



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:11 pm BST

PDB ID : 1LLZ
Title : Structural studies on the synchronization of catalytic centers in glutamate synthase: reduced enzyme
Authors : van den Heuvel, R.H.; Ferrari, D.; Bossi, R.T.; Ravasio, S.; Curti, B.; Vanoni, M.A.; Florencio, F.J.; Mattevi, A.
Deposited on : 2002-04-30
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

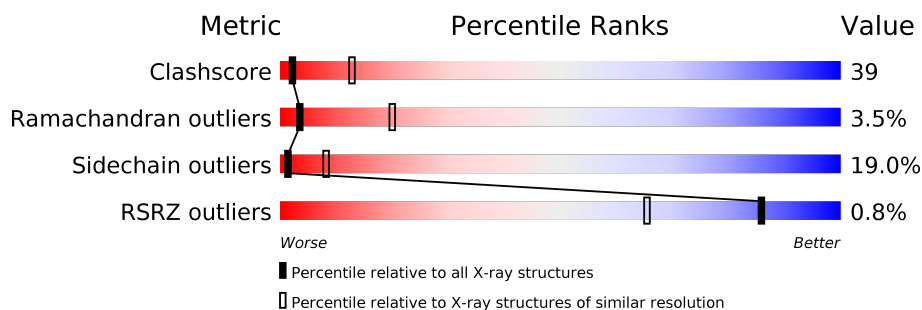
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1520	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 44%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 44%; width: 40%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 84%; width: 12%; height: 10px; background-color: orange;"></div> <div style="position: absolute; top: 0; left: 96%; width: 4%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: 0; left: 100%; width: 0; height: 0; border-left: 5px solid transparent; border-right: 5px solid transparent; border-bottom: 10px solid grey;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%; font-size: small;"> 44% 40% 12% .. </div> </div>

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
3	F3S	A	2072	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11349 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.

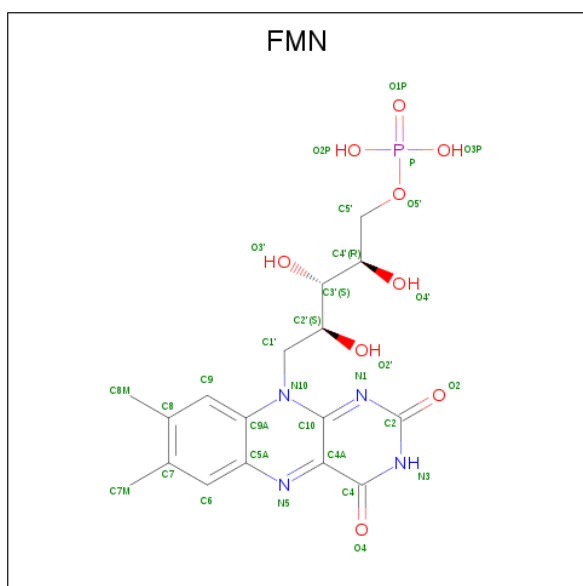
- Molecule 1 is a protein called Ferredoxin-dependent glutamate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1475	11311	7137	1970	2148	56	0	0	0

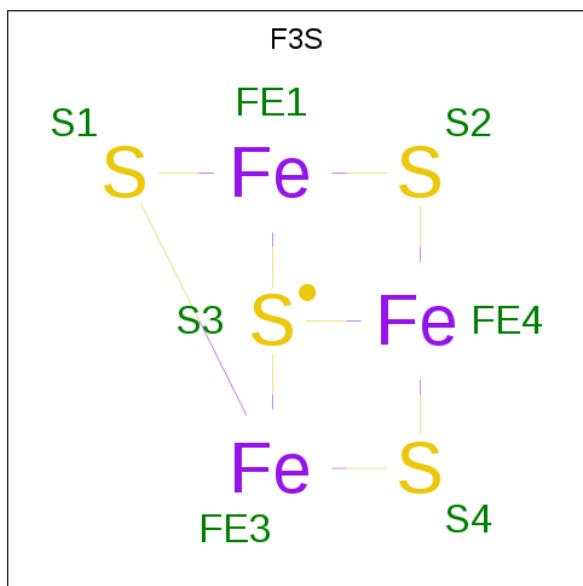
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	578	ASP	THR	CONFLICT	UNP P55038
A	581	THR	ASP	CONFLICT	UNP P55038
A	1507	ASN	GLY	CONFLICT	UNP P55038

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



- Molecule 3 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).

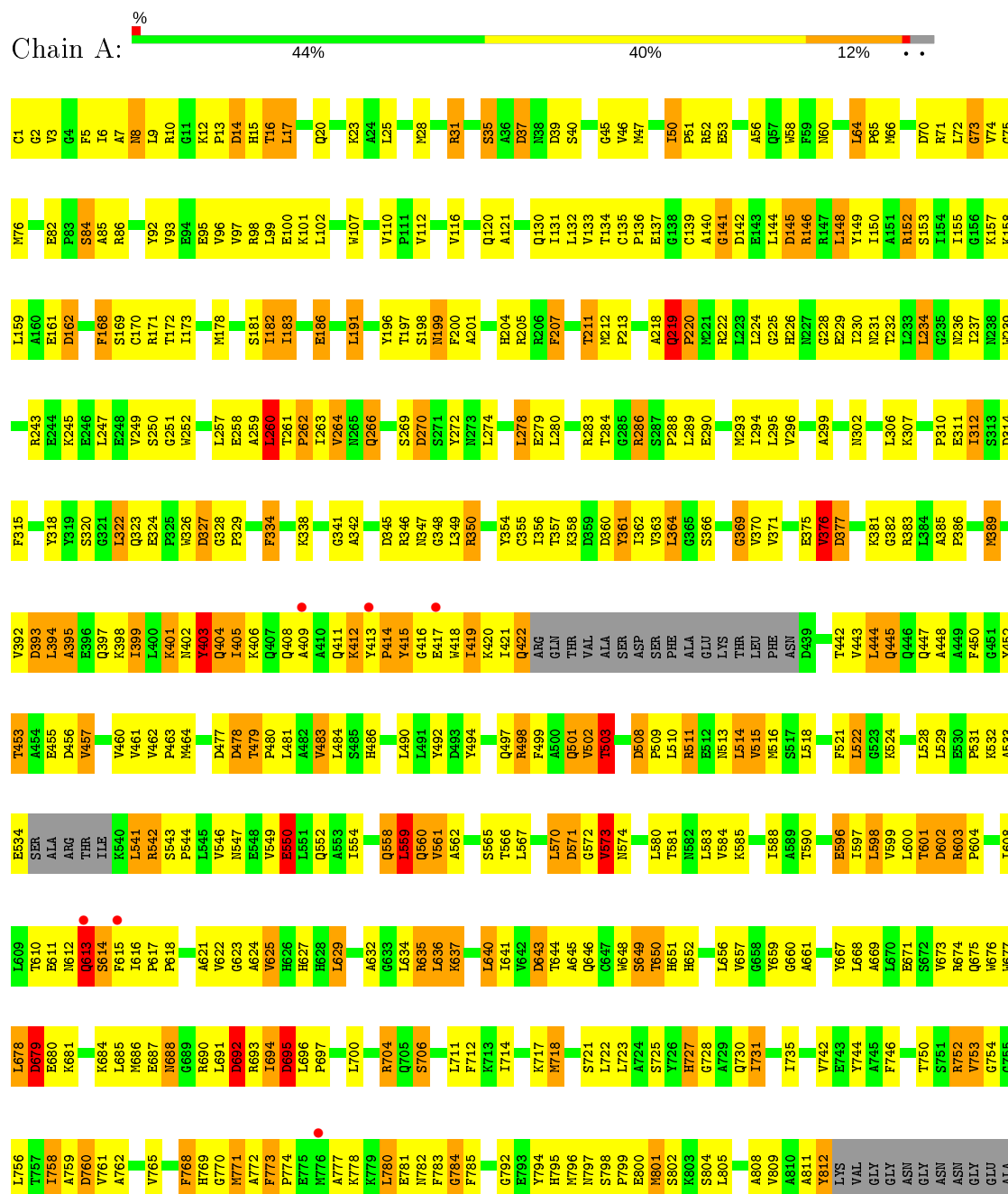


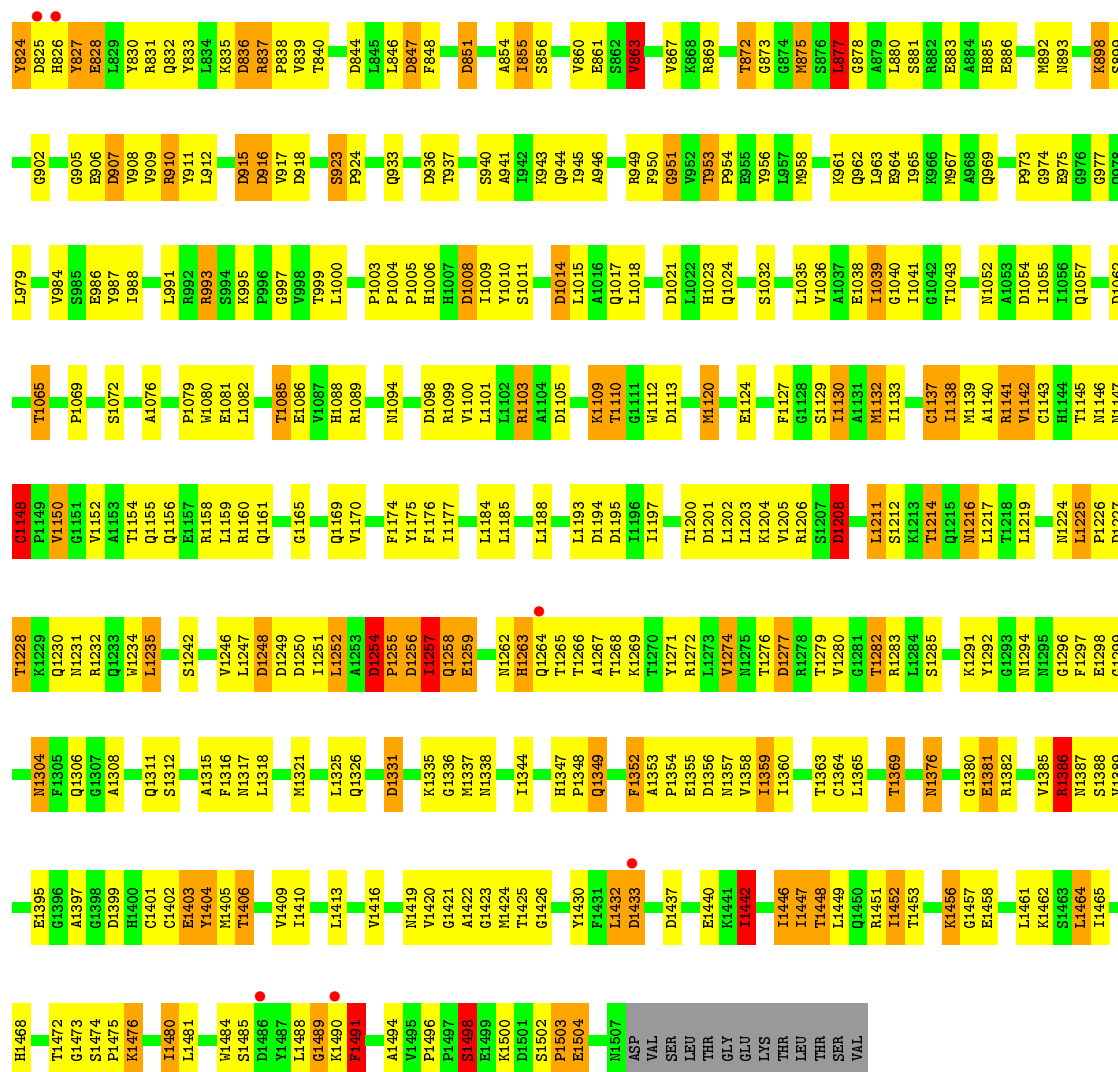
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			7	3	4		

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 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: Ferredoxin-dependent glutamate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	167.00Å 167.00Å 221.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	129.10 – 3.00 55.24 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (129.10-3.00) 96.6 (55.24-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.1.06	Depositor
R, R_{free}	0.217 , 0.269 0.213 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	68.4	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11349	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, F3S

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	0.82	6/11533 (0.1%)	1.07	58/15639 (0.4%)

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	12

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	796	MET	CG-SD	7.39	2.00	1.81
1	A	1433	ASP	CB-CG	7.00	1.66	1.51
1	A	550	GLU	CD-OE2	5.97	1.32	1.25
1	A	875	MET	CG-SD	-5.86	1.66	1.81
1	A	1148	CYS	CB-SG	5.62	1.91	1.82
1	A	552	GLN	CG-CD	5.38	1.63	1.51

