



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:23 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

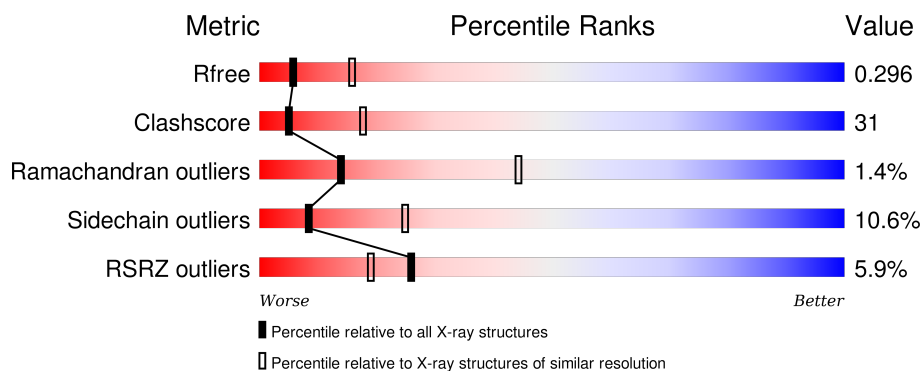
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

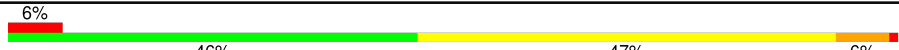
The reported resolution of this entry is 2.90 Å.

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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	715	

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 [i](#)

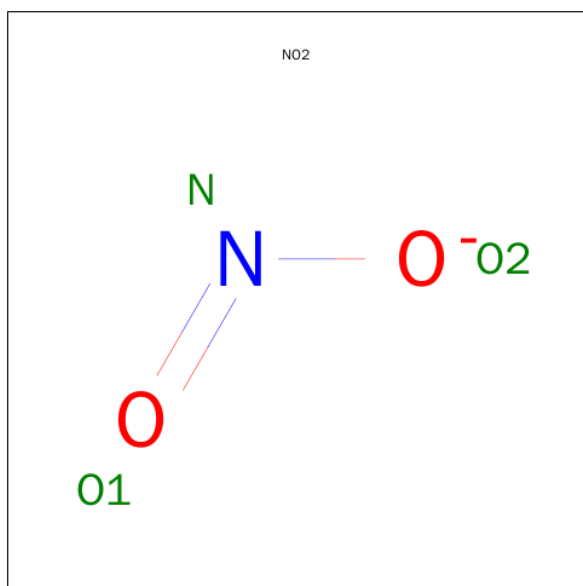
There are 6 unique types of molecules in this entry. The entry contains 5743 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

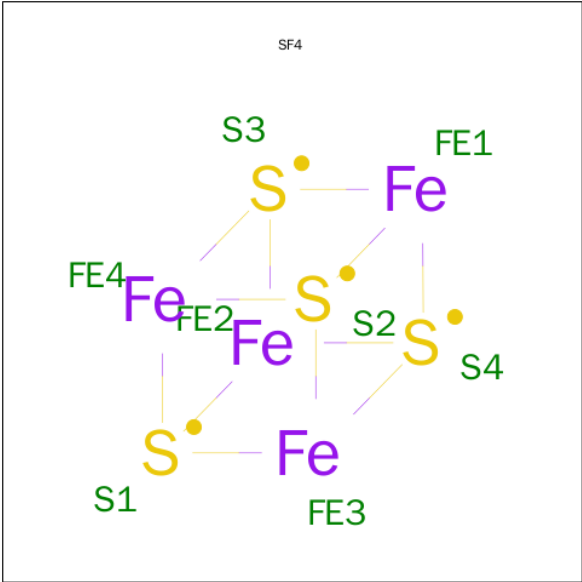
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	715	5575	3508	973	1060	33	1	0	0	0

- Molecule 2 is NITRITE ION (three-letter code: NO2) (formula: NO<sub>2</sub>).



