



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:05 AM UTC

PDB ID : 5XA1 / pdb_00005xa1
Title : Crystal structure of inositol 1,4,5-trisphosphate receptor cytosolic domain with inositol 1,4,5-trisphosphate
Authors : Hamada, K.; Miyatake, H.; Terauchi, A.; Mikoshiba, K.
Deposited on : 2017-03-10
Resolution : 6.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

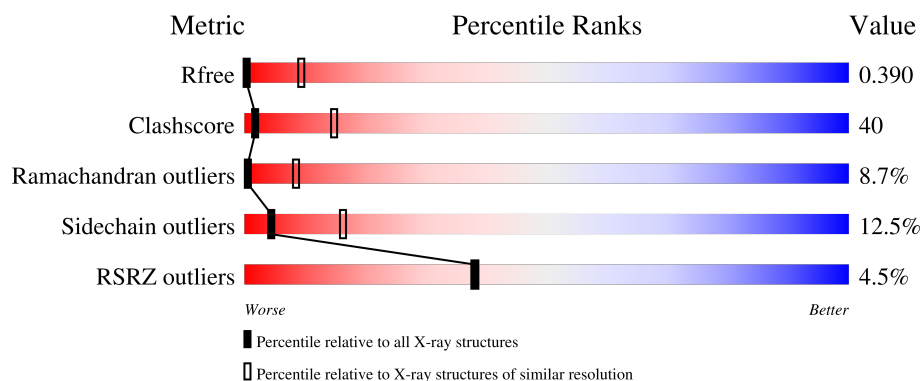
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.20 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}	180053	1148 (8.40-4.00)
Clashscore	190562	1008 (8.30-4.02)
Ramachandran outliers	187476	1037 (8.40-4.00)
Sidechain outliers	187428	1003 (8.40-4.00)
RSRZ outliers	180081	1141 (8.40-4.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1581	
1	B	1581	

2 Entry composition [i](#)

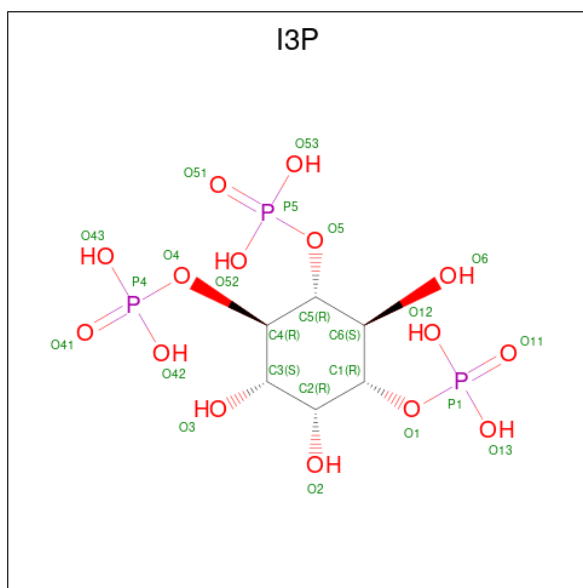
There are 2 unique types of molecules in this entry. The entry contains 25536 atoms, of which 10338 are hydrogens and 0 are deuteriums.

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.

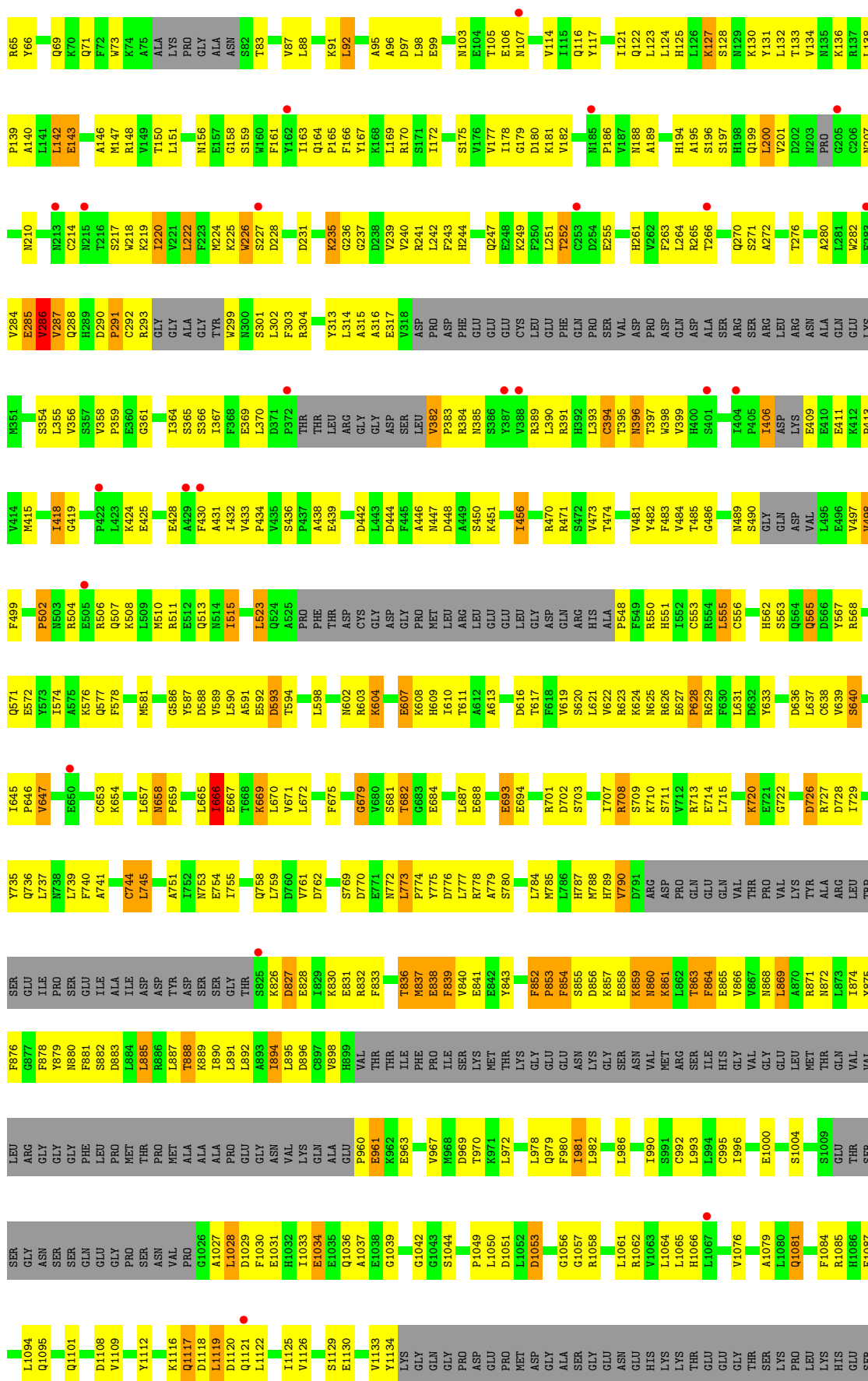
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 1.

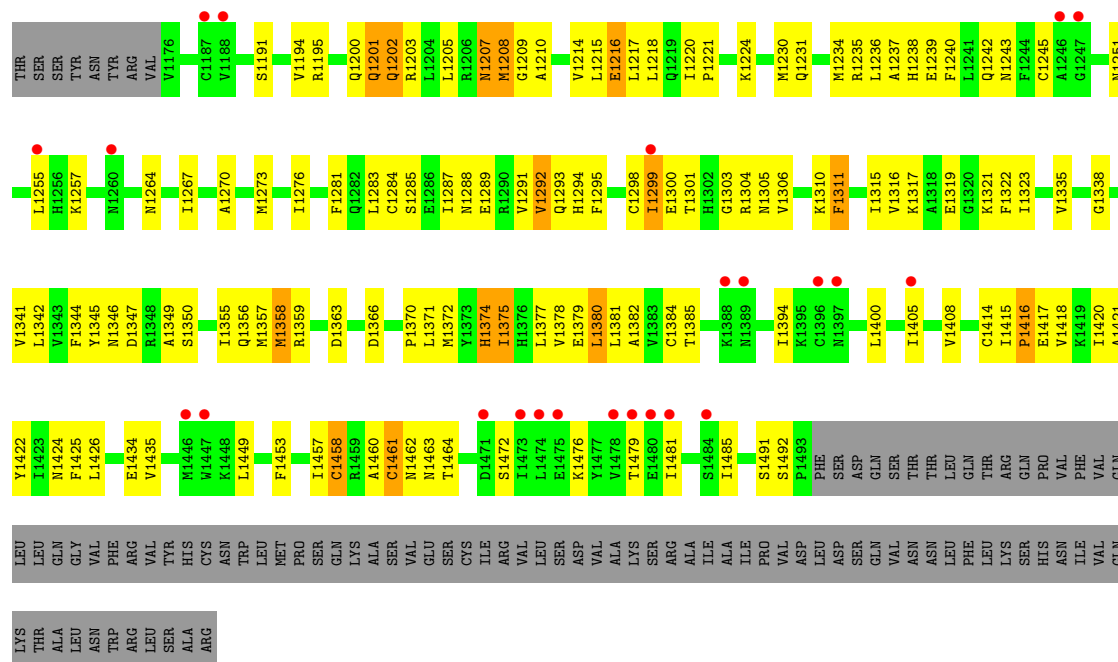
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1257	Total	C	H	N	O	S	0	0	0
			12735	4648	5160	1435	1475	17			
1	B	1257	Total	C	H	N	O	S	0	0	0
			12735	4648	5160	1435	1475	17			

- Molecule 2 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (CCD ID: I3P) (formula: $C_6H_{15}O_{15}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			33	6	9	15	3		
2	B	1	Total	C	H	O	P	0	0
			33	6	9	15	3		





4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	126.80Å 126.80Å 367.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.50 – 6.20 48.50 – 6.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.50-6.20) 99.7 (48.50-6.20)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 6.15Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.360 , 0.382 0.352 , 0.390	Depositor DCC
R_{free} test set	651 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	91.1	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 626.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.21$, $\langle L^2 \rangle = 0.07$	Xtriage
Estimated twinning fraction	0.377 for h,-k,-l	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	25536	wwPDB-VP
Average B, all atoms (Å ²)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: I3P

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	1.12	27/7637 (0.4%)	1.26	52/10494 (0.5%)
1	B	1.01	5/7637 (0.1%)	1.13	12/10494 (0.1%)
All	All	1.06	32/15274 (0.2%)	1.20	64/20988 (0.3%)

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	10
1	B	0	7
All	All	0	17

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1491	SER	C-N	13.28	1.61	1.33
1	A	116	GLN	CB-CG	11.39	1.86	1.52
1	A	175	SER	CA-C	10.37	1.65	1.52
1	A	109	LYS	CB-CG	9.79	1.81	1.52
1	A	1393	GLU	N-CA	9.75	1.58	1.46
1	A	175	SER	N-CA	9.08	1.57	1.46
1	A	116	GLN	CG-CD	8.62	1.73	1.52
1	A	109	LYS	CG-CD	8.55	1.78	1.52
1	A	1391	TYR	C-N	7.95	1.44	1.33
1	A	1392	THR	N-CA	7.60	1.55	1.45
1	B	868	ASN	C-N	7.41	1.44	1.33
1	A	109	LYS	CD-CE	6.93	1.73	1.52
1	A	1393	GLU	C-N	6.71	1.42	1.33
1	A	176	VAL	N-CA	6.58	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	PRO	CA-C	-6.55	1.47	1.52
1	A	1394	ILE	C-N	6.25	1.42	1.33
1	A	1411	HIS	CA-C	6.11	1.60	1.52
1	A	553	CYS	N-CA	5.86	1.53	1.46
1	A	55	ASP	CB-CG	-5.83	1.37	1.52
1	A	1393	GLU	CA-C	5.77	1.60	1.52
1	B	382	VAL	C-N	5.66	1.47	1.33
1	A	1192	ALA	N-CA	5.62	1.53	1.46
1	A	174	ASP	C-N	5.47	1.41	1.33
1	A	1392	THR	CA-C	5.39	1.59	1.52
1	A	1400	LEU	C-N	5.38	1.40	1.33
1	A	56	CYS	CB-SG	5.29	1.98	1.81
1	A	428	GLU	CB-CG	-5.23	1.36	1.52
1	A	899	HIS	N-CA	5.17	1.56	1.46
1	A	116	GLN	C-N	5.06	1.40	1.33
1	A	116	GLN	CD-NE2	5.04	1.43	1.33
1	B	666	ILE	N-CA	-5.02	1.40	1.46
1	B	1205	LEU	CA-C	5.01	1.59	1.52

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1393	GLU	CA-C-N	11.19	142.11	121.97
1	A	1393	GLU	C-N-CA	11.19	142.11	121.97
1	A	232	ASP	N-CA-C	-10.54	102.61	114.62
1	A	116	GLN	CB-CG-CD	9.93	129.49	112.60
1	A	175	SER	N-CA-C	9.51	124.08	108.96
1	B	869	LEU	CA-C-O	-9.04	107.59	120.51
1	A	174	ASP	CA-C-O	-8.63	112.15	121.99
1	A	175	SER	CA-CB-OG	8.58	128.27	111.10
1	A	109	LYS	CG-CD-CE	8.30	130.40	111.30
1	B	869	LEU	O-C-N	8.29	133.61	122.59
1	A	1287	ILE	CA-C-N	7.80	136.45	121.54
1	A	1287	ILE	C-N-CA	7.80	136.45	121.54
1	A	116	GLN	CB-CA-C	7.78	125.08	109.68
1	A	109	LYS	CB-CG-CD	7.61	128.80	111.30
1	A	1395	LYS	CB-CA-C	-7.45	95.59	110.42
1	A	1391	TYR	CA-C-O	-7.18	112.67	121.58
1	A	1393	GLU	O-C-N	-6.97	113.31	122.59
1	A	56	CYS	CA-CB-SG	6.89	130.24	114.40
1	A	317	GLU	CA-C-N	6.66	133.69	121.70
1	A	317	GLU	C-N-CA	6.66	133.69	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1395	LYS	N-CA-CB	6.64	121.72	110.49
1	A	553	CYS	N-CA-C	6.53	119.55	108.90
1	A	174	ASP	CA-C-N	6.46	131.02	122.30
1	A	174	ASP	C-N-CA	6.46	131.02	122.30
1	A	1392	THR	N-CA-C	6.43	118.96	109.24
1	B	1374	HIS	CA-C-N	6.36	130.93	121.77
1	B	1374	HIS	C-N-CA	6.36	130.93	121.77
1	B	1460	ALA	CA-C-N	6.34	133.65	121.54
1	B	1460	ALA	C-N-CA	6.34	133.65	121.54
1	A	109	LYS	CA-CB-CG	6.10	126.30	114.10
1	A	1394	ILE	CA-C-N	5.98	132.97	121.54
1	A	1394	ILE	C-N-CA	5.98	132.97	121.54
1	A	1288	ASN	N-CA-C	5.96	123.49	110.80
1	A	463	GLY	N-CA-C	5.81	117.72	110.29
1	A	162	TYR	CA-CB-CG	5.77	124.29	113.90
1	A	1461	CYS	N-CA-C	-5.68	98.70	110.80
1	A	174	ASP	O-C-N	-5.68	115.72	122.65
1	B	894	ILE	CA-C-N	5.63	132.56	121.58
1	B	894	ILE	C-N-CA	5.63	132.56	121.58
1	A	1393	GLU	N-CA-C	5.60	122.73	110.80
1	A	1391	TYR	N-CA-C	5.60	117.81	107.73
1	A	989	ARG	N-CA-C	5.58	117.80	109.59
1	A	1392	THR	O-C-N	-5.57	116.42	123.17
1	A	370	LEU	CA-C-N	5.47	135.15	121.80
1	A	370	LEU	C-N-CA	5.47	135.15	121.80
1	A	116	GLN	N-CA-CB	-5.44	101.28	111.13
1	A	1470	ALA	N-CA-C	-5.43	99.24	110.80
1	A	1460	ALA	CA-C-N	5.40	131.85	121.54
1	A	1460	ALA	C-N-CA	5.40	131.85	121.54
1	A	1461	CYS	CA-C-N	5.34	131.75	121.54
1	A	1461	CYS	C-N-CA	5.34	131.75	121.54
1	A	1345	TYR	N-CA-C	-5.32	104.53	111.02
1	A	745	LEU	N-CA-C	-5.31	99.48	110.80
1	A	174	ASP	N-CA-CB	-5.30	103.12	110.38
1	B	1462	ASN	N-CA-C	-5.26	105.14	112.03
1	A	607	GLU	N-CA-C	5.22	119.12	112.34
1	B	1033	ILE	CA-C-N	5.18	130.37	122.24
1	B	1033	ILE	C-N-CA	5.18	130.37	122.24
1	A	253	CYS	CA-CB-SG	5.13	126.20	114.40
1	A	1349	ALA	N-CA-C	-5.09	99.95	110.80
1	A	1263	LEU	CA-C-N	5.07	134.17	121.80
1	A	1263	LEU	C-N-CA	5.07	134.17	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	VAL	N-CA-C	-5.04	98.85	109.34
1	A	124	LEU	N-CA-C	5.01	116.58	108.41

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1034	GLU	Peptide
1	A	1203	ARG	Peptide
1	A	1228	THR	Peptide
1	A	1342	LEU	Peptide
1	A	1375	ILE	Peptide
1	A	1382	ALA	Peptide
1	A	1393	GLU	Peptide
1	A	173	GLY	Peptide
1	A	174	ASP	Mainchain
1	A	707	ILE	Peptide
1	B	1034	GLU	Peptide
1	B	1375	ILE	Peptide
1	B	1380	LEU	Peptide
1	B	1461	CYS	Peptide
1	B	679	GLY	Peptide
1	B	708	ARG	Peptide
1	B	744	CYS	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	7575	5160	5277	544	8
1	B	7575	5160	5277	497	0
2	A	24	9	9	0	0
2	B	24	9	9	0	0
All	All	15198	10338	10572	1041	8

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 40.

