Full wwPDB X-ray Structure Validation Report ⓘ

Jan 29, 2024 – 08:36 PM EST

PDB ID	:	1FDI
Title	:	OXIDIZED FORM OF FORMATE DEHYDROGENASE H FROM E. COLI COMPLEXED WITH THE INHIBITOR NITRITE
Authors	:	Sun, P.D.; Boyington, J.C.
Deposited on	:	1997-01-28
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

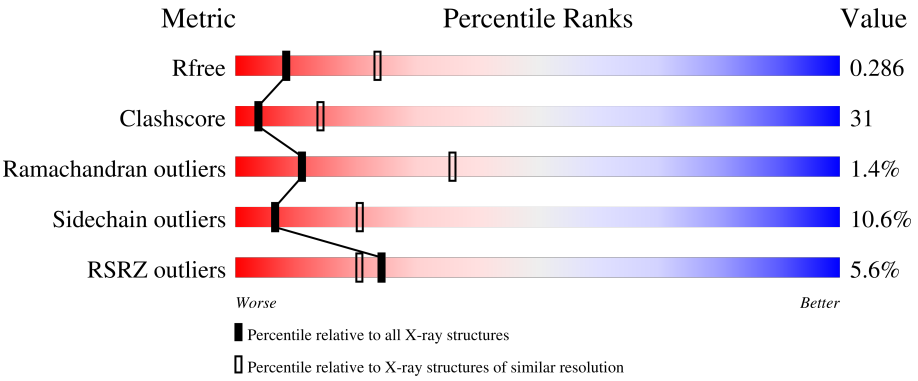
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	715	6% 46% 47% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NO2	A	804	-	-	X	-

2 Entry composition

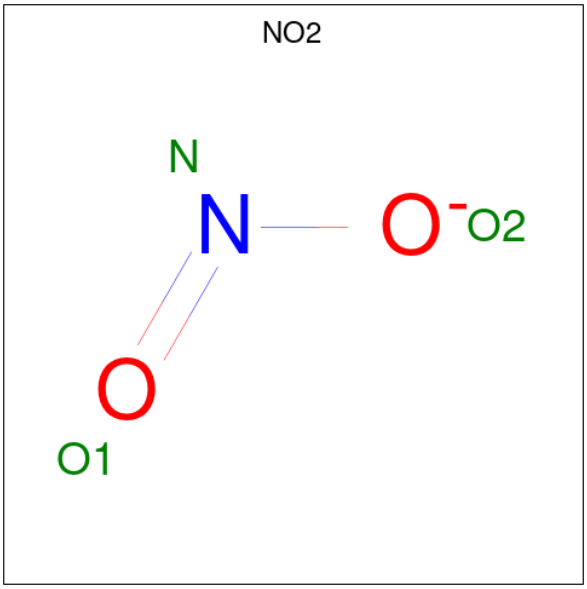
There are 6 unique types of molecules in this entry. The entry contains 5743 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FORMATE DEHYDROGENASE H.

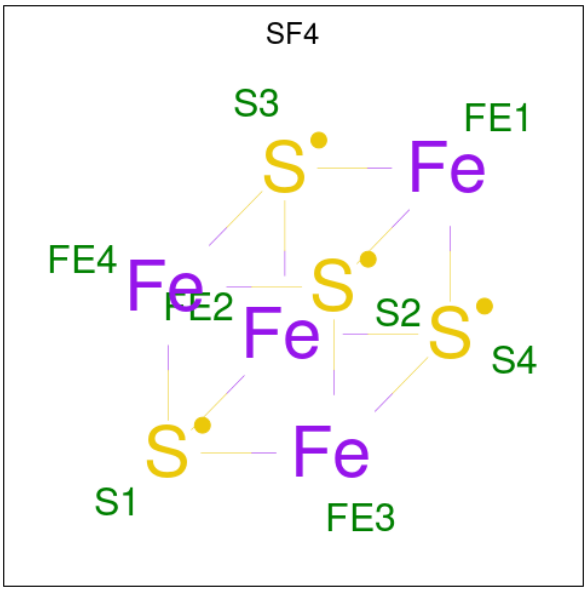
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	715	5575	3508	973	1060	33	1	0	0	0

- Molecule 2 is NITRITE ION (three-letter code: NO2) (formula: NO_2).



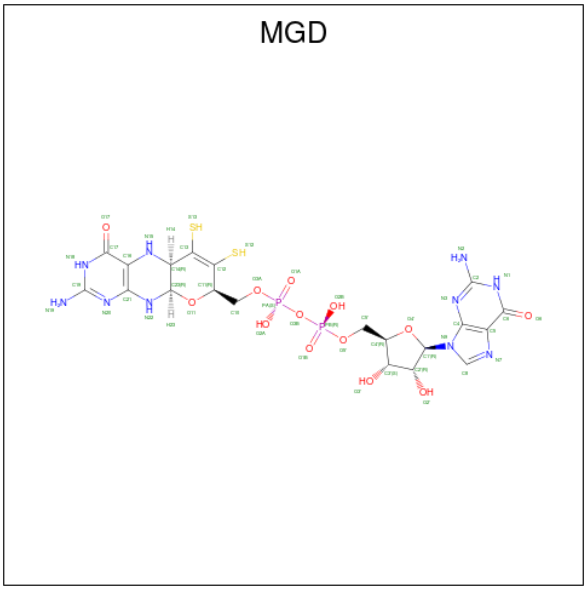
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	N	O			
2	A	1	3	1	2		0	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- 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	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 5 is MOLYBDENUM(VI) ION (three-letter code: 6MO) (formula: Mo).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mo 1 1	0	0

- Molecule 6 is water.