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	327	ASP	CB-CG-OD2	8.84	126.25	118.30
1	A	14	ASP	CB-CG-OD2	8.53	125.97	118.30
1	A	1248	ASP	CB-CG-OD2	7.95	125.45	118.30
1	A	679	ASP	CB-CG-OD2	7.74	125.27	118.30
1	A	1062	ASP	CB-CG-OD1	-7.51	111.54	118.30
1	A	1008	ASP	CB-CG-OD2	7.36	124.92	118.30
1	A	1062	ASP	CB-CG-OD2	7.21	124.79	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1277	ASP	CB-CG-OD2	7.10	124.69	118.30
1	A	1098	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	145	ASP	CB-CG-OD2	6.95	124.56	118.30
1	A	877	LEU	CA-CB-CG	-6.88	99.47	115.30
1	A	191	LEU	CA-CB-CG	6.87	131.10	115.30
1	A	695	ASP	CB-CG-OD2	6.84	124.46	118.30
1	A	1148	CYS	N-CA-CB	6.53	122.34	110.60
1	A	875	MET	CA-CB-CG	-6.50	102.26	113.30
1	A	694	ILE	CG1-CB-CG2	-6.47	97.16	111.40
1	A	643	ASP	CB-CG-OD2	6.35	124.02	118.30
1	A	270	ASP	CB-CG-OD2	6.33	123.99	118.30
1	A	1399	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	1227	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	907	ASP	CB-CG-OD2	6.24	123.91	118.30
1	A	501	GLN	C-N-CA	-6.23	106.12	121.70
1	A	918	ASP	CB-CG-OD2	6.06	123.76	118.30
1	A	1014	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	847	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	1250	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	1256	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	692	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	98	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	A	573	VAL	N-CA-C	-5.83	95.25	111.00
1	A	220	PRO	N-CD-CG	-5.78	94.53	103.20
1	A	844	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	1433	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	760	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	1105	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	836	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	162	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	498	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	851	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	1008	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	A	1252	LEU	CA-CB-CG	5.45	127.83	115.30
1	A	1201	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	1254	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	1437	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	37	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	1195	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	910	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	350	ARG	NE-CZ-NH1	-5.25	117.68	120.30
1	A	1208	ASP	CB-CG-OD2	5.21	122.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	GLY	N-CA-C	-5.15	100.22	113.10
1	A	219	GLN	N-CA-C	5.14	124.89	111.00
1	A	508	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	559	LEU	CB-CG-CD1	5.09	119.65	111.00
1	A	1138	ILE	CG1-CB-CG2	5.09	122.59	111.40
1	A	219	GLN	CB-CA-C	-5.08	100.25	110.40
1	A	1386	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	70	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	142	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1137	CYS	Peptide
1	A	218	ALA	Peptide
1	A	219	GLN	Peptide
1	A	369	GLY	Peptide
1	A	403	TYR	Peptide
1	A	445	GLN	Peptide
1	A	502	VAL	Peptide
1	A	560	GLN	Peptide
1	A	572	GLY	Peptide
1	A	873	GLY	Peptide
1	A	951	GLY	Peptide
1	A	997	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	11311	0	11256	889	0
2	A	31	0	19	0	0
3	A	7	0	0	12	0
All	All	11349	0	11275	889	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 39.