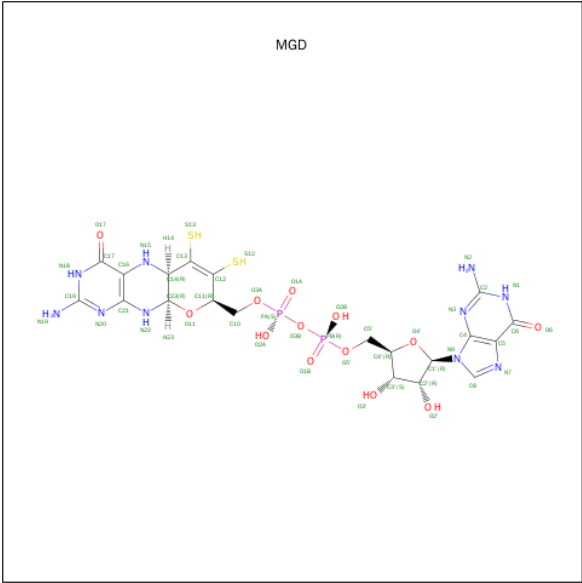
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
2	A	1	3	1	2	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).



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 1	Mo 1	0	0

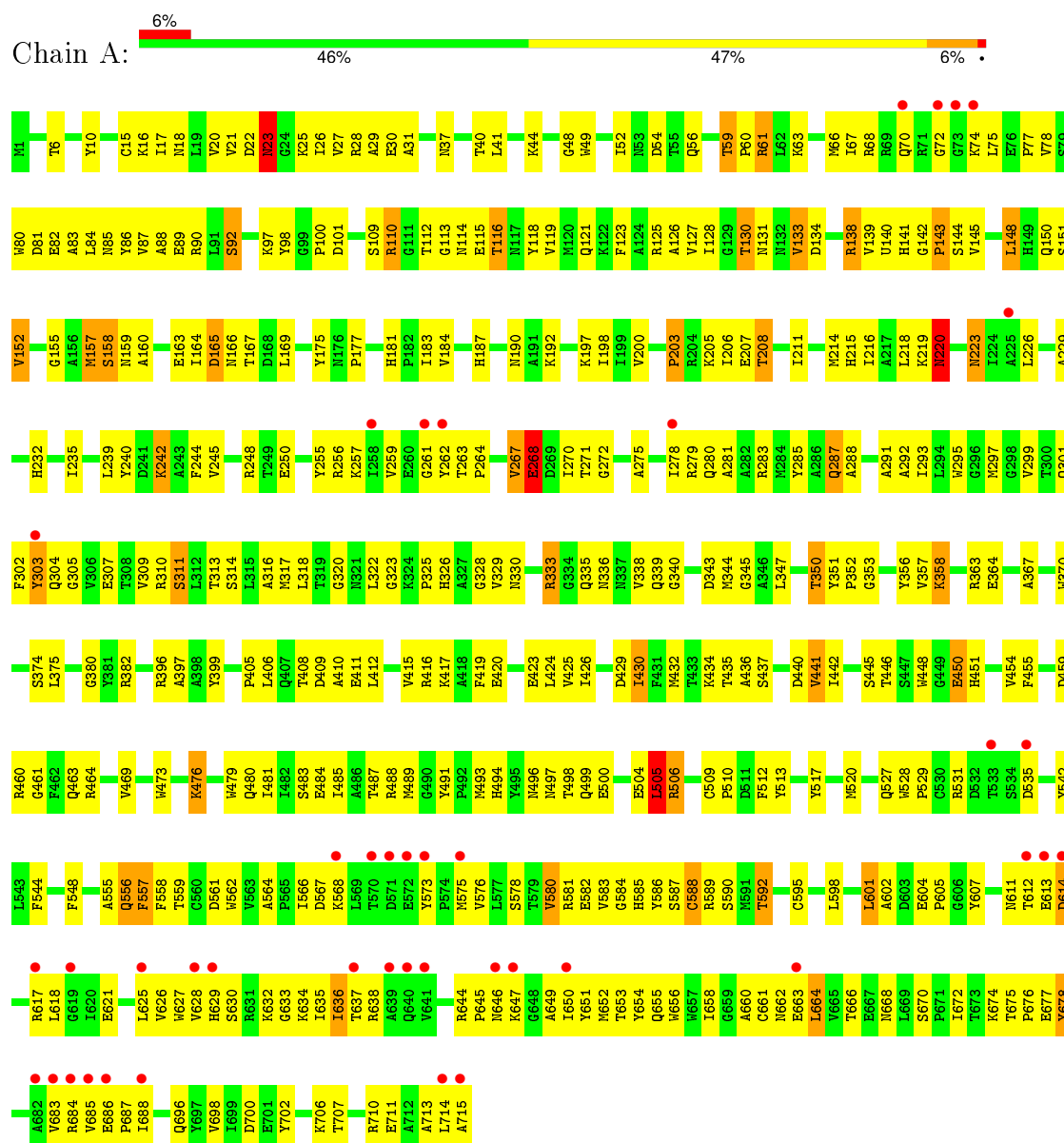
- Molecule 6 is water.

