



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:50 AM UTC

PDB ID : 4OVV / pdb_00004ovv
Title : Crystal Structure of PI3Kalpha in complex with diC4-PIP2
Authors : Gabelli, S.B.; Vogelstein, B.; Miller, M.; Amzel, L.M.
Deposited on : 2014-01-14
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

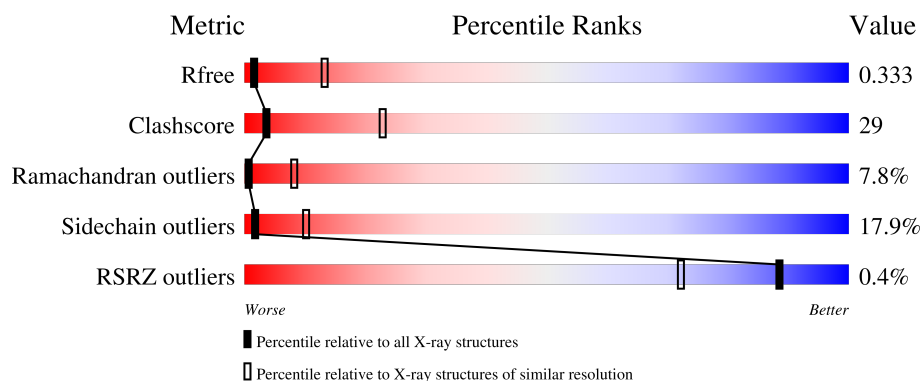
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	1096	
2	B	279	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10671 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1042	Total	C	N	O	S	0	0	0
			8525	5451	1457	1548	69			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	expression tag	UNP P42336
A	-27	SER	-	expression tag	UNP P42336
A	-26	TYR	-	expression tag	UNP P42336
A	-25	TYR	-	expression tag	UNP P42336
A	-24	HIS	-	expression tag	UNP P42336
A	-23	HIS	-	expression tag	UNP P42336
A	-22	HIS	-	expression tag	UNP P42336
A	-21	HIS	-	expression tag	UNP P42336
A	-20	HIS	-	expression tag	UNP P42336
A	-19	HIS	-	expression tag	UNP P42336
A	-18	ASP	-	expression tag	UNP P42336
A	-17	TYR	-	expression tag	UNP P42336
A	-16	ASP	-	expression tag	UNP P42336
A	-15	ILE	-	expression tag	UNP P42336
A	-14	PRO	-	expression tag	UNP P42336
A	-13	THR	-	expression tag	UNP P42336
A	-12	THR	-	expression tag	UNP P42336
A	-10	GLU	-	expression tag	UNP P42336
A	-9	ASN	-	expression tag	UNP P42336
A	-8	LEU	-	expression tag	UNP P42336
A	-7	TYR	-	expression tag	UNP P42336
A	-6	PHE	-	expression tag	UNP P42336
A	-5	GLN	-	expression tag	UNP P42336
A	-4	GLY	-	expression tag	UNP P42336
A	-3	ALA	-	expression tag	UNP P42336
A	-2	MET	-	expression tag	UNP P42336

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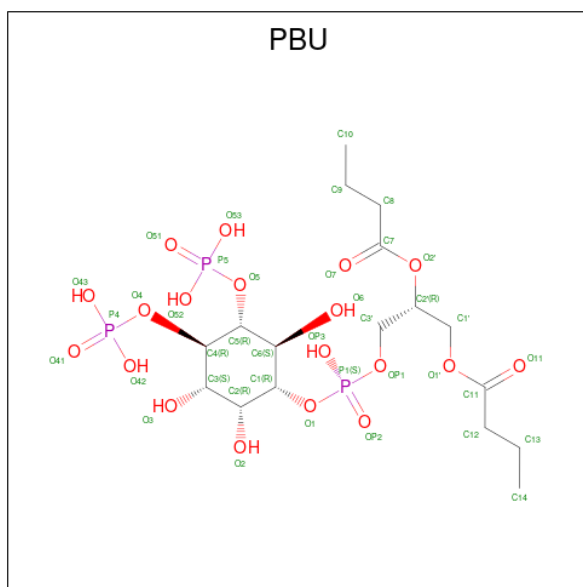
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

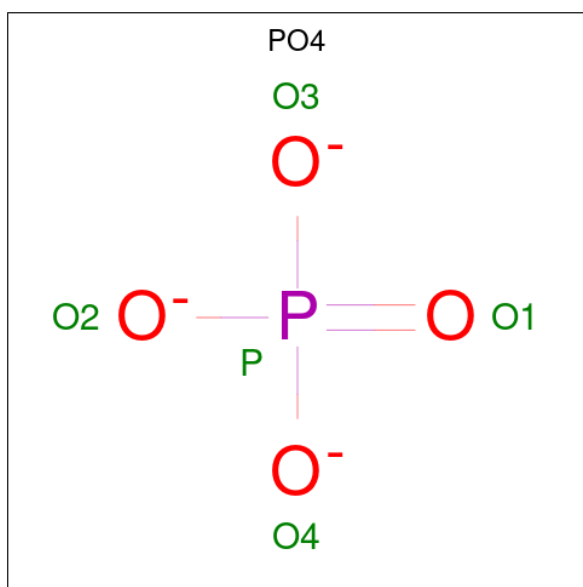
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			2059	1290	363	400	6			

- Molecule 3 is (2R)-3-{[(R)-HYDROXY{[(1R,2R,3S,4R,5R,6S)-2,3,6-TRIHYDROXY-4,5-BIS(PHOSPHONOOXY)CYCLOHEXYL]OXY}PHOSPHORYL]OXY}PROPANE-1,2-DIYL DIBUTANOATE (CCD ID: PBU) (formula: C₁₇H₃₃O₁₉P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			39	17	19	3		