All (889) 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:559:LEU:CD2	1:A:560:GLN:O	1.67	1.42
1:A:1263:HIS:CE1	1:A:1297:PHE:HA	1.60	1.37
1:A:413:TYR:O	1:A:415:TYR:N	1.62	1.32
1:A:263:ILE:HD12	1:A:280:LEU:HD22	1.27	1.15
1:A:686:MET:O	1:A:692:ASP:HB2	1.44	1.15
1:A:1347:HIS:ND1	1:A:1348:PRO:HD2	1.63	1.14
1:A:1024:GLN:HE22	1:A:1246:VAL:HG11	1.09	1.10
1:A:377:ASP:O	1:A:377:ASP:OD1	1.68	1.10
1:A:768:PHE:HE2	1:A:771:MET:HG2	1.04	1.10
1:A:583:LEU:HD12	1:A:616:ILE:HD13	1.33	1.10
1:A:312:ILE:HG21	1:A:405:ILE:CD1	1.80	1.10
1:A:1254:ASP:HB2	1:A:1255:PRO:CD	1.82	1.09
1:A:559:LEU:HD23	1:A:560:GLN:O	1.44	1.09
1:A:558:GLN:HA	1:A:558:GLN:OE1	1.32	1.09
1:A:1347:HIS:CG	1:A:1348:PRO:HD2	1.88	1.08
1:A:768:PHE:CE2	1:A:771:MET:HG2	1.88	1.08
1:A:559:LEU:HD21	1:A:560:GLN:O	1.33	1.07
1:A:453:THR:HB	1:A:456:ASP:OD2	1.54	1.07
1:A:312:ILE:HG21	1:A:405:ILE:HD12	1.09	1.07
1:A:611:GLU:C	1:A:613:GLN:H	1.43	1.06
1:A:182:ILE:HD13	1:A:182:ILE:H	1.17	1.06
1:A:1263:HIS:HE1	1:A:1297:PHE:CA	1.67	1.05
1:A:773:PHE:HB2	1:A:774:PRO:HD3	1.36	1.05
1:A:559:LEU:HG	1:A:560:GLN:N	1.70	1.05
1:A:953:THR:CG2	1:A:1294:ASN:HD21	1.70	1.03
1:A:1491:PHE:HD1	1:A:1491:PHE:O	1.39	1.03
1:A:1432:LEU:O	1:A:1432:LEU:HG	1.59	1.03
1:A:1254:ASP:CB	1:A:1255:PRO:HD2	1.89	1.02
1:A:993:ARG:HH11	1:A:993:ARG:HG3	1.24	1.01
1:A:608:ILE:HG21	1:A:615:PHE:HZ	1.26	1.01
1:A:358:LYS:HD2	1:A:377:ASP:OD2	1.61	1.00
1:A:768:PHE:CD2	1:A:771:MET:HB2	1.96	0.99
1:A:878:GLY:HA2	1:A:988:ILE:HD12	1.40	0.99
1:A:953:THR:HG21	1:A:1294:ASN:HD21	1.23	0.99
1:A:760:ASP:OD2	1:A:1214:THR:HG23	1.63	0.99
1:A:445:GLN:HG3	1:A:777:ALA:HB1	1.44	0.98
1:A:443:VAL:HG11	1:A:675:GLN:HG3	1.43	0.98
1:A:1148:CYS:SG	3:A:2072:F3S:S3	2.61	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1355:GLU:HG2	1:A:1476:LYS:CB	1.93	0.97
1:A:369:GLY:HA3	1:A:1308:ALA:CB	1.92	0.97
1:A:676:TRP:HE1	1:A:690:ARG:HH12	1.05	0.96
1:A:311:GLU:HB3	1:A:409:ALA:HB1	1.48	0.95
1:A:1154:THR:HG22	1:A:1156:GLN:H	1.32	0.95
1:A:415:TYR:CD1	1:A:416:GLY:N	2.35	0.95
1:A:444:LEU:O	1:A:445:GLN:HG2	1.67	0.94
1:A:182:ILE:HD13	1:A:182:ILE:N	1.82	0.94
1:A:657:VAL:HG11	1:A:723:LEU:HD11	1.48	0.94
1:A:480:PRO:HB3	1:A:840:THR:HA	1.49	0.94
1:A:1254:ASP:HB2	1:A:1255:PRO:HD2	0.96	0.94
1:A:611:GLU:C	1:A:613:GLN:N	2.19	0.93
1:A:1355:GLU:HG2	1:A:1476:LYS:HB2	1.47	0.93
1:A:186:GLU:HA	1:A:186:GLU:OE1	1.66	0.93
1:A:312:ILE:CG2	1:A:405:ILE:HD12	1.97	0.93
1:A:1387:ASN:HB3	1:A:1405:MET:CE	1.98	0.93
1:A:383:ARG:NH1	1:A:1380:GLY:CA	2.33	0.92
1:A:100:GLU:O	1:A:102:LEU:N	2.03	0.91
1:A:182:ILE:H	1:A:182:ILE:CD1	1.83	0.91
1:A:1140:ALA:HB3	3:A:2072:F3S:S1	2.10	0.91
1:A:1259:GLU:HA	1:A:1265:THR:HB	1.53	0.90
1:A:954:PRO:HG2	1:A:1318:LEU:HD21	1.52	0.90
1:A:567:LEU:HD21	1:A:615:PHE:CE2	2.07	0.90
1:A:383:ARG:HG2	1:A:1358:VAL:HG21	1.54	0.89
1:A:1263:HIS:HE1	1:A:1297:PHE:HA	0.76	0.89
1:A:1338:ASN:HA	1:A:1369:THR:HG22	1.54	0.89
1:A:1262:ASN:O	1:A:1264:GLN:N	2.05	0.88
1:A:1491:PHE:CD1	1:A:1491:PHE:O	2.26	0.88
1:A:1263:HIS:NE2	1:A:1298:GLU:HG3	1.89	0.88
1:A:1347:HIS:CE1	1:A:1348:PRO:HD2	2.08	0.87
1:A:773:PHE:CB	1:A:774:PRO:HD3	2.04	0.87
1:A:478:ASP:OD2	1:A:1141:ARG:NH2	2.05	0.87
1:A:404:GLN:HA	1:A:404:GLN:OE1	1.75	0.87
1:A:338:LYS:O	1:A:394:LEU:HD23	1.75	0.87
1:A:1138:ILE:HG22	1:A:1139:MET:N	1.89	0.86
1:A:1387:ASN:HB3	1:A:1405:MET:HE2	1.55	0.86
1:A:635:ARG:CG	1:A:635:ARG:HH11	1.88	0.86
1:A:311:GLU:CB	1:A:409:ALA:HB1	2.05	0.86
1:A:509:PRO:HA	1:A:516:MET:CE	2.04	0.86
1:A:802:SER:HB2	1:A:1133:ILE:HG23	1.58	0.86
1:A:567:LEU:HD21	1:A:615:PHE:HE2	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:PHE:HE2	1:A:771:MET:CG	1.87	0.85
1:A:383:ARG:NH1	1:A:1380:GLY:HA2	1.90	0.84
1:A:450:PHE:CD2	1:A:645:ALA:HB3	2.13	0.84
1:A:152:ARG:HH12	1:A:168:PHE:N	1.76	0.84
1:A:418:TRP:CE3	1:A:418:TRP:O	2.30	0.84
1:A:524:LYS:HB2	1:A:637:LYS:O	1.78	0.84
1:A:559:LEU:HD22	1:A:596:GLU:H	1.42	0.84
1:A:258:GLU:O	1:A:261:THR:OG1	1.96	0.83
1:A:768:PHE:HD2	1:A:771:MET:HB2	1.39	0.83
1:A:878:GLY:HA2	1:A:988:ILE:CD1	2.07	0.83
1:A:1081:GLU:HG3	1:A:1120:MET:HE1	1.61	0.83
1:A:773:PHE:HB2	1:A:774:PRO:CD	2.07	0.83
1:A:28:MET:CE	1:A:31:ARG:HD2	2.08	0.82
1:A:152:ARG:HH12	1:A:168:PHE:H	1.26	0.82
1:A:376:VAL:HA	1:A:1349:GLN:O	1.80	0.82
1:A:1360:ILE:HG23	1:A:1364:CYS:SG	2.20	0.81
1:A:608:ILE:HG21	1:A:615:PHE:CZ	2.15	0.81
1:A:660:GLY:O	1:A:727:HIS:HE1	1.63	0.81
1:A:1103:ARG:HH11	1:A:1103:ARG:HG3	1.46	0.81
1:A:419:ILE:HG22	1:A:420:LYS:N	1.94	0.81
1:A:676:TRP:HE1	1:A:690:ARG:NH1	1.78	0.80
1:A:1130:ILE:H	1:A:1130:ILE:HD13	1.44	0.80
1:A:1387:ASN:HD22	1:A:1405:MET:HE1	1.44	0.80
1:A:611:GLU:O	1:A:613:GLN:N	2.14	0.80
1:A:445:GLN:HG3	1:A:777:ALA:CB	2.11	0.80
1:A:804:SER:O	1:A:826:HIS:HB3	1.82	0.80
1:A:616:ILE:CG2	1:A:621:ALA:HB2	2.13	0.79
1:A:770:GLY:O	1:A:774:PRO:HD2	1.83	0.79
1:A:768:PHE:CE2	1:A:771:MET:CG	2.65	0.79
1:A:261:THR:HB	1:A:262:PRO:HD3	1.64	0.78
1:A:414:PRO:O	1:A:418:TRP:N	2.13	0.78
1:A:1101:LEU:HD21	1:A:1124:GLU:HG3	1.63	0.78
1:A:847:ASP:HB2	1:A:1206:ARG:HG3	1.66	0.78
1:A:1387:ASN:HD22	1:A:1405:MET:CE	1.96	0.78
1:A:886:GLU:HA	1:A:910:ARG:NH2	1.97	0.78
1:A:768:PHE:HE1	1:A:783:PHE:HZ	1.30	0.77
1:A:1355:GLU:HG2	1:A:1476:LYS:HB3	1.67	0.77
1:A:1024:GLN:NE2	1:A:1246:VAL:HG11	1.94	0.77
1:A:383:ARG:NH2	1:A:1381:GLU:OE2	2.18	0.77
1:A:1424:MET:O	1:A:1446:ILE:HD11	1.86	0.76
1:A:608:ILE:CG2	1:A:615:PHE:HZ	1.98	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:ARG:HG3	1:A:635:ARG:NH1	2.00	0.76
1:A:383:ARG:NH1	1:A:1380:GLY:HA3	1.98	0.76
1:A:447:GLN:O	1:A:452:TYR:HB2	1.85	0.76
1:A:514:LEU:HD12	1:A:515:VAL:N	1.99	0.76
1:A:501:GLN:HE22	1:A:1035:LEU:HB3	1.50	0.76
1:A:237:ILE:HG23	1:A:264:VAL:HG13	1.68	0.76
1:A:417:GLU:O	1:A:421:ILE:HD12	1.84	0.76
1:A:478:ASP:HB3	1:A:795:HIS:ND1	2.01	0.76
1:A:635:ARG:HG3	1:A:635:ARG:HH11	1.51	0.75
1:A:613:GLN:O	1:A:614:SER:OG	2.04	0.75
1:A:885:HIS:HD2	1:A:910:ARG:NH2	1.84	0.75
1:A:1337:MET:CE	1:A:1365:LEU:HD21	2.17	0.75
1:A:558:GLN:CA	1:A:558:GLN:OE1	2.24	0.75
1:A:677:TRP:NE1	1:A:694:ILE:O	2.17	0.75
1:A:1447:ILE:HD11	1:A:1494:ALA:HB1	1.68	0.75
1:A:450:PHE:CZ	1:A:608:ILE:HD13	2.22	0.75
1:A:1142:VAL:N	3:A:2072:F3S:S4	2.60	0.75
1:A:290:GLU:CD	1:A:408:GLN:HG3	2.06	0.75
1:A:318:TYR:HD1	1:A:418:TRP:CZ2	2.05	0.75
1:A:1468:HIS:O	1:A:1472:THR:HB	1.87	0.74
1:A:886:GLU:HG3	1:A:910:ARG:HE	1.51	0.74
1:A:460:VAL:HG12	1:A:464:MET:CE	2.18	0.74
1:A:1079:PRO:HD2	1:A:1082:LEU:HD12	1.68	0.74
1:A:1024:GLN:HE22	1:A:1246:VAL:CG1	1.97	0.74
1:A:411:GLN:O	1:A:413:TYR:N	2.20	0.74
1:A:1318:LEU:N	1:A:1318:LEU:HD23	2.01	0.74
1:A:413:TYR:C	1:A:415:TYR:H	1.85	0.74
1:A:837:ARG:HD2	1:A:838:PRO:O	1.89	0.73
1:A:1462:LYS:HB2	1:A:1484:TRP:CZ2	2.23	0.73
1:A:993:ARG:HH11	1:A:993:ARG:CG	1.98	0.73
1:A:404:GLN:OE1	1:A:404:GLN:CA	2.34	0.73
1:A:450:PHE:HZ	1:A:608:ILE:HD13	1.54	0.73
1:A:657:VAL:HG11	1:A:723:LEU:CD1	2.19	0.73
1:A:45:GLY:HA3	1:A:220:PRO:HD3	1.70	0.72
1:A:566:THR:HB	1:A:601:THR:O	1.87	0.72
1:A:1263:HIS:CE1	1:A:1297:PHE:CA	2.53	0.72
1:A:686:MET:C	1:A:692:ASP:HB2	2.10	0.72
1:A:773:PHE:CB	1:A:774:PRO:CD	2.67	0.72
1:A:945:ILE:N	1:A:945:ILE:HD12	2.04	0.72
1:A:354:TYR:HB3	1:A:364:LEU:HD12	1.71	0.72
1:A:457:VAL:O	1:A:462:VAL:HG23	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1419:ASN:ND2	1:A:1422:ALA:HB2	2.04	0.71
1:A:1137:CYS:SG	3:A:2072:F3S:S3	2.88	0.71
1:A:1420:VAL:O	1:A:1420:VAL:CG1	2.38	0.71
1:A:383:ARG:HH11	1:A:1380:GLY:CA	2.01	0.71
1:A:898:LYS:HB3	1:A:941:ALA:HB3	1.72	0.71
1:A:1263:HIS:CE1	1:A:1296:GLY:O	2.44	0.71
1:A:414:PRO:CB	1:A:418:TRP:HB3	2.21	0.71
1:A:315:PHE:CE1	1:A:413:TYR:HA	2.26	0.71
1:A:1387:ASN:ND2	1:A:1405:MET:HE1	2.05	0.71
1:A:511:ARG:HG3	1:A:1422:ALA:HB1	1.73	0.70
1:A:768:PHE:HE1	1:A:783:PHE:CZ	2.09	0.70
1:A:171:ARG:NH1	1:A:338:LYS:HD2	2.07	0.70
1:A:418:TRP:CD2	1:A:418:TRP:C	2.63	0.70
1:A:802:SER:HB2	1:A:1133:ILE:CG2	2.20	0.70
1:A:314:ASP:OD2	1:A:415:TYR:CD1	2.43	0.70
1:A:783:PHE:O	1:A:785:PHE:N	2.25	0.70
1:A:1147:ASN:O	1:A:1148:CYS:C	2.29	0.70
1:A:445:GLN:OE1	1:A:777:ALA:HB2	1.92	0.70
1:A:1146:ASN:O	1:A:1154:THR:HG23	1.92	0.69
1:A:1387:ASN:HB3	1:A:1405:MET:HE3	1.72	0.69
1:A:1387:ASN:ND2	1:A:1405:MET:CE	2.55	0.69
1:A:1491:PHE:CD1	1:A:1491:PHE:C	2.65	0.69
1:A:178:MET:HG3	1:A:213:PRO:HB2	1.73	0.69
1:A:314:ASP:HB2	1:A:415:TYR:HB2	1.75	0.69
1:A:329:PRO:HB3	1:A:349:LEU:HB2	1.73	0.69
1:A:484:LEU:HD13	1:A:839:VAL:HG12	1.74	0.69
1:A:808:ALA:HB2	1:A:826:HIS:HB2	1.74	0.69
1:A:243:ARG:HG2	1:A:636:LEU:HD21	1.73	0.69
1:A:1419:ASN:HD21	1:A:1422:ALA:HB2	1.57	0.69
1:A:686:MET:O	1:A:692:ASP:CB	2.32	0.69
1:A:965:ILE:HD13	1:A:1018:LEU:HD23	1.73	0.69
1:A:263:ILE:CD1	1:A:280:LEU:HD22	2.15	0.69
1:A:559:LEU:CG	1:A:560:GLN:N	2.53	0.69
1:A:613:GLN:HG3	1:A:769:HIS:CE1	2.28	0.69
1:A:1142:VAL:O	1:A:1142:VAL:HG12	1.91	0.69
1:A:1272:ARG:NH1	1:A:1306:GLN:HG2	2.08	0.69
1:A:625:VAL:O	1:A:629:LEU:HB2	1.93	0.68
1:A:1382:ARG:HB3	1:A:1385:VAL:HG22	1.75	0.68
1:A:399:ILE:HG22	1:A:404:GLN:HG2	1.76	0.68
1:A:414:PRO:HB2	1:A:418:TRP:HB3	1.75	0.68
1:A:768:PHE:CD2	1:A:771:MET:CB	2.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1403:GLU:HG2	1:A:1404:TYR:CE1	2.28	0.68
1:A:448:ALA:HB3	1:A:772:ALA:HB2	1.74	0.68
1:A:629:LEU:HD23	1:A:635:ARG:HD3	1.76	0.67
1:A:583:LEU:HD12	1:A:616:ILE:CD1	2.19	0.67
1:A:616:ILE:HG22	1:A:621:ALA:HB2	1.76	0.67
1:A:1251:ILE:HD13	1:A:1271:TYR:CE1	2.30	0.67
1:A:1360:ILE:CG2	1:A:1364:CYS:SG	2.83	0.67
1:A:695:ASP:HB2	1:A:697:PRO:HD2	1.75	0.67
1:A:518:LEU:HB3	1:A:544:PRO:HD3	1.77	0.67
1:A:1279:THR:HG22	1:A:1282:THR:HB	1.77	0.67
1:A:12:LYS:HB3	1:A:13:PRO:HD2	1.77	0.67
1:A:598:LEU:N	1:A:598:LEU:HD12	2.10	0.66
1:A:509:PRO:HA	1:A:516:MET:HE1	1.75	0.66
1:A:1103:ARG:NH1	1:A:1124:GLU:OE1	2.29	0.66
1:A:875:MET:SD	1:A:1132:MET:HE1	2.35	0.66
1:A:883:GLU:OE1	1:A:1160:ARG:HD2	1.95	0.66
1:A:601:THR:HG22	1:A:603:ARG:H	1.60	0.66
1:A:561:VAL:HG13	1:A:597:ILE:HG22	1.78	0.66
1:A:1337:MET:HE2	1:A:1365:LEU:HD21	1.78	0.66
1:A:1491:PHE:HD1	1:A:1491:PHE:C	1.97	0.66
1:A:418:TRP:HB2	1:A:533:ALA:HB1	1.76	0.66
1:A:768:PHE:CE2	1:A:771:MET:CB	2.79	0.66
1:A:916:ASP:HB2	1:A:924:PRO:HD2	1.78	0.66
1:A:1208:ASP:N	1:A:1208:ASP:OD1	2.29	0.65
1:A:953:THR:HG23	1:A:1294:ASN:HD21	1.59	0.65
1:A:314:ASP:CB	1:A:415:TYR:HB2	2.27	0.65
1:A:1138:ILE:CG2	1:A:1139:MET:N	2.58	0.65
1:A:13:PRO:HB2	1:A:197:THR:OG1	1.95	0.65
1:A:616:ILE:HG21	1:A:621:ALA:HB2	1.76	0.65
1:A:827:TYR:HE1	1:A:1176:PHE:CD1	2.14	0.65
1:A:1225:LEU:HB3	1:A:1226:PRO:HD2	1.78	0.65
1:A:1259:GLU:CD	1:A:1267:ALA:HB2	2.17	0.65
1:A:762:ALA:O	1:A:765:VAL:HG22	1.97	0.65
1:A:64:LEU:HD12	1:A:65:PRO:CD	2.27	0.65
1:A:908:VAL:HG22	1:A:911:TYR:CE1	2.32	0.65
1:A:1420:VAL:O	1:A:1420:VAL:HG12	1.95	0.65
1:A:462:VAL:HB	1:A:463:PRO:HD3	1.77	0.65
1:A:1004:PRO:HB2	1:A:1005:PRO:HD3	1.79	0.65
1:A:560:GLN:OE1	1:A:560:GLN:HA	1.96	0.65
1:A:908:VAL:HG22	1:A:911:TYR:HE1	1.62	0.65
1:A:415:TYR:CG	1:A:416:GLY:N	2.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ARG:NH1	1:A:528:LEU:HB2	2.12	0.65
1:A:1447:ILE:CD1	1:A:1494:ALA:HB1	2.26	0.65
1:A:315:PHE:CZ	1:A:413:TYR:HA	2.32	0.65
1:A:878:GLY:CA	1:A:988:ILE:HD12	2.22	0.65
1:A:369:GLY:HA3	1:A:1308:ALA:HB1	1.78	0.64
1:A:600:LEU:HD21	1:A:625:VAL:HG11	1.78	0.64
1:A:800:GLU:HG3	1:A:833:TYR:CE2	2.32	0.64
1:A:261:THR:CB	1:A:262:PRO:HD3	2.27	0.64
1:A:809:VAL:HG11	1:A:1169:GLN:O	1.97	0.64
1:A:677:TRP:HE3	1:A:678:LEU:HD23	1.61	0.64
1:A:828:GLU:O	1:A:832:GLN:HB2	1.97	0.64
1:A:1318:LEU:H	1:A:1321:MET:CE	2.10	0.64
1:A:100:GLU:HB2	1:A:102:LEU:HD12	1.80	0.64
1:A:1140:ALA:CB	3:A:2072:F3S:S1	2.83	0.64
1:A:1456:LYS:HB3	1:A:1503:PRO:O	1.97	0.64
1:A:294:ILE:HG21	1:A:528:LEU:HD11	1.80	0.64
1:A:490:LEU:N	1:A:490:LEU:HD23	2.11	0.63
1:A:444:LEU:O	1:A:444:LEU:HD12	1.98	0.63
1:A:71:ARG:HG2	1:A:71:ARG:O	1.98	0.63
1:A:1141:ARG:HA	3:A:2072:F3S:S2	2.39	0.63
1:A:307:LYS:HE3	1:A:1440:GLU:OE1	1.99	0.63
1:A:484:LEU:HD23	1:A:1211:LEU:CD1	2.29	0.63
1:A:1009:ILE:HA	1:A:1014:ASP:HB3	1.79	0.63
1:A:567:LEU:HD12	1:A:604:PRO:HD2	1.80	0.63
1:A:881:SER:HB2	1:A:1160:ARG:HD3	1.80	0.63
1:A:149:TYR:CG	1:A:283:ARG:HG3	2.34	0.63
1:A:677:TRP:CE3	1:A:678:LEU:HD23	2.34	0.63
1:A:954:PRO:O	1:A:958:MET:HG2	1.98	0.63
1:A:573:VAL:O	1:A:573:VAL:HG12	1.99	0.63
1:A:412:LYS:C	1:A:414:PRO:HD2	2.20	0.63
1:A:296:VAL:O	1:A:296:VAL:HG12	1.98	0.62
1:A:567:LEU:HD12	1:A:604:PRO:CD	2.28	0.62
1:A:953:THR:CG2	1:A:1294:ASN:ND2	2.53	0.62
1:A:1424:MET:O	1:A:1446:ILE:CD1	2.47	0.62
1:A:377:ASP:OD1	1:A:377:ASP:C	2.36	0.62
1:A:827:TYR:HD2	1:A:831:ARG:HG3	1.64	0.62
1:A:794:TYR:CZ	1:A:837:ARG:HB3	2.35	0.62
1:A:45:GLY:HA3	1:A:220:PRO:CD	2.29	0.62
1:A:1387:ASN:CB	1:A:1405:MET:CE	2.77	0.62
1:A:1130:ILE:CD1	1:A:1130:ILE:H	2.09	0.62
1:A:413:TYR:C	1:A:415:TYR:N	2.49	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:ARG:HH11	1:A:635:ARG:CB	2.13	0.61
1:A:1502:SER:O	1:A:1504:GLU:N	2.31	0.61
1:A:1103:ARG:NH1	1:A:1103:ARG:HG3	2.10	0.61
1:A:1023:HIS:HE1	1:A:1054:ASP:OD2	1.83	0.61
1:A:75:GLY:O	1:A:130:GLN:HA	2.01	0.61
1:A:1318:LEU:H	1:A:1321:MET:HE1	1.66	0.61
1:A:419:ILE:CG2	1:A:420:LYS:N	2.64	0.61
1:A:51:PRO:HG3	1:A:196:TYR:CZ	2.36	0.61
1:A:484:LEU:HD13	1:A:839:VAL:CG1	2.30	0.61
