-O1A

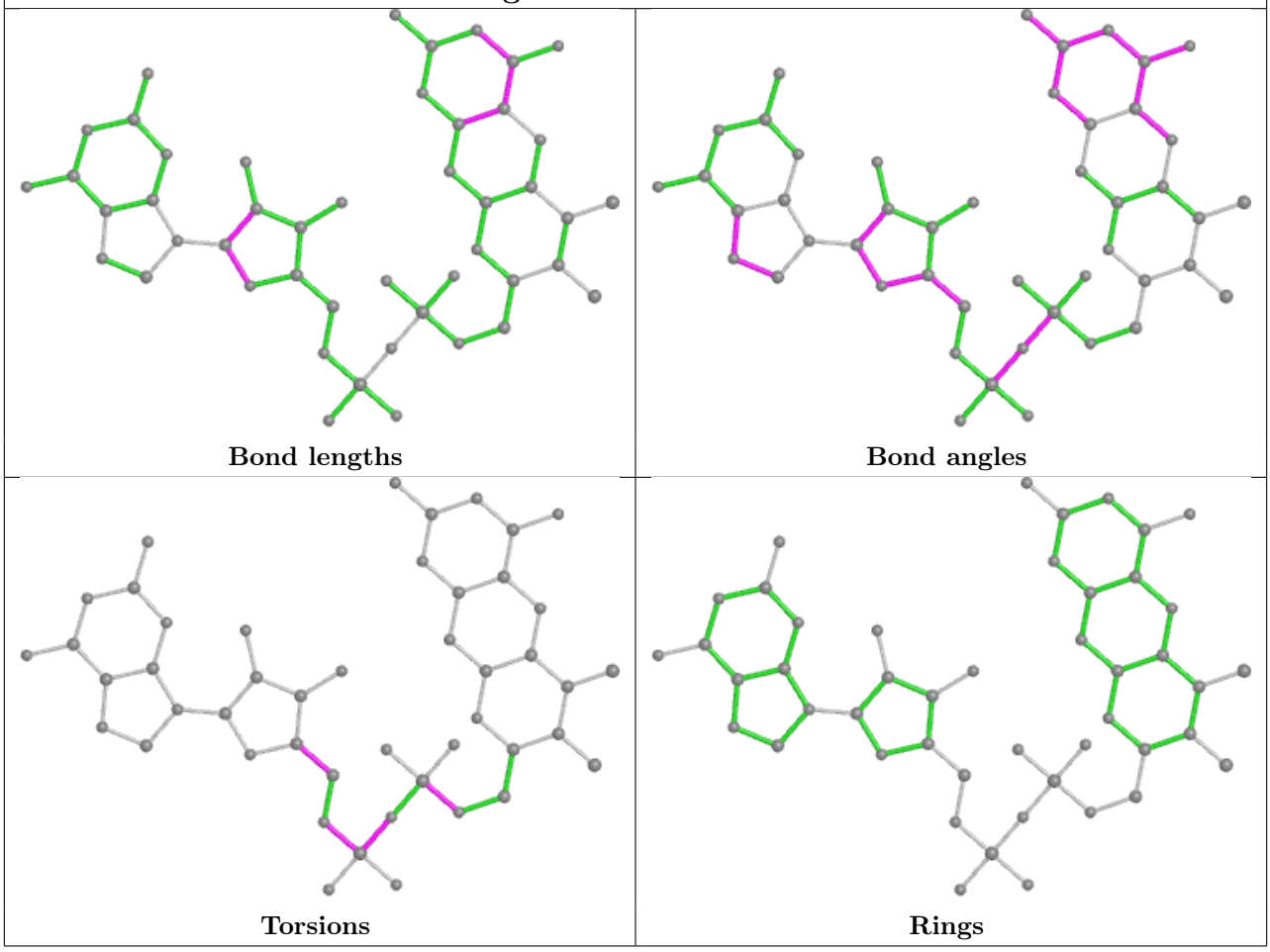
There are no ring outliers.