All (1041) 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:109:LYS:CD	1:A:109:LYS:CG	1.78	1.61
1:A:109:LYS:CG	1:A:109:LYS:CB	1.81	1.54
1:A:116:GLN:CG	1:A:116:GLN:CB	1.86	1.52
1:B:856:ASP:O	1:B:860:ASN:CB	1.89	1.20
1:A:1214:VAL:O	1:A:1218:LEU:CB	1.92	1.17
1:A:1281:PHE:O	1:A:1285:SER:CB	1.95	1.12
1:B:1116:LYS:O	1:B:1119:LEU:N	1.84	1.09
1:B:1281:PHE:O	1:B:1285:SER:CB	2.03	1.06
1:B:1371:LEU:O	1:B:1375:ILE:N	1.91	1.02
1:A:1371:LEU:O	1:A:1375:ILE:N	1.93	1.01
1:A:1125:ILE:O	1:A:1129:SER:CB	2.09	1.01
1:B:892:LEU:O	1:B:896:ASP:CB	2.10	1.00
1:B:1341:VAL:O	1:B:1345:TYR:N	1.95	0.99
1:A:1422:TYR:O	1:A:1426:LEU:CB	2.12	0.97
1:B:1377:LEU:O	1:B:1381:LEU:CB	2.12	0.97
1:A:705:LYS:HA	1:A:736:GLN:CB	1.94	0.97
1:A:1377:LEU:O	1:A:1381:LEU:CB	2.13	0.97
1:B:654:LYS:O	1:B:658:ASN:N	1.97	0.97
1:B:885:LEU:O	1:B:888:THR:N	1.97	0.96
1:A:1231:GLN:O	1:A:1235:ARG:CB	2.15	0.94
1:B:610:ILE:O	1:B:613:ALA:N	2.01	0.93
1:B:882:SER:O	1:B:885:LEU:N	2.00	0.93
1:B:1118:ASP:O	1:B:1120:ASP:N	2.03	0.91
1:B:840:VAL:O	1:B:843:TYR:N	2.04	0.90
1:A:755:ILE:O	1:A:758:GLN:N	2.03	0.90
1:B:653:CYS:O	1:B:657:LEU:N	2.04	0.90
1:A:885:LEU:O	1:A:888:THR:N	2.06	0.89
1:B:978:LEU:O	1:B:981:ILE:N	2.05	0.89
1:B:1472:SER:O	1:B:1476:LYS:CB	2.19	0.89
1:B:888:THR:O	1:B:891:LEU:N	2.06	0.88
1:A:1126:VAL:O	1:A:1130:GLU:CB	2.21	0.88
1:A:1421:ALA:O	1:A:1425:PHE:CB	2.21	0.87
1:B:777:LEU:O	1:B:780:SER:N	2.07	0.87
1:A:1381:LEU:HA	1:A:1384:CYS:CB	2.05	0.87
1:A:1459:ARG:O	1:A:1461:CYS:N	2.08	0.86
1:B:1270:ALA:HB2	1:B:1319:GLU:CB	2.05	0.86
1:A:603:ARG:O	1:A:605:LEU:N	2.08	0.85
1:A:574:ILE:O	1:A:578:PHE:N	2.09	0.84
1:A:1191:SER:CB	1:A:1236:LEU:O	2.25	0.84
1:B:285:GLU:O	1:B:287:VAL:N	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ALA:N	1:B:146:ALA:O	2.09	0.84
1:B:18:TYR:OH	1:B:45:ASP:OD1	1.95	0.83
1:A:1111:ASN:O	1:A:1114:GLN:N	2.12	0.83
1:B:963:GLU:O	1:B:967:VAL:CB	2.27	0.83
1:A:277:SER:OG	1:A:512:GLU:OE1	1.96	0.82
1:B:622:VAL:HA	1:B:631:LEU:CB	2.09	0.82
1:A:703:SER:CB	1:A:710:LYS:CB	2.57	0.82
1:B:624:LYS:O	1:B:626:ARG:N	2.12	0.82
1:B:865:GLU:O	1:B:869:LEU:CB	2.29	0.81
1:B:598:LEU:O	1:B:602:ASN:N	2.13	0.81
1:B:1231:GLN:O	1:B:1235:ARG:CB	2.29	0.81
1:B:1421:ALA:O	1:B:1425:PHE:CB	2.28	0.80
1:B:237:GLY:N	1:B:284:VAL:O	2.15	0.80
1:A:20:GLU:N	1:A:217:SER:O	2.14	0.80
1:A:618:PHE:O	1:A:622:VAL:N	2.15	0.80
1:A:586:GLY:O	1:A:588:ASP:N	2.16	0.79
1:A:49:PRO:HG2	1:A:291:PRO:HG2	1.64	0.79
1:A:595:ILE:O	1:A:598:LEU:CB	2.32	0.79
1:B:1125:ILE:O	1:B:1129:SER:CB	2.30	0.79
1:A:859:LYS:O	1:A:863:THR:CB	2.31	0.78
1:A:15:CYS:SG	1:A:222:LEU:HA	2.23	0.78
1:B:838:GLU:O	1:B:841:GLU:N	2.16	0.78
1:A:140:ALA:N	1:A:146:ALA:O	2.17	0.78
1:B:276:THR:O	1:B:508:LYS:NZ	2.13	0.77
1:A:200:LEU:HD21	1:A:208:GLU:HB2	1.67	0.77
1:B:1049:PRO:O	1:B:1053:ASP:N	2.18	0.77
1:B:1287:ILE:HA	1:B:1344:PHE:CB	2.14	0.77
1:A:1417:GLU:O	1:A:1419:LYS:N	2.17	0.77
1:B:669:LYS:O	1:B:671:VAL:N	2.18	0.77
1:A:755:ILE:O	1:A:759:LEU:N	2.17	0.76
1:A:1294:HIS:O	1:A:1298:CYS:N	2.17	0.76
1:B:49:PRO:HG2	1:B:291:PRO:HG2	1.67	0.76
1:A:595:ILE:O	1:A:599:LEU:N	2.19	0.76
1:A:1121:GLN:O	1:A:1124:SER:N	2.19	0.75
1:A:863:THR:O	1:A:866:VAL:N	2.18	0.75
1:A:20:GLU:O	1:A:217:SER:OG	2.05	0.75
1:B:47:ASN:O	1:B:49:PRO:HD3	1.86	0.75
1:B:885:LEU:O	1:B:888:THR:CB	2.35	0.74
1:B:607:GLU:O	1:B:611:THR:HA	1.87	0.74
1:A:1376:HIS:O	1:A:1380:LEU:CB	2.35	0.74
1:A:707:ILE:CB	1:A:737:LEU:N	2.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HD21	1:B:128:SER:HA	1.71	0.73
1:B:1335:VAL:O	1:B:1384:CYS:CB	2.36	0.73
1:A:1437:MET:O	1:A:1440:ILE:N	2.17	0.73
1:A:1341:VAL:O	1:A:1345:TYR:N	2.19	0.73
1:B:969:ASP:O	1:B:972:LEU:N	2.20	0.73
1:B:1207:ASN:O	1:B:1209:GLY:N	2.22	0.72
1:A:724:LYS:O	1:A:726:ASP:N	2.22	0.72
1:A:601:ASN:O	1:A:603:ARG:N	2.22	0.72
1:A:16:SER:N	1:A:221:VAL:O	2.19	0.72
1:B:29:THR:HG22	1:B:151:LEU:HD11	1.72	0.72
1:A:1134:TYR:O	1:A:1230:MET:N	2.21	0.72
1:A:224:MET:SD	1:A:228:ASP:HB3	2.30	0.72
1:A:581:MET:HA	1:A:591:ALA:HB1	1.72	0.71
1:A:963:GLU:O	1:A:967:VAL:CB	2.36	0.71
1:B:18:TYR:OH	1:B:24:ASN:HB3	1.89	0.71
1:B:857:LYS:O	1:B:861:LYS:CB	2.39	0.70
1:B:874:ILE:O	1:B:878:PHE:CB	2.39	0.70
1:B:1291:VAL:O	1:B:1293:GLN:N	2.24	0.70
1:A:316:ALA:HB3	1:A:392:HIS:ND1	2.06	0.70
1:A:1435:VAL:CB	1:A:1492:SER:CB	2.70	0.70
1:B:1420:ILE:O	1:B:1424:ASN:CB	2.39	0.70
1:A:871:ARG:HA	1:A:980:PHE:CB	2.21	0.70
1:B:885:LEU:O	1:B:888:THR:CA	2.40	0.70
1:A:523:LEU:HD12	1:A:553:CYS:SG	2.32	0.70
1:B:485:THR:HG21	1:B:562:HIS:CE1	2.26	0.70
1:B:128:SER:HB2	1:B:130:LYS:HE3	1.74	0.70
1:A:1270:ALA:HB2	1:A:1319:GLU:CB	2.22	0.70
1:A:230:LYS:HA	1:A:232:ASP:N	2.06	0.69
1:B:860:ASN:O	1:B:863:THR:N	2.25	0.69
1:A:450:SER:OG	1:A:513:GLN:O	2.09	0.69
1:A:981:ILE:O	1:A:985:ARG:CB	2.40	0.69
1:B:1291:VAL:O	1:B:1294:HIS:N	2.26	0.69
1:B:1381:LEU:HA	1:B:1384:CYS:CB	2.22	0.69
1:A:756:SER:O	1:A:760:ASP:N	2.26	0.69
1:A:264:LEU:HG	1:A:418:ILE:HD11	1.73	0.69
1:B:301:SER:O	1:B:303:PHE:CE1	2.46	0.69
1:A:1215:LEU:O	1:A:1219:GLN:N	2.23	0.68
1:B:290:ASP:O	1:B:292:CYS:N	2.25	0.68
1:B:483:PHE:O	1:B:506:ARG:NH1	2.26	0.68
1:B:755:ILE:O	1:B:758:GLN:N	2.26	0.68
1:A:162:TYR:HB3	1:A:164:GLN:NE2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ILE:HG23	1:B:367:ILE:O	1.91	0.68
1:A:72:PHE:CG	1:A:72:PHE:O	2.47	0.68
1:B:15:CYS:SG	1:B:222:LEU:HA	2.34	0.68
1:A:1096:ALA:O	1:A:1100:VAL:N	2.27	0.68
1:B:29:THR:HG22	1:B:151:LEU:CD1	2.24	0.68
1:B:194:HIS:CE1	1:B:214:CYS:SG	2.87	0.68
1:B:1203:ARG:CB	1:B:1207:ASN:CB	2.72	0.67
1:A:842:GLU:O	1:A:845:ARG:N	2.27	0.67
1:A:960:PRO:O	1:A:961:GLU:CB	2.41	0.67
1:B:855:SER:O	1:B:859:LYS:CB	2.43	0.67
1:B:1338:GLY:O	1:B:1342:LEU:CB	2.42	0.67
1:B:1449:LEU:O	1:B:1453:PHE:CB	2.42	0.67
1:A:55:ASP:OD1	1:A:127:LYS:HD3	1.94	0.67
1:A:1459:ARG:C	1:A:1461:CYS:H	2.01	0.67
1:A:610:ILE:O	1:A:613:ALA:HB3	1.95	0.67
1:B:863:THR:O	1:B:866:VAL:N	2.28	0.67
1:A:705:LYS:C	1:A:707:ILE:H	2.03	0.67
1:B:39:VAL:HG21	1:B:195:ALA:HB1	1.77	0.66
1:B:1085:ARG:C	1:B:1087:PHE:H	2.02	0.66
1:B:236:GLY:HA2	1:B:286:VAL:H	1.59	0.66
1:B:1380:LEU:O	1:B:1384:CYS:CB	2.43	0.66
1:A:1472:SER:O	1:A:1476:LYS:CB	2.43	0.66
1:A:469:GLU:O	1:A:473:VAL:HG23	1.96	0.66
1:A:243:PHE:O	1:A:430:PHE:HA	1.94	0.66
1:A:1285:SER:O	1:A:1341:VAL:CB	2.44	0.66
1:B:313:TYR:CD2	1:B:361:GLY:HA3	2.30	0.66
1:A:29:THR:HG22	1:A:151:LEU:CD1	2.26	0.66
1:A:863:THR:O	1:A:864:PHE:C	2.37	0.66
1:A:1251:ASN:CB	1:A:1283:LEU:O	2.44	0.66
1:B:1118:ASP:O	1:B:1119:LEU:C	2.39	0.66
1:B:510:MET:HA	1:B:515:ILE:HG13	1.78	0.65
1:B:138:LEU:O	1:B:147:MET:HA	1.97	0.65
1:A:703:SER:O	1:A:733:TYR:HA	1.97	0.65
1:A:477:LEU:O	1:A:555:LEU:HD21	1.97	0.65
1:A:1187:CYS:O	1:A:1191:SER:CB	2.45	0.65
1:A:117:TYR:CZ	1:A:165:PRO:HB3	2.32	0.64
1:A:32:LEU:HD21	1:A:128:SER:HA	1.79	0.64
1:A:581:MET:CA	1:A:591:ALA:HB1	2.26	0.64
1:B:31:GLY:HA3	1:B:448:ASP:OD2	1.96	0.64
1:B:726:ASP:O	1:B:729:ILE:N	2.30	0.64
1:A:196:SER:HB2	1:A:208:GLU:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:LEU:O	1:A:888:THR:CB	2.46	0.64
1:A:584:GLN:O	1:A:588:ASP:O	2.15	0.64
1:B:769:SER:CB	1:B:779:ALA:HA	2.28	0.64
1:A:117:TYR:O	1:A:172:ILE:HG12	1.97	0.64
1:B:439:GLU:HA	1:B:442:ASP:OD2	1.96	0.64
1:B:891:LEU:O	1:B:895:LEU:CB	2.46	0.64
1:A:20:GLU:HB2	1:A:217:SER:O	1.97	0.64
1:A:162:TYR:CE2	1:A:187:VAL:HA	2.33	0.64
1:A:871:ARG:CB	1:A:980:PHE:CA	2.75	0.64
1:A:1417:GLU:O	1:A:1420:ILE:N	2.31	0.64
1:B:65:ARG:N	1:B:103:ASN:OD1	2.31	0.63
1:B:252:THR:OG1	1:B:265:ARG:HB2	1.98	0.63
1:B:130:LYS:HD2	1:B:151:LEU:HB3	1.81	0.63
1:B:224:MET:SD	1:B:228:ASP:HB3	2.39	0.63
1:B:617:THR:O	1:B:621:LEU:CB	2.46	0.63
1:A:1178:GLU:O	1:A:1182:ARG:CB	2.47	0.63
1:B:852:PHE:O	1:B:856:ASP:N	2.26	0.63
1:A:240:VAL:HG12	1:A:434:PRO:HA	1.79	0.63
1:A:261:HIS:ND1	1:A:406:ILE:HD13	2.14	0.63
1:A:1200:GLN:O	1:A:1201:GLN:C	2.41	0.63
1:A:1245:CYS:CB	1:A:1285:SER:O	2.46	0.63
1:B:32:LEU:CD2	1:B:128:SER:HA	2.28	0.63
1:B:1315:ILE:O	1:B:1319:GLU:CB	2.47	0.63
1:A:397:THR:HB	1:A:420:THR:OG1	1.99	0.63
1:A:744:CYS:HA	1:A:1077:SER:CB	2.28	0.63
1:B:241:ARG:HG2	1:B:280:ALA:O	1.99	0.63
1:B:1126:VAL:O	1:B:1130:GLU:CB	2.46	0.63
1:B:225:LYS:C	1:B:227:SER:H	2.06	0.62
1:B:364:ILE:HG22	1:B:394:CYS:SG	2.39	0.62
1:A:671:VAL:O	1:A:674:ARG:N	2.32	0.62
1:A:1335:VAL:O	1:A:1384:CYS:CB	2.47	0.62
1:B:1210:ALA:O	1:B:1214:VAL:CB	2.46	0.62
1:A:1344:PHE:O	1:A:1347:ASP:N	2.31	0.62
1:B:313:TYR:CG	1:B:361:GLY:HA3	2.34	0.62
1:A:230:LYS:HA	1:A:232:ASP:H	1.63	0.62
1:A:1381:LEU:O	1:A:1385:THR:CB	2.47	0.62
1:A:69:GLN:NE2	1:A:73:TRP:HZ2	1.98	0.62
1:A:142:LEU:HB2	1:A:208:GLU:CD	2.24	0.62
1:A:701:ARG:CB	1:A:729:ILE:CB	2.78	0.62
1:A:1074:PRO:C	1:A:1076:VAL:H	2.07	0.62
1:B:1345:TYR:O	1:B:1350:SER:CB	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:ARG:CB	1:A:980:PHE:HA	2.30	0.62
1:A:244:HIS:CE1	1:A:428:GLU:HA	2.35	0.62
1:A:398:TRP:CZ2	1:A:424:LYS:HD2	2.35	0.61
1:A:761:VAL:O	1:A:762:ASP:C	2.44	0.61
1:B:367:ILE:O	1:B:367:ILE:CG2	2.49	0.61
1:B:755:ILE:O	1:B:759:LEU:N	2.32	0.61
1:B:863:THR:O	1:B:864:PHE:C	2.42	0.61
1:A:253:CYS:HB2	1:A:307:HIS:CE1	2.36	0.61
1:B:116:GLN:HA	1:B:175:SER:HA	1.81	0.61
1:B:1118:ASP:O	1:B:1121:GLN:N	2.34	0.61
1:B:240:VAL:HG12	1:B:434:PRO:HA	1.81	0.61
1:A:701:ARG:O	1:A:703:SER:N	2.33	0.61
1:A:769:SER:CB	1:A:779:ALA:HA	2.30	0.61
1:B:313:TYR:CE2	1:B:361:GLY:HA3	2.35	0.61
1:A:761:VAL:O	1:A:764:ILE:N	2.27	0.61
1:B:134:VAL:HG21	1:B:186:PRO:HG3	1.81	0.61
1:A:243:PHE:HB3	1:A:431:ALA:HB3	1.82	0.61
1:A:761:VAL:O	1:A:763:LEU:N	2.34	0.61
1:A:1273:MET:O	1:A:1276:ILE:N	2.33	0.61
1:B:982:LEU:O	1:B:986:LEU:CB	2.49	0.61
1:A:581:MET:O	1:A:585:ILE:N	2.34	0.60
1:B:117:TYR:OH	1:B:180:ASP:OD2	2.13	0.60
1:A:245:ALA:N	1:A:429:ALA:O	2.34	0.60
1:A:755:ILE:O	1:A:758:GLN:CA	2.49	0.60
1:B:369:GLU:HG2	1:B:370:LEU:N	2.17	0.60
1:B:751:ALA:O	1:B:754:GLU:N	2.34	0.60
1:B:1374:HIS:HA	1:B:1377:LEU:CB	2.32	0.60
1:A:281:LEU:O	1:A:308:LEU:CB	2.49	0.60
1:A:1471:ASP:O	1:A:1474:LEU:N	2.34	0.60
1:A:20:GLU:OE1	1:A:181:LYS:HD3	2.01	0.60
1:B:568:ARG:NH1	1:B:572:GLU:OE1	2.35	0.60
1:B:594:THR:O	1:B:598:LEU:N	2.34	0.60
1:A:196:SER:CB	1:A:208:GLU:O	2.50	0.60
1:A:224:MET:HA	1:A:293:ARG:CB	2.32	0.60
1:A:470:ARG:HD2	1:A:471:ARG:HH21	1.65	0.60
1:A:841:GLU:O	1:A:844:LEU:N	2.34	0.60
1:B:36:ARG:NH1	1:B:200:LEU:HD13	2.17	0.60
1:B:639:VAL:O	1:B:640:SER:CB	2.49	0.60
1:B:860:ASN:O	1:B:861:LYS:C	2.45	0.60
1:A:20:GLU:OE2	1:A:181:LYS:NZ	2.34	0.60
1:B:1215:LEU:O	1:B:1217:LEU:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:ASP:CB	1:A:865:GLU:O	2.50	0.59
1:A:1200:GLN:C	1:A:1202:GLN:N	2.56	0.59
1:A:15:CYS:CB	1:A:222:LEU:HA	2.32	0.59
1:A:249:LYS:O	1:A:264:LEU:HD22	2.02	0.59
1:A:16:SER:O	1:A:221:VAL:N	2.23	0.59
1:B:134:VAL:N	1:B:158:GLY:O	2.35	0.59
1:A:1203:ARG:CB	1:A:1207:ASN:CB	2.80	0.59
1:B:243:PHE:HB3	1:B:431:ALA:HB3	1.84	0.59
1:A:31:GLY:HA3	1:A:448:ASP:OD2	2.02	0.59
1:B:1405:ILE:O	1:B:1408:VAL:N	2.36	0.59
1:A:423:LEU:HD22	1:A:425:GLU:OE1	2.02	0.59
1:A:1310:LYS:O	1:A:1311:PHE:CB	2.50	0.59
1:B:264:LEU:HG	1:B:418:ILE:HD11	1.85	0.59
1:A:11:ILE:O	1:A:112:GLY:N	2.35	0.59
1:A:456:ILE:HG12	1:A:473:VAL:HG21	1.84	0.59
1:A:313:TYR:CD2	1:A:361:GLY:HA3	2.37	0.59
1:A:439:GLU:HA	1:A:442:ASP:OD2	2.03	0.59