3	B	1	Total	C	O	P	0	0
			39	17	19	3		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

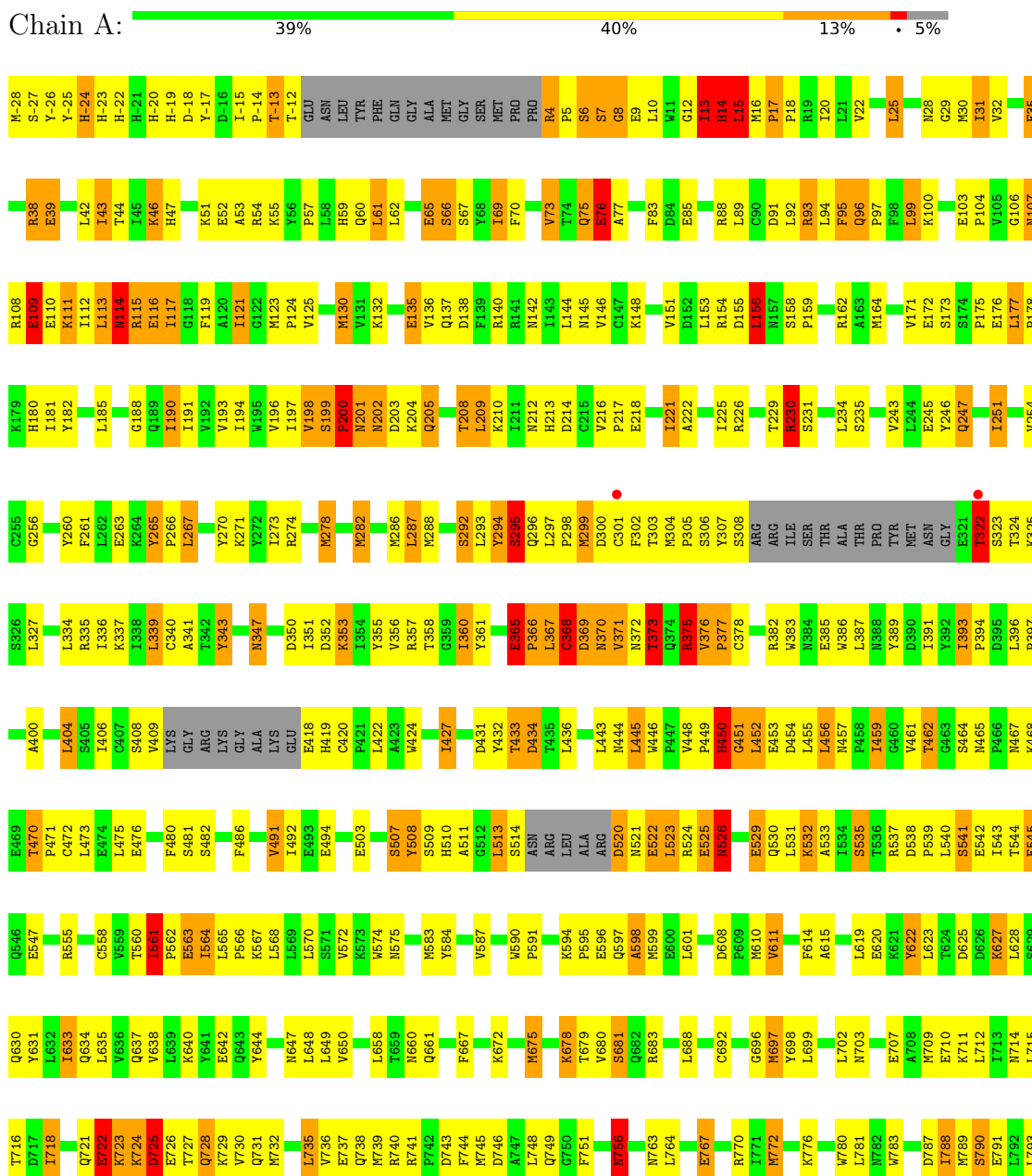
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.26Å 116.08Å 148.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.51 – 3.50 91.51 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (91.51-3.50) 99.8 (91.51-3.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.82 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.237 , 0.339 0.230 , 0.333	Depositor DCC
R_{free} test set	1494 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	97.4	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10671	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: PBU, PO4

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	15/8723 (0.2%)	1.23	55/11792 (0.5%)
2	B	0.86	1/2088 (0.0%)	1.09	5/2792 (0.2%)
All	All	1.08	16/10811 (0.1%)	1.20	60/14584 (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	4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	936	HIS	CG-CD2	6.65	1.43	1.35
1	A	450	HIS	CG-CD2	6.59	1.43	1.35
1	A	59	HIS	CG-CD2	6.40	1.42	1.35
1	A	322	THR	N-CA	6.37	1.54	1.46
1	A	-24	HIS	CG-CD2	6.11	1.42	1.35
1	A	1048	HIS	CG-CD2	5.91	1.42	1.35
1	A	917	HIS	CG-CD2	5.86	1.42	1.35
1	A	-13	THR	CA-C	5.62	1.59	1.53
1	A	17	PRO	C-O	-5.58	1.20	1.25
1	A	945	PHE	CA-CB	5.50	1.62	1.53
1	A	450	HIS	ND1-CE1	5.45	1.38	1.32
2	B	367	ASP	CA-C	5.44	1.56	1.53
1	A	420	CYS	CA-C	5.21	1.59	1.52
1	A	710	GLU	CA-C	-5.21	1.46	1.52
1	A	59	HIS	ND1-CE1	5.18	1.37	1.32
1	A	945	PHE	N-CA	5.17	1.52	1.46

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	590	TRP	CA-C-N	9.33	129.99	120.38
1	A	590	TRP	C-N-CA	9.33	129.99	120.38
1	A	486	PHE	CA-C-N	8.92	130.99	119.84
1	A	486	PHE	C-N-CA	8.92	130.99	119.84
1	A	510	HIS	N-CA-C	8.75	122.07	107.20
1	A	888	GLU	N-CA-C	-8.30	102.60	112.89
1	A	265	TYR	CA-C-N	-8.26	111.47	119.90
1	A	265	TYR	C-N-CA	-8.26	111.47	119.90
1	A	199	SER	CA-C-N	8.06	146.34	127.00
1	A	199	SER	C-N-CA	8.06	146.34	127.00