4 monomers are involved in 32 short contacts:

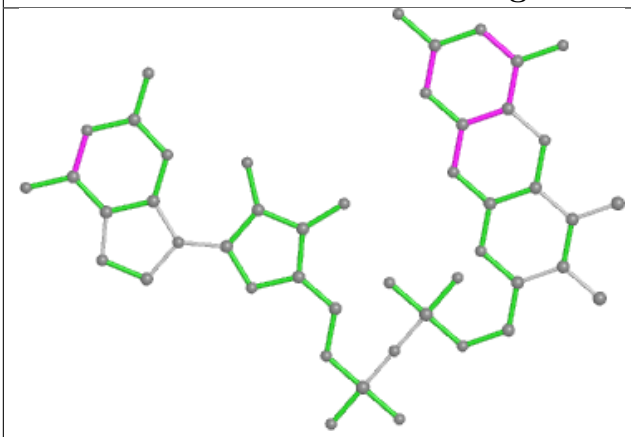
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3001	MGD	7	0
4	F	7001	MGD	8	0
4	F	6001	MGD	9	0
4	A	4001	MGD	8	0

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

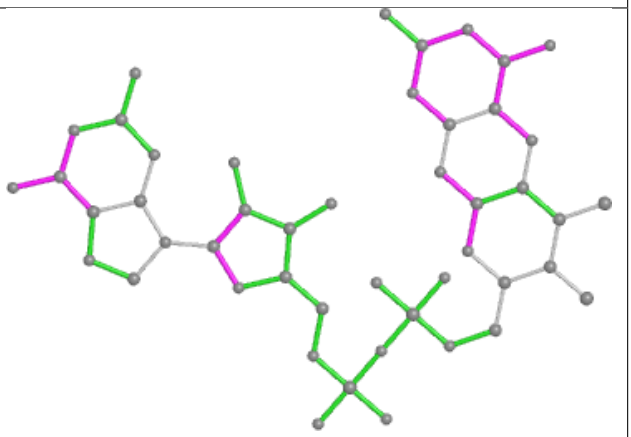