1:B:1317:LYS:HA	1:B:1323:ILE:CB	2.33	0.59
1:A:477:LEU:HB3	1:A:555:LEU:HD22	1.84	0.58
1:B:65:ARG:H	1:B:103:ASN:CG	2.11	0.58
1:A:313:TYR:CG	1:A:361:GLY:HA3	2.38	0.58
1:A:1061:LEU:HA	1:A:1101:GLN:CB	2.33	0.58
1:A:1438:LYS:O	1:A:1441:TYR:N	2.36	0.58
1:A:836:THR:O	1:A:839:PHE:N	2.36	0.58
1:B:54:ARG:CZ	1:B:127:LYS:HG3	2.32	0.58
1:B:1000:GLU:CB	1:B:1004:SER:O	2.51	0.58
1:A:839:PHE:O	1:A:842:GLU:CB	2.51	0.58
1:B:852:PHE:O	1:B:853:PRO:O	2.22	0.58
1:B:592:GLU:O	1:B:594:THR:N	2.36	0.58
1:B:1200:GLN:O	1:B:1202:GLN:N	2.36	0.58
1:A:398:TRP:CD2	1:A:424:LYS:HG3	2.38	0.58
1:A:1203:ARG:O	1:A:1207:ASN:CB	2.51	0.58
1:A:1203:ARG:O	1:A:1207:ASN:N	2.37	0.58
1:B:313:TYR:CD1	1:B:361:GLY:HA3	2.38	0.58
1:A:220:ILE:HG23	1:A:220:ILE:O	2.03	0.58
1:A:600:HIS:O	1:A:603:ARG:CB	2.52	0.58
1:A:282:TRP:CH2	1:A:314:LEU:HD22	2.39	0.58
1:B:571:GLN:O	1:B:574:ILE:N	2.36	0.58
1:B:1298:CYS:O	1:B:1299:ILE:CB	2.51	0.58
1:B:772:ASN:O	1:B:773:LEU:C	2.46	0.57
1:B:286:VAL:O	1:B:288:GLN:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1379:GLU:HA	1:B:1382:ALA:HB3	1.86	0.57
1:A:489:ASN:OD1	1:A:499:PHE:O	2.23	0.57
1:A:1210:ALA:O	1:A:1214:VAL:CB	2.53	0.57
1:A:1188:VAL:HA	1:A:1236:LEU:CB	2.34	0.57
1:A:1201:GLN:O	1:A:1202:GLN:C	2.47	0.57
1:B:450:SER:OG	1:B:513:GLN:O	2.22	0.57
1:A:364:ILE:O	1:A:394:CYS:SG	2.63	0.57
1:B:669:LYS:C	1:B:671:VAL:N	2.62	0.57
1:A:772:ASN:O	1:A:773:LEU:C	2.48	0.57
1:A:1375:ILE:HA	1:A:1378:VAL:CB	2.35	0.57
1:A:113:THR:O	1:A:114:VAL:C	2.44	0.57
1:A:555:LEU:HD23	1:A:555:LEU:O	2.05	0.57
1:A:246:GLU:HB2	1:A:427:LYS:HB3	1.86	0.57
1:B:1273:MET:O	1:B:1276:ILE:N	2.38	0.57
1:B:1116:LYS:O	1:B:1117:GLN:C	2.48	0.57
1:B:313:TYR:CZ	1:B:361:GLY:HA3	2.40	0.56
1:B:1122:LEU:O	1:B:1125:ILE:N	2.38	0.56
1:A:71:GLN:HB3	1:A:92:LEU:CD2	2.35	0.56
1:A:264:LEU:HG	1:A:418:ILE:CD1	2.35	0.56
1:A:753:ASN:O	1:A:754:GLU:C	2.48	0.56
1:A:1294:HIS:O	1:A:1298:CYS:CB	2.54	0.56
1:A:39:VAL:O	1:A:41:PRO:HD3	2.04	0.56
1:A:400:HIS:HA	1:A:428:GLU:HG2	1.87	0.56
1:A:447:ASN:O	1:A:448:ASP:C	2.45	0.56
1:A:744:CYS:O	1:A:1077:SER:CB	2.53	0.56
1:B:55:ASP:OD1	1:B:127:LYS:HD3	2.06	0.56
1:B:1108:ASP:O	1:B:1112:TYR:CB	2.53	0.56
1:B:1435:VAL:CB	1:B:1492:SER:CB	2.83	0.56
1:A:767:CYS:O	1:A:771:GLU:CB	2.54	0.56
1:B:616:ASP:O	1:B:620:SER:CB	2.54	0.56
1:B:669:LYS:C	1:B:671:VAL:H	2.13	0.56
1:A:1207:ASN:O	1:A:1210:ALA:N	2.37	0.56
1:B:20:GLU:OE2	1:B:181:LYS:NZ	2.36	0.56
1:B:64:ASN:HB2	1:B:66:TYR:CE2	2.40	0.56
1:A:1215:LEU:O	1:A:1218:LEU:N	2.39	0.56
1:B:859:LYS:O	1:B:860:ASN:C	2.49	0.56
1:B:871:ARG:CB	1:B:980:PHE:HA	2.36	0.56
1:B:1200:GLN:C	1:B:1202:GLN:H	2.14	0.56
1:B:194:HIS:CD2	1:B:214:CYS:HB2	2.41	0.56
1:A:861:LYS:O	1:A:862:LEU:C	2.47	0.56
1:B:20:GLU:HB2	1:B:217:SER:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:PRO:HB2	1:B:170:ARG:O	2.06	0.56
1:B:888:THR:O	1:B:889:LYS:C	2.49	0.56
1:A:19:ALA:HB2	1:A:218:TRP:CZ3	2.41	0.56
1:A:368:PHE:CD1	1:A:392:HIS:HA	2.41	0.56
1:A:975:ILE:O	1:A:979:GLN:CB	2.54	0.56
1:A:1436:GLU:CB	1:A:1493:PRO:C	2.79	0.56
1:B:1203:ARG:O	1:B:1207:ASN:CB	2.54	0.56
1:A:871:ARG:CA	1:A:980:PHE:CB	2.83	0.55
1:B:170:ARG:NH2	1:B:180:ASP:OD1	2.38	0.55
1:B:769:SER:O	1:B:773:LEU:CB	2.54	0.55
1:B:1434:GLU:O	1:B:1492:SER:CB	2.55	0.55
1:A:708:ARG:O	1:A:712:VAL:N	2.39	0.55
1:A:610:ILE:O	1:A:613:ALA:CB	2.53	0.55
1:A:1434:GLU:O	1:A:1492:SER:CB	2.54	0.55
1:B:30:LEU:HD12	1:B:36:ARG:NH2	2.20	0.55
1:B:142:LEU:HD21	1:B:200:LEU:HA	1.88	0.55
1:A:1361:GLU:O	1:A:1364:ARG:CB	2.54	0.55
1:B:20:GLU:N	1:B:217:SER:O	2.38	0.55
1:B:633:TYR:O	1:B:636:ASP:N	2.40	0.55
1:B:1245:CYS:CB	1:B:1341:VAL:H	2.20	0.55
1:B:1284:CYS:CB	1:B:1295:PHE:CB	2.85	0.55
1:A:312:HIS:CB	1:A:357:SER:OG	2.54	0.55
1:B:1200:GLN:C	1:B:1202:GLN:N	2.62	0.55
1:A:66:TYR:O	1:A:157:GLU:OE2	2.23	0.55
1:A:364:ILE:O	1:A:367:ILE:HG22	2.07	0.55
1:B:609:HIS:O	1:B:610:ILE:C	2.50	0.55
1:B:726:ASP:O	1:B:728:ASP:N	2.40	0.55
1:B:1207:ASN:O	1:B:1208:MET:C	2.49	0.55
1:B:1245:CYS:CB	1:B:1285:SER:O	2.55	0.55
1:A:142:LEU:HB2	1:A:208:GLU:OE2	2.06	0.55
1:A:181:LYS:HA	1:A:218:TRP:O	2.07	0.55
1:A:671:VAL:O	1:A:674:ARG:CB	2.55	0.55
1:B:1422:TYR:O	1:B:1426:LEU:CB	2.55	0.55
1:B:1245:CYS:CB	1:B:1285:SER:CB	2.84	0.55
1:A:645:ILE:O	1:A:646:PRO:C	2.50	0.55
1:A:1375:ILE:C	1:A:1378:VAL:H	2.15	0.55
1:B:136:LYS:HB3	1:B:189:ALA:HA	1.89	0.55
1:B:1285:SER:HA	1:B:1341:VAL:CB	2.37	0.55
1:A:861:LYS:O	1:A:864:PHE:N	2.40	0.54
1:A:885:LEU:O	1:A:888:THR:CA	2.55	0.54
1:A:844:LEU:HA	1:A:847:VAL:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASN:O	1:B:49:PRO:C	2.49	0.54
1:B:1215:LEU:O	1:B:1216:GLU:C	2.50	0.54
1:B:13:ASP:OD1	1:B:226:TRP:N	2.40	0.54
1:B:511:ARG:HG2	1:B:511:ARG:O	2.07	0.54
1:A:244:HIS:CD2	1:A:264:LEU:HD11	2.43	0.54
1:A:788:MET:O	1:A:790:VAL:N	2.41	0.54
1:B:389:ARG:CZ	1:B:425:GLU:O	2.55	0.54
1:B:1234:MET:O	1:B:1237:ALA:HB3	2.08	0.54
1:A:999:ARG:HA	1:A:1007:GLN:HA	1.88	0.54
1:A:223:PHE:CD1	1:A:292:CYS:HA	2.43	0.54
1:B:34:ASP:OD2	1:B:36:ARG:HB2	2.08	0.54
1:B:270:GLN:NE2	1:B:1257:LYS:HA	2.22	0.54
1:A:1315:ILE:O	1:A:1319:GLU:CB	2.56	0.54
1:B:18:TYR:HA	1:B:25:GLY:O	2.08	0.54
1:B:777:LEU:C	1:B:780:SER:H	2.14	0.54
1:A:20:GLU:OE1	1:A:219:LYS:HB2	2.08	0.54
1:A:142:LEU:HD21	1:A:200:LEU:HA	1.88	0.54
1:A:142:LEU:HD23	1:A:200:LEU:HD23	1.90	0.54
1:B:235:LYS:O	1:B:236:GLY:C	2.51	0.54
1:A:39:VAL:HG21	1:A:195:ALA:HB1	1.89	0.54
1:A:162:TYR:HB3	1:A:164:GLN:CD	2.33	0.54
1:A:477:LEU:O	1:A:555:LEU:CD2	2.56	0.54
1:A:756:SER:HA	1:A:759:LEU:CB	2.37	0.54
1:A:789:HIS:O	1:A:790:VAL:CB	2.56	0.54
1:B:130:LYS:HB2	1:B:151:LEU:HD22	1.90	0.54
1:B:744:CYS:CB	1:B:1081:GLN:O	2.56	0.54
1:A:879:TYR:H	1:A:884:LEU:CB	2.21	0.54
1:B:225:LYS:O	1:B:227:SER:N	2.38	0.54
1:B:270:GLN:HE22	1:B:1257:LYS:HA	1.73	0.54
1:B:836:THR:O	1:B:838:GLU:N	2.41	0.54
1:A:1096:ALA:O	1:A:1097:PHE:C	2.50	0.53
1:A:29:THR:HG22	1:A:151:LEU:HD11	1.90	0.53
1:A:108:ARG:O	1:A:111:LEU:HB2	2.08	0.53
1:A:977:ILE:C	1:A:979:GLN:H	2.16	0.53
1:A:257:ARG:O	1:A:259:LYS:HG3	2.08	0.53
1:A:316:ALA:HA	1:A:354:SER:O	2.09	0.53
1:A:1251:ASN:CB	1:A:1283:LEU:HA	2.39	0.53
1:A:1416:PRO:O	1:A:1417:GLU:C	2.50	0.53
1:B:14:ILE:HG22	1:B:57:LEU:HD22	1.91	0.53
1:B:19:ALA:O	1:B:24:ASN:HA	2.08	0.53
1:B:654:LYS:O	1:B:657:LEU:C	2.50	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:TYR:CE1	1:B:361:GLY:HA3	2.43	0.53
1:A:10:HIS:HA	1:A:113:THR:O	2.09	0.53
1:A:115:ILE:CG2	1:A:116:GLN:N	2.71	0.53
1:A:196:SER:OG	1:A:197:SER:N	2.41	0.53
1:A:371:ASP:HB3	1:A:389:ARG:O	2.09	0.53
1:B:285:GLU:C	1:B:287:VAL:N	2.66	0.53
1:A:707:ILE:CB	1:A:733:TYR:O	2.57	0.53
1:A:871:ARG:HA	1:A:980:PHE:HA	1.89	0.53
1:A:1207:ASN:O	1:A:1209:GLY:N	2.41	0.53
1:B:186:PRO:HB2	1:B:189:ALA:HB3	1.91	0.53
1:B:739:LEU:O	1:B:740:PHE:C	2.49	0.53
1:A:705:LYS:C	1:A:707:ILE:N	2.67	0.53
1:B:856:ASP:HA	1:B:859:LYS:CB	2.39	0.53
1:B:882:SER:O	1:B:885:LEU:CA	2.56	0.53
1:B:1191:SER:CB	1:B:1236:LEU:O	2.57	0.53
1:B:1207:ASN:C	1:B:1209:GLY:N	2.64	0.53
1:A:40:GLN:CB	1:A:43:ALA:CB	2.87	0.53
1:A:63:MET:SD	1:A:120:VAL:HG21	2.48	0.53
1:A:755:ILE:O	1:A:756:SER:C	2.50	0.53
1:A:867:VAL:CB	1:A:976:GLU:CB	2.87	0.53
1:B:194:HIS:CD2	1:B:214:CYS:CB	2.92	0.53
1:B:856:ASP:C	1:B:860:ASN:CB	2.79	0.53
1:A:38:VAL:HG11	1:A:200:LEU:HD11	1.90	0.53
1:B:523:LEU:HD12	1:B:553:CYS:SG	2.49	0.53
1:A:353:TYR:O	1:A:420:THR:HG22	2.08	0.52
1:B:484:VAL:HG11	1:B:562:HIS:HB3	1.91	0.52
1:A:142:LEU:HD12	1:A:198:HIS:HB3	1.91	0.52
1:A:225:LYS:O	1:A:227:SER:N	2.39	0.52
1:A:657:LEU:O	1:A:659:PRO:N	2.41	0.52
1:A:992:CYS:O	1:A:993:LEU:C	2.51	0.52
1:A:1189:GLN:C	1:A:1191:SER:H	2.18	0.52
1:B:744:CYS:C	1:B:745:LEU:O	2.51	0.52
1:A:1438:LYS:HA	1:A:1441:TYR:CB	2.39	0.52
1:A:369:GLU:OE2	1:A:391:ARG:NH2	2.33	0.52
1:A:581:MET:O	1:A:585:ILE:CB	2.57	0.52
1:B:701:ARG:O	1:B:703:SER:N	2.43	0.52
1:B:853:PRO:O	1:B:854:PHE:C	2.51	0.52
1:B:1476:LYS:O	1:B:1479:THR:N	2.42	0.52
1:B:1207:ASN:O	1:B:1210:ALA:N	2.43	0.52
1:B:1245:CYS:CB	1:B:1341:VAL:N	2.72	0.52
1:A:15:CYS:HA	1:A:223:PHE:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:TRP:CZ2	1:A:372:PRO:HD3	2.45	0.52
1:A:671:VAL:O	1:A:672:LEU:C	2.52	0.52
1:A:511:ARG:O	1:A:511:ARG:HG2	2.10	0.52
1:A:871:ARG:CB	1:A:980:PHE:N	2.72	0.52
1:B:69:GLN:HG2	1:B:73:TRP:CZ2	2.45	0.52
1:B:124:LEU:HD13	1:B:131:TYR:CE1	2.45	0.52
1:A:117:TYR:CE2	1:A:165:PRO:HB3	2.43	0.52
1:A:1379:GLU:HA	1:A:1382:ALA:HB3	1.92	0.52
1:B:288:GLN:CD	1:B:293:ARG:C	2.78	0.52
1:B:830:LYS:O	1:B:833:PHE:CB	2.58	0.52
1:A:514:ASN:ND2	1:A:517:LYS:HD3	2.25	0.52
1:B:134:VAL:HG23	1:B:161:PHE:CZ	2.45	0.52
1:B:470:ARG:NH2	1:B:548:PRO:HA	2.25	0.52
1:B:992:CYS:O	1:B:995:CYS:N	2.43	0.52
1:A:772:ASN:O	1:A:774:PRO:N	2.43	0.52
1:B:1064:LEU:CB	1:B:1101:GLN:CB	2.87	0.52
1:A:891:LEU:O	1:A:892:LEU:C	2.53	0.51
1:B:627:GLU:O	1:B:629:ARG:N	2.43	0.51
1:B:1085:ARG:C	1:B:1087:PHE:N	2.66	0.51
1:A:727:ARG:O	1:A:730:LEU:N	2.43	0.51
1:B:485:THR:CG2	1:B:562:HIS:ND1	2.73	0.51
1:B:1289:GLU:C	1:B:1291:VAL:H	2.18	0.51
1:A:1338:GLY:O	1:A:1342:LEU:CB	2.59	0.51
1:A:15:CYS:SG	1:A:222:LEU:HG	2.51	0.51
1:A:1346:ASN:O	1:A:1348:ARG:N	2.44	0.51
1:A:69:GLN:CD	1:A:73:TRP:HZ2	2.18	0.51
1:A:148:ARG:HG2	1:A:150:THR:HG22	1.93	0.51
1:A:551:HIS:C	1:A:552:ILE:HG13	2.34	0.51
1:B:980:PHE:O	1:B:981:ILE:C	2.53	0.51
1:A:14:ILE:O	1:A:222:LEU:HD23	2.10	0.51
1:B:288:GLN:HG3	1:B:292:CYS:O	2.11	0.51
1:B:669:LYS:O	1:B:672:LEU:N	2.43	0.51
1:B:860:ASN:O	1:B:863:THR:CB	2.59	0.51
1:B:967:VAL:HA	1:B:970:THR:CB	2.40	0.51
1:A:20:GLU:OE2	1:A:181:LYS:CE	2.58	0.51
1:A:460:LEU:HD13	1:A:465:ILE:HG23	1.93	0.51
1:A:843:TYR:O	1:A:847:VAL:CB	2.59	0.51
1:A:998:LYS:CB	1:A:1008:SER:CB	2.89	0.51
1:B:1094:LEU:O	1:B:1095:GLN:C	2.54	0.51
1:B:1251:ASN:O	1:B:1255:LEU:CB	2.58	0.51
1:A:66:TYR:CD1	1:A:69:GLN:OE1	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ALA:HB2	1:A:147:MET:O	2.11	0.51
1:A:697:TRP:CB	1:A:726:ASP:CB	2.89	0.51
1:B:194:HIS:CG	1:B:214:CYS:HG	2.29	0.51
1:B:1084:PHE:O	1:B:1087:PHE:CB	2.59	0.51
1:A:11:ILE:HG21	1:A:62:PRO:HG3	1.93	0.50
1:A:241:ARG:NH2	1:A:439:GLU:OE1	2.42	0.50
1:A:715:LEU:O	1:A:716:ALA:C	2.54	0.50
1:A:992:CYS:C	1:A:994:LEU:N	2.65	0.50
1:B:122:GLN:HG2	1:B:159:SER:O	2.10	0.50
1:B:196:SER:OG	1:B:197:SER:N	2.44	0.50
1:B:665:LEU:O	1:B:666:ILE:CB	2.59	0.50
1:A:21:GLY:HA3	1:A:216:THR:HA	1.94	0.50
1:A:225:LYS:C	1:A:227:SER:H	2.19	0.50
1:A:398:TRP:CH2	1:A:424:LYS:HE3	2.46	0.50
1:A:473:VAL:O	1:A:476:LEU:N	2.44	0.50
1:A:708:ARG:O	1:A:712:VAL:CB	2.58	0.50
1:A:999:ARG:HA	1:A:1007:GLN:CA	2.40	0.50
1:A:1034:GLU:HA	1:A:1037:ALA:HB3	1.93	0.50
1:B:1215:LEU:O	1:B:1218:LEU:N	2.45	0.50
1:A:8:PHE:O	1:A:10:HIS:CE1	2.64	0.50
1:A:255:GLU:HA	1:A:259:LYS:O	2.11	0.50
1:A:596:THR:C	1:A:598:LEU:N	2.66	0.50
1:B:18:TYR:CD1	1:B:25:GLY:C	2.90	0.50
1:A:224:MET:SD	1:A:228:ASP:CB	2.99	0.50
1:A:502:PRO:HG3	1:A:565:GLN:HG2	1.93	0.50
1:B:38:VAL:HG11	1:B:200:LEU:HD11	1.93	0.50
1:B:194:HIS:CD2	1:B:214:CYS:SG	3.05	0.50
1:A:224:MET:HE2	1:A:293:ARG:O	2.12	0.50
1:A:306:LYS:HB2	1:A:313:TYR:CZ	2.47	0.50
1:A:852:PHE:O	1:A:856:ASP:CB	2.60	0.50
1:A:856:ASP:O	1:A:860:ASN:CB	2.60	0.50
1:B:711:SER:CB	1:B:737:LEU:CB	2.89	0.50
1:B:1061:LEU:O	1:B:1065:LEU:N	2.31	0.50