1	A	370	ASN	N-CA-C	8.04	121.62	108.99
1	A	396	LEU	CA-C-N	7.36	127.28	119.85
1	A	396	LEU	C-N-CA	7.36	127.28	119.85
1	A	115	ARG	N-CA-C	-7.32	103.33	111.82
2	B	409	ARG	N-CA-C	-7.22	104.33	113.72
1	A	918	ASN	N-CA-C	7.18	126.10	110.80
1	A	591	PRO	CA-C-N	-7.17	112.59	119.76
1	A	591	PRO	C-N-CA	-7.17	112.59	119.76
1	A	199	SER	C-N-CD	-7.12	104.94	120.60
1	A	-13	THR	N-CA-C	6.93	120.41	109.39
1	A	594	LYS	CA-C-N	6.90	128.47	119.84
1	A	594	LYS	C-N-CA	6.90	128.47	119.84
1	A	304	MET	CA-C-N	6.77	126.71	120.21
1	A	304	MET	C-N-CA	6.77	126.71	120.21
2	B	397	THR	N-CA-C	-6.56	106.02	112.97
1	A	756	ASN	CA-C-N	6.47	126.60	119.87
1	A	756	ASN	C-N-CA	6.47	126.60	119.87
2	B	486	ALA	N-CA-C	-6.42	105.26	113.23
1	A	667	PHE	N-CA-C	-6.18	104.08	111.69
1	A	445	LEU	N-CA-C	6.18	118.69	110.53
1	A	365	GLU	N-CA-C	5.98	123.02	109.81
1	A	322	THR	N-CA-C	5.92	123.40	110.80
1	A	299	MET	N-CA-C	5.88	118.98	110.28
1	A	455	LEU	N-CA-C	5.87	118.91	111.69
2	B	541	SER	N-CA-C	5.85	117.74	111.36
1	A	507	SER	N-CA-C	5.82	123.20	110.80
1	A	200	PRO	N-CA-C	5.81	127.21	112.10
1	A	420	CYS	N-CA-C	5.80	122.64	109.81
1	A	622	TYR	N-CA-C	5.77	118.68	111.24
1	A	751	PHE	N-CA-C	5.74	116.67	108.74
1	A	611	VAL	CB-CA-C	-5.71	104.67	111.81
1	A	-22	HIS	N-CA-C	5.67	118.58	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	866	LEU	N-CA-C	5.66	122.85	110.80
1	A	15	LEU	N-CA-C	-5.57	99.21	108.34
1	A	419	HIS	N-CA-C	5.56	118.25	109.96
1	A	598	ALA	N-CA-C	-5.55	106.46	113.18
1	A	1024	LYS	N-CA-C	-5.43	105.46	112.68
1	A	17	PRO	CA-C-N	5.42	124.94	119.19
1	A	17	PRO	C-N-CA	5.42	124.94	119.19
1	A	295	SER	N-CA-C	-5.33	104.36	112.04
1	A	907	ALA	N-CA-C	-5.28	105.43	111.07
1	A	76	GLU	N-CA-C	-5.26	102.40	110.30
1	A	156	LEU	N-CA-C	5.23	116.67	111.07
1	A	46	LYS	N-CA-C	-5.22	105.49	111.07
1	A	7	SER	N-CA-C	-5.20	104.32	111.81
1	A	367	LEU	N-CA-C	5.14	116.81	109.14
1	A	162	ARG	N-CA-C	-5.10	105.81	112.23
1	A	937	PHE	N-CA-C	5.08	117.37	109.60
2	B	378	ASN	N-CA-C	5.04	117.45	109.24
1	A	524	ARG	N-CA-C	-5.03	107.10	114.39

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	LEU	Peptide