1:A:660:GLY:O	1:A:727:HIS:CE1	2.50	0.61
1:A:1142:VAL:O	1:A:1142:VAL:CG1	2.48	0.61
1:A:1311:GLN:OE1	1:A:1331:ASP:HB2	2.01	0.61
1:A:243:ARG:NH1	1:A:528:LEU:HD22	2.15	0.61
1:A:1403:GLU:HG2	1:A:1404:TYR:CD1	2.35	0.61
1:A:306:LEU:HD13	1:A:312:ILE:CD1	2.31	0.61
1:A:542:ARG:O	1:A:542:ARG:HD2	2.01	0.61
1:A:421:ILE:O	1:A:422:GLN:O	2.18	0.60
1:A:1085:THR:HG22	1:A:1086:GLU:N	2.15	0.60
1:A:561:VAL:HG12	1:A:599:VAL:HG23	1.82	0.60
1:A:768:PHE:CE1	1:A:783:PHE:HZ	2.16	0.60
1:A:383:ARG:HH11	1:A:1380:GLY:HA3	1.65	0.60
1:A:1355:GLU:H	1:A:1355:GLU:CD	2.03	0.60
1:A:1251:ILE:HD13	1:A:1271:TYR:CZ	2.35	0.60
1:A:412:LYS:O	1:A:414:PRO:HD2	2.01	0.60
1:A:358:LYS:CD	1:A:377:ASP:OD2	2.45	0.60
1:A:502:VAL:CG2	1:A:967:MET:HG3	2.32	0.60
1:A:140:ALA:O	1:A:141:GLY:C	2.40	0.60
1:A:278:LEU:HD12	1:A:295:LEU:HD12	1.83	0.60
1:A:917:VAL:HG21	1:A:933:GLN:O	2.02	0.60
1:A:1447:ILE:HD11	1:A:1494:ALA:CB	2.32	0.60
1:A:550:GLU:OE2	1:A:704:ARG:NH2	2.35	0.59
1:A:969:GLN:NE2	1:A:1065:THR:HG23	2.17	0.59
1:A:1325:LEU:HB3	1:A:1344:ILE:HG23	1.84	0.59
1:A:64:LEU:HD12	1:A:65:PRO:HD3	1.85	0.59
1:A:877:LEU:O	1:A:880:LEU:O	2.19	0.59
1:A:1140:ALA:N	3:A:2072:F3S:S1	2.76	0.59
1:A:250:SER:O	1:A:252:TRP:N	2.34	0.59
1:A:514:LEU:CD1	1:A:514:LEU:C	2.71	0.59
1:A:1347:HIS:ND1	1:A:1348:PRO:CD	2.54	0.59
1:A:885:HIS:CD2	1:A:910:ARG:NH2	2.68	0.59
1:A:514:LEU:CD1	1:A:515:VAL:N	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:THR:CB	1:A:601:THR:O	2.50	0.59
1:A:608:ILE:CG2	1:A:615:PHE:CZ	2.83	0.59
1:A:395:ALA:O	1:A:397:GLN:HG3	2.03	0.59
1:A:718:MET:HG2	1:A:731:ILE:HG21	1.85	0.59
1:A:524:LYS:CB	1:A:637:LYS:O	2.51	0.59
1:A:946:ALA:O	1:A:949:ARG:HD3	2.03	0.59
1:A:1352:PHE:O	1:A:1354:PRO:HD3	2.02	0.58
1:A:369:GLY:HA3	1:A:1308:ALA:HB2	1.85	0.58
1:A:110:VAL:O	1:A:112:VAL:HG13	2.03	0.58
1:A:632:ALA:HB1	1:A:634:LEU:HD12	1.85	0.58
1:A:1403:GLU:O	1:A:1422:ALA:O	2.21	0.58
1:A:207:PHE:CD2	1:A:207:PHE:C	2.75	0.58
1:A:547:ASN:OD1	1:A:549:VAL:HB	2.02	0.58
1:A:1256:ASP:C	1:A:1258:GLN:H	2.07	0.58
1:A:289:LEU:HB3	1:A:389:MET:CE	2.34	0.58
1:A:559:LEU:HG	1:A:560:GLN:H	1.66	0.58
1:A:581:THR:CG2	1:A:585:LYS:HE3	2.33	0.58
1:A:501:GLN:NE2	1:A:1036:VAL:H	2.01	0.58
1:A:182:ILE:HG12	1:A:183:ILE:HD13	1.84	0.58
1:A:357:THR:HB	1:A:377:ASP:OD1	2.03	0.58
1:A:550:GLU:O	1:A:554:ILE:HD13	2.03	0.58
1:A:1472:THR:HG22	1:A:1474:SER:N	2.19	0.58
1:A:827:TYR:HA	1:A:830:TYR:HB3	1.86	0.58
1:A:953:THR:HG21	1:A:1294:ASN:ND2	2.07	0.58
1:A:1130:ILE:HD13	1:A:1130:ILE:N	2.16	0.58
1:A:1405:MET:HG3	1:A:1406:THR:H	1.68	0.58
1:A:230:ILE:HD12	1:A:270:ASP:HB2	1.86	0.58
1:A:35:SER:HB2	1:A:120:GLN:NE2	2.18	0.58
1:A:1154:THR:HG21	1:A:1156:GLN:HB2	1.84	0.57
1:A:1347:HIS:CE1	1:A:1348:PRO:CD	2.86	0.57
1:A:501:GLN:NE2	1:A:1035:LEU:HB3	2.17	0.57
1:A:798:SER:OG	1:A:800:GLU:HG2	2.04	0.57
1:A:7:ALA:HB3	1:A:362:ILE:HG23	1.86	0.57
1:A:1138:ILE:HG22	1:A:1139:MET:H	1.66	0.57
1:A:1447:ILE:HG12	1:A:1448:THR:N	2.17	0.57
1:A:799:PRO:HD2	1:A:800:GLU:OE1	2.04	0.57
1:A:668:LEU:O	1:A:668:LEU:HD23	2.04	0.57
1:A:1397:ALA:HB3	1:A:1416:VAL:HG22	1.86	0.57
1:A:152:ARG:NH1	1:A:168:PHE:H	1.99	0.57
1:A:1154:THR:HG21	1:A:1159:LEU:HD12	1.85	0.57
1:A:1344:ILE:HG22	1:A:1359:ILE:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:ASP:OD1	1:A:681:LYS:N	2.37	0.57
1:A:1347:HIS:CD2	1:A:1348:PRO:HD2	2.37	0.57
1:A:635:ARG:HH11	1:A:635:ARG:HB3	1.68	0.57
1:A:418:TRP:HE3	1:A:418:TRP:O	1.87	0.57
1:A:546:VAL:HB	1:A:550:GLU:HB2	1.87	0.57
1:A:886:GLU:CA	1:A:910:ARG:HH21	2.18	0.57
1:A:1489:GLY:O	1:A:1491:PHE:HB3	2.04	0.56
1:A:583:LEU:CD1	1:A:616:ILE:HD13	2.21	0.56
1:A:825:ASP:O	1:A:828:GLU:HB3	2.05	0.56
1:A:886:GLU:HA	1:A:910:ARG:HH21	1.67	0.56
1:A:461:VAL:HA	1:A:464:MET:HE3	1.87	0.56
1:A:452:TYR:CZ	1:A:668:LEU:HD22	2.40	0.56
1:A:847:ASP:HB2	1:A:1206:ARG:CG	2.34	0.56
1:A:6:ILE:HG22	1:A:17:LEU:CD2	2.36	0.56
1:A:186:GLU:CA	1:A:186:GLU:OE1	2.44	0.56
1:A:522:LEU:N	1:A:522:LEU:HD23	2.20	0.56
1:A:362:ILE:HG13	1:A:363:VAL:N	2.20	0.56
1:A:634:LEU:O	1:A:637:LYS:HB2	2.05	0.56
1:A:445:GLN:CG	1:A:777:ALA:CB	2.83	0.56
1:A:1103:ARG:HH11	1:A:1103:ARG:CG	2.16	0.56
1:A:1081:GLU:CG	1:A:1120:MET:HE1	2.34	0.56
1:A:207:PHE:HD2	1:A:207:PHE:C	2.09	0.56
1:A:800:GLU:HG3	1:A:833:TYR:HE2	1.70	0.56
1:A:97:VAL:O	1:A:102:LEU:HB2	2.06	0.56
1:A:599:VAL:CG1	1:A:643:ASP:HB2	2.36	0.56
1:A:969:GLN:NE2	1:A:1065:THR:CG2	2.69	0.56
1:A:1137:CYS:SG	1:A:1138:ILE:O	2.62	0.56
1:A:447:GLN:HB3	1:A:780:LEU:HD21	1.87	0.56
1:A:284:THR:OG1	1:A:529:LEU:HD22	2.06	0.56
1:A:375:GLU:O	1:A:377:ASP:N	2.38	0.56
1:A:383:ARG:HH21	1:A:385:ALA:HA	1.70	0.56
1:A:1461:LEU:HD21	1:A:1491:PHE:CZ	2.40	0.56
1:A:1054:ASP:C	1:A:1055:ILE:HG13	2.25	0.56
1:A:832:GLN:HA	1:A:835:LYS:HG3	1.88	0.56
1:A:338:LYS:O	1:A:394:LEU:CD2	2.52	0.55
1:A:116:VAL:HG21	1:A:186:GLU:HB3	1.88	0.55
1:A:311:GLU:HB2	1:A:409:ALA:HB1	1.87	0.55
1:A:1363:THR:HG23	1:A:1385:VAL:HG21	1.88	0.55
1:A:1285:SER:HA	1:A:1321:MET:HE2	1.89	0.55
1:A:418:TRP:C	1:A:418:TRP:CE3	2.80	0.55
1:A:419:ILE:O	1:A:422:GLN:HG2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:LEU:O	1:A:693:ARG:N	2.38	0.55
1:A:444:LEU:O	1:A:445:GLN:CG	2.50	0.55
1:A:561:VAL:CG1	1:A:599:VAL:HG23	2.36	0.55
1:A:1145:THR:CG2	1:A:1147:ASN:ND2	2.69	0.55
1:A:381:LYS:N	1:A:1357:ASN:OD1	2.39	0.55
1:A:460:VAL:HG12	1:A:464:MET:HE1	1.87	0.55
1:A:855:ILE:HG23	1:A:856:SER:H	1.71	0.55
1:A:1263:HIS:CE1	1:A:1298:GLU:N	2.74	0.55
1:A:1388:SER:HA	1:A:1406:THR:HG22	1.88	0.55
1:A:1421:GLY:HA3	1:A:1447:ILE:HG21	1.89	0.55
1:A:486:HIS:CD2	1:A:1212:SER:OG	2.60	0.55
1:A:243:ARG:NH1	1:A:323:GLN:HE21	2.05	0.55
1:A:1318:LEU:HB2	1:A:1321:MET:CE	2.37	0.55
1:A:375:GLU:C	1:A:377:ASP:H	2.11	0.54
1:A:342:ALA:O	1:A:389:MET:HA	2.07	0.54
1:A:1141:ARG:N	3:A:2072:F3S:S2	2.81	0.54
1:A:1154:THR:CG2	1:A:1156:GLN:H	2.15	0.54
1:A:1024:GLN:HA	1:A:1283:ARG:HH21	1.73	0.54
1:A:668:LEU:C	1:A:668:LEU:HD23	2.27	0.54
1:A:345:ASP:OD2	1:A:348:GLY:N	2.41	0.54
1:A:768:PHE:CE2	1:A:771:MET:HB2	2.41	0.54
1:A:263:ILE:HD12	1:A:280:LEU:CD2	2.19	0.54
1:A:753:VAL:HG13	1:A:1217:LEU:HG	1.89	0.54
1:A:135:CYS:CB	1:A:139:CYS:HB2	2.38	0.54
1:A:685:LEU:HD12	1:A:690:ARG:HD2	1.88	0.54
1:A:886:GLU:HG3	1:A:910:ARG:NE	2.22	0.54
1:A:211:THR:HG21	1:A:1094:ASN:O	2.08	0.54
1:A:1110:THR:HG22	1:A:1113:ASP:H	1.73	0.54
1:A:1247:LEU:HD12	1:A:1247:LEU:O	2.08	0.54
1:A:770:GLY:O	1:A:774:PRO:CD	2.55	0.53
1:A:995:LYS:HE2	1:A:1426:GLY:HA3	1.90	0.53
1:A:1039:ILE:HD12	1:A:1040:GLY:N	2.24	0.53
1:A:993:ARG:HG3	1:A:993:ARG:NH1	2.05	0.53
1:A:414:PRO:HB3	1:A:418:TRP:HB3	1.89	0.53
1:A:486:HIS:HD2	1:A:1212:SER:OG	1.91	0.53
1:A:613:GLN:O	1:A:614:SER:CB	2.57	0.53
1:A:650:THR:CG2	1:A:651:HIS:N	2.72	0.53
1:A:687:GLU:O	1:A:688:ASN:HB3	2.08	0.53
1:A:759:ALA:O	1:A:762:ALA:HB3	2.09	0.53
1:A:107:TRP:CZ2	1:A:131:ILE:HD12	2.43	0.53
1:A:199:ASN:H	1:A:199:ASN:ND2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:MET:HB3	1:A:721:SER:O	2.08	0.53
1:A:1197:ILE:O	1:A:1232:ARG:NH2	2.42	0.53
1:A:239:TRP:HH2	1:A:635:ARG:HH22	1.55	0.53
1:A:648:TRP:H	1:A:652:HIS:HD2	1.57	0.53
1:A:1205:VAL:HG22	1:A:1219:LEU:HD12	1.91	0.53
1:A:1228:THR:CG2	1:A:1228:THR:O	2.56	0.53
1:A:145:ASP:O	1:A:149:TYR:N	2.31	0.53
1:A:307:LYS:CE	1:A:1440:GLU:OE1	2.56	0.53
1:A:464:MET:HG2	1:A:706:SER:OG	2.09	0.53
1:A:805:LEU:O	1:A:805:LEU:HG	2.09	0.53
1:A:10:ARG:HH11	1:A:10:ARG:HG2	1.74	0.53
1:A:290:GLU:OE1	1:A:408:GLN:HG3	2.08	0.53
1:A:622:VAL:HG11	1:A:661:ALA:H	1.74	0.53
1:A:306:LEU:HD13	1:A:312:ILE:HD11	1.91	0.52
1:A:315:PHE:HE1	1:A:413:TYR:HA	1.73	0.52
1:A:603:ARG:HD2	1:A:667:TYR:CE2	2.44	0.52
1:A:855:ILE:HG23	1:A:856:SER:N	2.24	0.52
1:A:969:GLN:HE22	1:A:1065:THR:CG2	2.23	0.52
1:A:403:TYR:H	1:A:403:TYR:HD1	1.55	0.52
1:A:674:ARG:O	1:A:678:LEU:HB2	2.10	0.52
1:A:1457:GLY:O	1:A:1458:GLU:C	2.46	0.52
1:A:146:ARG:O	1:A:150:ILE:HG13	2.10	0.52
1:A:73:GLY:HA2	1:A:170:CYS:HA	1.92	0.52
1:A:676:TRP:NE1	1:A:690:ARG:NH1	2.52	0.52
1:A:1279:THR:HG22	1:A:1282:THR:CB	2.39	0.52
1:A:561:VAL:HG13	1:A:597:ILE:CG2	2.38	0.52
1:A:497:GLN:NE2	1:A:714:ILE:HD13	2.24	0.52
1:A:445:GLN:HB3	1:A:772:ALA:HB1	1.91	0.52
1:A:809:VAL:CG1	1:A:1169:GLN:O	2.57	0.52
1:A:1395:GLU:HG2	1:A:1413:LEU:HD12	1.91	0.52
1:A:650:THR:CG2	1:A:651:HIS:H	2.23	0.52
1:A:886:GLU:HG3	1:A:910:ARG:HH21	1.74	0.52
1:A:1228:THR:HG23	1:A:1232:ARG:HE	1.74	0.52
1:A:509:PRO:HA	1:A:516:MET:HE3	1.90	0.52
1:A:944:GLN:C	1:A:945:ILE:HD12	2.30	0.52
1:A:1401:CYS:O	1:A:1402:CYS:HB2	2.10	0.51
1:A:483:VAL:HG23	1:A:494:TYR:HE2	1.76	0.51
1:A:514:LEU:HD12	1:A:515:VAL:H	1.75	0.51
1:A:234:LEU:C	1:A:234:LEU:CD1	2.78	0.51
1:A:224:LEU:HD23	1:A:278:LEU:HD22	1.93	0.51
1:A:975:GLU:OE1	1:A:1069:PRO:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1010:TYR:O	1:A:1011:SER:HB3	2.09	0.51
1:A:47:MET:O	1:A:201:ALA:HA	2.11	0.51
1:A:28:MET:HE1	1:A:31:ARG:HD2	1.87	0.51
1:A:1292:TYR:HB3	1:A:1296:GLY:HA3	1.92	0.51
1:A:1318:LEU:HB2	1:A:1321:MET:HE3	1.91	0.51
1:A:228:GLY:O	1:A:229:GLU:HG2	2.11	0.51
1:A:907:ASP:OD2	1:A:909:VAL:HG23	2.11	0.51
1:A:290:GLU:O	1:A:294:ILE:HD12	2.11	0.51
1:A:1089:ARG:NH1	1:A:1224:ASN:O	2.44	0.51
1:A:9:LEU:HD12	1:A:360:ASP:HB3	1.93	0.51
1:A:1142:VAL:HB	3:A:2072:F3S:S4	2.50	0.51
1:A:885:HIS:CD2	1:A:910:ARG:HH22	2.29	0.51
1:A:383:ARG:HH11	1:A:1380:GLY:HA2	1.62	0.51
1:A:562:ALA:HB3	1:A:590:THR:HG21	1.91	0.51
1:A:877:LEU:O	1:A:878:GLY:C	2.47	0.51
1:A:886:GLU:CA	1:A:910:ARG:NH2	2.69	0.51
1:A:1145:THR:HG22	1:A:1147:ASN:ND2	2.26	0.51
1:A:848:PHE:HB3	1:A:1188:LEU:HD21	1.92	0.51
1:A:484:LEU:HD23	1:A:1211:LEU:HD13	1.92	0.51
1:A:1376:ASN:ND2	1:A:1376:ASN:H	2.08	0.51
1:A:691:LEU:C	1:A:693:ARG:H	2.13	0.51
1:A:954:PRO:HG3	1:A:1316:PHE:HB3	1.92	0.51
1:A:610:THR:HG22	1:A:610:THR:O	2.10	0.51
1:A:855:ILE:CG2	1:A:856:SER:N	2.73	0.50
1:A:1251:ILE:CD1	1:A:1271:TYR:CE1	2.94	0.50
1:A:1476:LYS:O	1:A:1480:ILE:HG13	2.11	0.50
1:A:310:PRO:O	1:A:314:ASP:OD2	2.28	0.50
1:A:460:VAL:CG1	1:A:464:MET:CE	2.89	0.50
1:A:546:VAL:HA	1:A:550:GLU:HG3	1.94	0.50
1:A:599:VAL:HA	1:A:641:ILE:O	2.10	0.50
1:A:602:ASP:C	1:A:604:PRO:HD3	2.30	0.50
1:A:781:GLU:HG3	1:A:782:ASN:N	2.26	0.50
1:A:892:MET:CE	1:A:1174:PHE:CE1	2.95	0.50
1:A:1451:ARG:HH12	1:A:1490:LYS:HD2	1.76	0.50
1:A:414:PRO:C	1:A:418:TRP:HD1	2.15	0.50
1:A:1154:THR:HG22	1:A:1155:GLN:N	2.26	0.50
1:A:1315:ALA:HA	1:A:1335:LYS:O	2.11	0.50
1:A:399:ILE:HG22	1:A:404:GLN:CG	2.40	0.50
1:A:64:LEU:HD12	1:A:65:PRO:HD2	1.92	0.50
1:A:993:ARG:NH1	1:A:993:ARG:CG	2.65	0.50
1:A:677:TRP:NE1	1:A:686:MET:HE1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:GLU:O	1:A:1085:THR:HB	2.11	0.50
1:A:953:THR:HG23	1:A:1294:ASN:ND2	2.23	0.50
1:A:2:GLY:HA3	1:A:28:MET:HG3	1.94	0.50
1:A:1259:GLU:CA	1:A:1265:THR:HB	2.36	0.50
1:A:1263:HIS:CE1	1:A:1298:GLU:H	2.30	0.50
1:A:1496:PRO:O	1:A:1498:SER:N	2.45	0.50
1:A:418:TRP:CZ2	1:A:419:ILE:HG13	2.47	0.50
1:A:581:THR:O	1:A:585:LYS:HG3	2.11	0.50
1:A:1262:ASN:C	1:A:1264:GLN:H	2.05	0.49
1:A:1353:ALA:HB3	1:A:1356:ASP:HB2	1.94	0.49
1:A:318:TYR:HD1	1:A:418:TRP:CE2	2.29	0.49
1:A:1129:SER:O	1:A:1133:ILE:HG13	2.12	0.49
1:A:1472:THR:HG22	1:A:1474:SER:H	1.76	0.49
1:A:14:ASP:O	1:A:197:THR:HB	2.11	0.49
1:A:566:THR:CG2	1:A:616:ILE:HB	2.42	0.49
1:A:497:GLN:OE1	1:A:717:LYS:HE3	2.11	0.49
1:A:944:GLN:NE2	1:A:964:GLU:OE1	2.45	0.49
1:A:1110:THR:HG22	1:A:1112:TRP:N	2.27	0.49
1:A:1256:ASP:O	1:A:1258:GLN:N	2.46	0.49
1:A:1008:ASP:HB3	1:A:1009:ILE:HG13	1.95	0.49
1:A:1252:LEU:O	1:A:1257:ILE:HD11	2.13	0.49
1:A:1256:ASP:C	1:A:1258:GLN:N	2.65	0.49
1:A:362:ILE:HG13	1:A:363:VAL:H	1.77	0.49
1:A:566:THR:HG23	1:A:616:ILE:HB	1.95	0.49
1:A:693:ARG:C	1:A:694:ILE:HG12	2.33	0.49
1:A:805:LEU:O	1:A:809:VAL:HG23	2.12	0.49
1:A:945:ILE:N	1:A:945:ILE:CD1	2.75	0.49
1:A:581:THR:HG23	1:A:585:LYS:HE3	1.94	0.49
1:A:1344:ILE:HD12	1:A:1360:ILE:HD11	1.94	0.49
1:A:603:ARG:HG2	1:A:603:ARG:O	2.12	0.49
1:A:314:ASP:OD2	1:A:415:TYR:HD1	1.92	0.48
1:A:501:GLN:HE22	1:A:1035:LEU:CB	2.23	0.48
1:A:559:LEU:CD2	1:A:596:GLU:H	2.19	0.48
1:A:933:GLN:N	1:A:936:ASP:OD2	2.42	0.48
1:A:1376:ASN:H	1:A:1376:ASN:HD22	1.59	0.48
1:A:898:LYS:HB3	1:A:941:ALA:CB	2.39	0.48
1:A:518:LEU:HD13	1:A:712:PHE:CE2	2.48	0.48
1:A:1158:ARG:HH21	1:A:1159:LEU:HD21	1.78	0.48
1:A:1292:TYR:CE1	1:A:1297:PHE:HD1	2.32	0.48
1:A:1311:GLN:O	1:A:1312:SER:HB2	2.12	0.48
1:A:1472:THR:HG22	1:A:1473:GLY:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:GLN:OE1	1:A:777:ALA:CB	2.61	0.48
1:A:832:GLN:O	1:A:835:LYS:HG3	2.14	0.48
1:A:986:GLU:O	1:A:987:TYR:C	2.52	0.48
1:A:385:ALA:HB1	1:A:386:PRO:CD	2.44	0.48
1:A:392:VAL:HG12	1:A:393:ASP:N	2.28	0.48
1:A:1347:HIS:CG	1:A:1348:PRO:CD	2.80	0.48
1:A:1057:GLN:HA	1:A:1103:ARG:O	2.13	0.48
1:A:243:ARG:NH2	1:A:322:LEU:O	2.47	0.48
1:A:455:GLU:OE1	1:A:785:PHE:HB2	2.14	0.48
1:A:6:ILE:HG22	1:A:17:LEU:HD22	1.96	0.47
1:A:408:GLN:O	1:A:408:GLN:CD	2.53	0.47
1:A:418:TRP:CE2	1:A:419:ILE:HG13	2.49	0.47
1:A:1141:ARG:CA	3:A:2072:F3S:S2	3.03	0.47
1:A:1216:ASN:HD22	1:A:1216:ASN:C	2.16	0.47
1:A:1376:ASN:OD1	1:A:1472:THR:CG2	2.62	0.47
1:A:453:THR:CB	1:A:456:ASP:OD2	2.45	0.47
1:A:636:LEU:HA	1:A:636:LEU:HD12	1.56	0.47
1:A:742:VAL:HG13	1:A:746:PHE:O	2.15	0.47
1:A:1081:GLU:HG3	1:A:1120:MET:CE	2.41	0.47
1:A:239:TRP:CZ3	1:A:635:ARG:NH1	2.82	0.47