Ligand MGD A 3001



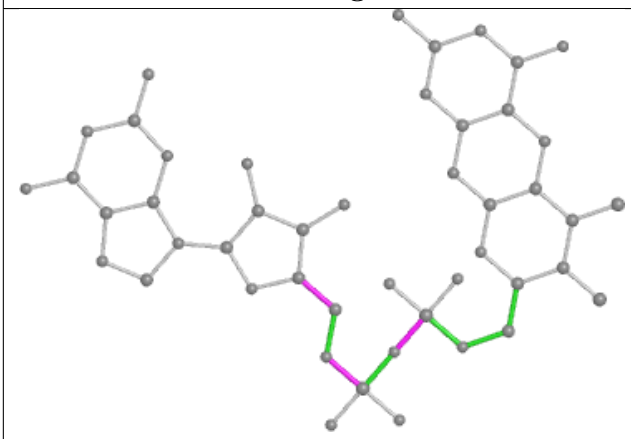
Ligand MGD F 7001



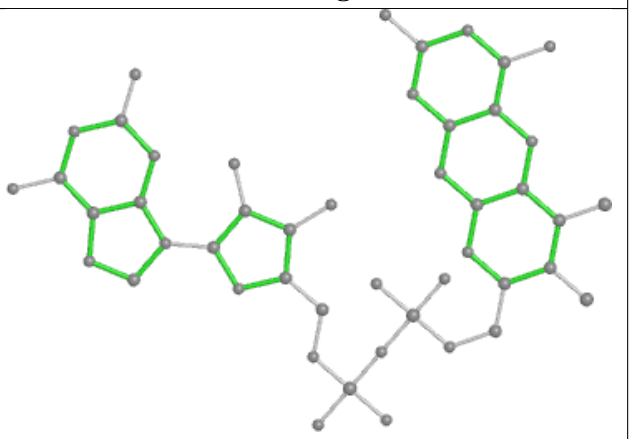
Bond lengths



Bond angles

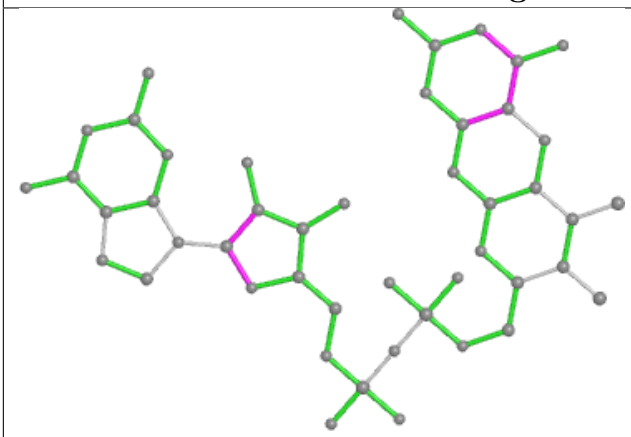


Torsions

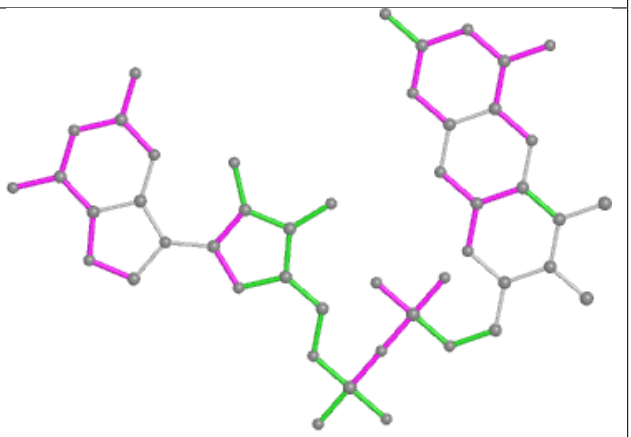


Rings