1	A	201	ASN	Peptide
1	A	375	ARG	Peptide
1	A	377	PRO	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8525	0	8494	527	0
2	B	2059	0	2020	123	0
3	A	39	0	28	0	0
3	B	39	0	28	1	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	0	0	0
All	All	10671	0	10570	623	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 29.

All (623) 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:924:LYS:NZ	1:A:928:GLN:HB3	1.59	1.15
1:A:924:LYS:HB2	1:A:924:LYS:HZ2	1.08	1.14
1:A:13:ILE:O	1:A:14:HIS:HB2	1.45	1.09
2:B:355:PHE:HE1	2:B:427:PRO:HA	1.09	1.09
1:A:642:GLU:HG2	1:A:647:ASN:CG	1.78	1.08
1:A:772:MET:HE2	1:A:772:MET:HA	1.37	1.05
2:B:355:PHE:CE1	2:B:427:PRO:HA	1.92	1.05
1:A:353:LYS:HG3	1:A:377:PRO:HB3	1.39	1.04
1:A:31:ILE:HG12	2:B:531:LEU:HD13	1.37	1.04
1:A:924:LYS:HZ2	1:A:924:LYS:CB	1.72	1.02
2:B:461:ARG:O	2:B:465:ARG:HG3	1.58	1.01
1:A:508:TYR:HD1	1:A:508:TYR:C	1.68	1.01
1:A:956:LEU:H	1:A:1047:HIS:HE1	1.03	1.00
1:A:177:LEU:HD12	1:A:178:PRO:HD2	1.43	1.00
1:A:508:TYR:HD1	1:A:508:TYR:O	1.42	0.99
1:A:352:ASP:HB2	1:A:409:VAL:O	1.64	0.97
1:A:910:ILE:HA	1:A:1025:THR:HG21	1.47	0.96
1:A:278:MET:HE2	1:A:278:MET:HA	1.46	0.96
1:A:30:MET:HG2	2:B:527:ASN:HD21	1.31	0.95
1:A:924:LYS:HZ3	1:A:928:GLN:HB3	1.31	0.95
1:A:30:MET:HG2	2:B:527:ASN:ND2	1.83	0.93
1:A:523:LEU:O	1:A:523:LEU:HD23	1.68	0.92
1:A:243:VAL:O	1:A:247:GLN:HB2	1.70	0.90
2:B:398:PHE:HB2	2:B:399:SER:HA	1.54	0.89
2:B:439:GLU:O	2:B:445:VAL:HG23	1.71	0.89
1:A:772:MET:HA	1:A:772:MET:CE	2.04	0.88
1:A:956:LEU:H	1:A:1047:HIS:CE1	1.91	0.87
1:A:130:MET:HE3	1:A:130:MET:HA	1.55	0.87
1:A:924:LYS:NZ	1:A:924:LYS:CB	2.29	0.87
1:A:6:SER:HB3	2:B:479:MET:HE1	1.57	0.87
2:B:398:PHE:CB	2:B:399:SER:HA	2.06	0.85
1:A:767:GLU:H	1:A:767:GLU:CD	1.84	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:LEU:O	1:A:739:MET:HG3	1.78	0.84
1:A:35:GLU:O	1:A:35:GLU:HG3	1.77	0.84
2:B:330:ASP:O	2:B:332:GLU:N	2.10	0.84
1:A:358:THR:HG22	1:A:404:LEU:HB3	1.57	0.83
1:A:965:SER:O	1:A:967:GLY:N	2.10	0.83
2:B:441:ASN:HB3	2:B:444:ALA:H	1.43	0.83
1:A:545:GLU:OE2	1:A:545:GLU:HA	1.80	0.81
1:A:508:TYR:O	1:A:508:TYR:CD1	2.31	0.81