1:A:650:THR:HG23	1:A:651:HIS:N	2.29	0.47
1:A:1000:LEU:HA	1:A:1000:LEU:HD23	1.39	0.47
1:A:6:ILE:CG2	1:A:17:LEU:HD22	2.45	0.47
1:A:243:ARG:HH12	1:A:323:GLN:HE21	1.60	0.47
1:A:349:LEU:O	1:A:350:ARG:NH1	2.46	0.47
1:A:289:LEU:HB3	1:A:389:MET:HE3	1.96	0.47
1:A:419:ILE:HG22	1:A:420:LYS:H	1.75	0.47
1:A:445:GLN:O	1:A:772:ALA:HB1	2.14	0.47
1:A:513:ASN:O	1:A:515:VAL:N	2.48	0.47
1:A:152:ARG:HH12	1:A:168:PHE:CB	2.27	0.47
1:A:224:LEU:HD13	1:A:226:HIS:HB2	1.96	0.47
1:A:243:ARG:HG2	1:A:636:LEU:CD2	2.44	0.47
1:A:547:ASN:H	1:A:550:GLU:HG3	1.80	0.47
1:A:770:GLY:C	1:A:771:MET:SD	2.93	0.47
1:A:784:GLY:H	1:A:792:GLY:HA3	1.79	0.47
1:A:1234:TRP:CZ3	1:A:1235:LEU:HD13	2.50	0.47
1:A:1387:ASN:CB	1:A:1405:MET:HE2	2.34	0.47
1:A:559:LEU:O	1:A:561:VAL:HG22	2.14	0.47
1:A:694:ILE:HG23	1:A:694:ILE:HD12	1.43	0.47
1:A:1145:THR:HG21	1:A:1147:ASN:ND2	2.30	0.47
1:A:484:LEU:HD23	1:A:1211:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1263:HIS:NE2	1:A:1298:GLU:CG	2.71	0.47
1:A:460:VAL:CG1	1:A:464:MET:HE2	2.45	0.47
1:A:602:ASP:OD2	1:A:644:THR:HA	2.14	0.47
1:A:6:ILE:HG22	1:A:17:LEU:HD21	1.96	0.47
1:A:100:GLU:HB2	1:A:102:LEU:CD1	2.44	0.47
1:A:1317:ASN:C	1:A:1318:LEU:HD23	2.34	0.47
1:A:1442:ILE:HD12	1:A:1449:LEU:HD22	1.96	0.47
1:A:1:CYS:HA	1:A:205:ARG:O	2.14	0.47
1:A:231:ASN:OD1	1:A:232:THR:HG23	2.14	0.46
1:A:637:LYS:HA	1:A:637:LYS:HD3	1.59	0.46
1:A:1416:VAL:CG1	1:A:1420:VAL:HG21	2.46	0.46
1:A:293:MET:SD	1:A:405:ILE:HG22	2.55	0.46
1:A:40:SER:HB3	1:A:121:ALA:HB2	1.97	0.46
1:A:872:THR:HG22	1:A:899:SER:HA	1.96	0.46
1:A:560:GLN:HA	1:A:561:VAL:HG23	1.97	0.46
1:A:770:GLY:O	1:A:774:PRO:HG2	2.16	0.46
1:A:1376:ASN:OD1	1:A:1472:THR:HG21	2.16	0.46
1:A:411:GLN:C	1:A:413:TYR:N	2.63	0.46
1:A:1150:VAL:HG13	1:A:1152:VAL:HG23	1.97	0.46
1:A:1282:THR:OG1	1:A:1315:ALA:HB3	2.16	0.46
1:A:14:ASP:C	1:A:197:THR:HB	2.36	0.46
1:A:64:LEU:HA	1:A:65:PRO:HD3	1.83	0.46
1:A:660:GLY:O	1:A:661:ALA:C	2.51	0.46
1:A:6:ILE:HD11	1:A:371:VAL:HG21	1.98	0.46
1:A:1038:GLU:O	1:A:1041:ILE:HG22	2.16	0.46
1:A:542:ARG:CD	1:A:542:ARG:O	2.62	0.46
1:A:239:TRP:HH2	1:A:635:ARG:NH2	2.13	0.46
1:A:1246:VAL:O	1:A:1249:ASP:HB2	2.16	0.46
1:A:152:ARG:HH12	1:A:168:PHE:CA	2.28	0.46
1:A:16:THR:O	1:A:20:GLN:HG3	2.16	0.46
1:A:399:ILE:HG22	1:A:399:ILE:O	2.16	0.46
1:A:490:LEU:HD11	1:A:648:TRP:CH2	2.50	0.46
1:A:848:PHE:O	1:A:1204:LYS:HE3	2.15	0.46
1:A:881:SER:HB2	1:A:1160:ARG:CD	2.46	0.46
1:A:912:LEU:HD23	1:A:912:LEU:HA	1.76	0.46
1:A:1405:MET:CG	1:A:1406:THR:N	2.79	0.46
1:A:141:GLY:HA3	1:A:171:ARG:NH2	2.31	0.46
1:A:1498:SER:H	1:A:1500:LYS:H	1.62	0.46
1:A:462:VAL:HB	1:A:463:PRO:CD	2.44	0.46
1:A:72:LEU:O	1:A:133:VAL:O	2.34	0.45
1:A:610:THR:O	1:A:613:GLN:CD	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:ILE:H	1:A:758:ILE:HG13	1.33	0.45
1:A:946:ALA:O	1:A:949:ARG:CD	2.64	0.45
1:A:905:GLY:CA	1:A:951:GLY:HA3	2.47	0.45
1:A:314:ASP:CG	1:A:415:TYR:HD1	2.18	0.45
1:A:369:GLY:HA3	1:A:1308:ALA:HB3	1.90	0.45
1:A:14:ASP:O	1:A:197:THR:HA	2.16	0.45
1:A:157:LYS:NZ	1:A:261:THR:HB	2.31	0.45
1:A:232:THR:HG21	1:A:725:SER:HB3	1.98	0.45
1:A:347:ASN:C	1:A:386:PRO:HB3	2.36	0.45
1:A:405:ILE:HG13	1:A:406:LYS:H	1.82	0.45
1:A:414:PRO:O	1:A:417:GLU:N	2.49	0.45
1:A:632:ALA:CB	1:A:634:LEU:HD12	2.46	0.45
1:A:892:MET:HE2	1:A:1174:PHE:CE1	2.51	0.45
1:A:646:GLN:HG2	1:A:646:GLN:O	2.17	0.45
1:A:696:LEU:N	1:A:697:PRO:CD	2.79	0.45
1:A:1256:ASP:HA	1:A:1259:GLU:HG2	1.99	0.45
1:A:229:GLU:O	1:A:328:GLY:HA3	2.17	0.45
1:A:354:TYR:CZ	1:A:382:GLY:HA3	2.52	0.45
1:A:1316:PHE:CE2	1:A:1336:GLY:HA3	2.52	0.45
1:A:412:LYS:NZ	1:A:531:PRO:HD2	2.32	0.45
1:A:6:ILE:O	1:A:200:PHE:HA	2.17	0.45
1:A:826:HIS:O	1:A:830:TYR:CB	2.65	0.45
1:A:314:ASP:HB3	1:A:415:TYR:HB2	1.99	0.45
1:A:96:VAL:HG21	1:A:155:ILE:HG13	1.98	0.45
1:A:334:PHE:N	1:A:334:PHE:CD2	2.85	0.45
1:A:547:ASN:OD1	1:A:550:GLU:HG2	2.16	0.45
1:A:727:HIS:O	1:A:728:GLY:C	2.51	0.45
1:A:1006:HIS:C	1:A:1008:ASP:H	2.20	0.44
1:A:1442:ILE:HD11	1:A:1449:LEU:HD13	1.98	0.44
1:A:1143:CYS:N	3:A:2072:F3S:S4	2.90	0.44
1:A:318:TYR:CD1	1:A:418:TRP:CE2	3.05	0.44
1:A:243:ARG:HH12	1:A:528:LEU:HD22	1.82	0.44
1:A:1347:HIS:O	1:A:1349:GLN:N	2.51	0.44
1:A:349:LEU:O	1:A:350:ARG:HD2	2.17	0.44
1:A:602:ASP:OD2	1:A:667:TYR:HE2	1.99	0.44
1:A:649:SER:O	1:A:652:HIS:HB2	2.18	0.44
1:A:688:ASN:O	1:A:688:ASN:CG	2.54	0.44
1:A:800:GLU:HG2	1:A:801:MET:H	1.83	0.44
1:A:413:TYR:HB2	1:A:415:TYR:HD2	1.83	0.44
1:A:53:GLU:O	1:A:56:ALA:HB3	2.18	0.44
1:A:875:MET:HG3	1:A:875:MET:H	1.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1404:TYR:N	1:A:1404:TYR:CD1	2.85	0.44
1:A:28:MET:HA	1:A:28:MET:CE	2.47	0.44
1:A:567:LEU:CD2	1:A:615:PHE:CE2	2.90	0.44
1:A:1032:SER:CB	1:A:1055:ILE:HB	2.48	0.44
1:A:1274:VAL:O	1:A:1277:ASP:HB2	2.17	0.44
1:A:375:GLU:C	1:A:377:ASP:N	2.70	0.44
1:A:567:LEU:HA	1:A:567:LEU:HD23	1.72	0.44
1:A:479:THR:HG22	1:A:795:HIS:CE1	2.53	0.44
1:A:1148:CYS:C	1:A:1150:VAL:H	2.20	0.44
1:A:1265:THR:HG22	1:A:1266:THR:O	2.17	0.44
1:A:499:PHE:CD2	1:A:499:PHE:N	2.85	0.44
1:A:826:HIS:O	1:A:830:TYR:N	2.36	0.44
1:A:401:LYS:O	1:A:404:GLN:HB2	2.18	0.44
1:A:659:TYR:CE2	1:A:730:GLN:HG2	2.53	0.44
1:A:478:ASP:CB	1:A:795:HIS:ND1	2.79	0.44
1:A:1081:GLU:HA	1:A:1120:MET:CE	2.48	0.44
1:A:1228:THR:HG23	1:A:1228:THR:O	2.17	0.44
1:A:358:LYS:HE3	1:A:377:ASP:HB2	2.00	0.43
1:A:346:ARG:HD2	1:A:721:SER:OG	2.17	0.43
1:A:828:GLU:HG2	1:A:832:GLN:NE2	2.33	0.43
1:A:84:SER:OG	1:A:85:ALA:N	2.50	0.43
1:A:963:LEU:HA	1:A:963:LEU:HD23	1.71	0.43
1:A:1023:HIS:CE1	1:A:1054:ASP:OD2	2.68	0.43
1:A:846:LEU:HD13	1:A:1203:LEU:HD13	2.01	0.43
1:A:1297:PHE:CZ	1:A:1299:GLY:HA3	2.53	0.43
1:A:236:ASN:HB3	1:A:326:TRP:CE2	2.53	0.43
1:A:521:PHE:C	1:A:522:LEU:HD23	2.38	0.43
1:A:450:PHE:CE2	1:A:645:ALA:HB3	2.53	0.43
1:A:1021:ASP:OD2	1:A:1335:LYS:NZ	2.34	0.43
1:A:1306:GLN:HA	1:A:1326:GLN:O	2.18	0.43
1:A:144:LEU:HG	1:A:148:LEU:HD22	1.99	0.43
1:A:266:GLN:HE21	1:A:266:GLN:HB3	1.69	0.43
1:A:598:LEU:N	1:A:598:LEU:CD1	2.79	0.43
1:A:679:ASP:OD1	1:A:679:ASP:C	2.57	0.43
1:A:744:TYR:CD2	1:A:744:TYR:C	2.92	0.43
1:A:950:PHE:CZ	1:A:1000:LEU:HD13	2.53	0.43
1:A:1085:THR:CG2	1:A:1086:GLU:N	2.82	0.43
1:A:8:ASN:OD1	1:A:361:TYR:CZ	2.71	0.43
1:A:1451:ARG:O	1:A:1452:ILE:C	2.56	0.43
1:A:15:HIS:HD2	1:A:196:TYR:O	2.01	0.43
1:A:260:LEU:O	1:A:263:ILE:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ILE:C	1:A:422:GLN:O	2.57	0.43
1:A:522:LEU:HA	1:A:522:LEU:HD22	1.78	0.43
1:A:584:VAL:O	1:A:588:ILE:HG13	2.18	0.43
1:A:71:ARG:CG	1:A:71:ARG:O	2.65	0.43
1:A:288:PRO:HB2	1:A:334:PHE:CD1	2.53	0.43
1:A:671:GLU:OE1	1:A:674:ARG:NH1	2.52	0.43
1:A:12:LYS:HA	1:A:12:LYS:HD3	1.62	0.43
1:A:695:ASP:CB	1:A:697:PRO:HD2	2.45	0.43
1:A:908:VAL:HA	1:A:911:TYR:CE1	2.53	0.43
1:A:1137:CYS:SG	3:A:2072:F3S:S1	3.17	0.43
1:A:565:SER:OG	1:A:567:LEU:HB2	2.19	0.43
1:A:811:ALA:O	1:A:812:TYR:HB2	2.18	0.43
1:A:907:ASP:O	1:A:910:ARG:HB2	2.18	0.43
1:A:869:ARG:HD2	1:A:1193:LEU:HD23	2.01	0.43
1:A:230:ILE:HA	1:A:327:ASP:O	2.19	0.43
1:A:797:ASN:HA	1:A:801:MET:HE3	2.01	0.43
1:A:941:ALA:HB1	1:A:961:LYS:HD2	2.00	0.43
1:A:1088:HIS:HD2	1:A:1225:LEU:CD1	2.31	0.43
1:A:1386:ARG:HG2	1:A:1404:TYR:HB2	2.00	0.43
1:A:668:LEU:O	1:A:671:GLU:HB3	2.18	0.43
1:A:832:GLN:CA	1:A:835:LYS:HG3	2.48	0.43
1:A:885:HIS:HD2	1:A:910:ARG:CZ	2.32	0.43
1:A:1021:ASP:O	1:A:1024:GLN:HB3	2.19	0.42
1:A:1282:THR:O	1:A:1285:SER:HB3	2.19	0.42
1:A:1285:SER:HA	1:A:1321:MET:CE	2.49	0.42
1:A:1405:MET:CG	1:A:1406:THR:H	2.32	0.42
1:A:711:LEU:O	1:A:712:PHE:C	2.57	0.42
1:A:893:ASN:ND2	1:A:937:THR:HG23	2.34	0.42
1:A:92:TYR:O	1:A:93:VAL:C	2.56	0.42
1:A:1202:LEU:HA	1:A:1202:LEU:HD23	1.80	0.42
1:A:25:LEU:HB3	1:A:181:SER:HB2	2.02	0.42
1:A:477:ASP:OD1	1:A:479:THR:HG23	2.19	0.42
1:A:58:TRP:CZ3	1:A:132:LEU:HD12	2.53	0.42
1:A:211:THR:O	1:A:211:THR:HG23	2.19	0.42
1:A:401:LYS:NZ	1:A:402:ASN:OD1	2.44	0.42
1:A:691:LEU:C	1:A:693:ARG:N	2.71	0.42
1:A:497:GLN:CD	1:A:714:ILE:HD13	2.39	0.42
1:A:1039:ILE:HD12	1:A:1040:GLY:H	1.82	0.42
1:A:1230:GLN:O	1:A:1232:ARG:N	2.51	0.42
1:A:1354:PRO:HB2	1:A:1355:GLU:OE2	2.20	0.42
1:A:1355:GLU:HG3	1:A:1395:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1474:SER:HA	1:A:1475:PRO:HD3	1.86	0.42
1:A:8:ASN:N	1:A:199:ASN:O	2.52	0.42
1:A:9:LEU:CD2	1:A:392:VAL:HG11	2.50	0.42
1:A:541:LEU:HA	1:A:541:LEU:HD12	1.81	0.42
1:A:824:TYR:HD2	1:A:824:TYR:HA	1.73	0.42
1:A:1255:PRO:O	1:A:1258:GLN:HG2	2.20	0.42
1:A:247:LEU:HD22	1:A:529:LEU:HD12	2.01	0.42
1:A:640:LEU:N	1:A:640:LEU:HD13	2.35	0.42
1:A:668:LEU:O	1:A:669:ALA:C	2.58	0.42
1:A:678:LEU:HA	1:A:678:LEU:HD22	1.87	0.42
1:A:686:MET:HB3	1:A:692:ASP:HA	2.01	0.42
1:A:863:VAL:HG13	1:A:1175:TYR:CD2	2.55	0.42
1:A:1268:THR:O	1:A:1269:LYS:HG2	2.19	0.42
1:A:234:LEU:HD12	1:A:234:LEU:C	2.38	0.42
1:A:403:TYR:CD1	1:A:403:TYR:N	2.77	0.42
1:A:1254:ASP:CB	1:A:1255:PRO:CD	2.64	0.42
1:A:412:LYS:HZ3	1:A:531:PRO:HD2	1.84	0.42
1:A:769:HIS:CD2	1:A:769:HIS:C	2.93	0.42
1:A:892:MET:HE1	1:A:1174:PHE:CE1	2.55	0.42
1:A:74:VAL:HG22	1:A:132:LEU:HD23	2.01	0.42
1:A:204:HIS:CG	1:A:219:GLN:O	2.73	0.42
1:A:450:PHE:CG	1:A:645:ALA:HB3	2.54	0.42
1:A:627:HIS:CE1	1:A:730:GLN:HE22	2.38	0.42
1:A:659:TYR:CD2	1:A:730:GLN:HG2	2.54	0.42
1:A:770:GLY:O	1:A:774:PRO:CG	2.67	0.42
1:A:827:TYR:O	1:A:831:ARG:N	2.49	0.42
1:A:828:GLU:HG2	1:A:832:GLN:HE22	1.85	0.42
1:A:979:LEU:HD23	1:A:984:VAL:HG22	2.01	0.42
1:A:1451:ARG:NH1	1:A:1490:LYS:HG3	2.35	0.42
1:A:314:ASP:OD2	1:A:415:TYR:CE1	2.72	0.42
1:A:5:PHE:CE2	1:A:341:GLY:HA2	2.55	0.42
1:A:456:ASP:O	1:A:460:VAL:HB	2.19	0.42
1:A:561:VAL:CG1	1:A:597:ILE:HG22	2.48	0.42
1:A:940:SER:HB2	1:A:943:LYS:HE3	2.02	0.42
1:A:1004:PRO:HB2	1:A:1005:PRO:CD	2.49	0.41
1:A:157:LYS:HZ3	1:A:261:THR:HB	1.85	0.41
1:A:559:LEU:O	1:A:561:VAL:CG2	2.68	0.41
1:A:802:SER:CB	1:A:1133:ILE:HD13	2.51	0.41
1:A:283:ARG:HA	1:A:283:ARG:HD3	1.93	0.41
1:A:286:ARG:NH2	1:A:529:LEU:HA	2.35	0.41
1:A:514:LEU:HD13	1:A:514:LEU:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HA	1:A:51:PRO:HD3	1.86	0.41
1:A:286:ARG:NH2	1:A:528:LEU:O	2.44	0.41
1:A:1312:SER:OG	1:A:1335:LYS:HE3	2.21	0.41
1:A:1387:ASN:CB	1:A:1405:MET:HE3	2.44	0.41
1:A:673:VAL:HG11	1:A:700:LEU:HD23	2.02	0.41
1:A:1185:LEU:HD23	1:A:1185:LEU:HA	1.92	0.41
1:A:1206:ARG:NH2	1:A:1208:ASP:OD2	2.52	0.41
1:A:1464:LEU:HD12	1:A:1464:LEU:HA	1.96	0.41
1:A:28:MET:HA	1:A:28:MET:HE2	2.01	0.41
1:A:322:LEU:HD12	1:A:322:LEU:HA	1.89	0.41
1:A:570:LEU:HD13	1:A:571:ASP:OD1	2.21	0.41
1:A:917:VAL:HA	1:A:923:SER:HB2	2.03	0.41
1:A:1285:SER:OG	1:A:1318:LEU:HG	2.21	0.41
1:A:1337:MET:CE	1:A:1365:LEU:CD2	2.95	0.41
1:A:1409:VAL:O	1:A:1410:ILE:HD13	2.20	0.41
1:A:211:THR:HB	1:A:1094:ASN:OD1	2.20	0.41
1:A:28:MET:HE3	1:A:31:ARG:HD2	1.94	0.41
1:A:797:ASN:HB3	1:A:1139:MET:HG3	2.01	0.41
1:A:1081:GLU:CG	1:A:1120:MET:CE	2.99	0.41
1:A:752:ARG:NH1	1:A:1086:GLU:OE2	2.54	0.41
1:A:299:ALA:HB2	1:A:346:ARG:NH2	2.35	0.41
1:A:377:ASP:CG	1:A:377:ASP:O	2.48	0.41
1:A:731:ILE:HG22	1:A:731:ILE:O	2.20	0.41
1:A:1363:THR:HG23	1:A:1385:VAL:CG2	2.51	0.41
1:A:152:ARG:NH1	1:A:168:PHE:CB	2.84	0.41
1:A:560:GLN:C	1:A:561:VAL:CG2	2.89	0.41
1:A:508:ASP:HA	1:A:1004:PRO:HG2	2.03	0.41
1:A:1304:ASN:N	1:A:1304:ASN:ND2	2.69	0.41
1:A:1337:MET:HE2	1:A:1365:LEU:CD2	2.50	0.41
1:A:399:ILE:HG22	1:A:404:GLN:CD	2.41	0.41
1:A:973:PRO:HD2	1:A:1076:ALA:CB	2.51	0.41
1:A:1032:SER:HA	1:A:1055:ILE:O	2.21	0.41
1:A:1325:LEU:HA	1:A:1325:LEU:HD12	1.65	0.41
1:A:693:ARG:O	1:A:694:ILE:HG12	2.21	0.41
1:A:499:PHE:CE1	1:A:973:PRO:HB3	2.56	0.41
1:A:1130:ILE:CD1	1:A:1130:ILE:N	2.79	0.41
1:A:1150:VAL:CG1	1:A:1152:VAL:HG23	2.51	0.41
1:A:1442:ILE:CD1	1:A:1449:LEU:HD13	2.51	0.41
1:A:229:GLU:HG3	1:A:503:THR:O	2.20	0.41
1:A:269:SER:O	1:A:270:ASP:C	2.59	0.41
1:A:411:GLN:O	1:A:413:TYR:CA	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:TYR:CD2	1:A:652:HIS:HA	2.56	0.41
1:A:574:ASN:C	1:A:574:ASN:OD1	2.59	0.41
1:A:583:LEU:HD21	1:A:600:LEU:HD23	2.03	0.41
1:A:623:GLY:O	1:A:624:ALA:C	2.59	0.41
1:A:717:LYS:HG2	1:A:974:GLY:HA3	2.03	0.41
1:A:135:CYS:HA	1:A:136:PRO:HD3	1.81	0.40
1:A:257:LEU:C	1:A:259:ALA:H	2.24	0.40
1:A:685:LEU:HD12	1:A:690:ARG:CD	2.51	0.40
1:A:771:MET:N	1:A:771:MET:SD	2.94	0.40
1:A:860:VAL:HG12	1:A:861:GLU:O	2.21	0.40
1:A:953:THR:H	1:A:956:TYR:HB3	1.85	0.40
1:A:1165:GLY:HA2	1:A:1169:GLN:NE2	2.36	0.40
1:A:1338:ASN:OD1	1:A:1369:THR:CG2	2.70	0.40
1:A:20:GLN:HB3	1:A:371:VAL:HG13	2.03	0.40
1:A:289:LEU:CB	1:A:389:MET:HE3	2.51	0.40
1:A:413:TYR:O	1:A:415:TYR:CA	2.61	0.40
1:A:617:PRO:HA	1:A:618:PRO:HD3	1.81	0.40
1:A:872:THR:O	1:A:1127:PHE:O	2.39	0.40
1:A:1268:THR:C	1:A:1269:LYS:HG2	2.41	0.40
1:A:1318:LEU:H	1:A:1321:MET:HE3	1.83	0.40
1:A:1461:LEU:HG	1:A:1465:ILE:HD12	2.04	0.40
1:A:483:VAL:HG23	1:A:494:TYR:CE2	2.54	0.40
1:A:915:ASP:O	1:A:917:VAL:N	2.54	0.40
1:A:999:THR:O	1:A:1000:LEU:HD23	2.22	0.40
1:A:1109:LYS:HB2	1:A:1130:ILE:HG21	2.04	0.40
1:A:406:LYS:HA	1:A:409:ALA:HB3	2.03	0.40
1:A:722:LEU:O	1:A:725:SER:N	2.46	0.40
1:A:1003:PRO:HB3	1:A:1404:TYR:CZ	2.56	0.40
1:A:232:THR:C	1:A:236:ASN:ND2	2.75	0.40
1:A:58:TRP:CE3	1:A:132:LEU:HD12	2.56	0.40
1:A:544:PRO:HB3	1:A:723:LEU:HD21	2.04	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	1467/1520 (96%)	1218 (83%)	197 (13%)	52 (4%)	3	20