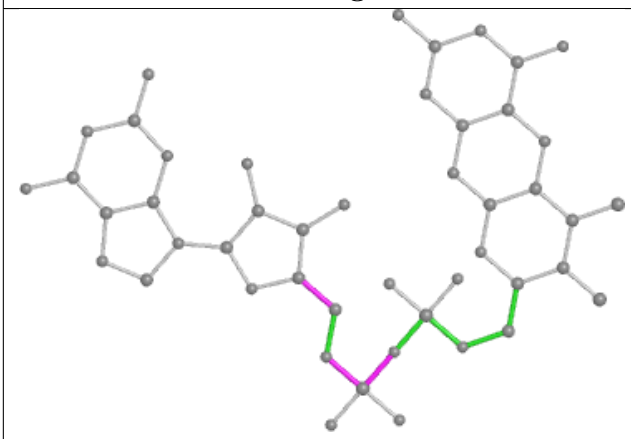
Ligand MGD F 6001



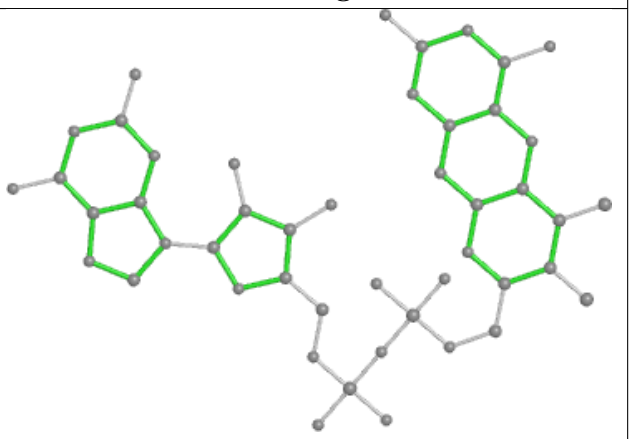
Bond lengths



Bond angles

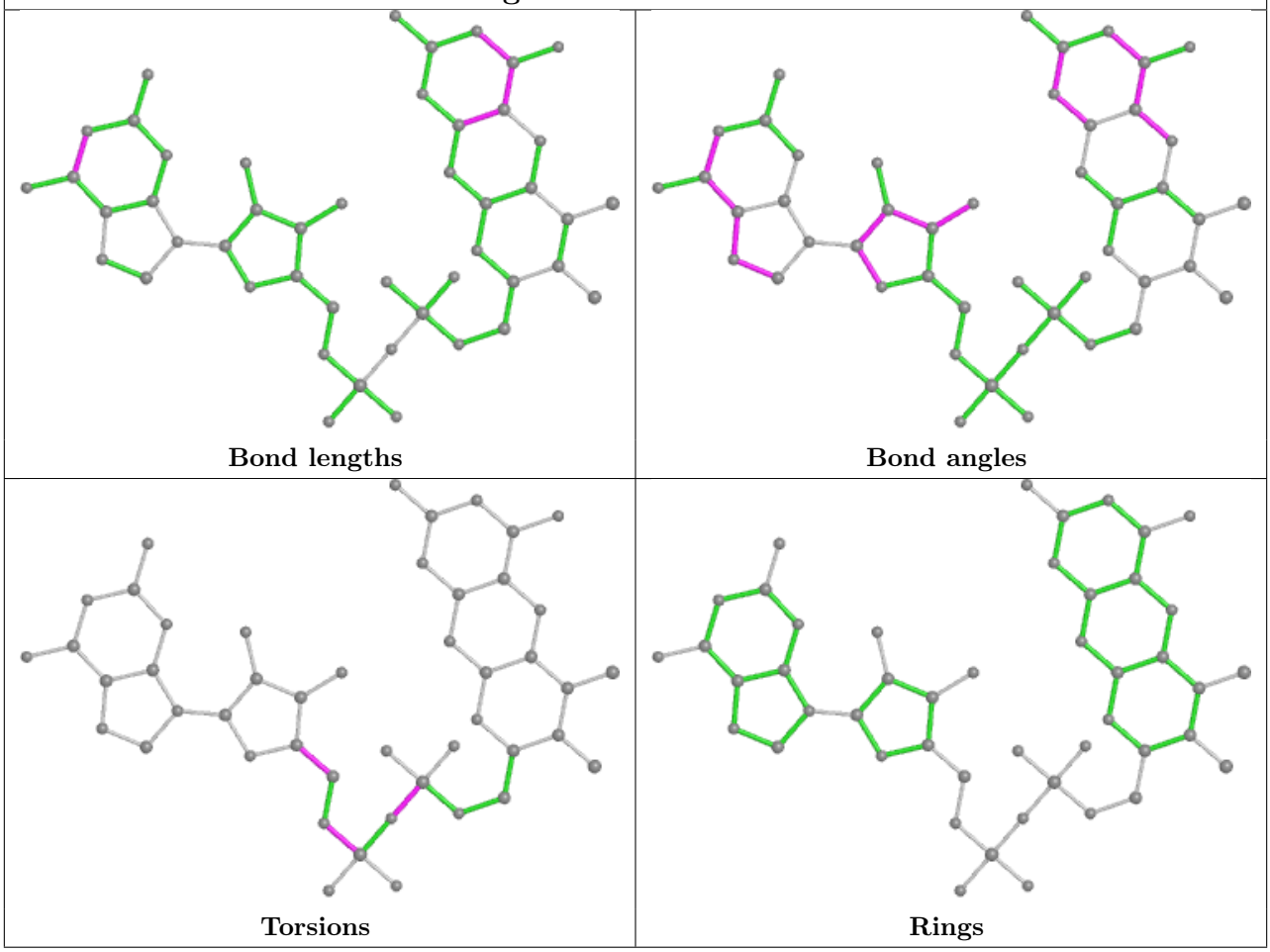


Torsions



Rings

Ligand MGD A 4001



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 monosaccharides in this entry.