1:A:475:LYS:NZ	1:A:479:ASP:OD1	2.42	0.50
1:A:581:MET:HA	1:A:591:ALA:CB	2.39	0.50
1:A:730:LEU:O	1:A:733:TYR:N	2.45	0.50
1:B:836:THR:O	1:B:837:MET:C	2.55	0.50
1:B:891:LEU:HA	1:B:894:ILE:H	1.77	0.50
1:B:1355:ILE:C	1:B:1357:MET:H	2.20	0.50
1:A:9:LEU:HD13	1:A:178:ILE:CD1	2.42	0.50
1:A:245:ALA:HB2	1:A:429:ALA:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:TYR:HB2	1:A:420:THR:CG2	2.42	0.50
1:A:751:ALA:O	1:A:752:ILE:C	2.55	0.50
1:A:871:ARG:CA	1:A:980:PHE:HA	2.42	0.50
1:B:36:ARG:HH12	1:B:200:LEU:HD13	1.76	0.50
1:B:194:HIS:CG	1:B:214:CYS:SG	3.05	0.50
1:B:313:TYR:CG	1:B:361:GLY:CA	2.94	0.50
1:B:853:PRO:C	1:B:855:SER:N	2.69	0.50
1:B:1371:LEU:O	1:B:1375:ILE:CA	2.60	0.50
1:B:1375:ILE:HA	1:B:1378:VAL:CB	2.42	0.50
1:A:998:LYS:C	1:A:1007:GLN:HA	2.37	0.50
1:B:39:VAL:HG23	1:B:207:ASN:HB2	1.94	0.50
1:B:263:PHE:CE2	1:B:415:MET:HG2	2.46	0.50
1:B:1357:MET:O	1:B:1359:ARG:N	2.44	0.50
1:B:140:ALA:HB3	1:B:143:GLU:O	2.12	0.49
1:B:395:THR:O	1:B:396:ASN:C	2.55	0.49
1:B:502:PRO:HG3	1:B:565:GLN:HG2	1.93	0.49
1:B:978:LEU:O	1:B:981:ILE:CA	2.60	0.49
1:A:40:GLN:CB	1:A:43:ALA:HB2	2.42	0.49
1:B:608:LYS:O	1:B:611:THR:CB	2.60	0.49
1:A:554:ARG:CB	1:A:557:TYR:CB	2.91	0.49
1:B:456:ILE:HG12	1:B:473:VAL:HG21	1.94	0.49
1:B:523:LEU:CD1	1:B:553:CYS:SG	3.01	0.49
1:B:1134:TYR:O	1:B:1230:MET:CB	2.61	0.49
1:B:1201:GLN:O	1:B:1202:GLN:C	2.55	0.49
1:B:1371:LEU:O	1:B:1372:MET:C	2.55	0.49
1:B:1382:ALA:HA	1:B:1385:THR:CB	2.42	0.49
1:A:632:ASP:O	1:A:635:SER:N	2.45	0.49
1:A:840:VAL:O	1:A:841:GLU:C	2.52	0.49
1:A:1381:LEU:C	1:A:1385:THR:H	2.20	0.49
1:B:127:LYS:HG2	1:B:127:LYS:O	2.12	0.49
1:B:196:SER:C	1:B:207:ASN:HD22	2.21	0.49
1:B:1027:ALA:O	1:B:1029:ASP:N	2.38	0.49
1:A:103:ASN:O	1:A:107:ASN:ND2	2.46	0.49
1:A:601:ASN:C	1:A:603:ARG:N	2.70	0.49
1:A:753:ASN:O	1:A:755:ILE:N	2.46	0.49
1:A:1037:ALA:C	1:A:1039:GLY:N	2.70	0.49
1:A:1094:LEU:O	1:A:1095:GLN:C	2.56	0.49
1:B:603:ARG:O	1:B:604:LYS:CB	2.61	0.49
1:B:720:LYS:O	1:B:722:GLY:N	2.44	0.49
1:B:1310:LYS:O	1:B:1311:PHE:CB	2.61	0.49
1:A:125:HIS:O	1:A:129:ASN:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLY:O	1:A:180:ASP:C	2.55	0.49
1:A:1215:LEU:O	1:A:1216:GLU:C	2.56	0.49
1:A:1371:LEU:O	1:A:1372:MET:C	2.56	0.49
1:B:354:SER:HA	1:B:419:GLY:HA2	1.95	0.49
1:B:576:LYS:O	1:B:578:PHE:N	2.45	0.49
1:B:761:VAL:O	1:B:762:ASP:C	2.55	0.49
1:B:836:THR:O	1:B:839:PHE:N	2.46	0.49
1:B:1200:GLN:O	1:B:1201:GLN:C	2.56	0.49
1:B:735:TYR:C	1:B:737:LEU:H	2.21	0.49
1:B:831:GLU:O	1:B:832:ARG:C	2.55	0.49
1:A:125:HIS:CE1	1:A:127:LYS:HB3	2.48	0.49
1:A:428:GLU:CA	1:A:428:GLU:OE2	2.58	0.49
1:A:514:ASN:O	1:A:518:GLN:HG2	2.12	0.49
1:A:549:PHE:O	1:A:552:ILE:N	2.45	0.49
1:B:140:ALA:HB2	1:B:147:MET:O	2.13	0.49
1:A:96:ALA:O	1:A:100:LYS:HB2	2.13	0.48
1:A:598:LEU:O	1:A:599:LEU:C	2.56	0.48
1:A:841:GLU:O	1:A:844:LEU:CB	2.60	0.48
1:B:18:TYR:CE1	1:B:25:GLY:CA	2.96	0.48
1:B:242:LEU:HD23	1:B:432:ILE:HD13	1.94	0.48
1:B:391:ARG:HD2	1:B:396:ASN:OD1	2.13	0.48
1:A:125:HIS:HE1	1:A:127:LYS:HB3	1.79	0.48
1:A:735:TYR:O	1:A:738:ASN:O	2.32	0.48
1:B:236:GLY:CA	1:B:286:VAL:H	2.25	0.48
1:A:20:GLU:OE1	1:A:181:LYS:CD	2.61	0.48
1:A:20:GLU:OE2	1:A:181:LYS:HE2	2.12	0.48
1:B:888:THR:O	1:B:890:ILE:N	2.46	0.48
1:A:725:GLU:CB	1:A:865:GLU:CB	2.91	0.48
1:B:47:ASN:O	1:B:49:PRO:CD	2.58	0.48
1:B:188:ASN:OD1	1:B:189:ALA:N	2.46	0.48
1:B:504:ARG:HD2	1:B:567:TYR:CZ	2.49	0.48
1:A:254:ASP:O	1:A:260:GLN:HA	2.14	0.48
1:A:773:LEU:CB	1:A:779:ALA:N	2.77	0.48
1:B:20:GLU:OE1	1:B:219:LYS:HB2	2.13	0.48
1:B:863:THR:O	1:B:865:GLU:N	2.46	0.48
1:A:1362:ARG:O	1:A:1363:ASP:C	2.55	0.48
1:B:484:VAL:CG1	1:B:562:HIS:HB3	2.43	0.48
1:B:681:SER:O	1:B:682:THR:C	2.57	0.48
1:A:20:GLU:C	1:A:217:SER:H	2.22	0.48
1:A:759:LEU:O	1:A:760:ASP:O	2.32	0.48
1:A:1076:VAL:O	1:A:1079:ALA:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLY:H	1:B:286:VAL:CB	2.26	0.48
1:B:271:SER:O	1:B:272:ALA:C	2.56	0.48
1:B:627:GLU:O	1:B:628:PRO:C	2.57	0.48
1:B:49:PRO:O	1:B:50:PRO:C	2.55	0.48
1:B:165:PRO:CB	1:B:170:ARG:O	2.62	0.48
1:A:680:VAL:C	1:A:682:THR:H	2.20	0.48
1:A:680:VAL:C	1:A:682:THR:N	2.68	0.48
1:B:666:ILE:N	1:B:667:GLU:HA	2.29	0.48
1:A:586:GLY:O	1:A:587:TYR:C	2.54	0.48
1:B:18:TYR:CE1	1:B:25:GLY:N	2.82	0.48
1:B:32:LEU:HD22	1:B:128:SER:HB2	1.96	0.48
1:B:166:PHE:HE1	1:B:167:TYR:CE1	2.32	0.48
1:A:69:GLN:CD	1:A:73:TRP:CZ2	2.92	0.47
1:A:235:LYS:HD3	1:A:235:LYS:HA	1.64	0.47
1:A:703:SER:O	1:A:733:TYR:CA	2.60	0.47
1:B:1291:VAL:C	1:B:1293:GLN:N	2.72	0.47
1:A:30:LEU:HB2	1:A:34:ASP:OD2	2.14	0.47
1:A:179:GLY:H	1:A:220:ILE:HG23	1.79	0.47
1:A:1420:ILE:O	1:A:1424:ASN:CB	2.62	0.47
1:B:588:ASP:C	1:B:590:LEU:H	2.21	0.47
1:B:1076:VAL:O	1:B:1079:ALA:HB3	2.14	0.47
1:A:20:GLU:HB2	1:A:217:SER:OG	2.14	0.47
1:A:704:ASN:O	1:A:736:GLN:CB	2.62	0.47
1:A:891:LEU:O	1:A:894:ILE:N	2.45	0.47
1:B:166:PHE:CE1	1:B:167:TYR:CE1	3.02	0.47
1:B:978:LEU:O	1:B:979:GLN:C	2.55	0.47
1:B:1357:MET:O	1:B:1358:MET:C	2.57	0.47
1:A:39:VAL:HG23	1:A:207:ASN:HB2	1.96	0.47
1:A:753:ASN:C	1:A:755:ILE:N	2.70	0.47
1:A:1298:CYS:O	1:A:1299:ILE:CB	2.63	0.47
1:A:1369:SER:O	1:A:1370:PRO:C	2.56	0.47
1:B:1417:GLU:O	1:B:1420:ILE:N	2.44	0.47
1:B:1481:ILE:O	1:B:1485:ILE:CB	2.62	0.47
1:A:162:TYR:HB3	1:A:164:GLN:HE22	1.78	0.47
1:B:95:ALA:O	1:B:96:ALA:C	2.55	0.47
1:B:482:TYR:HD1	1:B:489:ASN:O	1.98	0.47
1:B:571:GLN:C	1:B:574:ILE:H	2.21	0.47
1:B:1215:LEU:C	1:B:1217:LEU:N	2.73	0.47
1:A:98:LEU:HD23	1:A:101:LYS:HE2	1.97	0.47
1:A:115:ILE:CG2	1:A:116:GLN:H	2.27	0.47
1:A:286:VAL:O	1:A:288:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:VAL:O	1:A:474:THR:C	2.57	0.47
1:A:707:ILE:CB	1:A:736:GLN:CB	2.92	0.47
1:A:847:VAL:CB	1:A:897:CYS:O	2.63	0.47
1:B:64:ASN:CB	1:B:66:TYR:CE2	2.98	0.47
1:B:626:ARG:C	1:B:628:PRO:N	2.71	0.47
1:B:883:ASP:O	1:B:887:LEU:CB	2.63	0.47
1:B:1134:TYR:C	1:B:1230:MET:CB	2.87	0.47
1:A:1344:PHE:C	1:A:1347:ASP:H	2.23	0.47
1:B:447:ASN:O	1:B:448:ASP:C	2.57	0.47
1:A:595:ILE:C	1:A:598:LEU:CB	2.88	0.47
1:A:115:ILE:HG22	1:A:116:GLN:N	2.30	0.47
1:A:1078:GLY:O	1:A:1081:GLN:CB	2.63	0.47
1:A:1415:ILE:O	1:A:1416:PRO:C	2.58	0.47
1:B:1061:LEU:O	1:B:1064:LEU:CB	2.62	0.47
1:B:1415:ILE:O	1:B:1416:PRO:C	2.57	0.47
1:A:113:THR:O	1:A:115:ILE:N	2.47	0.46
1:A:510:MET:SD	1:A:515:ILE:HG21	2.55	0.46
1:A:1273:MET:O	1:A:1274:GLN:C	2.58	0.46
1:B:1363:ASP:O	1:B:1366:ASP:CB	2.63	0.46
1:A:20:GLU:CB	1:A:217:SER:OG	2.64	0.46
1:A:69:GLN:HA	1:A:96:ALA:HB2	1.97	0.46
1:A:580:PHE:O	1:A:581:MET:C	2.57	0.46
1:A:724:LYS:C	1:A:726:ASP:H	2.23	0.46
1:A:871:ARG:HA	1:A:980:PHE:CA	2.45	0.46
1:B:49:PRO:O	1:B:50:PRO:O	2.34	0.46
1:B:470:ARG:HH22	1:B:548:PRO:HA	1.79	0.46
1:B:872:ASN:O	1:B:875:TYR:CB	2.63	0.46
1:A:160:TRP:O	1:A:186:PRO:HA	2.16	0.46
1:A:1354:LEU:O	1:A:1355:ILE:C	2.58	0.46
1:B:409:GLU:O	1:B:409:GLU:HG3	2.14	0.46
1:B:510:MET:SD	1:B:515:ILE:HG21	2.55	0.46
1:B:485:THR:O	1:B:486:GLY:C	2.57	0.46
1:B:687:LEU:O	1:B:688:GLU:C	2.59	0.46
1:A:769:SER:O	1:A:773:LEU:CB	2.64	0.46
1:A:1437:MET:O	1:A:1438:LYS:C	2.57	0.46
1:A:1477:TYR:O	1:A:1481:ILE:CB	2.63	0.46
1:A:68:ALA:HA	1:A:71:GLN:HB2	1.98	0.46
1:A:162:TYR:HB2	1:A:185:ASN:O	2.15	0.46
1:A:727:ARG:O	1:A:728:ASP:C	2.57	0.46
1:A:842:GLU:C	1:A:844:LEU:N	2.73	0.46
1:B:60:LEU:HD13	1:B:123:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ARG:NH2	1:B:425:GLU:H	2.14	0.46
1:B:826:LYS:O	1:B:827:ASP:C	2.58	0.46
1:B:891:LEU:HA	1:B:894:ILE:CB	2.45	0.46
1:A:40:GLN:CB	1:A:43:ALA:HB3	2.46	0.46
1:A:72:PHE:O	1:A:72:PHE:CD1	2.69	0.46
1:A:479:ASP:O	1:A:482:TYR:HB3	2.16	0.46
1:B:49:PRO:C	1:B:50:PRO:O	2.57	0.46
1:A:1065:LEU:HA	1:A:1104:VAL:CB	2.46	0.46
1:B:32:LEU:CD2	1:B:128:SER:HB2	2.46	0.46
1:B:231:ASP:OD2	1:B:434:PRO:HG3	2.16	0.46
1:B:993:LEU:HA	1:B:996:ILE:CB	2.46	0.46
1:B:1028:LEU:O	1:B:1031:GLU:N	2.48	0.46
1:B:1034:GLU:HA	1:B:1037:ALA:HB3	1.98	0.46
1:A:581:MET:O	1:A:591:ALA:CB	2.64	0.46
1:B:707:ILE:CB	1:B:736:GLN:CB	2.94	0.46
1:B:1238:HIS:O	1:B:1240:PHE:N	2.49	0.46
1:A:1378:VAL:O	1:A:1382:ALA:HB2	2.16	0.45
1:B:139:PRO:O	1:B:148:ARG:HB2	2.16	0.45
1:B:194:HIS:NE2	1:B:214:CYS:SG	2.89	0.45
1:B:498:VAL:HB	1:B:499:PHE:CD1	2.51	0.45
1:A:1001:PHE:O	1:A:1002:ASP:CB	2.63	0.45
1:B:65:ARG:HH22	1:B:106:GLU:HG2	1.81	0.45
1:B:622:VAL:CA	1:B:631:LEU:CB	2.89	0.45
1:B:315:ALA:HB1	1:B:365:SER:OG	2.16	0.45
1:A:1489:PHE:O	1:A:1490:PHE:C	2.60	0.45
1:B:220:ILE:HG23	1:B:220:ILE:O	2.17	0.45
1:B:1303:GLY:O	1:B:1304:ARG:C	2.59	0.45
1:A:477:LEU:HD11	1:A:556:CYS:SG	2.57	0.45
1:A:485:THR:HB	1:A:501:LYS:O	2.17	0.45
1:A:833:PHE:O	1:A:836:THR:CB	2.65	0.45
1:A:1207:ASN:C	1:A:1209:GLY:N	2.73	0.45
1:A:1405:ILE:O	1:A:1406:VAL:C	2.58	0.45
1:B:58:PHE:CZ	1:B:125:HIS:CD2	3.05	0.45
1:B:88:LEU:C	1:B:88:LEU:HD23	2.42	0.45
1:A:32:LEU:CD2	1:A:128:SER:HA	2.46	0.45
1:A:39:VAL:O	1:A:41:PRO:CD	2.65	0.45
1:A:121:ILE:HD13	1:A:161:PHE:O	2.16	0.45
1:B:316:ALA:HA	1:B:354:SER:O	2.16	0.45
1:A:85:ASP:HB2	1:A:88:LEU:HB3	1.99	0.45
1:A:769:SER:HA	1:A:773:LEU:CB	2.47	0.45
1:B:860:ASN:O	1:B:863:THR:CA	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:889:LYS:O	1:B:892:LEU:CB	2.65	0.45
1:B:1085:ARG:O	1:B:1087:PHE:N	2.50	0.45
1:B:1201:GLN:O	1:B:1203:ARG:N	2.50	0.45
1:B:1457:ILE:O	1:B:1458:CYS:O	2.34	0.45
1:A:245:ALA:CB	1:A:429:ALA:O	2.65	0.45
1:A:977:ILE:O	1:A:979:GLN:N	2.50	0.45
1:A:1207:ASN:O	1:A:1208:MET:C	2.59	0.45
1:A:1437:MET:C	1:A:1439:GLU:N	2.75	0.45
1:B:124:LEU:CD1	1:B:131:TYR:CE1	3.00	0.45
1:B:840:VAL:O	1:B:841:GLU:C	2.59	0.45
1:A:67:SER:O	1:A:71:GLN:OE1	2.34	0.45
1:B:315:ALA:CB	1:B:365:SER:O	2.64	0.45
1:A:196:SER:OG	1:A:198:HIS:N	2.39	0.45
1:A:222:LEU:HD21	1:A:224:MET:O	2.16	0.45
1:A:353:TYR:CZ	1:A:395:THR:HG22	2.52	0.45
1:A:628:PRO:O	1:A:629:ARG:C	2.59	0.45
1:A:1074:PRO:C	1:A:1076:VAL:N	2.74	0.45
1:B:961:GLU:CB	1:B:963:GLU:H	2.30	0.45
1:B:1251:ASN:CB	1:B:1283:LEU:HA	2.47	0.45
1:A:224:MET:HG3	1:A:293:ARG:CB	2.47	0.44
1:A:1083:LEU:O	1:A:1084:PHE:C	2.59	0.44
1:B:143:GLU:HB2	1:B:210:ASN:ND2	2.32	0.44
1:B:143:GLU:HB2	1:B:210:ASN:HD21	1.82	0.44
1:B:882:SER:O	1:B:883:ASP:C	2.60	0.44
1:A:589:VAL:O	1:A:592:GLU:CB	2.65	0.44
1:A:596:THR:HA	1:A:599:LEU:CB	2.47	0.44
1:A:687:LEU:O	1:A:688:GLU:C	2.60	0.44
1:A:701:ARG:O	1:A:702:ASP:C	2.60	0.44
1:A:1229:LYS:O	1:A:1230:MET:C	2.59	0.44
1:B:228:ASP:CG	1:B:228:ASP:O	2.60	0.44
1:B:444:ASP:C	1:B:446:ALA:H	2.25	0.44
1:B:576:LYS:C	1:B:578:PHE:N	2.74	0.44
1:B:775:TYR:O	1:B:776:ASP:C	2.60	0.44
1:B:1316:VAL:O	1:B:1317:LYS:C	2.59	0.44
1:B:1374:HIS:CA	1:B:1377:LEU:CB	2.95	0.44
1:B:243:PHE:O	1:B:430:PHE:HA	2.18	0.44
1:B:304:ARG:CB	1:B:366:SER:O	2.65	0.44
1:B:444:ASP:C	1:B:446:ALA:N	2.76	0.44
1:B:646:PRO:O	1:B:647:VAL:C	2.60	0.44
1:B:709:SER:O	1:B:713:ARG:CB	2.65	0.44
1:B:1242:GLN:O	1:B:1243:ASN:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LEU:O	1:A:457:ALA:HB3	2.17	0.44
1:A:1253:ALA:HA	1:A:1256:HIS:CB	2.48	0.44
1:B:18:TYR:CZ	1:B:24:ASN:HB3	2.52	0.44
1:B:769:SER:HA	1:B:773:LEU:CB	2.48	0.44
1:B:788:MET:O	1:B:790:VAL:N	2.50	0.44
1:A:249:LYS:HB2	1:A:264:LEU:HD13	1.99	0.44
1:A:313:TYR:CD1	1:A:313:TYR:N	2.84	0.44
1:A:457:ALA:HB1	1:A:521:LYS:O	2.17	0.44
1:A:853:PRO:O	1:A:854:PHE:C	2.59	0.44
1:B:484:VAL:HG13	1:B:485:THR:HG23	2.00	0.44