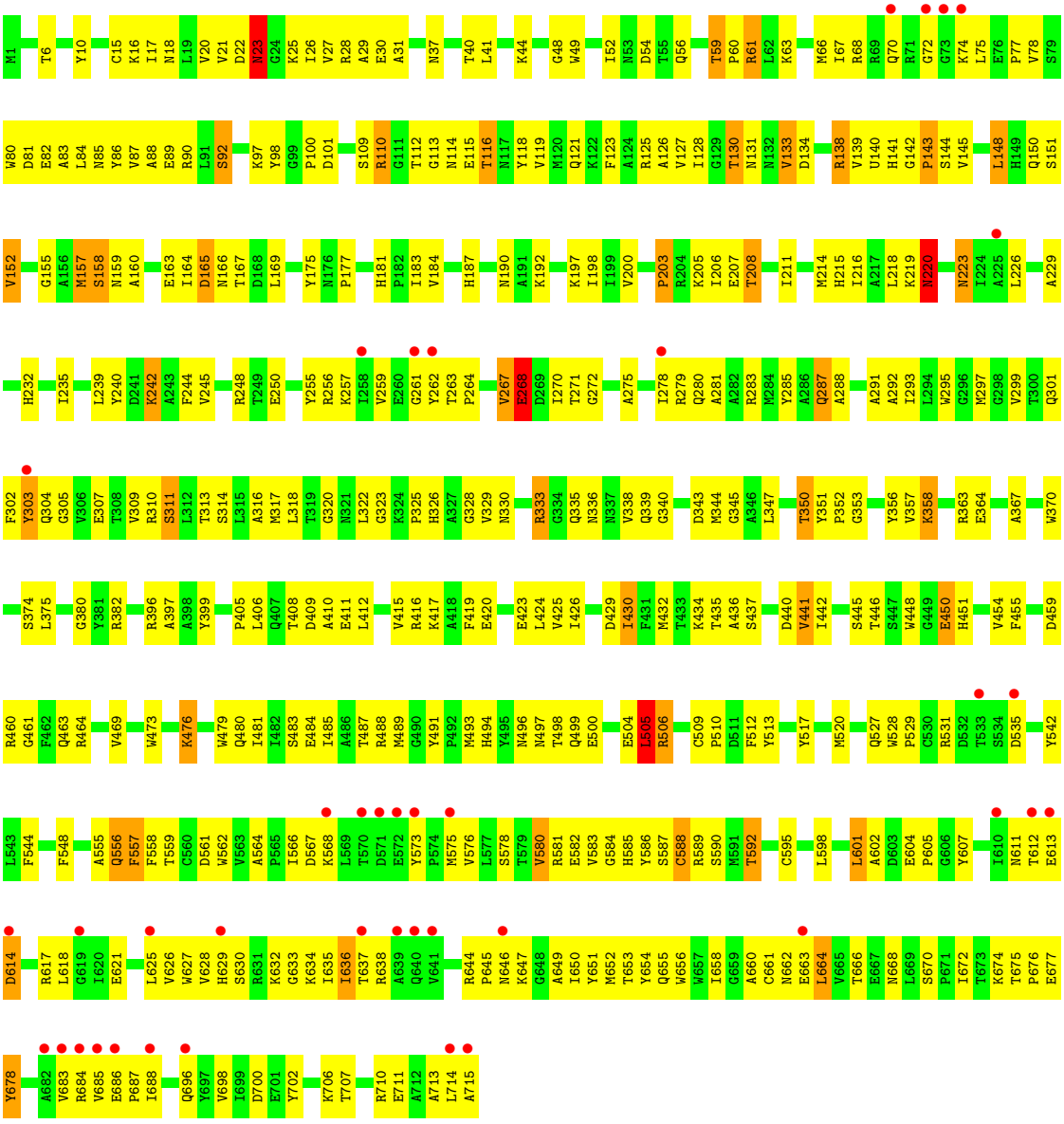
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	62	Total O 62 62	0	0

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: FORMATE DEHYDROGENASE H

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	146.80Å 146.80Å 81.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.90 40.71 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.3 (6.00-2.90) 94.4 (40.71-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.10 (at 2.90Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.192 , 0.284 0.224 , 0.286	Depositor DCC
R_{free} test set	869 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 74.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	5743	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6MO, SEC, MGD, SF4, NO2

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	0.61	1/5690 (0.0%)	0.85	3/7719 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	509	CYS	CB-SG	-5.18	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	505	LEU	CA-CB-CG	7.33	132.15	115.30
1	A	75	LEU	CA-CB-CG	5.89	128.85	115.30
1	A	506	ARG	NE-CZ-NH2	-5.15	117.72	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	678	TYR	Sidechain

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	5575	0	5453	347	0
2	A	3	0	0	3	0
3	A	8	0	0	1	0
4	A	94	0	44	8	0
5	A	1	0	0	0	0
6	A	62	0	0	10	0
All	All	5743	0	5497	347	0

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 31.