6.4 Ligands (i)

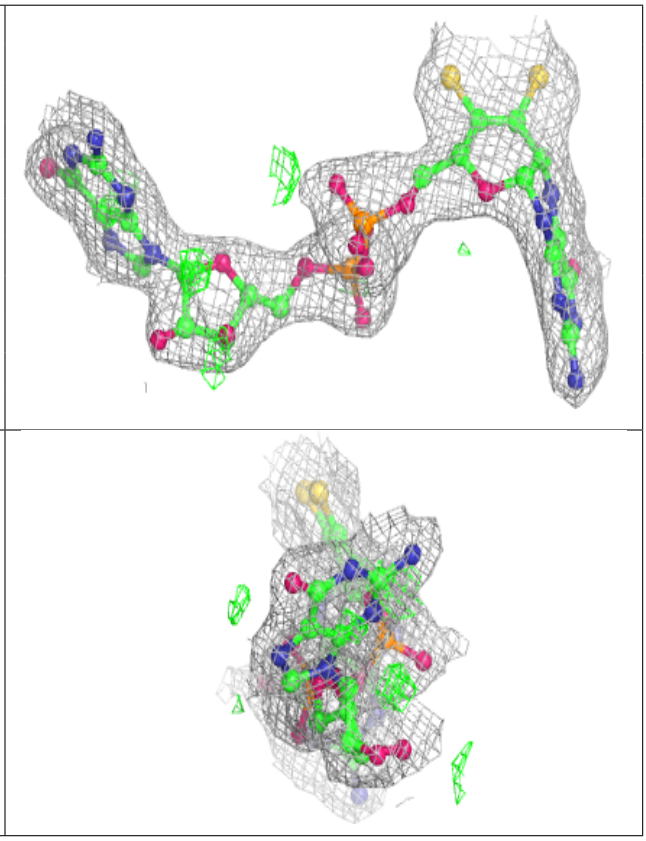
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

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

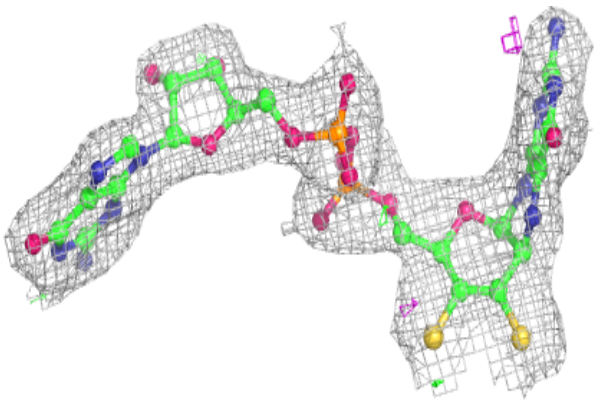
Electron density around MGD F 7001:

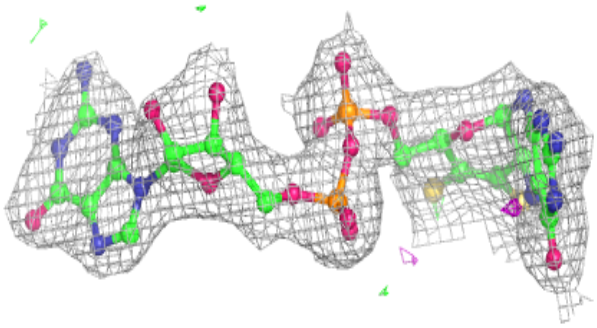
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