1:B:523:LEU:HD11	1:B:556:CYS:SG	2.58	0.44
1:B:735:TYR:C	1:B:737:LEU:N	2.76	0.44
1:B:1116:LYS:O	1:B:1119:LEU:CA	2.63	0.44
1:A:756:SER:O	1:A:759:LEU:C	2.60	0.44
1:A:854:PHE:O	1:A:855:SER:C	2.60	0.44
1:B:701:ARG:CB	1:B:729:ILE:CB	2.95	0.44
1:B:1289:GLU:C	1:B:1291:VAL:N	2.75	0.44
1:B:1371:LEU:O	1:B:1375:ILE:CB	2.65	0.44
1:A:248:GLU:O	1:A:249:LYS:HG3	2.17	0.44
1:A:701:ARG:CB	1:A:729:ILE:C	2.91	0.44
1:B:54:ARG:O	1:B:54:ARG:HG2	2.18	0.44
1:B:286:VAL:O	1:B:287:VAL:C	2.59	0.44
1:B:299:TRP:HB2	1:B:382:VAL:CB	2.48	0.44
1:B:741:ALA:CB	1:B:876:PHE:HA	2.47	0.44
1:A:21:GLY:CA	1:A:216:THR:HA	2.47	0.44
1:A:353:TYR:HB2	1:A:420:THR:HG21	1.99	0.44
1:A:484:VAL:HG13	1:A:485:THR:HG23	2.00	0.44
1:A:612:ALA:O	1:A:613:ALA:C	2.59	0.44
1:A:1245:CYS:CB	1:A:1341:VAL:H	2.30	0.44
1:B:99:GLU:O	1:B:103:ASN:ND2	2.51	0.44
1:B:507:GLN:HG2	1:B:563:SER:HA	2.00	0.44
1:B:555:LEU:O	1:B:555:LEU:HD23	2.17	0.44
1:B:784:LEU:O	1:B:785:MET:C	2.60	0.44
1:A:69:GLN:HG2	1:A:73:TRP:NE1	2.32	0.44
1:A:264:LEU:CG	1:A:418:ILE:HD11	2.46	0.44
1:A:773:LEU:CB	1:A:779:ALA:H	2.31	0.44
1:B:364:ILE:O	1:B:394:CYS:SG	2.76	0.44
1:A:760:ASP:O	1:A:761:VAL:C	2.61	0.43
1:A:166:PHE:CD1	1:A:167:TYR:CE2	3.06	0.43
1:A:237:GLY:N	1:A:284:VAL:O	2.48	0.43
1:A:306:LYS:HD2	1:A:313:TYR:OH	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:GLU:N	1:A:354:SER:O	2.51	0.43
1:A:364:ILE:HG22	1:A:394:CYS:SG	2.59	0.43
1:A:581:MET:CB	1:A:591:ALA:HB1	2.47	0.43
1:A:602:ASN:O	1:A:606:LEU:CB	2.66	0.43
1:B:166:PHE:CD1	1:B:166:PHE:C	2.96	0.43
1:B:451:LYS:HE2	1:B:451:LYS:HA	2.00	0.43
1:B:753:ASN:O	1:B:754:GLU:C	2.61	0.43
1:B:1049:PRO:O	1:B:1050:LEU:C	2.61	0.43
1:B:1284:CYS:O	1:B:1292:VAL:CB	2.66	0.43
1:A:57:LEU:HD21	1:A:223:PHE:HB2	2.00	0.43
1:A:142:LEU:CD2	1:A:200:LEU:HD23	2.48	0.43
1:A:498:VAL:HG12	1:A:499:PHE:HD1	1.82	0.43
1:A:707:ILE:CB	1:A:737:LEU:H	2.26	0.43
1:B:32:LEU:CD2	1:B:128:SER:CB	2.96	0.43
1:B:69:GLN:O	1:B:73:TRP:CE2	2.71	0.43
1:B:156:ASN:O	1:B:159:SER:OG	2.28	0.43
1:A:621:LEU:O	1:A:625:ASN:CB	2.66	0.43
1:A:682:THR:O	1:A:686:ALA:HB3	2.19	0.43
1:B:313:TYR:CD1	1:B:361:GLY:CA	3.00	0.43
1:B:316:ALA:HB2	1:B:355:LEU:HD12	2.00	0.43
1:B:1292:VAL:HA	1:B:1295:PHE:CB	2.49	0.43
1:A:549:PHE:O	1:A:551:HIS:N	2.52	0.43
1:B:12:GLY:O	1:B:13:ASP:C	2.61	0.43
1:B:177:VAL:HG12	1:B:178:ILE:N	2.33	0.43
1:B:826:LYS:O	1:B:828:GLU:N	2.51	0.43
1:B:960:PRO:O	1:B:961:GLU:CB	2.66	0.43
1:B:1299:ILE:O	1:B:1300:GLU:C	2.61	0.43
1:A:9:LEU:C	1:A:10:HIS:CG	2.96	0.43
1:A:73:TRP:CD1	1:A:73:TRP:N	2.87	0.43
1:A:114:VAL:CG1	1:A:175:SER:HB3	2.49	0.43
1:A:196:SER:HB3	1:A:208:GLU:O	2.18	0.43
1:A:479:ASP:O	1:A:482:TYR:N	2.52	0.43
1:A:483:PHE:O	1:A:506:ARG:NH1	2.48	0.43
1:B:18:TYR:CE1	1:B:25:GLY:HA2	2.53	0.43
1:B:586:GLY:O	1:B:588:ASP:N	2.52	0.43
1:B:1293:GLN:CB	1:B:1345:TYR:O	2.67	0.43
1:A:40:GLN:O	1:A:41:PRO:C	2.61	0.43
1:A:231:ASP:OD2	1:A:434:PRO:HG3	2.19	0.43
1:A:1459:ARG:C	1:A:1461:CYS:N	2.66	0.43
1:B:133:THR:HG21	1:B:156:ASN:HD21	1.84	0.43
1:B:224:MET:SD	1:B:228:ASP:CB	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:THR:HG21	1:B:562:HIS:ND1	2.33	0.43
1:B:960:PRO:O	1:B:963:GLU:CB	2.67	0.43
1:A:95:ALA:O	1:A:99:GLU:HB2	2.18	0.43
1:A:315:ALA:HB1	1:A:365:SER:OG	2.18	0.43
1:A:1098:LYS:C	1:A:1100:VAL:N	2.75	0.43
1:B:38:VAL:CG1	1:B:200:LEU:HD11	2.49	0.43
1:B:270:GLN:CD	1:B:1257:LYS:HA	2.44	0.43
1:A:232:ASP:C	1:A:233:ILE:HG13	2.44	0.43
1:A:701:ARG:O	1:A:703:SER:O	2.36	0.43
1:B:10:HIS:CE1	1:B:114:VAL:HG22	2.53	0.43
1:B:134:VAL:HB	1:B:189:ALA:CB	2.49	0.43
1:B:484:VAL:O	1:B:484:VAL:HG22	2.19	0.43
1:A:15:CYS:HA	1:A:223:PHE:H	1.84	0.43
1:A:18:TYR:HA	1:A:25:GLY:O	2.19	0.43
1:A:69:GLN:O	1:A:73:TRP:CD1	2.71	0.43
1:A:402:THR:O	1:A:403:ASN:OD1	2.37	0.43
1:A:853:PRO:O	1:A:856:ASP:N	2.51	0.43
1:B:576:LYS:C	1:B:578:PHE:H	2.26	0.43
1:A:744:CYS:CB	1:A:1075:LEU:HA	2.48	0.42
1:A:1000:GLU:CB	1:A:1005:ASN:HA	2.49	0.42
1:A:1103:LEU:O	1:A:1105:THR:N	2.52	0.42
1:B:592:GLU:O	1:B:593:ASP:C	2.61	0.42
1:B:1285:SER:O	1:B:1341:VAL:CB	2.67	0.42
1:A:361:GLY:O	1:A:366:SER:OG	2.36	0.42
1:A:316:ALA:HB3	1:A:392:HIS:CE1	2.54	0.42
1:B:1062:ARG:O	1:B:1066:HIS:N	2.50	0.42
1:A:755:ILE:O	1:A:758:GLN:CB	2.68	0.42
1:A:1133:VAL:O	1:A:1134:TYR:CB	2.66	0.42
1:B:35:ASP:OD1	1:B:35:ASP:C	2.63	0.42
1:B:42:GLU:O	1:B:43:ALA:C	2.62	0.42
1:B:62:PRO:HB2	1:B:107:ASN:OD1	2.19	0.42
1:A:73:TRP:CZ3	1:A:156:ASN:HB3	2.55	0.42
1:A:163:ILE:O	1:A:164:GLN:OE1	2.38	0.42
1:A:188:ASN:O	1:A:190:GLY:N	2.52	0.42
1:A:248:GLU:C	1:A:249:LYS:HG3	2.45	0.42
1:A:253:CYS:SG	1:A:262:VAL:HG22	2.60	0.42
1:A:1122:LEU:HA	1:A:1125:ILE:CB	2.50	0.42
1:B:143:GLU:CB	1:B:210:ASN:ND2	2.83	0.42
1:B:389:ARG:NE	1:B:425:GLU:O	2.53	0.42
1:A:520:PHE:CE2	1:A:560:LEU:HD21	2.53	0.42
1:A:647:VAL:O	1:A:648:THR:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:THR:O	1:A:866:VAL:CB	2.67	0.42
1:B:167:TYR:HE2	1:B:181:LYS:HD2	1.85	0.42
1:B:772:ASN:C	1:B:774:PRO:N	2.77	0.42
1:B:1036:GLN:C	1:B:1039:GLY:H	2.27	0.42
1:B:1305:ASN:O	1:B:1306:VAL:C	2.62	0.42
1:B:1378:VAL:O	1:B:1382:ALA:HB2	2.20	0.42
1:A:398:TRP:CE2	1:A:424:LYS:HD2	2.54	0.42
1:B:179:GLY:H	1:B:220:ILE:HG23	1.84	0.42
1:A:15:CYS:HA	1:A:222:LEU:HA	2.01	0.42
1:A:128:SER:HB2	1:A:130:LYS:HE3	2.00	0.42
1:A:1280:ASN:O	1:A:1281:PHE:C	2.62	0.42
1:B:398:TRP:CD2	1:B:424:LYS:HG3	2.54	0.42
1:B:438:ALA:O	1:B:442:ASP:OD1	2.37	0.42
1:B:1224:LYS:CB	1:B:1319:GLU:O	2.68	0.42
1:A:38:VAL:CG1	1:A:200:LEU:HD11	2.50	0.42
1:A:1354:LEU:C	1:A:1355:ILE:O	2.62	0.42
1:A:1476:LYS:C	1:A:1478:VAL:N	2.77	0.42
1:B:58:PHE:CE2	1:B:125:HIS:HB2	2.54	0.42
1:B:239:VAL:HA	1:B:282:TRP:O	2.20	0.42
1:B:261:HIS:CD2	1:B:406:ILE:HD13	2.55	0.42
1:B:391:ARG:HH22	1:B:393:LEU:HD12	1.85	0.42
1:A:200:LEU:HG	1:A:206:CYS:O	2.20	0.42
1:A:268:GLY:C	1:A:269:ARG:O	2.62	0.42
1:B:270:GLN:OE1	1:B:1257:LYS:HA	2.20	0.42
1:B:286:VAL:HA	1:B:303:PHE:CD2	2.55	0.42
1:B:314:LEU:O	1:B:315:ALA:HB2	2.20	0.42
1:B:1321:LYS:O	1:B:1323:ILE:N	2.43	0.42
1:B:1415:ILE:C	1:B:1416:PRO:O	2.62	0.42
1:A:69:GLN:HA	1:A:96:ALA:CB	2.50	0.41
1:A:594:THR:O	1:A:598:LEU:N	2.50	0.41
1:A:701:ARG:C	1:A:703:SER:N	2.77	0.41
1:A:1200:GLN:O	1:A:1202:GLN:N	2.53	0.41
1:A:1342:LEU:O	1:A:1343:VAL:C	2.61	0.41
1:B:316:ALA:HA	1:B:355:LEU:HA	2.02	0.41
1:B:770:ASP:C	1:B:772:ASN:N	2.78	0.41
1:A:26:PHE:HB3	1:A:56:CYS:SG	2.60	0.41
1:A:460:LEU:O	1:A:460:LEU:HG	2.20	0.41
1:A:1361:GLU:O	1:A:1364:ARG:N	2.52	0.41
1:B:607:GLU:O	1:B:611:THR:CA	2.62	0.41
1:B:755:ILE:O	1:B:758:GLN:CA	2.68	0.41
1:A:441:ARG:HA	1:A:444:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:LEU:HD12	1:A:463:GLY:O	2.21	0.41
1:A:1253:ALA:O	1:A:1256:HIS:CB	2.69	0.41
1:B:88:LEU:CD2	1:B:92:LEU:HD12	2.51	0.41
1:B:199:GLN:C	1:B:200:LEU:O	2.63	0.41
1:B:292:CYS:O	1:B:293:ARG:C	2.64	0.41
1:B:693:GLU:O	1:B:694:GLU:C	2.61	0.41
1:B:1304:ARG:O	1:B:1305:ASN:C	2.60	0.41
1:A:15:CYS:O	1:A:57:LEU:CD2	2.69	0.41
1:A:222:LEU:CD2	1:A:224:MET:O	2.68	0.41
1:A:302:LEU:N	1:A:302:LEU:CD1	2.83	0.41
1:A:514:ASN:CG	1:A:517:LYS:HD3	2.46	0.41
1:A:1030:PHE:O	1:A:1033:ILE:N	2.52	0.41
1:B:236:GLY:HA2	1:B:284:VAL:HG12	2.02	0.41
1:B:244:HIS:CD2	1:B:264:LEU:HD11	2.56	0.41
1:B:446:ALA:HB1	1:B:515:ILE:HD11	2.02	0.41
1:B:666:ILE:CB	1:B:669:LYS:N	2.83	0.41
1:A:13:ASP:OD1	1:A:226:TRP:N	2.48	0.41
1:A:617:THR:O	1:A:621:LEU:CB	2.68	0.41
1:A:776:ASP:O	1:A:777:LEU:C	2.63	0.41
1:A:842:GLU:O	1:A:843:TYR:C	2.63	0.41
1:B:27:ILE:HG12	1:B:218:TRP:CZ3	2.56	0.41
1:B:484:VAL:HG11	1:B:562:HIS:CB	2.50	0.41
1:B:637:LEU:O	1:B:639:VAL:N	2.53	0.41
1:A:10:HIS:HB3	1:A:112:GLY:O	2.21	0.41
1:A:234:LEU:HD13	1:A:432:ILE:HG21	2.02	0.41
1:A:523:LEU:CD1	1:A:553:CYS:SG	3.07	0.41
1:A:756:SER:O	1:A:759:LEU:N	2.54	0.41
1:A:842:GLU:O	1:A:844:LEU:N	2.54	0.41
1:A:977:ILE:C	1:A:979:GLN:N	2.79	0.41
1:B:235:LYS:HA	1:B:235:LYS:HD3	1.83	0.41
1:B:675:PHE:O	1:B:679:GLY:N	2.54	0.41
1:B:772:ASN:O	1:B:774:PRO:N	2.53	0.41
1:B:879:TYR:C	1:B:881:PHE:H	2.27	0.41
1:B:1042:GLY:C	1:B:1044:SER:N	2.77	0.41
1:B:1381:LEU:O	1:B:1385:THR:CB	2.69	0.41
1:A:166:PHE:CE1	1:A:167:TYR:CZ	3.09	0.41
1:A:313:TYR:N	1:A:313:TYR:HD1	2.18	0.41
1:A:841:GLU:O	1:A:844:LEU:CA	2.67	0.41
1:B:136:LYS:O	1:B:147:MET:HG2	2.21	0.41
1:B:619:VAL:O	1:B:623:ARG:CB	2.69	0.41
1:B:831:GLU:C	1:B:833:PHE:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:TRP:O	1:A:226:TRP:CE3	2.73	0.41
1:A:276:THR:O	1:A:508:LYS:NZ	2.34	0.41
1:A:1079:ALA:C	1:A:1081:GLN:N	2.77	0.41
1:A:1251:ASN:CB	1:A:1283:LEU:CA	2.99	0.41
1:B:249:LYS:HZ2	1:B:266:THR:HA	1.85	0.41
1:B:777:LEU:O	1:B:778:ARG:C	2.62	0.41
1:B:1056:GLY:O	1:B:1057:GLY:C	2.64	0.41
1:A:398:TRP:CZ3	1:A:424:LYS:HE3	2.56	0.41
1:A:555:LEU:O	1:A:559:VAL:HG23	2.20	0.41
1:A:560:LEU:O	1:A:564:GLN:HG2	2.21	0.41
1:A:647:VAL:O	1:A:649:GLN:N	2.54	0.41
1:A:723:GLN:O	1:A:862:LEU:CB	2.68	0.41
1:A:836:THR:O	1:A:837:MET:C	2.63	0.41
1:A:863:THR:O	1:A:866:VAL:CA	2.69	0.41
1:A:1039:GLY:O	1:A:1040:ILE:C	2.64	0.41
1:A:1362:ARG:C	1:A:1364:ARG:N	2.78	0.41
1:A:1374:HIS:O	1:A:1377:LEU:CB	2.69	0.41
1:B:28:SER:O	1:B:37:CYS:HA	2.21	0.41
1:B:95:ALA:O	1:B:98:LEU:N	2.53	0.41
1:B:179:GLY:O	1:B:180:ASP:C	2.64	0.41
1:B:369:GLU:HG2	1:B:370:LEU:H	1.84	0.41
1:B:852:PHE:O	1:B:856:ASP:CB	2.69	0.41
1:A:19:ALA:HB2	1:A:218:TRP:CH2	2.56	0.41
1:B:69:GLN:NE2	1:B:73:TRP:HZ2	2.18	0.41
1:B:707:ILE:HA	1:B:710:LYS:CB	2.50	0.41
1:A:510:MET:CE	1:A:515:ILE:HG13	2.51	0.40
1:A:888:THR:O	1:A:889:LYS:C	2.63	0.40
1:A:999:ARG:O	1:A:1006:SER:O	2.39	0.40
1:A:1079:ALA:O	1:A:1081:GLN:N	2.54	0.40
1:A:1436:GLU:O	1:A:1439:GLU:CB	2.69	0.40
1:B:358:VAL:HA	1:B:359:PRO:HD3	1.91	0.40
1:A:143:GLU:HG3	1:A:198:HIS:HE1	1.87	0.40
1:A:367:ILE:O	1:A:367:ILE:HG23	2.21	0.40
1:A:403:ASN:HA	1:A:416:LEU:HD22	2.04	0.40
1:A:847:VAL:C	1:A:849:CYS:N	2.78	0.40
1:A:1112:TYR:HA	1:A:1115:ILE:CB	2.51	0.40
1:B:384:ARG:O	1:B:385:ASN:C	2.64	0.40
1:B:838:GLU:O	1:B:840:VAL:N	2.53	0.40
1:B:1194:VAL:O	1:B:1195:ARG:C	2.65	0.40
1:A:142:LEU:HD23	1:A:200:LEU:CD2	2.50	0.40
1:A:166:PHE:HD1	1:A:167:TYR:CD2	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:ASP:O	1:A:1109:VAL:C	2.63	0.40
1:B:18:TYR:HD1	1:B:26:PHE:CD1	2.39	0.40
1:B:194:HIS:ND1	1:B:214:CYS:SG	2.93	0.40
1:B:251:LEU:HD13	1:B:418:ILE:HD12	2.02	0.40
1:B:836:THR:C	1:B:838:GLU:N	2.79	0.40
1:B:969:ASP:O	1:B:972:LEU:CB	2.68	0.40
1:A:71:GLN:HB3	1:A:92:LEU:HD22	2.03	0.40
1:A:701:ARG:HA	1:A:730:LEU:HA	2.03	0.40
1:A:1316:VAL:HA	1:A:1319:GLU:CB	2.51	0.40
1:B:166:PHE:HD1	1:B:167:TYR:CD2	2.39	0.40
1:B:481:VAL:HB	1:B:490:SER:O	2.21	0.40
1:A:66:TYR:HD1	1:A:69:GLN:OE1	2.03	0.40
1:B:29:THR:HG23	1:B:125:HIS:CD2	2.56	0.40
1:B:88:LEU:O	1:B:92:LEU:HD12	2.21	0.40
1:B:148:ARG:HG2	1:B:150:THR:HG22	2.03	0.40
1:B:315:ALA:O	1:B:355:LEU:HA	2.22	0.40
1:B:1028:LEU:O	1:B:1030:PHE:N	2.54	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ASP:O	1:A:1393:GLU:N[2_655]	1.65	0.55
1:A:116:GLN:NE2	1:A:1391:TYR:O[2_655]	1.85	0.35
1:A:117:TYR:H	1:A:1392:THR:O[2_655]	1.45	0.15
1:A:174:ASP:O	1:A:1392:THR:C[2_655]	2.11	0.09
1:A:175:SER:H	1:A:1395:LYS:N[2_655]	1.51	0.09
1:A:117:TYR:N	1:A:1392:THR:O[2_655]	2.14	0.06
1:A:116:GLN:HE21	1:A:1391:TYR:O[2_655]	1.55	0.05
1:A:109:LYS:N	1:A:1288:ASN:O[2_655]	2.18	0.02