All (347) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:SEC:SE	2:A:804:NO2:N	2.28	1.16
1:A:614:ASP:HB3	1:A:647:LYS:HE3	1.28	1.09
1:A:582:GLU:HG2	1:A:655:GLN:HE22	1.07	1.08
1:A:302:PHE:HA	1:A:677:GLU:HG3	1.39	0.99
1:A:140:SEC:SE	2:A:804:NO2:O1	2.35	0.94
1:A:588:CYS:HB3	4:A:801:MGD:O1B	1.68	0.94
1:A:116:THR:HG22	1:A:479:TRP:HD1	1.36	0.90
1:A:582:GLU:HG2	1:A:655:GLN:NE2	1.86	0.90
1:A:140:SEC:SE	1:A:141:HIS:HD2	2.08	0.86
1:A:635:ILE:HG12	1:A:664:LEU:HD21	1.56	0.85
1:A:121:GLN:NE2	1:A:352:PRO:HD3	1.95	0.82
1:A:660:ALA:O	1:A:663:GLU:HB2	1.79	0.82
1:A:613:GLU:HB3	1:A:647:LYS:HZ3	1.45	0.81
1:A:614:ASP:HB2	1:A:617:ARG:HH22	1.44	0.81
1:A:59:THR:HG21	1:A:432:MET:O	1.80	0.81
1:A:151:SER:OG	1:A:310:ARG:HD3	1.82	0.80
1:A:630:SER:HB3	1:A:664:LEU:HB3	1.62	0.80
1:A:148:LEU:HD21	1:A:329:VAL:HG11	1.65	0.78
1:A:614:ASP:CB	1:A:647:LYS:HE3	2.12	0.76
1:A:702:TYR:CZ	1:A:706:LYS:HD2	2.21	0.75
1:A:232:HIS:CE1	1:A:263:THR:HG22	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ALA:HB2	1:A:41:LEU:HG	1.69	0.75
1:A:613:GLU:HB3	1:A:647:LYS:NZ	2.03	0.74
1:A:256:ARG:HH22	1:A:257:LYS:HZ1	1.35	0.74
1:A:305:GLY:O	1:A:309:VAL:HG23	1.88	0.74
1:A:140:SEC:SE	2:A:804:NO2:O2	2.57	0.73
1:A:144:SER:O	1:A:148:LEU:HB2	1.89	0.73
1:A:256:ARG:HH11	1:A:256:ARG:HB3	1.54	0.73
1:A:580:VAL:HG22	1:A:581:ARG:H	1.53	0.72
1:A:244:PHE:CE1	1:A:248:ARG:HD3	2.25	0.71
1:A:586:TYR:H	1:A:592:THR:HG21	1.54	0.71
1:A:169:LEU:HD12	1:A:197:LYS:HE3	1.72	0.71
1:A:333:ARG:NH1	1:A:333:ARG:HB3	2.06	0.71
1:A:396:ARG:O	1:A:423:GLU:HB2	1.91	0.70
1:A:499:GLN:HB2	1:A:517:TYR:CE2	2.26	0.70
1:A:333:ARG:HB3	1:A:333:ARG:HH11	1.57	0.69
1:A:115:GLU:HG2	1:A:498:THR:HB	1.74	0.69
1:A:614:ASP:HB3	1:A:647:LYS:CE	2.17	0.69
1:A:628:VAL:HG13	1:A:683:VAL:HB	1.75	0.69
1:A:223:ASN:HD22	1:A:223:ASN:H	1.40	0.68
1:A:605:PRO:HD3	1:A:698:VAL:HG11	1.76	0.67
1:A:628:VAL:HG22	1:A:685:VAL:HG22	1.76	0.67
1:A:78:VAL:HG13	1:A:82:GLU:HB3	1.76	0.67
1:A:350:THR:HA	1:A:356:TYR:HA	1.75	0.67
1:A:167:THR:HG22	1:A:326:HIS:O	1.95	0.67
1:A:295:TRP:CZ2	1:A:309:VAL:HG13	2.31	0.66
1:A:283:ARG:HG3	1:A:283:ARG:HH11	1.60	0.66
1:A:255:TYR:HE1	1:A:559:THR:HG23	1.61	0.66
1:A:163:GLU:OE2	1:A:325:PRO:HA	1.97	0.65
1:A:205:LYS:HG3	1:A:644:ARG:O	1.96	0.65
1:A:279:ARG:HB3	1:A:283:ARG:NH1	2.12	0.65
1:A:235:ILE:HD12	1:A:259:VAL:HG21	1.78	0.65
1:A:625:LEU:O	1:A:688:ILE:HB	1.97	0.65
1:A:702:TYR:CE1	1:A:706:LYS:HD2	2.31	0.65
1:A:10:TYR:HB2	3:A:800:SF4:S3	2.37	0.64
1:A:479:TRP:HE1	1:A:498:THR:HG22	1.62	0.64
1:A:110:ARG:HD2	1:A:336:ASN:HD21	1.61	0.64
1:A:409:ASP:HB2	1:A:415:VAL:HG21	1.79	0.64
1:A:140:SEC:HA	1:A:297:MET:CE	2.28	0.64
1:A:85:ASN:O	1:A:89:GLU:HB2	1.98	0.63
1:A:408:THR:HG22	1:A:654:TYR:HD2	1.63	0.63
1:A:614:ASP:HB2	1:A:617:ARG:NH2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:THR:HG22	1:A:479:TRP:CD1	2.27	0.63
1:A:86:TYR:O	1:A:90:ARG:HG2	1.97	0.63
1:A:60:PRO:HG2	1:A:713:ALA:CB	2.28	0.63
1:A:335:GLN:HA	1:A:586:TYR:OH	1.98	0.63
1:A:367:ALA:HB2	1:A:375:LEU:HG	1.81	0.62
1:A:109:SER:OG	1:A:338:VAL:HA	1.99	0.62
1:A:229:ALA:HB2	1:A:267:VAL:HG21	1.81	0.62
1:A:86:TYR:CE2	1:A:90:ARG:NH2	2.68	0.62
1:A:121:GLN:HB2	1:A:125:ARG:HH11	1.64	0.62
1:A:248:ARG:NH1	1:A:548:PHE:CE2	2.68	0.62
1:A:607:TYR:CE1	1:A:638:ARG:HG2	2.35	0.62
1:A:301:GLN:O	1:A:677:GLU:HA	2.00	0.62
1:A:150:GLN:HB3	1:A:310:ARG:NH2	2.15	0.62
1:A:262:TYR:OH	1:A:561:ASP:HA	1.99	0.62
1:A:408:THR:HG22	1:A:654:TYR:CD2	2.34	0.61
1:A:658:ILE:HD11	1:A:702:TYR:HA	1.82	0.61
1:A:131:ASN:ND2	1:A:357:VAL:HG21	2.14	0.61
1:A:169:LEU:HD12	1:A:197:LYS:CE	2.31	0.61
1:A:220:ASN:HD22	1:A:220:ASN:H	1.46	0.61
1:A:344:MET:O	1:A:352:PRO:HB3	2.01	0.61
1:A:408:THR:HG21	4:A:801:MGD:O2A	2.01	0.61
1:A:152:VAL:HG13	1:A:544:PHE:CZ	2.34	0.61
1:A:214:MET:SD	1:A:280:GLN:HG2	2.40	0.61
1:A:416:ARG:HD2	6:A:866:HOH:O	2.00	0.61
1:A:696:GLN:HG3	1:A:700:ASP:OD2	2.01	0.61
1:A:628:VAL:HA	1:A:684:ARG:O	2.00	0.60
1:A:240:TYR:CZ	1:A:242:LYS:HE2	2.36	0.60
1:A:140:SEC:HA	1:A:297:MET:HE1	1.84	0.60
1:A:140:SEC:SE	1:A:297:MET:HE1	2.52	0.60
1:A:216:ILE:HD11	1:A:281:ALA:HB2	1.83	0.60
1:A:183:ILE:O	1:A:187:HIS:HD2	1.85	0.59
1:A:573:TYR:CE1	1:A:684:ARG:HD2	2.38	0.59
1:A:121:GLN:HA	1:A:133:VAL:HG11	1.85	0.58
1:A:67:ILE:HD11	1:A:83:ALA:HA	1.85	0.58
1:A:115:GLU:OE2	1:A:454:VAL:HG23	2.03	0.58
1:A:256:ARG:HH12	1:A:257:LYS:HZ2	1.50	0.58
1:A:479:TRP:NE1	1:A:498:THR:HG22	2.18	0.58
1:A:223:ASN:H	1:A:223:ASN:ND2	2.01	0.58
1:A:460:ARG:O	1:A:527:GLN:HA	2.03	0.58
1:A:318:LEU:HD13	1:A:557:PHE:CZ	2.39	0.58
1:A:256:ARG:HB3	1:A:256:ARG:NH1	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:HH22	1:A:257:LYS:NZ	2.01	0.58
1:A:479:TRP:CZ3	1:A:480:GLN:HG3	2.39	0.57
1:A:15:CYS:SG	1:A:183:ILE:HG12	2.43	0.57
1:A:446:THR:HB	1:A:450:GLU:HB2	1.87	0.57
1:A:141:HIS:HB3	1:A:144:SER:HB2	1.86	0.57
1:A:351:TYR:CZ	1:A:357:VAL:HG12	2.39	0.57
1:A:110:ARG:HA	1:A:336:ASN:HD21	1.70	0.56
1:A:485:ILE:O	1:A:489:MET:HG3	2.05	0.56
1:A:139:VAL:HG13	1:A:678:TYR:HE2	1.70	0.56
1:A:484:GLU:O	1:A:488:ARG:HG3	2.06	0.56
1:A:311:SER:OG	1:A:559:THR:HG22	2.05	0.56