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

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.80 Å   146.80 Å   81.80 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.10 (at 2.90 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.192   ,   0.284 0.215   ,   0.296	Depositor DCC
$R_{free}$ test set	757 reflections (4.71%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.4	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 74.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 19260 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	5743	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, SEC, NO2, 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	0.61	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(°)	Ideal(°)
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 ⓘ

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:144:SER:O	1:A:148:LEU:HB2	1.89	0.73
1:A:140:SEC:SE	2:A:804:NO2:O2	2.57	0.73
1:A:256:ARG:HB3	1:A:256:ARG:HH11	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:HB3	1:A:333:ARG:NH1	2.06	0.71
1:A:499:GLN:HB2	1:A:517:TYR:CE2	2.26	0.70
1:A:396:ARG:O	1:A:423:GLU:HB2	1.91	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:H	1:A:223:ASN:HD22	1.40	0.68
1:A:628:VAL:HG22	1:A:685:VAL:HG22	1.76	0.67
1:A:605:PRO:HD3	1:A:698:VAL:HG11	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:HH11	1:A:283:ARG:HG3	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:702:TYR:CE1	1:A:706:LYS:HD2	2.31	0.65
1:A:625:LEU:O	1:A:688:ILE:HB	1.97	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:408:THR:HG22	1:A:654:TYR:HD2	1.63	0.63
1:A:85:ASN:O	1:A:89:GLU:HB2	1.98	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:229:ALA:HB2	1:A:267:VAL:HG21	1.81	0.62
1:A:109:SER:OG	1:A:338:VAL:HA	1.99	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:86:TYR:CE2	1:A:90:ARG:NH2	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:408:THR:HG21	4:A:801:MGD:O2A	2.01	0.61
1:A:344:MET:O	1:A:352:PRO:HB3	2.01	0.61
1:A:169:LEU:HD12	1:A:197:LYS:CE	2.31	0.61
1:A:220:ASN:H	1:A:220:ASN:HD22	1.46	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:115:GLU:OE2	1:A:454:VAL:HG23	2.03	0.58
1:A:479:TRP:NE1	1:A:498:THR:HG22	2.18	0.58
1:A:256:ARG:HH12	1:A:257:LYS:HZ2	1.50	0.58
1:A:67:ILE:HD11	1:A:83:ALA:HA	1.85	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:NH1	1:A:256:ARG:HB3	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:484:GLU:O	1:A:488:ARG:HG3	2.06	0.56
1:A:139:VAL:HG13	1:A:678:TYR:HE2	1.70	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:661:CYS:SG	1:A:662:ASN:N	2.79	0.56
1:A:575:MET:SD	1:A:650:ILE:HG23	2.46	0.56
1:A:203:PRO:HB3	1:A:220:ASN:HD21	1.70	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:626:VAL:HG23	1:A:687:PRO:HA	1.87	0.55
1:A:239:LEU:HD22	1:A:287:GLN:HE22	1.71	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:585:HIS:HA	1:A:592:THR:HG21	1.90	0.54
1:A:192:LYS:HB2	1:A:198:ILE:HD11	1.89	0.54
1:A:626:VAL:HG22	1:A:627:TRP:H	1.73	0.54
1:A:110:ARG:HD2	1:A:336:ASN:ND2	2.23	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:163:GLU:HA	6:A:841:HOH:O	2.08	0.53