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	101	LYS
1	A	251	GLY
1	A	376	VAL
1	A	404	GLN
1	A	412	LYS
1	A	414	PRO
1	A	415	TYR
1	A	503	THR
1	A	573	VAL
1	A	612	ASN
1	A	613	GLN
1	A	614	SER
1	A	688	ASN
1	A	727	HIS
1	A	836	ASP
1	A	1255	PRO
1	A	1331	ASP
1	A	1403	GLU
1	A	1491	PHE
1	A	1498	SER
1	A	39	ASP
1	A	141	GLY
1	A	561	VAL
1	A	571	ASP
1	A	692	ASP
1	A	754	GLY
1	A	784	GLY
1	A	916	ASP
1	A	1142	VAL
1	A	1263	HIS
1	A	1489	GLY
1	A	395	ALA
1	A	773	PHE
1	A	828	GLU

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Mol	Chain	Res	Type
1	A	1231	ASN
1	A	1257	ILE
1	A	1503	PRO
1	A	260	LEU
1	A	1423	GLY
1	A	399	ILE
1	A	854	ALA
1	A	977	GLY
1	A	1254	ASP
1	A	1141	ARG
1	A	262	PRO
1	A	1389	VAL
1	A	731	ILE
1	A	902	GLY
1	A	1442	ILE
1	A	73	GLY
1	A	863	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	1200/1236 (97%)	972 (81%)	228 (19%)	1 8