1:A:410:ALA:HB2	1:A:678:TYR:CE1	2.41	0.56
1:A:203:PRO:HB3	1:A:220:ASN:HD21	1.70	0.56
1:A:575:MET:SD	1:A:650:ILE:HG23	2.46	0.56
1:A:661:CYS:SG	1:A:662:ASN:N	2.79	0.56
1:A:630:SER:N	1:A:633:GLY:O	2.39	0.56
1:A:629:HIS:HA	1:A:634:LYS:HA	1.88	0.56
1:A:576:VAL:HB	1:A:649:ALA:HB2	1.88	0.55
1:A:239:LEU:HD22	1:A:287:GLN:HE22	1.71	0.55
1:A:626:VAL:HG23	1:A:687:PRO:HA	1.87	0.55
1:A:436:ALA:O	1:A:442:ILE:HD11	2.06	0.55
1:A:317:MET:HE2	1:A:555:ALA:HB1	1.88	0.55
1:A:629:HIS:CE1	1:A:634:LYS:HE3	2.42	0.55
1:A:80:TRP:CE2	1:A:476:LYS:HD2	2.42	0.55
1:A:145:VAL:HG13	1:A:155:GLY:HA3	1.87	0.54
1:A:263:THR:O	1:A:267:VAL:HG23	2.07	0.54
1:A:67:ILE:HD12	1:A:78:VAL:HG11	1.89	0.54
1:A:239:LEU:HD22	1:A:287:GLN:NE2	2.23	0.54
1:A:192:LYS:HB2	1:A:198:ILE:HD11	1.89	0.54
1:A:585:HIS:HA	1:A:592:THR:HG21	1.90	0.54
1:A:110:ARG:HD2	1:A:336:ASN:ND2	2.23	0.54
1:A:626:VAL:HG22	1:A:627:TRP:H	1.73	0.54
1:A:134:ASP:OD2	1:A:138:ARG:HD2	2.07	0.54
1:A:585:HIS:CD2	1:A:602:ALA:HB3	2.43	0.54
1:A:48:GLY:HA2	1:A:595:CYS:SG	2.48	0.53
1:A:192:LYS:HB2	1:A:198:ILE:CD1	2.38	0.53
1:A:26:ILE:HD12	1:A:52:ILE:HD12	1.91	0.53
1:A:181:HIS:HB2	1:A:184:VAL:HB	1.90	0.53
1:A:63:LYS:HG2	1:A:473:TRP:CE2	2.43	0.53
1:A:163:GLU:HA	6:A:841:HOH:O	2.08	0.53
1:A:627:TRP:O	1:A:685:VAL:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:HG12	1:A:271:THR:HG23	1.89	0.53
1:A:16:LYS:HE2	1:A:463:GLN:NE2	2.24	0.53
1:A:208:THR:O	1:A:211:ILE:HG12	2.09	0.52
1:A:220:ASN:HD22	1:A:220:ASN:N	2.05	0.52
1:A:506:ARG:HD2	1:A:513:TYR:O	2.09	0.52
1:A:663:GLU:HB3	1:A:664:LEU:HD23	1.90	0.52
1:A:358:LYS:NZ	1:A:358:LYS:HB3	2.24	0.52
1:A:582:GLU:OE2	1:A:656:TRP:HZ2	1.93	0.52
1:A:66:MET:HE2	6:A:825:HOH:O	2.09	0.52
1:A:426:ILE:HG12	1:A:441:VAL:HG13	1.90	0.52
1:A:123:PHE:HZ	1:A:489:MET:HE1	1.75	0.52
1:A:293:ILE:HG22	1:A:295:TRP:HE3	1.75	0.52
1:A:358:LYS:O	1:A:363:ARG:NH2	2.42	0.52
1:A:528:TRP:HB2	1:A:529:PRO:HA	1.90	0.52
1:A:203:PRO:HB3	1:A:220:ASN:ND2	2.24	0.52
1:A:644:ARG:H	1:A:645:PRO:HD2	1.75	0.52
1:A:56:GLN:OE1	1:A:710:ARG:NH1	2.43	0.52
1:A:626:VAL:HG22	1:A:627:TRP:N	2.24	0.52
1:A:115:GLU:O	1:A:119:VAL:HG23	2.10	0.51
1:A:151:SER:HG	1:A:310:ARG:HD3	1.76	0.51
1:A:317:MET:CE	1:A:555:ALA:HB1	2.40	0.51
1:A:351:TYR:HB3	1:A:352:PRO:HD2	1.90	0.51
1:A:635:ILE:HG12	1:A:664:LEU:CD2	2.34	0.51
1:A:702:TYR:CE2	1:A:706:LYS:HD2	2.44	0.51
1:A:604:GLU:HG3	1:A:702:TYR:CD1	2.46	0.51
1:A:302:PHE:CA	1:A:677:GLU:HG3	2.28	0.51
1:A:426:ILE:HG12	1:A:441:VAL:CG1	2.41	0.51
1:A:676:PRO:HG2	1:A:678:TYR:CE2	2.46	0.51
1:A:350:THR:HG23	1:A:356:TYR:CD2	2.46	0.51
1:A:562:TRP:CH2	1:A:564:ALA:HB2	2.45	0.51
1:A:583:VAL:HA	4:A:802:MGD:N19	2.26	0.51
1:A:139:VAL:HG13	1:A:678:TYR:CE2	2.46	0.50
1:A:429:ASP:OD1	4:A:801:MGD:H1'	2.11	0.50
1:A:707:THR:O	1:A:711:GLU:HG3	2.11	0.50
1:A:244:PHE:CD2	1:A:320:GLY:HA2	2.46	0.50
1:A:248:ARG:HG2	6:A:845:HOH:O	2.11	0.50
1:A:270:ILE:HD13	1:A:562:TRP:CE3	2.47	0.50
1:A:279:ARG:HB3	1:A:283:ARG:HH12	1.75	0.50
1:A:483:SER:HA	1:A:493:MET:HE2	1.93	0.50
1:A:583:VAL:HA	4:A:802:MGD:H191	1.76	0.50
1:A:504:GLU:HG3	6:A:856:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:MET:SD	1:A:505:LEU:HD21	2.52	0.50
1:A:18:ASN:HB2	1:A:30:GLU:HG3	1.93	0.50
1:A:498:THR:HG23	6:A:853:HOH:O	2.12	0.50
1:A:279:ARG:O	1:A:283:ARG:HG3	2.12	0.50
1:A:318:LEU:CD1	1:A:557:PHE:HZ	2.24	0.50
1:A:654:TYR:HB2	1:A:662:ASN:ND2	2.27	0.50
1:A:140:SEC:SE	1:A:141:HIS:CD2	3.01	0.49
1:A:203:PRO:HG3	1:A:218:LEU:O	2.13	0.49
1:A:293:ILE:CG2	1:A:295:TRP:HE3	2.25	0.49
1:A:598:LEU:HA	1:A:601:LEU:HD12	1.95	0.49
1:A:322:LEU:HD23	1:A:328:GLY:HA2	1.94	0.49
1:A:581:ARG:CZ	4:A:802:MGD:H102	2.42	0.49
1:A:285:TYR:OH	1:A:316:ALA:HA	2.11	0.49
1:A:611:ASN:HB3	1:A:614:ASP:OD1	2.13	0.48
1:A:589:ARG:HG3	1:A:592:THR:HG22	1.96	0.48
1:A:21:VAL:HG13	1:A:25:LYS:O	2.13	0.48
1:A:461:GLY:HA2	1:A:527:GLN:HA	1.95	0.48
1:A:363:ARG:HG2	1:A:375:LEU:HB2	1.95	0.48
1:A:70:GLN:HG2	1:A:72:GLY:H	1.78	0.48
1:A:333:ARG:HH11	1:A:333:ARG:CB	2.24	0.48
1:A:617:ARG:HG2	1:A:617:ARG:O	2.14	0.48
1:A:479:TRP:CE3	1:A:480:GLN:HG3	2.48	0.48
1:A:646:ASN:OD1	1:A:649:ALA:HB3	2.14	0.48
1:A:463:GLN:NE2	6:A:830:HOH:O	2.46	0.48
1:A:6:THR:CG2	1:A:17:ILE:HB	2.44	0.47
1:A:513:TYR:HD2	1:A:531:ARG:O	1.96	0.47
1:A:98:TYR:CD2	1:A:396:ARG:HD3	2.49	0.47
1:A:37:ASN:HB2	1:A:40:THR:O	2.14	0.47
1:A:279:ARG:HG2	1:A:279:ARG:HH11	1.77	0.47
1:A:118:TYR:O	1:A:121:GLN:HG3	2.15	0.47
1:A:405:PRO:HA	1:A:409:ASP:OD1	2.13	0.47
1:A:629:HIS:CE1	1:A:634:LYS:HG3	2.49	0.47
1:A:169:LEU:HD12	1:A:197:LYS:NZ	2.29	0.47
1:A:29:ALA:HB2	1:A:49:TRP:CD1	2.49	0.47
1:A:261:GLY:O	1:A:263:THR:HG23	2.15	0.47
1:A:353:GLY:HA2	1:A:512:PHE:CZ	2.50	0.47
1:A:419:PHE:CZ	1:A:435:THR:HG23	2.49	0.47
1:A:586:TYR:N	1:A:592:THR:HG21	2.26	0.47
1:A:617:ARG:CZ	1:A:617:ARG:HB3	2.44	0.47
1:A:60:PRO:HG2	1:A:713:ALA:HB3	1.97	0.47
1:A:60:PRO:HB2	1:A:714:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:TRP:CD1	1:A:688:ILE:HD11	2.50	0.47
1:A:80:TRP:CZ2	1:A:476:LYS:HD2	2.50	0.47
1:A:338:VAL:HG13	1:A:339:GLN:N	2.29	0.47