1:A:508:TYR:C	1:A:508:TYR:CD1	2.45	0.81
1:A:427:ILE:HG13	1:A:443:LEU:HD22	1.62	0.81
1:A:10:LEU:HD21	1:A:97:PRO:HG3	1.63	0.79
1:A:357:ARG:NH1	1:A:371:VAL:HG13	1.97	0.79
1:A:924:LYS:NZ	1:A:924:LYS:HB2	1.83	0.78
1:A:-28:MET:C	1:A:-26:TYR:H	1.90	0.78
1:A:709:MET:HE1	1:A:847:LEU:HD21	1.64	0.78
1:A:116:GLU:HG2	1:A:703:ASN:ND2	1.98	0.78
1:A:194:ILE:CD1	1:A:209:LEU:HG	2.13	0.78
1:A:355:TYR:HE2	1:A:371:VAL:HG12	1.49	0.78
1:A:745:MET:HE2	1:A:745:MET:HA	1.66	0.78
1:A:724:LYS:O	1:A:725:ASP:HB2	1.83	0.77
1:A:343:TYR:O	1:A:343:TYR:CD1	2.38	0.77
1:A:739:MET:O	1:A:745:MET:HE3	1.84	0.77
1:A:924:LYS:HZ1	1:A:928:GLN:HB3	1.43	0.77
1:A:408:SER:OG	1:A:422:LEU:HD21	1.83	0.77
1:A:443:LEU:HD12	1:A:444:ASN:H	1.50	0.77
1:A:908:THR:HG21	1:A:954:PHE:HB2	1.64	0.77
1:A:942:LYS:CB	1:A:946:GLY:HA3	2.15	0.76
1:A:825:GLN:O	1:A:827:GLN:N	2.18	0.76
1:A:343:TYR:O	1:A:343:TYR:HD1	1.69	0.76
1:A:13:ILE:O	1:A:14:HIS:CB	2.31	0.76
1:A:985:TYR:CE1	1:A:1040:MET:HG2	2.21	0.75
2:B:333:TRP:CZ2	2:B:405:ILE:HG21	2.22	0.75
1:A:200:PRO:CB	1:A:201:ASN:HA	2.16	0.74
1:A:117:ILE:O	1:A:121:ILE:HG13	1.87	0.74
1:A:397:PRO:HG3	1:A:574:TRP:O	1.86	0.74
1:A:357:ARG:HH12	1:A:371:VAL:HG13	1.51	0.73
1:A:278:MET:HA	1:A:278:MET:CE	2.18	0.73
1:A:116:GLU:HG2	1:A:703:ASN:HD21	1.52	0.73
1:A:335:ARG:HB3	1:A:386:TRP:CE3	2.23	0.73
1:A:822:ASN:O	1:A:826:ASN:HB2	1.88	0.73
2:B:578:ASP:O	2:B:582:MET:HG2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:ASP:HB3	1:A:611:VAL:HG23	1.70	0.72
2:B:398:PHE:CB	2:B:399:SER:CA	2.67	0.72
1:A:8:GLY:HA3	1:A:14:HIS:O	1.89	0.72
1:A:30:MET:HE1	1:A:57:PRO:O	1.89	0.72
2:B:341:GLU:O	2:B:345:GLU:HG2	1.89	0.72
1:A:181:ILE:HG12	1:A:278:MET:HE3	1.72	0.72
1:A:544:THR:HG23	1:A:547:GLU:OE2	1.90	0.71
1:A:194:ILE:HD11	1:A:209:LEU:HG	1.70	0.71
1:A:1023:ARG:NH2	1:A:1029:ASP:OD1	2.24	0.71
1:A:193:VAL:HG22	1:A:208:THR:HG22	1.73	0.71
1:A:288:MET:HE3	1:A:288:MET:HA	1.73	0.71
1:A:375:ARG:NH2	1:A:385:GLU:HG3	2.06	0.70
1:A:83:PHE:CD1	1:A:109:GLU:OE1	2.45	0.70
1:A:198:VAL:H	1:A:201:ASN:ND2	1.90	0.70
1:A:936:HIS:CD2	1:A:1012:GLU:OE2	2.45	0.70