1:A:63:LYS:HG2	1:A:473:TRP:CE2	2.43	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:220:ASN:N	1:A:220:ASN:HD22	2.05	0.52
1:A:208:THR:O	1:A:211:ILE:HG12	2.09	0.52
1:A:663:GLU:HB3	1:A:664:LEU:HD23	1.90	0.52
1:A:506:ARG:HD2	1:A:513:TYR:O	2.09	0.52
1:A:582:GLU:OE2	1:A:656:TRP:HZ2	1.93	0.52
1:A:358:LYS:NZ	1:A:358:LYS:HB3	2.24	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:644:ARG:H	1:A:645:PRO:HD2	1.75	0.52
1:A:203:PRO:HB3	1:A:220:ASN:ND2	2.24	0.52
1:A:626:VAL:HG22	1:A:627:TRP:N	2.24	0.52
1:A:56:GLN:OE1	1:A:710:ARG:NH1	2.43	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:635:ILE:HG12	1:A:664:LEU:CD2	2.34	0.51
1:A:351:TYR:HB3	1:A:352:PRO:HD2	1.90	0.51
1:A:702:TYR:CE2	1:A:706:LYS:HD2	2.44	0.51
1:A:317:MET:CE	1:A:555:ALA:HB1	2.40	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:583:VAL:HA	4:A:802:MGD:N19	2.26	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:429:ASP:OD1	4:A:801:MGD:H1'	2.11	0.50
1:A:139:VAL:HG13	1:A:678:TYR:CE2	2.46	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:279:ARG:HB3	1:A:283:ARG:HH12	1.75	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: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:498:THR:HG23	6:A:853:HOH:O	2.12	0.50
1:A:18:ASN:HB2	1:A:30:GLU:HG3	1.93	0.50
1:A:654:TYR:HB2	1:A:662:ASN:ND2	2.27	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:140:SEC:SE	1:A:141:HIS:CD2	3.01	0.49
1:A:293:ILE:CG2	1:A:295:TRP:HE3	2.25	0.49
1:A:203:PRO:HG3	1:A:218:LEU:O	2.13	0.49
1:A:598:LEU:HA	1:A:601:LEU:HD12	1.95	0.49
1:A:581:ARG:CZ	4:A:802:MGD:H102	2.42	0.49
1:A:322:LEU:HD23	1:A:328:GLY:HA2	1.94	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:461:GLY:HA2	1:A:527:GLN:HA	1.95	0.48
1:A:21:VAL:HG13	1:A:25:LYS:O	2.13	0.48
1:A:363:ARG:HG2	1:A:375:LEU:HB2	1.95	0.48
1:A:617:ARG:O	1:A:617:ARG:HG2	2.14	0.48
1:A:333:ARG:HH11	1:A:333:ARG:CB	2.24	0.48
1:A:70:GLN:HG2	1:A:72:GLY:H	1.78	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:513:TYR:HD2	1:A:531:ARG:O	1.96	0.47
1:A:6:THR:CG2	1:A:17:ILE:HB	2.44	0.47
1:A:98:TYR:CD2	1:A:396:ARG:HD3	2.49	0.47
1:A:279:ARG:HH11	1:A:279:ARG:HG2	1.77	0.47
1:A:37:ASN:HB2	1:A:40:THR:O	2.14	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: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:29:ALA:HB2	1:A:49:TRP:CD1	2.49	0.47
1:A:617:ARG:HB3	1:A:617:ARG:CZ	2.44	0.47
1:A:586:TYR:N	1:A:592:THR:HG21	2.26	0.47
1:A:419:PHE:CZ	1:A:435:THR:HG23	2.49	0.47
1:A:627:TRP:CD1	1:A:688:ILE:HD11	2.50	0.47
1:A:60:PRO:HG2	1:A:713:ALA:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:PRO:HB2	1:A:714:LEU:HD21	1.97	0.47
1:A:338:VAL:HG13	1:A:339:GLN:N	2.29	0.47
1:A:80:TRP:CZ2	1:A:476:LYS:HD2	2.50	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:310:ARG:NH1	1:A:558:PHE:HB2	2.31	0.46
1:A:169:LEU:HD12	1:A:197:LYS:HZ1	1.80	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:654:TYR:CE2	4:A:801:MGD:O11	2.68	0.46
1:A:397:ALA:HA	1:A:424:LEU:O	2.16	0.46
1:A:630:SER:CB	1:A:664:LEU:HB3	2.39	0.46
1:A:430:ILE:HD12	1:A:445:SER:OG	2.16	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:614:ASP:HB2	1:A:617:ARG:HH12	1.81	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:148:LEU:HB3	1:A:155:GLY:HA2	1.97	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:158:SER:OG	1:A:159:ASN:OD1	2.29	0.46