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	1231/1581 (78%)	891 (72%)	234 (19%)	106 (9%)	0	8
1	B	1231/1581 (78%)	894 (73%)	228 (18%)	109 (9%)	0	8
All	All	2462/3162 (78%)	1785 (72%)	462 (19%)	215 (9%)	0	8

All (215) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	383	PRO
1	A	587	TYR
1	A	602	ASN
1	A	604	LYS
1	A	628	PRO
1	A	645	ILE
1	A	658	ASN
1	A	666	ILE
1	A	702	ASP
1	A	708	ARG
1	A	744	CYS
1	A	762	ASP
1	A	789	HIS
1	A	863	THR
1	A	961	GLU
1	A	977	ILE
1	A	990	ILE
1	A	994	LEU
1	A	1133	VAL
1	A	1239	GLU
1	A	1243	ASN
1	A	1264	ASN
1	A	1286	GLU
1	A	1288	ASN
1	A	1299	ILE
1	A	1343	VAL
1	A	1347	ASP
1	A	1370	PRO
1	A	1394	ILE
1	A	1400	LEU
1	A	1418	VAL
1	A	1435	VAL
1	A	1437	MET

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Mol	Chain	Res	Type
1	A	1458	CYS
1	A	1460	ALA
1	A	1461	CYS
1	B	48	ASN
1	B	200	LEU
1	B	286	VAL
1	B	383	PRO
1	B	587	TYR
1	B	625	ASN
1	B	628	PRO
1	B	640	SER
1	B	658	ASN
1	B	659	PRO
1	B	666	ILE
1	B	669	LYS
1	B	715	LEU
1	B	836	THR
1	B	838	GLU
1	B	853	PRO
1	B	859	LYS
1	B	860	ASN
1	B	863	THR
1	B	898	VAL
1	B	961	GLU
1	B	990	ILE
1	B	1119	LEU
1	B	1201	GLN
1	B	1202	GLN
1	B	1221	PRO
1	B	1264	ASN
1	B	1267	ILE
1	B	1288	ASN
1	B	1299	ILE
1	B	1346	ASN
1	B	1370	PRO
1	B	1394	ILE
1	B	1400	LEU
1	B	1418	VAL
1	B	1458	CYS
1	B	1461	CYS
1	B	1464	THR
1	A	105	THR