1:A:806:ASP:OD1	1:A:808:ARG:HG3	1.91	0.69
2:B:398:PHE:HB3	2:B:399:SER:C	2.17	0.69
1:A:300:ASP:HB2	1:A:696:GLY:CA	2.23	0.69
1:A:1038:TYR:O	1:A:1042:GLN:HG2	1.92	0.69
1:A:300:ASP:HB2	1:A:696:GLY:HA3	1.73	0.69
1:A:522:GLU:OE2	1:A:523:LEU:HD22	1.93	0.69
1:A:767:GLU:CD	1:A:767:GLU:N	2.51	0.69
1:A:130:MET:HA	1:A:130:MET:CE	2.24	0.68
1:A:980:PHE:O	1:A:983:MET:N	2.25	0.68
1:A:-18:ASP:HB3	1:A:889:ILE:HD11	1.75	0.68
1:A:-28:MET:H2	1:A:-25:TYR:H	1.41	0.67
1:A:198:VAL:H	1:A:201:ASN:HD22	1.41	0.67
1:A:522:GLU:OE1	1:A:522:GLU:HA	1.94	0.67
1:A:356:VAL:HB	1:A:372:ASN:HD21	1.59	0.67
1:A:154:ARG:C	1:A:156:LEU:H	2.03	0.67
1:A:942:LYS:HB3	1:A:946:GLY:HA3	1.74	0.67
1:A:38:ARG:HD3	1:A:39:GLU:OE1	1.96	0.66
1:A:542:GLU:CG	2:B:380:LEU:HD22	2.26	0.66
1:A:910:ILE:HA	1:A:1025:THR:CG2	2.24	0.66
2:B:562:ARG:HG2	2:B:566:ILE:HD12	1.78	0.66
1:A:229:THR:O	1:A:230:ARG:C	2.39	0.66
1:A:532:LYS:HE3	1:A:561:ILE:HG12	1.77	0.66
1:A:627:LYS:HG3	1:A:631:TYR:CE2	2.31	0.66
1:A:825:GLN:C	1:A:827:GLN:H	2.03	0.66
1:A:221:ILE:HG23	1:A:287:LEU:HD21	1.78	0.65
1:A:341:ALA:HB2	1:A:473:LEU:HD12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:972:THR:HG22	1:A:973:LYS:HD3	1.79	0.65
1:A:945:PHE:H	2:B:577:ARG:HH12	1.45	0.64
1:A:177:LEU:HD12	1:A:178:PRO:CD	2.23	0.64
1:A:159:PRO:HG2	1:A:294:TYR:CD2	2.32	0.64
2:B:562:ARG:HA	2:B:565:SER:HB2	1.79	0.64
1:A:15:LEU:HD21	1:A:738:GLN:NE2	2.13	0.64
1:A:361:TYR:HA	1:A:365:GLU:HA	1.78	0.64
1:A:159:PRO:HG2	1:A:294:TYR:CE2	2.33	0.64
3:B:2001:PBU:H82	3:B:2001:PBU:H1'2	1.78	0.64
1:A:103:GLU:HG3	1:A:104:PRO:CD	2.29	0.63
1:A:901:CYS:HA	1:A:929:LEU:HD21	1.79	0.63
1:A:903:GLY:C	1:A:905:CYS:H	2.07	0.63
2:B:518:GLU:HA	2:B:521:ILE:HD12	1.81	0.63
1:A:251:ILE:HD12	1:A:288:MET:HB3	1.80	0.63
2:B:542:ARG:O	2:B:542:ARG:HG2	1.98	0.63
1:A:8:GLY:CA	1:A:14:HIS:O	2.47	0.63
1:A:357:ARG:NH1	1:A:371:VAL:CG1	2.61	0.63
1:A:924:LYS:NZ	1:A:924:LYS:HB3	2.10	0.63
1:A:888:GLU:OE1	1:A:892:ALA:HB2	1.99	0.62
1:A:217:PRO:O	1:A:221:ILE:HG13	1.98	0.62
2:B:330:ASP:C	2:B:332:GLU:H	2.05	0.62
1:A:213:HIS:CE1	1:A:214:ASP:HB3	2.34	0.62
1:A:767:GLU:N	1:A:767:GLU:OE2	2.33	0.62