1:A:333:ARG:HG3	1:A:339:GLN:HE21	1.80	0.45
1:A:307:GLU:O	1:A:311:SER:HB2	2.16	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:582:GLU:HG3	1:A:583:VAL:O	2.17	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: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:581:ARG:NH2	4:A:801:MGD:O17	2.50	0.44
1:A:264:PRO:HG2	1:A:279:ARG:NH1	2.31	0.44
1:A:650:ILE:HD11	1:A:683:VAL:HG21	2.00	0.44
1:A:200:VAL:CG1	1:A:206:ILE:HD11	2.47	0.44
1:A:303:TYR:C	1:A:305:GLY:H	2.19	0.44
1:A:114:ASN:O	1:A:344:MET:HG3	2.16	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:632:LYS:HB2	1:A:664:LEU:HA	1.99	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:77:PRO:HD3	1:A:715:ALA:OXT	2.17	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: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: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:566:ILE:HG22	1:A:567:ASP:N	2.33	0.43
1:A:283:ARG:NH1	1:A:283:ARG:HG3	2.29	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: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:483:SER:HA	1:A:493:MET:CE	2.49	0.42
1:A:17:ILE:HG22	1:A:18:ASN:N	2.34	0.42
1:A:109:SER:CB	1:A:338:VAL:HA	2.48	0.42
1:A:676:PRO:CG	1:A:678:TYR:CE2	3.02	0.42
1:A:637:THR:HG21	1:A:652:MET:CE	2.49	0.42
1:A:160:ALA:HB3	1:A:163:GLU:HB2	2.00	0.42
1:A:110:ARG:HA	1:A:110:ARG:HD2	1.82	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:340:GLY:O	1:A:343:ASP:HB2	2.20	0.42
1:A:288:ALA:HB3	1:A:291:ALA:HB2	2.01	0.42
1:A:587:SER:O	1:A:655:GLN:HA	2.19	0.42
1:A:87:VAL:HG13	1:A:426:ILE:HD13	2.02	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:604:GLU:OE1	1:A:604:GLU:HA	2.20	0.42
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:310:ARG:HB3	1:A:558:PHE:HD2	1.85	0.41
1:A:232:HIS:CD2	1:A:264:PRO:HD3	2.55	0.41
1:A:152:VAL:HG22	1:A:548:PHE:CD1	2.55	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: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: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: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:126:ALA:HB2	1:A:370:TRP:CE3	2.55	0.41
1:A:101:ASP:HA	1:A:130:THR:CG2	2.50	0.41
1:A:632:LYS:HE3	1:A:666:THR:OG1	2.20	0.41
1:A:310:ARG:HD2	1:A:558:PHE:HB3	2.01	0.41
1:A:215:HIS:CD2	1:A:215:HIS:C	2.93	0.41
1:A:358:LYS:HZ3	1:A:358:LYS:HB3	1.85	0.41
1:A:566:ILE:CD1	1:A:668:ASN:HB3	2.50	0.41
1:A:22:ASP:O	1:A:23:ASN:HB2	2.20	0.41
1:A:497:ASN:N	1:A:497:ASN:OD1	2.54	0.41
1:A:607:TYR:HE1	1:A:638:ARG:HG2	1.85	0.41
1:A:417:LYS:HD2	1:A:420:GLU:OE1	2.21	0.41
1:A:584:GLY:O	1:A:598:LEU:HD13	2.20	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: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:633:GLY:C	1:A:664:LEU:HD22	2.41	0.40
1:A:68:ARG:NH2	1:A:437:SER:O	2.52	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:183:ILE:O	1:A:187:HIS:CD2	2.70	0.40
1:A:406:LEU:HD23	1:A:406:LEU:HA	1.77	0.40
1:A:451:HIS:C	1:A:451:HIS:CD2	2.94	0.40
1:A:20:VAL:HG21	1:A:28:ARG:CZ	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	14	44