1:A:670:SER:H	1:A:675:THR:H	1.63	0.47
1:A:636:ILE:HG12	1:A:637:THR:N	2.29	0.47
1:A:131:ASN:O	1:A:380:GLY:HA3	2.14	0.46
1:A:169:LEU:HD12	1:A:197:LYS:HZ1	1.80	0.46
1:A:310:ARG:NH1	1:A:558:PHE:HB2	2.31	0.46
1:A:123:PHE:HZ	1:A:489:MET:CE	2.28	0.46
1:A:140:SEC:HA	1:A:297:MET:HE3	1.96	0.46
1:A:397:ALA:HA	1:A:424:LEU:O	2.16	0.46
1:A:654:TYR:CE2	4:A:801:MGD:O11	2.68	0.46
1:A:430:ILE:HD12	1:A:445:SER:OG	2.16	0.46
1:A:630:SER:CB	1:A:664:LEU:HB3	2.39	0.46
1:A:78:VAL:HG22	1:A:82:GLU:OE1	2.16	0.46
1:A:100:PRO:HB3	1:A:128:ILE:O	2.16	0.46
1:A:15:CYS:SG	1:A:37:ASN:HB3	2.56	0.46
1:A:84:LEU:HD21	1:A:481:ILE:HG23	1.98	0.46
1:A:345:GLY:C	1:A:347:LEU:H	2.19	0.46
1:A:614:ASP:HB2	1:A:617:ARG:HH12	1.81	0.46
1:A:148:LEU:HB3	1:A:155:GLY:HA2	1.97	0.46
1:A:158:SER:OG	1:A:159:ASN:OD1	2.29	0.46
1:A:279:ARG:HH11	1:A:279:ARG:CG	2.29	0.46
1:A:626:VAL:HG21	1:A:685:VAL:HG12	1.97	0.46
1:A:307:GLU:O	1:A:311:SER:HB2	2.16	0.45
1:A:333:ARG:HG3	1:A:339:GLN:HE21	1.80	0.45
1:A:488:ARG:HD3	6:A:808:HOH:O	2.15	0.45
1:A:653:THR:O	1:A:661:CYS:SG	2.74	0.45
1:A:88:ALA:O	1:A:92:SER:HB2	2.15	0.45
1:A:207:GLU:HA	1:A:644:ARG:HH22	1.82	0.45
1:A:219:LYS:HE3	1:A:272:GLY:CA	2.47	0.45
1:A:582:GLU:HG3	1:A:583:VAL:O	2.17	0.45
1:A:430:ILE:HD11	1:A:446:THR:C	2.36	0.45
1:A:302:PHE:O	1:A:305:GLY:N	2.49	0.45
1:A:143:PRO:HD3	1:A:675:THR:OG1	2.17	0.45
1:A:200:VAL:CG1	1:A:206:ILE:HD11	2.47	0.44
1:A:264:PRO:HG2	1:A:279:ARG:NH1	2.31	0.44
1:A:581:ARG:NH2	4:A:801:MGD:O17	2.50	0.44
1:A:650:ILE:HD11	1:A:683:VAL:HG21	2.00	0.44
1:A:114:ASN:O	1:A:344:MET:HG3	2.16	0.44
1:A:303:TYR:C	1:A:305:GLY:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:THR:O	1:A:317:MET:HG3	2.18	0.44
1:A:576:VAL:HB	1:A:649:ALA:CB	2.46	0.44
1:A:411:GLU:CD	1:A:632:LYS:HD2	2.38	0.44
1:A:77:PRO:HD3	1:A:715:ALA:OXT	2.17	0.44
1:A:267:VAL:O	1:A:268:GLU:C	2.57	0.44
1:A:628:VAL:CG1	1:A:683:VAL:HB	2.47	0.44
1:A:632:LYS:HB2	1:A:664:LEU:HA	1.99	0.44
1:A:121:GLN:HB2	1:A:125:ARG:NH1	2.31	0.43
1:A:573:TYR:HE1	1:A:684:ARG:HD2	1.80	0.43
1:A:629:HIS:NE2	1:A:634:LYS:HE3	2.33	0.43
1:A:54:ASP:O	1:A:56:GLN:HG3	2.18	0.43
1:A:219:LYS:HE3	1:A:272:GLY:HA3	2.00	0.43
1:A:61:ARG:HH22	1:A:450:GLU:CD	2.22	0.43
1:A:226:LEU:CD1	1:A:278:ILE:HG12	2.48	0.43
1:A:297:MET:C	1:A:299:VAL:H	2.20	0.43
1:A:350:THR:HG23	1:A:356:TYR:CG	2.54	0.43
1:A:566:ILE:HG22	1:A:567:ASP:N	2.33	0.43
1:A:164:ILE:O	1:A:166:ASN:N	2.51	0.43
1:A:250:GLU:OE1	1:A:556:GLN:OE1	2.37	0.43
1:A:283:ARG:HG3	1:A:283:ARG:NH1	2.29	0.43
1:A:84:LEU:HD22	1:A:485:ILE:HG12	2.00	0.43
1:A:292:ALA:HA	6:A:811:HOH:O	2.19	0.43
1:A:80:TRP:O	1:A:81:ASP:C	2.57	0.43
1:A:113:GLY:HA2	1:A:455:PHE:CD1	2.53	0.43
1:A:459:ASP:O	1:A:527:GLN:HG2	2.18	0.43
1:A:17:ILE:HG22	1:A:18:ASN:N	2.34	0.42
1:A:483:SER:HA	1:A:493:MET:CE	2.49	0.42
1:A:109:SER:CB	1:A:338:VAL:HA	2.48	0.42
1:A:637:THR:HG21	1:A:652:MET:CE	2.49	0.42
1:A:676:PRO:CG	1:A:678:TYR:CE2	3.02	0.42
1:A:110:ARG:HD2	1:A:110:ARG:HA	1.82	0.42
1:A:160:ALA:HB3	1:A:163:GLU:HB2	2.00	0.42
1:A:44:LYS:HB2	1:A:44:LYS:HE3	1.69	0.42
1:A:264:PRO:CB	1:A:275:ALA:HB1	2.49	0.42
1:A:288:ALA:HB3	1:A:291:ALA:HB2	2.01	0.42
1:A:340:GLY:O	1:A:343:ASP:HB2	2.20	0.42
1:A:87:VAL:HG13	1:A:426:ILE:HD13	2.02	0.42
1:A:587:SER:O	1:A:655:GLN:HA	2.19	0.42
1:A:607:TYR:HA	1:A:638:ARG:O	2.20	0.42
1:A:123:PHE:CZ	1:A:489:MET:CE	3.03	0.42
1:A:434:LYS:O	1:A:437:SER:OG	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:VAL:CG1	1:A:544:PHE:CZ	3.03	0.42
1:A:464:ARG:HG2	1:A:520:MET:HE3	2.02	0.42
1:A:604:GLU:OE1	1:A:604:GLU:HA	2.20	0.42
1:A:310:ARG:HB3	1:A:558:PHE:HD2	1.85	0.41
1:A:113:GLY:HA2	1:A:455:PHE:CE1	2.54	0.41
1:A:127:VAL:HG22	1:A:491:TYR:CG	2.55	0.41
1:A:152:VAL:HG22	1:A:548:PHE:CD1	2.55	0.41
1:A:232:HIS:CD2	1:A:264:PRO:HD3	2.55	0.41
1:A:496:ASN:HB2	1:A:500:GLU:OE2	2.20	0.41
1:A:323:GLY:O	1:A:542:TYR:HE2	2.04	0.41
1:A:101:ASP:HA	1:A:130:THR:CG2	2.50	0.41
1:A:126:ALA:HB2	1:A:370:TRP:CE3	2.55	0.41
1:A:142:GLY:N	1:A:143:PRO:CD	2.84	0.41
1:A:157:MET:HE3	1:A:330:ASN:HB3	2.02	0.41
1:A:232:HIS:HB2	1:A:262:TYR:O	2.19	0.41
1:A:318:LEU:HD13	1:A:557:PHE:HZ	1.81	0.41
1:A:215:HIS:C	1:A:215:HIS:CD2	2.93	0.41
1:A:310:ARG:HD2	1:A:558:PHE:HB3	2.01	0.41
1:A:632:LYS:HE3	1:A:666:THR:OG1	2.20	0.41
1:A:22:ASP:O	1:A:23:ASN:HB2	2.20	0.41
1:A:358:LYS:HB3	1:A:358:LYS:HZ3	1.85	0.41
1:A:566:ILE:CD1	1:A:668:ASN:HB3	2.50	0.41
1:A:497:ASN:OD1	1:A:497:ASN:N	2.54	0.41
1:A:417:LYS:HD2	1:A:420:GLU:OE1	2.21	0.41
1:A:607:TYR:HE1	1:A:638:ARG:HG2	1.85	0.41
1:A:175:TYR:CE2	1:A:177:PRO:HG3	2.55	0.41
1:A:425:VAL:O	1:A:440:ASP:HB2	2.21	0.41
1:A:584:GLY:O	1:A:598:LEU:HD13	2.20	0.41
1:A:268:GLU:OE1	1:A:275:ALA:HB2	2.21	0.41
1:A:578:SER:HB3	1:A:651:TYR:CE2	2.56	0.41
1:A:68:ARG:NH2	1:A:437:SER:O	2.52	0.40
1:A:633:GLY:C	1:A:664:LEU:HD22	2.41	0.40
1:A:150:GLN:HB3	1:A:310:ARG:CZ	2.51	0.40
1:A:487:THR:HA	1:A:491:TYR:O	2.21	0.40
1:A:339:GLN:NE2	6:A:826:HOH:O	2.54	0.40
1:A:20:VAL:HG21	1:A:28:ARG:CZ	2.52	0.40
1:A:183:ILE:O	1:A:187:HIS:CD2	2.70	0.40
1:A:406:LEU:HA	1:A:406:LEU:HD23	1.77	0.40
1:A:451:HIS:C	1:A:451:HIS:CD2	2.94	0.40