1:A:860:ILE:HG21	1:A:877:LEU:HD12	1.81	0.62
1:A:355:TYR:CE2	1:A:371:VAL:HG12	2.34	0.62
1:A:503:GLU:CD	1:A:555:ARG:HH22	2.08	0.62
1:A:360:ILE:HD13	1:A:367:LEU:HD21	1.80	0.62
1:A:375:ARG:NH2	1:A:383:TRP:HB3	2.14	0.62
1:A:608:ASP:HB3	1:A:611:VAL:CG2	2.29	0.61
1:A:254:VAL:HG22	1:A:261:PHE:HE1	1.65	0.61
1:A:286:MET:HG3	1:A:789:MET:HE3	1.82	0.61
1:A:-28:MET:C	1:A:-26:TYR:N	2.59	0.61
1:A:35:GLU:O	1:A:35:GLU:CG	2.48	0.61
1:A:542:GLU:HG3	2:B:380:LEU:CD2	2.30	0.61
1:A:977:PHE:HE1	1:A:981:GLN:NE2	1.97	0.61
1:A:38:ARG:HD2	1:A:741:ARG:CZ	2.31	0.61
1:A:103:GLU:HG3	1:A:104:PRO:HD2	1.83	0.61
1:A:108:ARG:C	1:A:110:GLU:H	2.09	0.61
1:A:347:ASN:HB3	1:A:350:ASP:HB2	1.83	0.61
2:B:584:LEU:O	2:B:588:GLY:N	2.28	0.61
1:A:805:ASP:O	1:A:807:LEU:HD23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:544:ARG:O	2:B:547:GLU:HG2	2.01	0.60
1:A:450:HIS:CE1	2:B:464:ASP:OD1	2.54	0.60
1:A:60:GLN:HG2	1:A:61:LEU:HD12	1.83	0.60
1:A:135:GLU:HB2	1:A:432:TYR:CE1	2.36	0.60
1:A:542:GLU:HG3	2:B:380:LEU:HD22	1.84	0.60
1:A:431:ASP:C	1:A:431:ASP:OD1	2.44	0.60
1:A:660:ASN:OD1	1:A:660:ASN:C	2.44	0.60
1:A:896:LEU:HD21	1:A:928:GLN:HB2	1.84	0.60
1:A:745:MET:O	1:A:749:GLN:HB2	2.01	0.60
1:A:444:ASN:O	1:A:465:ASN:HB3	2.01	0.59
1:A:375:ARG:HH22	1:A:383:TRP:HB3	1.67	0.59
2:B:350:THR:HG21	2:B:428:VAL:HG11	1.85	0.59
1:A:365:GLU:OE2	1:A:365:GLU:N	2.36	0.59
2:B:398:PHE:HB3	2:B:399:SER:CA	2.33	0.59
2:B:509:ILE:C	2:B:511:LYS:H	2.09	0.59
1:A:642:GLU:HG2	1:A:647:ASN:CB	2.33	0.59
1:A:727:THR:O	1:A:730:VAL:N	2.32	0.59
1:A:200:PRO:HB2	1:A:201:ASN:HA	1.84	0.58
1:A:336:ILE:HB	1:A:389:TYR:HE2	1.67	0.58
1:A:367:LEU:CD2	1:A:389:TYR:HB3	2.33	0.58
1:A:526:ASN:O	1:A:529:GLU:HB2	2.03	0.58
1:A:977:PHE:HE1	1:A:981:GLN:HE21	1.51	0.58
1:A:138:ASP:O	1:A:142:ASN:ND2	2.36	0.58
2:B:445:VAL:HG12	2:B:584:LEU:HD21	1.85	0.58
1:A:637:GLN:OE1	1:A:640:LYS:NZ	2.36	0.58
1:A:721:GLN:O	1:A:722:GLU:C	2.46	0.58
1:A:948:LYS:O	1:A:950:GLU:N	2.36	0.58
1:A:873:ASN:HD22	1:A:876:THR:HG23	1.68	0.58
1:A:908:THR:HG21	1:A:954:PHE:CB	2.34	0.58
2:B:537:GLU:O	2:B:540:ASP:HB2	2.04	0.58