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

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%)	8	25

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

Some 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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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$
3	SF4	A	800	1	0,12,12	0.00	-	0,24,24	0.00	-
4	MGD	A	801	5	38,52,52	1.26	4 (10%)	43,81,81	2.81	15 (34%)
4	MGD	A	802	5	38,52,52	1.93	3 (7%)	43,81,81	2.31	14 (32%)
2	NO2	A	804	5	2,2,2	0.23	0	1,1,1	0.34	0

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	-	0/0/48/48	0/6/5/5
4	MGD	A	801	5	-	0/18/66/66	0/6/6/6
4	MGD	A	802	5	-	0/18/66/66	0/6/6/6
2	NO2	A	804	5	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	802	MGD	C23-C14	-9.45	1.46	1.53
4	A	801	MGD	O11-C11	-2.10	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	MGD	C23-C14	-2.04	1.52	1.53
4	A	801	MGD	C6-N1	2.58	1.37	1.33
4	A	802	MGD	C17-N18	2.76	1.38	1.33
4	A	802	MGD	C6-N1	3.21	1.39	1.33
4	A	801	MGD	C17-N18	3.68	1.39	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	802	MGD	C5-C6-N1	-6.45	114.77	123.59
4	A	801	MGD	C5-C6-N1	-5.96	115.44	123.59
4	A	801	MGD	N3-C2-N1	-4.77	120.18	127.44
4	A	802	MGD	C21-N22-C23	-4.58	114.69	123.67
4	A	801	MGD	N18-C19-N20	-3.78	119.34	125.53
4	A	801	MGD	C21-N22-C23	-3.76	116.30	123.67
4	A	802	MGD	N3-C2-N1	-3.56	122.03	127.44
4	A	802	MGD	N18-C19-N20	-3.44	119.90	125.53
4	A	802	MGD	C4'-O4'-C1'	-3.14	106.27	109.72
4	A	801	MGD	C6-C5-C4	-2.74	117.62	120.90
4	A	801	MGD	PA-O3B-PB	-2.67	125.24	132.73
4	A	802	MGD	C2'-C1'-N9	-2.65	110.25	114.29
4	A	802	MGD	C6-C5-C4	-2.56	117.84	120.90
4	A	801	MGD	C16-N15-C14	-2.01	113.23	118.65
4	A	802	MGD	N19-C19-N18	2.08	120.65	117.20
4	A	801	MGD	O5'-C5'-C4'	2.41	118.02	109.12
4	A	801	MGD	C4-C5-N7	2.95	112.19	109.48
4	A	802	MGD	O4'-C1'-N9	3.00	114.38	108.10
4	A	802	MGD	C17-N18-C19	3.16	120.32	115.94
4	A	801	MGD	C16-C21-N22	3.21	121.71	118.34
4	A	802	MGD	C16-C21-N22	3.27	121.76	118.34
4	A	801	MGD	C19-N20-C21	3.58	122.58	114.54
4	A	802	MGD	C19-N20-C21	3.61	122.66	114.54
4	A	802	MGD	C17-C16-C21	4.61	118.73	114.56
4	A	802	MGD	C6-N1-C2	4.91	122.75	115.94
4	A	801	MGD	C17-C16-C21	4.96	119.05	114.56
4	A	801	MGD	C17-N18-C19	5.32	123.32	115.94
4	A	801	MGD	C6-N1-C2	6.41	124.83	115.94
4	A	801	MGD	O11-C23-C14	8.26	114.61	108.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

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

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	714/715 (99%)	0.28	42 (5%) 26 19	5, 22, 51, 71	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	572	GLU	5.4
1	A	625	LEU	4.9
1	A	571	ASP	4.8
1	A	629	HIS	4.5
1	A	686	GLU	4.3
1	A	72	GLY	4.1
1	A	685	VAL	4.1
1	A	688	ILE	4.1
1	A	646	ASN	4.0
1	A	533	THR	3.8
1	A	683	VAL	3.6
1	A	714	LEU	3.5
1	A	641	VAL	3.4
1	A	613	GLU	3.4
1	A	715	ALA	3.3
1	A	568	LYS	3.3
1	A	575	MET	3.2
1	A	570	THR	3.0
1	A	225	ALA	2.8
1	A	70	GLN	2.7
1	A	663	GLU	2.7
1	A	303	TYR	2.5
1	A	684	ARG	2.5
1	A	639	ALA	2.4
1	A	573	TYR	2.3
1	A	640	GLN	2.3
1	A	682	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	637	THR	2.3
1	A	612	THR	2.3
1	A	278	ILE	2.3
1	A	261	GLY	2.3
1	A	535	ASP	2.2
1	A	619	GLY	2.2
1	A	262	TYR	2.2
1	A	74	LYS	2.1
1	A	650	ILE	2.1
1	A	73	GLY	2.1
1	A	647	LYS	2.1
1	A	258	ILE	2.1
1	A	628	VAL	2.0
1	A	617	ARG	2.0
1	A	614	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NO2	A	804	3/3	0.94	0.25	0.20	26,26,28,30	0
4	MGD	A	802	47/47	0.94	0.20	-0.63	21,25,28,32	0
4	MGD	A	801	47/47	0.93	0.19	-0.68	14,24,31,32	0
3	SF4	A	800	8/8	0.98	0.16	-1.06	13,13,14,14	0
5	6MO	A	803	1/1	0.92	0.11	-	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.