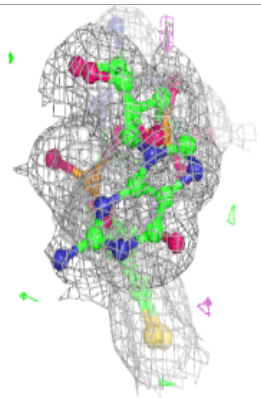


Electron density around MGD A 4001:

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

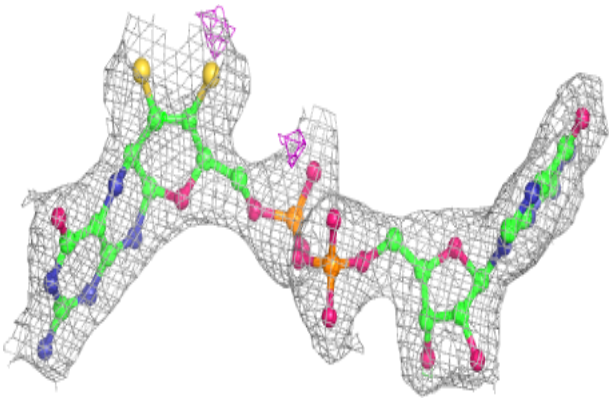


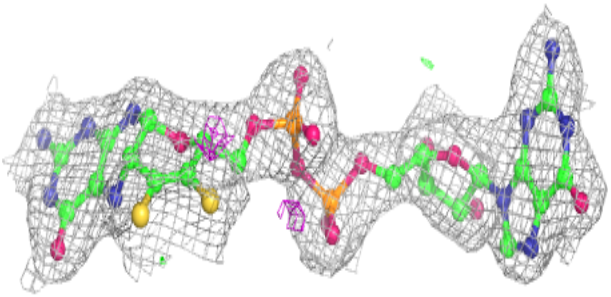


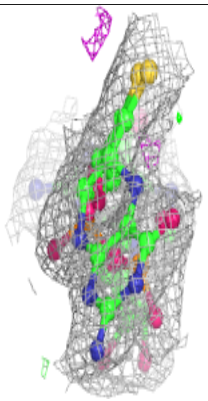


Electron density around MGD F 6001:

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

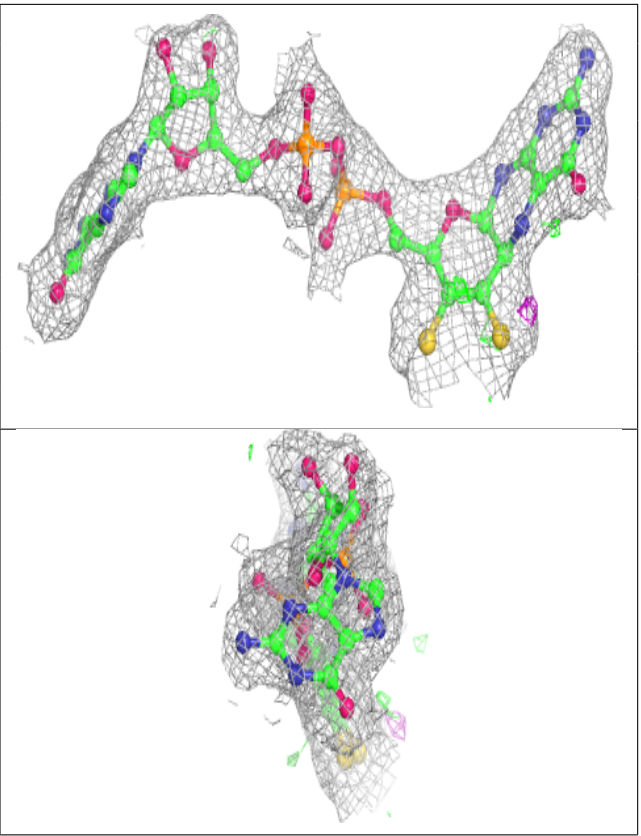






Electron density around MGD A 3001:

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



6.5 Other polymers (i)

There are no such residues in this entry.