There are no symmetry-related clashes.

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	712/715 (100%)	630 (88%)	72 (10%)	10 (1%)	11 36

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	GLU
1	A	165	ASP
1	A	580	VAL
1	A	672	ILE
1	A	220	ASN
1	A	412	LEU
1	A	612	THR
1	A	23	ASN
1	A	74	LYS
1	A	245	VAL

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	584/584 (100%)	522 (89%)	62 (11%)	6 20

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASN

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Mol	Chain	Res	Type
1	A	27	VAL
1	A	59	THR
1	A	61	ARG
1	A	92	SER
1	A	97	LYS
1	A	110	ARG
1	A	112	THR
1	A	116	THR
1	A	130	THR
1	A	133	VAL
1	A	138	ARG
1	A	143	PRO
1	A	148	LEU
1	A	152	VAL
1	A	157	MET
1	A	158	SER
1	A	165	ASP
1	A	190	ASN
1	A	203	PRO
1	A	208	THR
1	A	220	ASN
1	A	223	ASN
1	A	242	LYS
1	A	267	VAL
1	A	268	GLU
1	A	287	GLN
1	A	303	TYR
1	A	304	GLN
1	A	311	SER
1	A	314	SER
1	A	333	ARG
1	A	350	THR
1	A	358	LYS
1	A	364	GLU
1	A	374	SER
1	A	382	ARG
1	A	399	TYR
1	A	430	ILE
1	A	441	VAL
1	A	448	TRP
1	A	450	GLU
1	A	469	VAL

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Mol	Chain	Res	Type
1	A	476	LYS
1	A	494	HIS
1	A	505	LEU
1	A	510	PRO
1	A	535	ASP
1	A	556	GLN
1	A	557	PHE
1	A	568	LYS
1	A	588	CYS
1	A	590	SER
1	A	592	THR
1	A	601	LEU
1	A	614	ASP
1	A	618	LEU
1	A	621	GLU
1	A	636	ILE
1	A	664	LEU
1	A	674	LYS
1	A	686	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	166	ASN
1	A	220	ASN
1	A	223	ASN
1	A	280	GLN
1	A	336	ASN
1	A	339	GLN
1	A	463	GLN
1	A	527	GLN
1	A	696	GLN

5.3.3 RNA

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	NO2	A	804	5	1,2,2	1.01	0	0,1,1	-	-
4	MGD	A	802	5	41,52,52	1.73	4 (9%)	40,81,81	1.63	5 (12%)
4	MGD	A	801	5	41,52,52	1.28	5 (12%)	40,81,81	2.19	9 (22%)
3	SF4	A	800	1	0,12,12	-	-	-		

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
3	SF4	A	800	1	-	-	0/6/5/5
4	MGD	A	802	5	-	5/18/66/66	0/6/6/6
4	MGD	A	801	5	-	6/18/66/66	0/6/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	802	MGD	C23-C14	-8.87	1.46	1.53
4	A	801	MGD	C5-C6	-4.64	1.38	1.47
4	A	802	MGD	C5-C4	-2.68	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	802	MGD	C5-C6	-2.45	1.42	1.47
4	A	801	MGD	O11-C11	-2.31	1.40	1.43
4	A	801	MGD	C16-C21	2.31	1.42	1.38
4	A	801	MGD	C5-C4	-2.18	1.37	1.43
4	A	802	MGD	C8-N7	-2.13	1.31	1.35
4	A	801	MGD	O4'-C4'	-2.03	1.40	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	801	MGD	O11-C23-C14	8.46	114.61	108.96
4	A	801	MGD	O11-C23-N22	5.19	113.90	108.57
4	A	802	MGD	C19-N20-C21	5.11	122.66	113.43
4	A	801	MGD	C19-N20-C21	5.07	122.58	113.43
4	A	802	MGD	O11-C23-N22	4.90	113.60	108.57
4	A	801	MGD	C3'-C2'-C1'	-3.01	96.44	100.98
4	A	802	MGD	O17-C17-C16	-2.68	121.09	127.24
4	A	802	MGD	C19-N18-C17	-2.62	120.32	125.10
4	A	801	MGD	O5'-C5'-C4'	2.62	118.02	108.99
4	A	801	MGD	O6-C6-N1	2.52	123.62	120.65
4	A	801	MGD	O17-C17-C16	-2.37	121.82	127.24
4	A	801	MGD	PA-O3B-PB	-2.21	125.24	132.83
4	A	801	MGD	N18-C19-N20	-2.13	119.34	123.32
4	A	802	MGD	C16-C17-N18	2.12	118.64	112.31