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Mol	Chain	Res	Type
1	A	226	TRP
1	A	550	ARG
1	A	640	SER
1	A	647	VAL
1	A	669	LYS
1	A	684	GLU
1	A	755	ILE
1	A	760	ASP
1	A	787	HIS
1	A	790	VAL
1	A	836	THR
1	A	853	PRO
1	A	895	LEU
1	A	1108	ASP
1	A	1109	VAL
1	A	1208	MET
1	A	1267	ILE
1	A	1301	THR
1	A	1311	PHE
1	A	1349	ALA
1	A	1464	THR
1	B	226	TRP
1	B	396	ASN
1	B	550	ARG
1	B	638	CYS
1	B	670	LEU
1	B	708	ARG
1	B	839	PHE
1	B	861	LYS
1	B	864	PHE
1	B	888	THR
1	B	1028	LEU
1	B	1051	ASP
1	B	1053	ASP
1	B	1058	ARG
1	B	1109	VAL
1	B	1117	GLN
1	B	1208	MET
1	B	1216	GLU
1	B	1239	GLU
1	B	1292	VAL
1	B	1311	PHE

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Mol	Chain	Res	Type
1	B	1347	ASP
1	B	1463	ASN
1	A	428	GLU
1	A	575	ALA
1	A	610	ILE
1	A	660	THR
1	A	682	THR
1	A	716	ALA
1	A	719	ALA
1	A	725	GLU
1	A	827	ASP
1	A	1028	LEU
1	A	1207	ASN
1	A	1414	CYS
1	A	1463	ASN
1	A	1474	LEU
1	B	50	PRO
1	B	291	PRO
1	B	399	VAL
1	B	577	GLN
1	B	581	MET
1	B	589	VAL
1	B	591	ALA
1	B	604	LYS
1	B	693	GLU
1	B	714	GLU
1	B	726	ASP
1	B	727	ARG
1	B	787	HIS
1	B	789	HIS
1	B	790	VAL
1	B	827	ASP
1	B	837	MET
1	B	1133	VAL
1	B	1207	ASN
1	B	1301	THR
1	B	1322	PHE
1	B	1358	MET
1	B	1414	CYS
1	A	53	PHE
1	A	445	PHE
1	A	572	GLU

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Mol	Chain	Res	Type
1	A	607	GLU
1	A	659	PRO
1	A	698	LEU
1	A	715	LEU
1	A	773	LEU
1	A	978	LEU
1	A	1004	SER
1	A	1075	LEU
1	A	1104	VAL
1	A	1355	ILE
1	A	1462	ASN
1	B	47	ASN
1	B	413	PRO
1	B	607	GLU
1	B	682	THR
1	B	720	LYS
1	B	858	GLU
1	B	981	ILE
1	B	1081	GLN
1	B	1349	ALA
1	B	1356	GLN
1	B	1416	PRO
1	A	110	LEU
1	A	269	ARG
1	A	573	TYR
1	A	753	ASN
1	A	754	GLU
1	A	1074	PRO
1	A	1201	GLN
1	A	1202	GLN
1	A	1342	LEU
1	A	1397	ASN
1	A	1411	HIS
1	B	702	ASP
1	B	880	ASN
1	B	885	LEU
1	A	413	PRO
1	A	586	GLY
1	A	589	VAL
1	A	743	MET
1	B	593	ASP
1	B	645	ILE

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Mol	Chain	Res	Type
1	B	684	GLU
1	B	745	LEU
1	B	773	LEU
1	B	852	PHE
1	B	854	PHE
1	A	286	VAL
1	B	647	VAL
1	B	1220	ILE
1	A	1221	PRO
1	B	497	VAL
1	A	646	PRO
1	B	498	VAL
1	A	984	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	400/1427 (28%)	351 (88%)	49 (12%)	4	17
1	B	400/1427 (28%)	349 (87%)	51 (13%)	4	15
All	All	800/2854 (28%)	700 (88%)	100 (12%)	4	16

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	28	SER
1	A	38	VAL
1	A	39	VAL
1	A	42	GLU
1	A	71	GLN
1	A	83	THR
1	A	85	ASP
1	A	87	VAL
1	A	91	LYS

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Mol	Chain	Res	Type
1	A	102	GLN
1	A	105	THR
1	A	109	LYS
1	A	113	THR
1	A	121	ILE
1	A	127	LYS
1	A	142	LEU
1	A	150	THR
1	A	163	ILE
1	A	164	GLN
1	A	169	LEU
1	A	172	ILE
1	A	182	VAL
1	A	201	VAL
1	A	202	ASP
1	A	208	GLU
1	A	222	LEU
1	A	235	LYS
1	A	247	GLN
1	A	252	THR
1	A	255	GLU
1	A	289	HIS
1	A	302	LEU
1	A	317	GLU
1	A	356	VAL
1	A	390	LEU
1	A	394	CYS
1	A	406	ILE
1	A	418	ILE
1	A	423	LEU
1	A	428	GLU
1	A	433	VAL
1	A	456	ILE
1	A	465	ILE
1	A	471	ARG
1	A	515	ILE
1	A	523	LEU
1	A	551	HIS
1	A	555	LEU
1	B	27	ILE
1	B	38	VAL
1	B	39	VAL

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Mol	Chain	Res	Type
1	B	42	GLU
1	B	71	GLN
1	B	83	THR
1	B	87	VAL
1	B	91	LYS
1	B	92	LEU
1	B	97	ASP
1	B	105	THR
1	B	121	ILE
1	B	127	LYS
1	B	132	LEU
1	B	142	LEU
1	B	143	GLU
1	B	163	ILE
1	B	164	GLN
1	B	169	LEU
1	B	172	ILE
1	B	182	VAL
1	B	201	VAL
1	B	220	ILE
1	B	222	LEU
1	B	235	LYS
1	B	247	GLN
1	B	252	THR
1	B	255	GLU
1	B	285	GLU
1	B	287	VAL
1	B	302	LEU
1	B	317	GLU
1	B	356	VAL
1	B	390	LEU
1	B	394	CYS
1	B	397	THR
1	B	406	ILE
1	B	411	GLU
1	B	418	ILE
1	B	428	GLU
1	B	433	VAL
1	B	436	SER
1	B	456	ILE
1	B	471	ARG
1	B	474	THR

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Mol	Chain	Res	Type
1	B	502	PRO
1	B	515	ILE
1	B	523	LEU
1	B	551	HIS
1	B	555	LEU
1	B	565	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	64	ASN
1	A	93	HIS
1	A	107	ASN
1	A	116	GLN
1	A	122	GLN
1	A	129	ASN
1	A	145	ASN
1	A	194	HIS
1	A	198	HIS
1	A	513	GLN
1	B	10	HIS
1	B	64	ASN
1	B	69	GLN
1	B	194	HIS
1	B	198	HIS
1	B	207	ASN
1	B	210	ASN
1	B	215	ASN
1	B	244	HIS
1	B	400	HIS
1	B	447	ASN
1	B	503	ASN
1	B	513	GLN
1	B	524	GLN
1	B	564	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	I3P	A	3000	-	24,24,24	1.20	3 (12%)	39,39,39	1.14	4 (10%)
2	I3P	B	3000	-	24,24,24	1.15	1 (4%)	39,39,39	1.15	4 (10%)

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	I3P	A	3000	-	-	0/15/39/39	0/1/1/1
2	I3P	B	3000	-	-	0/15/39/39	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3000	I3P	P5-O53	-2.28	1.46	1.54
2	A	3000	I3P	P4-O42	-2.28	1.46	1.54
2	A	3000	I3P	P1-O13	-2.24	1.46	1.54
2	B	3000	I3P	P1-O13	-2.22	1.46	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3000	I3P	O5-P5-O51	-2.59	100.10	109.33
2	A	3000	I3P	O13-P1-O12	2.54	117.31	107.80
2	B	3000	I3P	O43-P4-O42	2.38	116.74	107.80
2	B	3000	I3P	O53-P5-O52	2.31	116.45	107.80
2	A	3000	I3P	O1-C1-C2	2.27	113.55	108.73
2	B	3000	I3P	O1-C1-C2	2.26	113.53	108.73
2	B	3000	I3P	O5-P5-O51	-2.10	101.85	109.33
2	A	3000	I3P	O53-P5-O52	2.01	115.34	107.80