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	8	ASN
1	A	16	THR
1	A	17	LEU
1	A	23	LYS
1	A	31	ARG
1	A	35	SER
1	A	46	VAL
1	A	50	ILE

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Mol	Chain	Res	Type
1	A	52	ARG
1	A	60	ASN
1	A	64	LEU
1	A	66	MET
1	A	76	MET
1	A	82	GLU
1	A	84	SER
1	A	86	ARG
1	A	95	GLU
1	A	99	LEU
1	A	134	THR
1	A	137	GLU
1	A	146	ARG
1	A	148	LEU
1	A	152	ARG
1	A	153	SER
1	A	158	LYS
1	A	159	LEU
1	A	161	GLU
1	A	162	ASP
1	A	168	PHE
1	A	169	SER
1	A	172	THR
1	A	173	ILE
1	A	182	ILE
1	A	183	ILE
1	A	186	GLU
1	A	191	LEU
1	A	198	SER
1	A	199	ASN
1	A	207	PHE
1	A	211	THR
1	A	212	MET
1	A	219	GLN
1	A	222	ARG
1	A	234	LEU
1	A	245	LYS
1	A	249	VAL
1	A	260	LEU
1	A	264	VAL
1	A	266	GLN
1	A	272	TYR

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Mol	Chain	Res	Type
1	A	274	LEU
1	A	278	LEU
1	A	279	GLU
1	A	286	ARG
1	A	302	ASN
1	A	312	ILE
1	A	320	SER
1	A	322	LEU
1	A	324	GLU
1	A	334	PHE
1	A	355	CYS
1	A	356	ILE
1	A	361	TYR
1	A	364	LEU
1	A	366	SER
1	A	370	VAL
1	A	376	VAL
1	A	377	ASP
1	A	389	MET
1	A	393	ASP
1	A	394	LEU
1	A	398	LYS
1	A	401	LYS
1	A	403	TYR
1	A	405	ILE
1	A	419	ILE
1	A	422	GLN
1	A	442	THR
1	A	444	LEU
1	A	453	THR
1	A	457	VAL
1	A	478	ASP
1	A	479	THR
1	A	481	LEU
1	A	483	VAL
1	A	498	ARG
1	A	503	THR
1	A	510	LEU
1	A	511	ARG
1	A	514	LEU
1	A	515	VAL
1	A	522	LEU