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	MGD	C5'-O5'-PB-O2B
4	A	801	MGD	O3A-C10-C11-O11
4	A	801	MGD	O3A-C10-C11-C12
4	A	802	MGD	C5'-O5'-PB-O1B
4	A	802	MGD	PB-O3B-PA-O1A
4	A	801	MGD	C5'-O5'-PB-O3B
4	A	802	MGD	C5'-O5'-PB-O3B
4	A	801	MGD	C5'-O5'-PB-O1B
4	A	802	MGD	O4'-C4'-C5'-O5'
4	A	802	MGD	PB-O3B-PA-O2A
4	A	801	MGD	O4'-C4'-C5'-O5'

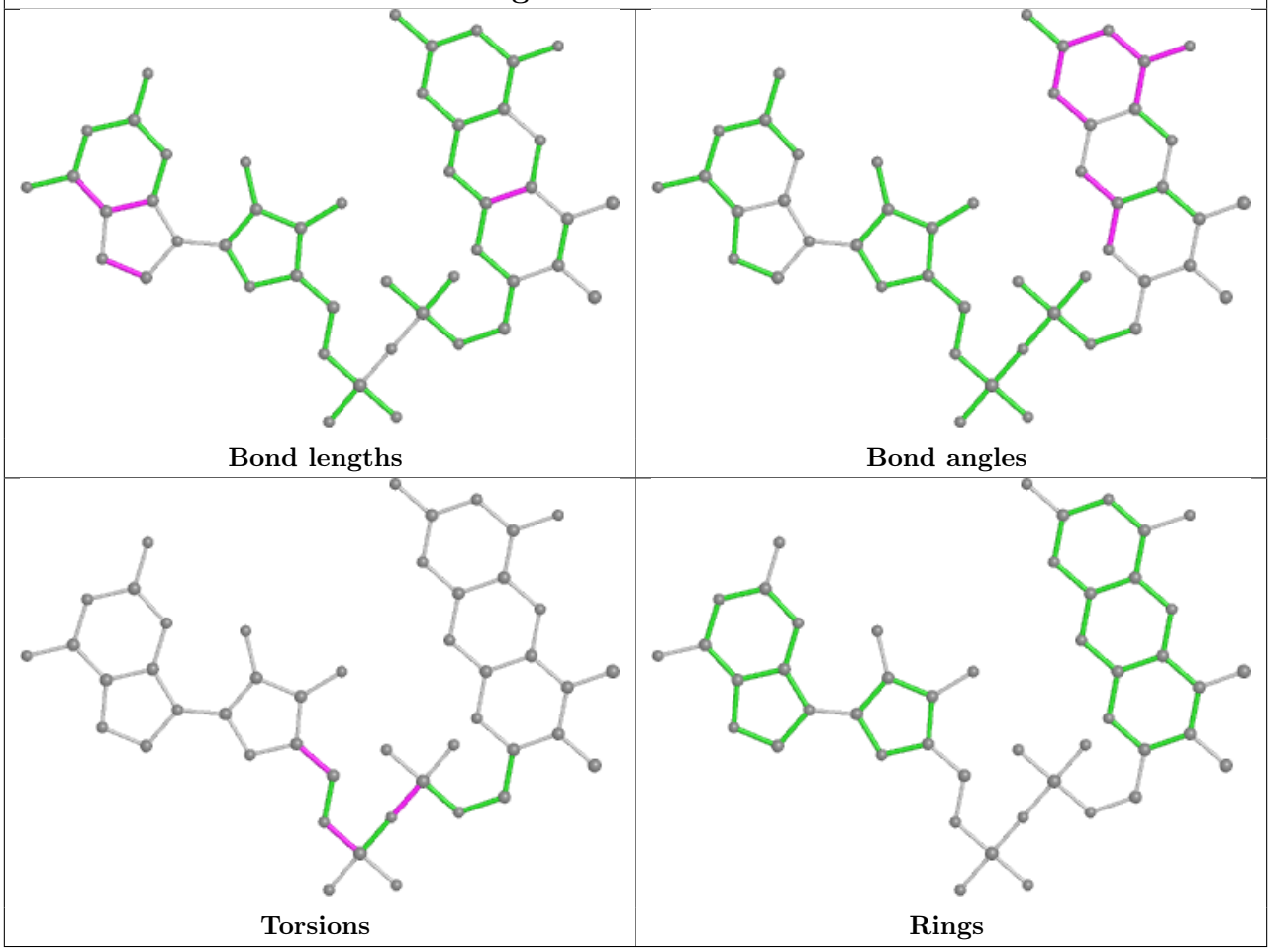
There are no ring outliers.

4 monomers are involved in 12 short contacts:

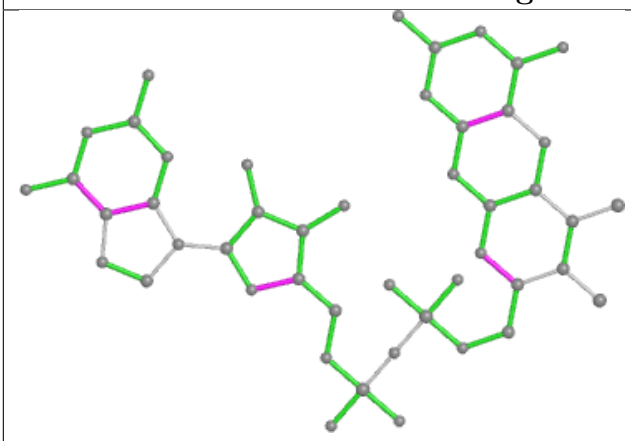
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	804	NO2	3	0
4	A	802	MGD	3	0
4	A	801	MGD	5	0
3	A	800	SF4	1	0