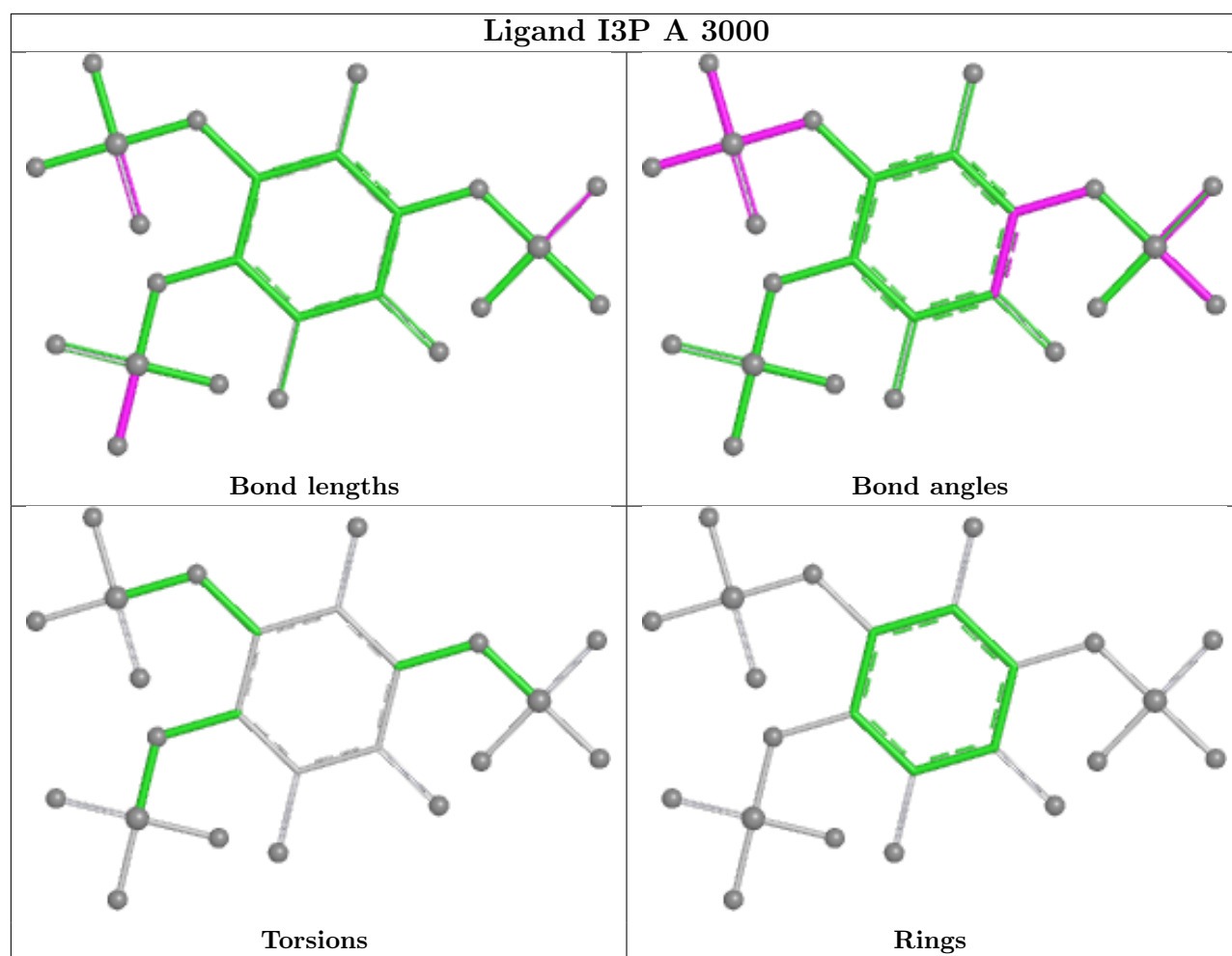
There are no chirality outliers.

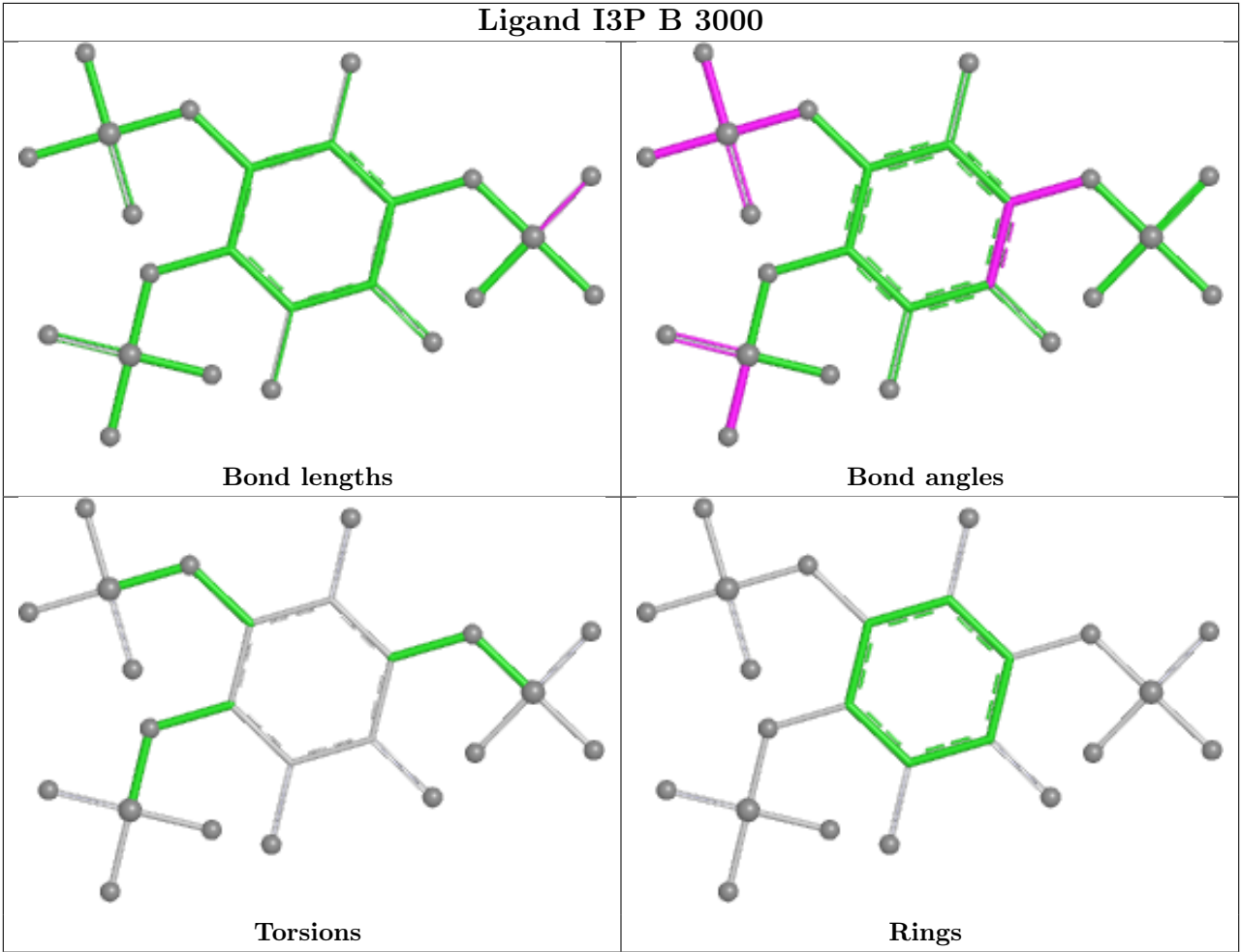
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1491:SER	C	1492:SER	N	1.61

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	1257/1581 (79%)	-0.05	60 (4%)	35	36	168, 174, 177, 179	0
1	B	1257/1581 (79%)	-0.10	52 (4%)	41	40	168, 174, 177, 179	0
All	All	2514/3162 (79%)	-0.07	112 (4%)	38	38	168, 174, 177, 179	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1242	GLN	14.7
1	A	1243	ASN	12.3
1	A	159	SER	8.0
1	A	1414	CYS	7.7
1	B	1481	ILE	6.6
1	B	1397	ASN	6.0
1	B	1299	ILE	5.4
1	A	1415	ILE	5.0
1	B	429	ALA	5.0
1	B	22	SER	4.7
1	A	176	VAL	4.6
1	A	215	ASN	4.4
1	B	1471	ASP	4.4
1	A	1239	GLU	4.1
1	A	266	THR	4.1
1	A	1241	LEU	3.9
1	B	1484	SER	3.9
1	A	216	THR	3.9
1	A	64	ASN	3.8
1	A	211	SER	3.8
1	A	1244	PHE	3.7
1	B	1246	ALA	3.7
1	B	162	TYR	3.7
1	A	22	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	160	TRP	3.6
1	B	825	SER	3.6
1	B	1478	VAL	3.4
1	A	667	GLU	3.4
1	B	1473	ILE	3.4
1	B	1479	THR	3.4
1	B	1446	MET	3.4
1	B	205	GLY	3.3
1	B	372	PRO	3.3
1	A	7	SER	3.3
1	B	1405	ILE	3.2
1	A	770	ASP	3.2
1	B	387	TYR	3.1
1	A	1432	ASP	3.1
1	A	1392	THR	3.0
1	B	185	ASN	3.0
1	A	1393	GLU	3.0
1	B	283	GLU	3.0
1	A	28	SER	3.0
1	A	495	LEU	3.0
1	A	237	GLY	3.0
1	A	1240	PHE	3.0
1	A	1451	GLU	3.0
1	B	1388	LYS	2.9
1	B	1447	TRP	2.9
1	A	1430	TYR	2.9
1	B	47	ASN	2.9
1	B	215	ASN	2.9
1	A	131	TYR	2.8
1	B	1396	CYS	2.8
1	B	1188	VAL	2.8
1	A	133	THR	2.8
1	A	252	THR	2.8
1	A	265	ARG	2.8
1	A	51	LYS	2.7
1	B	253	CYS	2.7
1	A	117	TYR	2.6
1	B	1247	GLY	2.6
1	A	285	GLU	2.6
1	A	504	ARG	2.6
1	A	496	GLU	2.5
1	B	40	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1310	LYS	2.5
1	A	1405	ILE	2.5
1	A	1401	PRO	2.5
1	A	1319	GLU	2.5
1	A	1320	GLY	2.5
1	A	753	ASN	2.4
1	A	1433	THR	2.4
1	B	266	THR	2.4
1	B	650	GLU	2.4
1	B	1255	LEU	2.4
1	A	1479	THR	2.4
1	A	1457	ILE	2.4
1	B	61	CYS	2.4
1	B	388	VAL	2.4
1	A	140	ALA	2.3
1	B	1187	CYS	2.3
1	A	1195	ARG	2.3
1	B	1260	ASN	2.3
1	B	1121	GLN	2.3
1	B	213	ASN	2.3
1	B	1067	LEU	2.3
1	B	227	SER	2.3
1	B	401	SER	2.3
1	A	289	HIS	2.2
1	A	570	ASN	2.2
1	B	1474	LEU	2.2
1	A	360	GLU	2.2
1	B	505	GLU	2.2
1	A	183	VAL	2.2
1	A	1046	GLU	2.2
1	B	1475	GLU	2.2
1	A	212	VAL	2.1
1	B	1480	GLU	2.1
1	A	1369	SER	2.1
1	B	62	PRO	2.1
1	B	1389	ASN	2.1
1	B	430	PHE	2.0
1	A	668	THR	2.0
1	B	107	ASN	2.0
1	B	422	PRO	2.0
1	A	962	LYS	2.0
1	A	1410	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	51	LYS	2.0
1	B	404	ILE	2.0
1	A	182	VAL	2.0
1	A	1296	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

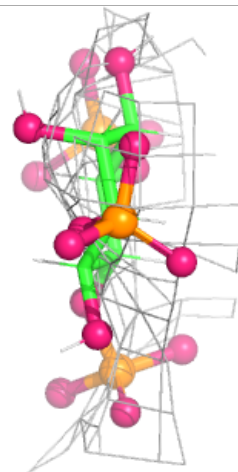
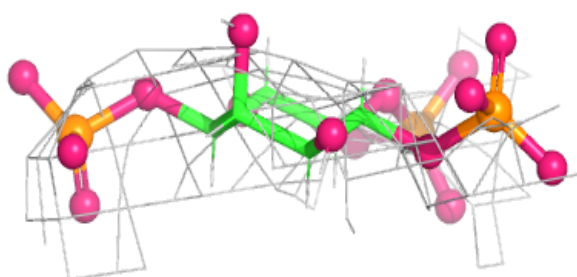
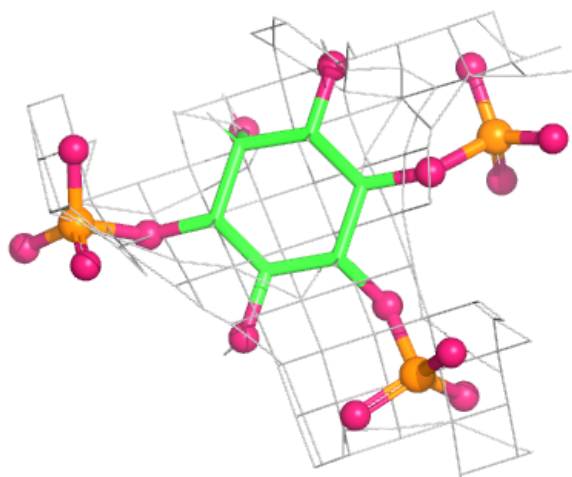
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	I3P	A	3000	24/24	0.96	0.08	174,174,174,174	0
2	I3P	B	3000	24/24	0.98	0.04	174,174,174,174	0

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

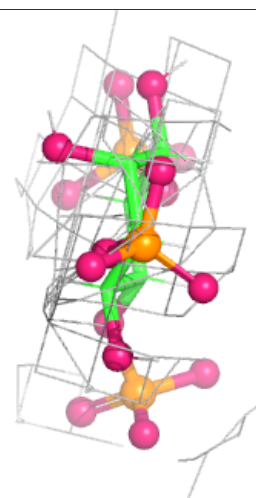
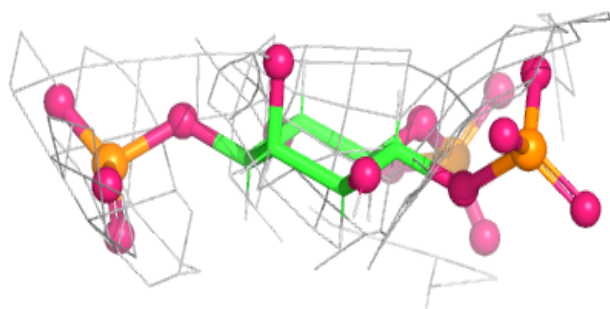
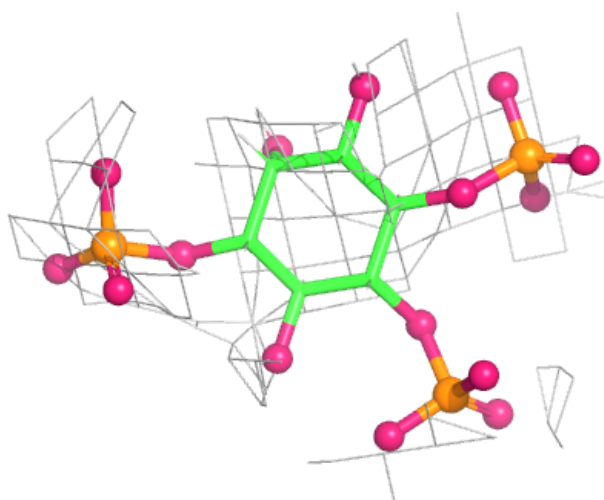
Electron density around I3P A 3000:

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



Electron density around I3P B 3000:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.