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Mol	Chain	Res	Type
1	A	532	LYS
1	A	534	GLU
1	A	541	LEU
1	A	542	ARG
1	A	543	SER
1	A	550	GLU
1	A	558	GLN
1	A	559	LEU
1	A	570	LEU
1	A	580	LEU
1	A	596	GLU
1	A	598	LEU
1	A	601	THR
1	A	602	ASP
1	A	603	ARG
1	A	613	GLN
1	A	625	VAL
1	A	629	LEU
1	A	635	ARG
1	A	636	LEU
1	A	637	LYS
1	A	640	LEU
1	A	649	SER
1	A	650	THR
1	A	656	LEU
1	A	678	LEU
1	A	679	ASP
1	A	680	GLU
1	A	684	LYS
1	A	695	ASP
1	A	704	ARG
1	A	706	SER
1	A	718	MET
1	A	735	ILE
1	A	750	THR
1	A	752	ARG
1	A	753	VAL
1	A	756	LEU
1	A	758	ILE
1	A	761	VAL
1	A	768	PHE
1	A	771	MET

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Mol	Chain	Res	Type
1	A	778	LYS
1	A	780	LEU
1	A	801	MET
1	A	812	TYR
1	A	824	TYR
1	A	827	TYR
1	A	837	ARG
1	A	851	ASP
1	A	855	ILE
1	A	863	VAL
1	A	867	VAL
1	A	872	THR
1	A	877	LEU
1	A	898	LYS
1	A	906	GLU
1	A	915	ASP
1	A	923	SER
1	A	953	THR
1	A	962	GLN
1	A	991	LEU
1	A	993	ARG
1	A	1015	LEU
1	A	1017	GLN
1	A	1039	ILE
1	A	1043	THR
1	A	1052	ASN
1	A	1065	THR
1	A	1072	SER
1	A	1080	TRP
1	A	1085	THR
1	A	1099	ARG
1	A	1100	VAL
1	A	1103	ARG
1	A	1109	LYS
1	A	1110	THR
1	A	1120	MET
1	A	1130	ILE
1	A	1132	MET
1	A	1148	CYS
1	A	1150	VAL
1	A	1161	GLN
1	A	1170	VAL

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Mol	Chain	Res	Type
1	A	1177	ILE
1	A	1184	LEU
1	A	1194	ASP
1	A	1200	THR
1	A	1208	ASP
1	A	1211	LEU
1	A	1214	THR
1	A	1216	ASN
1	A	1225	LEU
1	A	1228	THR
1	A	1235	LEU
1	A	1242	SER
1	A	1248	ASP
1	A	1257	ILE
1	A	1258	GLN
1	A	1259	GLU
1	A	1274	VAL
1	A	1276	THR
1	A	1280	VAL
1	A	1282	THR
1	A	1291	LYS
1	A	1304	ASN
1	A	1349	GLN
1	A	1352	PHE
1	A	1359	ILE
1	A	1369	THR
1	A	1376	ASN
1	A	1381	GLU
1	A	1386	ARG
1	A	1404	TYR
1	A	1406	THR
1	A	1425	THR
1	A	1430	TYR
1	A	1432	LEU
1	A	1433	ASP
1	A	1442	ILE
1	A	1446	ILE
1	A	1447	ILE
1	A	1448	THR
1	A	1452	ILE
1	A	1453	THR
1	A	1456	LYS

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Mol	Chain	Res	Type
1	A	1464	LEU
1	A	1476	LYS
1	A	1480	ILE
1	A	1481	LEU
1	A	1485	SER
1	A	1488	LEU
1	A	1491	PHE
1	A	1498	SER
1	A	1504	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	15	HIS
1	A	120	GLN
1	A	199	ASN
1	A	236	ASN
1	A	266	GLN
1	A	323	GLN
1	A	486	HIS
1	A	501	GLN
1	A	552	GLN
1	A	651	HIS
1	A	652	HIS
1	A	727	HIS
1	A	730	GLN
1	A	832	GLN
1	A	885	HIS
1	A	944	GLN
1	A	1023	HIS
1	A	1052	ASN
1	A	1147	ASN
1	A	1216	ASN
1	A	1294	ASN
1	A	1304	ASN
1	A	1306	GLN
1	A	1347	HIS
1	A	1372	ASN
1	A	1493	GLN
1	A	1506	ASN

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 ⓘ

2 ligands are modelled in this entry.

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	FMN	A	2070	-	31,33,33	1.50	4 (12%)	40,50,50	1.93	8 (20%)
3	F3S	A	2072	1	0,9,9	0.00	-	-		

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	FMN	A	2070	-	-	3/18/18/18	0/3/3/3
3	F3S	A	2072	1	-	-	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2070	FMN	C4A-N5	3.70	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2070	FMN	C4-N3	3.49	1.39	1.33
2	A	2070	FMN	C10-N1	2.58	1.36	1.33
2	A	2070	FMN	O2'-C2'	-2.21	1.38	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2070	FMN	C4-N3-C2	7.94	121.85	115.14
2	A	2070	FMN	C4A-C4-N3	-3.96	118.02	123.43
2	A	2070	FMN	C5A-C9A-N10	3.44	120.21	117.72
2	A	2070	FMN	C1'-N10-C9A	3.37	120.95	118.29
2	A	2070	FMN	O3P-P-O5'	2.90	114.46	106.73
2	A	2070	FMN	C4A-N5-C5A	2.37	119.14	116.77
2	A	2070	FMN	O4'-C4'-C5'	-2.37	104.59	109.92
2	A	2070	FMN	C4-C4A-N5	2.08	120.98	118.60

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2070	FMN	C4'-C5'-O5'-P
2	A	2070	FMN	C5'-O5'-P-O1P
2	A	2070	FMN	C5'-O5'-P-O3P

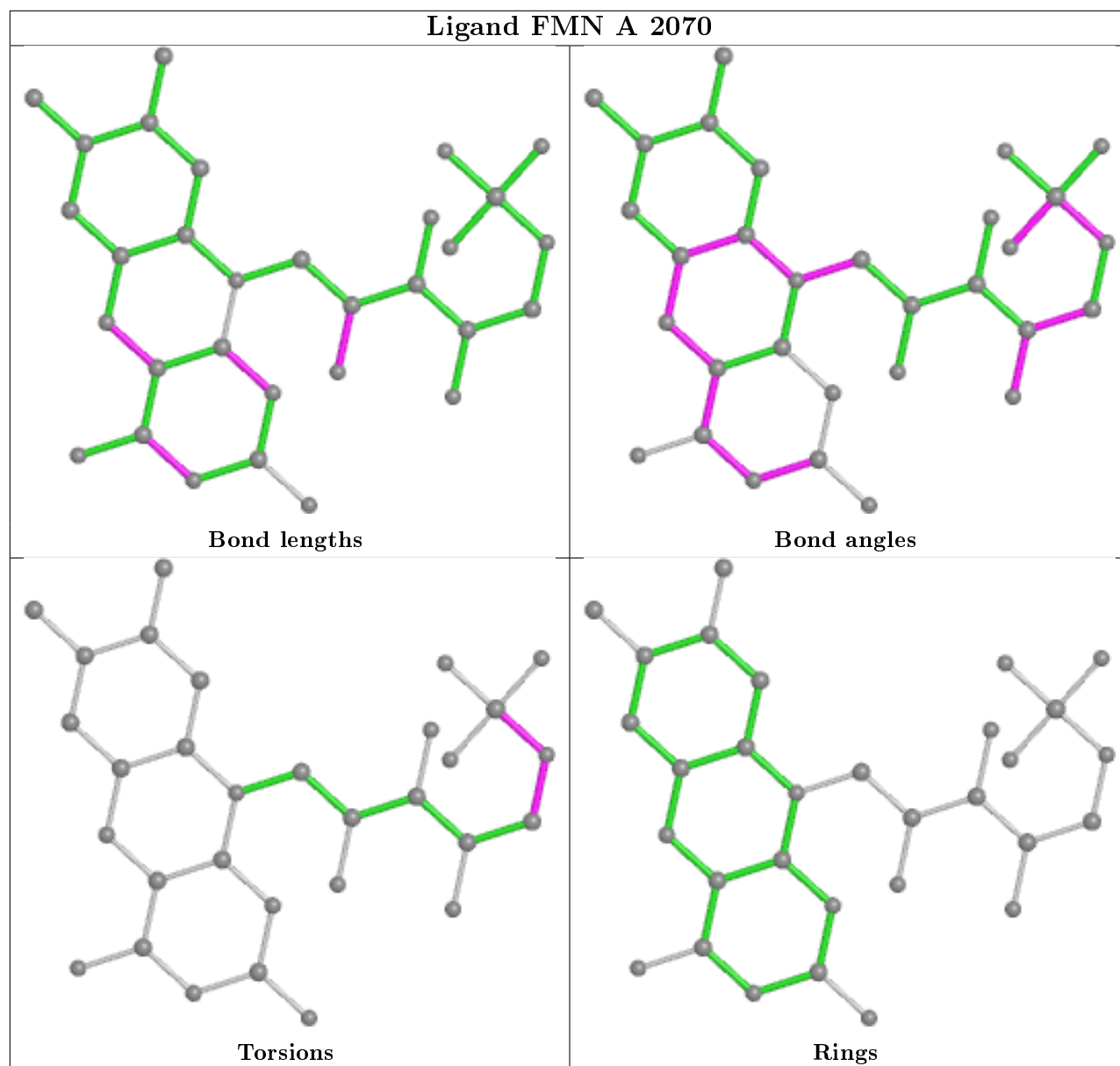
There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2072	F3S	12	0

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

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1475/1520 (97%)	-0.34	12 (0%) 86 65	9, 33, 55, 100	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	613	GLN	3.4
1	A	1490	LYS	3.0
1	A	1486	ASP	2.6
1	A	825	ASP	2.6
1	A	776	MET	2.5
1	A	826	HIS	2.4
1	A	413	TYR	2.2
1	A	417	GLU	2.2
1	A	409	ALA	2.1
1	A	615	PHE	2.1
1	A	1264	GLN	2.0
1	A	1433	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.

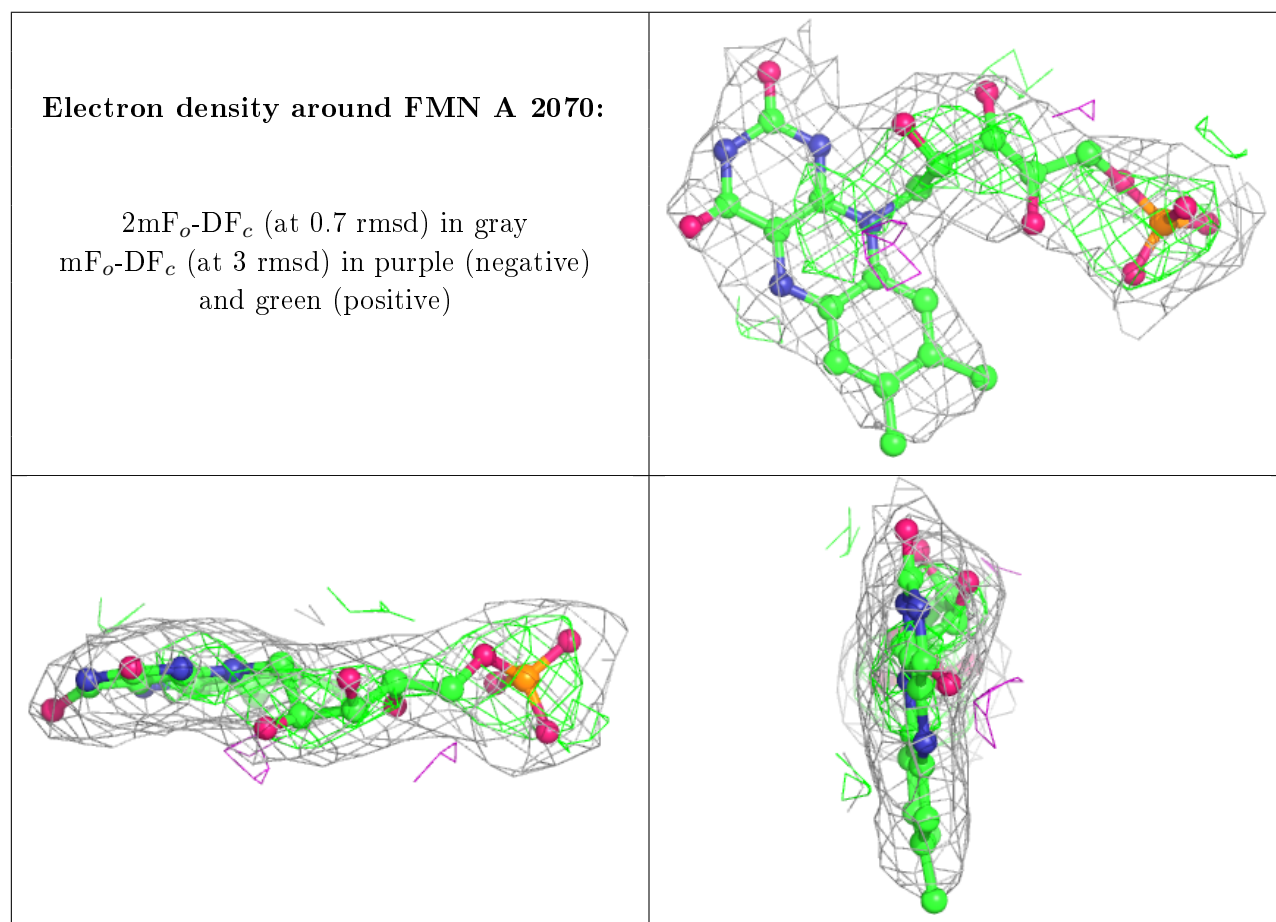
6.4 Ligands [i](#)

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. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	F3S	A	2072	7/7	0.89	0.24	82,94,99,100	0
2	FMN	A	2070	31/31	0.97	0.31	76,87,90,90	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.