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

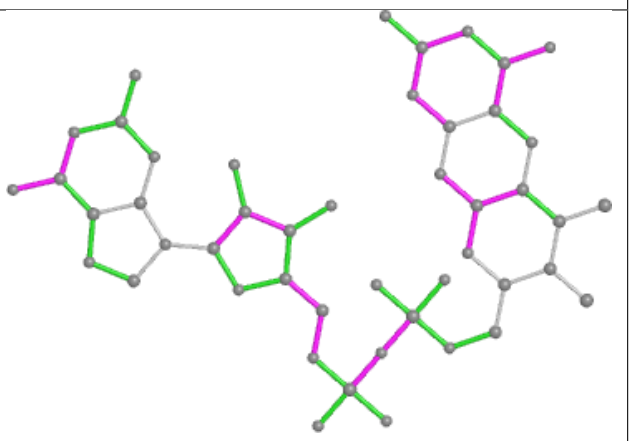
Ligand MGD A 802



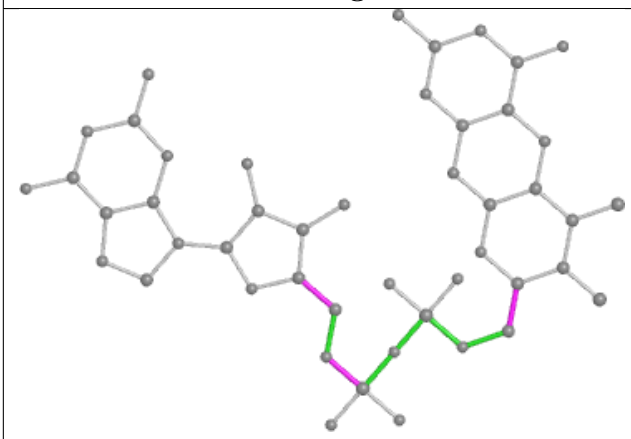
Ligand MGD A 801



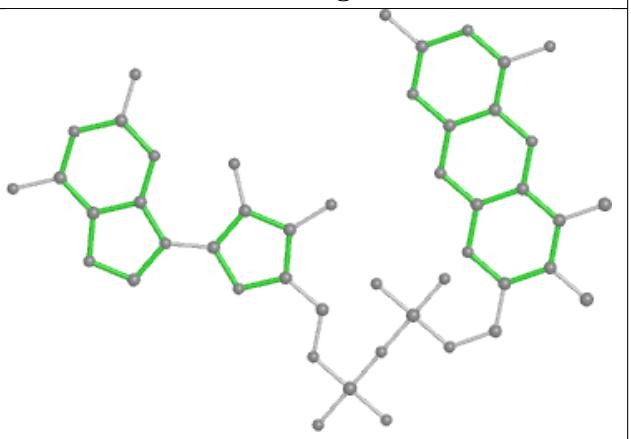
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	714/715 (99%)	0.27	40 (5%)	24	20	5, 22, 51, 71	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	625	LEU	5.2
1	A	572	GLU	5.1
1	A	571	ASP	4.9
1	A	629	HIS	4.9
1	A	686	GLU	4.4
1	A	72	GLY	4.1
1	A	685	VAL	4.1
1	A	688	ILE	3.9
1	A	646	ASN	3.8
1	A	533	THR	3.8
1	A	683	VAL	3.7
1	A	714	LEU	3.6
1	A	641	VAL	3.6
1	A	715	ALA	3.4
1	A	568	LYS	3.3
1	A	613	GLU	3.2
1	A	575	MET	3.2
1	A	570	THR	2.8
1	A	225	ALA	2.7
1	A	70	GLN	2.6
1	A	684	ARG	2.6
1	A	663	GLU	2.6
1	A	261	GLY	2.5
1	A	303	TYR	2.5
1	A	682	ALA	2.3
1	A	612	THR	2.3
1	A	610	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	573	TYR	2.3
1	A	639	ALA	2.2
1	A	262	TYR	2.2
1	A	619	GLY	2.2
1	A	535	ASP	2.2
1	A	614	ASP	2.2
1	A	637	THR	2.1
1	A	73	GLY	2.1
1	A	258	ILE	2.1
1	A	278	ILE	2.0
1	A	74	LYS	2.0
1	A	640	GLN	2.0
1	A	696	GLN	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)

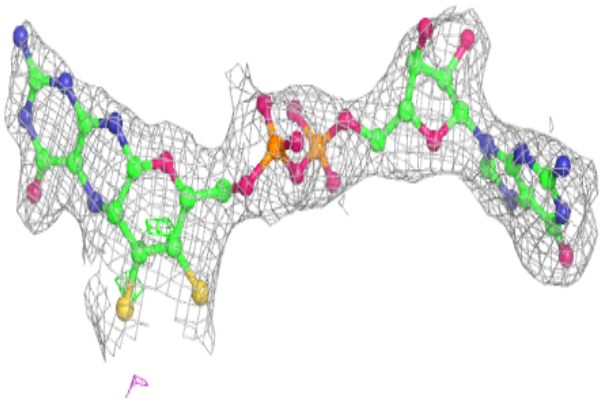
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

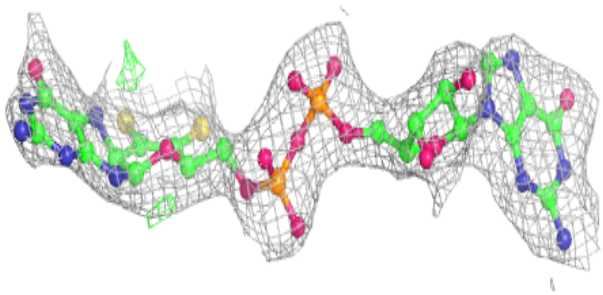
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	6MO	A	803	1/1	0.92	0.11	30,30,30,30	0
4	MGD	A	801	47/47	0.93	0.20	14,24,31,32	0
4	MGD	A	802	47/47	0.94	0.19	21,25,28,32	0
2	NO2	A	804	3/3	0.94	0.26	26,26,28,30	0
3	SF4	A	800	8/8	0.98	0.16	13,13,14,14	0

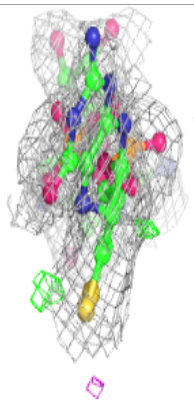
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MGD A 801:

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

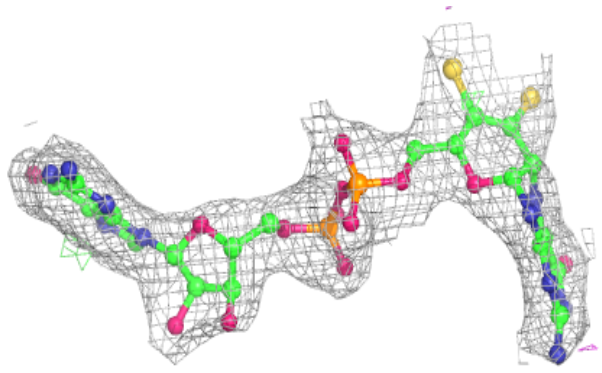


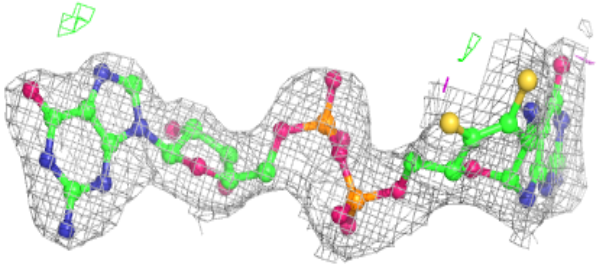


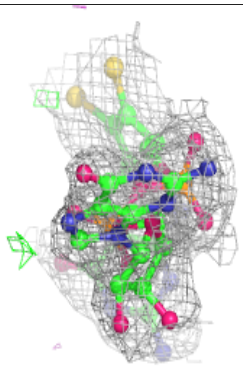


Electron density around MGD A 802:

$2mF_o$-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.