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.40	0.57
1:A:336:ILE:O	1:A:387:LEU:N	2.29	0.57
1:A:870:LEU:O	1:A:871:GLN:HB2	2.04	0.57
1:A:514:SER:O	1:A:522:GLU:HG2	2.05	0.57
1:A:60:GLN:H	1:A:60:GLN:CD	2.11	0.57
1:A:198:VAL:N	1:A:201:ASN:HD22	2.02	0.57
1:A:367:LEU:C	1:A:367:LEU:HD12	2.30	0.57
1:A:1036:LEU:O	1:A:1040:MET:HG3	2.04	0.57
1:A:111:LYS:HE2	1:A:306:SER:H	1.70	0.57
1:A:182:TYR:O	1:A:185:LEU:HB2	2.04	0.57
2:B:338:ILE:HB	2:B:342:GLU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:THR:O	1:A:728:GLN:C	2.48	0.56
1:A:956:LEU:N	1:A:1047:HIS:HE1	1.88	0.56
1:A:567:LYS:O	1:A:568:LEU:C	2.49	0.56
1:A:642:GLU:HG2	1:A:647:ASN:OD1	2.05	0.56
1:A:800:ILE:CD1	1:A:850:VAL:HG22	2.36	0.56
1:A:404:LEU:HD11	1:A:443:LEU:HD23	1.86	0.56
1:A:977:PHE:O	1:A:980:PHE:HB3	2.05	0.56
1:A:108:ARG:C	1:A:110:GLU:N	2.63	0.56
1:A:461:VAL:HG22	1:A:462:THR:N	2.21	0.56
2:B:566:ILE:CG2	2:B:566:ILE:O	2.53	0.56
1:A:293:LEU:C	1:A:295:SER:H	2.13	0.56
1:A:375:ARG:HH21	1:A:385:GLU:HG3	1.69	0.56
1:A:828:GLY:O	1:A:829:LEU:HB2	2.04	0.56
1:A:929:LEU:O	1:A:929:LEU:HD23	2.06	0.56
1:A:185:LEU:HD13	1:A:188:GLY:HA2	1.88	0.55
1:A:361:TYR:CE2	1:A:365:GLU:HG3	2.42	0.55
1:A:558:CYS:HB3	1:A:564:ILE:HG21	1.88	0.55
1:A:265:TYR:O	1:A:266:PRO:C	2.49	0.55
1:A:46:LYS:HE3	1:A:65:GLU:HB3	1.89	0.55
2:B:483:ALA:O	2:B:486:ALA:N	2.39	0.55
1:A:634:GLN:HG2	1:A:1001:LEU:HD22	1.88	0.55
1:A:961:LEU:HD22	1:A:977:PHE:HE2	1.71	0.55
1:A:996:ASN:H	1:A:996:ASN:HD22	1.53	0.55
1:A:357:ARG:HG2	1:A:456:LEU:HD13	1.87	0.55
1:A:25:LEU:CD1	1:A:25:LEU:N	2.70	0.55
1:A:60:GLN:OE1	1:A:60:GLN:N	2.25	0.55
1:A:83:PHE:HD1	1:A:109:GLU:OE1	1.89	0.55
1:A:341:ALA:HB2	1:A:473:LEU:CD1	2.37	0.55
1:A:542:GLU:HG2	2:B:380:LEU:HD22	1.87	0.55
1:A:856:THR:O	1:A:857:ILE:C	2.48	0.55
2:B:343:VAL:HG21	2:B:358:ARG:HH11	1.70	0.55
2:B:554:ALA:HA	2:B:557:ARG:CZ	2.37	0.55
1:A:945:PHE:H	2:B:577:ARG:NH1	2.04	0.54
1:A:433:THR:O	1:A:434:ASP:HB2	2.07	0.54
1:A:809:GLN:HG2	1:A:1012:GLU:OE2	2.07	0.54
1:A:977:PHE:CE1	1:A:981:GLN:NE2	2.74	0.54
1:A:1027:ALA:HB1	1:A:1030:LYS:HD2	1.88	0.54
1:A:897:PHE:O	1:A:901:CYS:HB2	2.07	0.54
1:A:564:ILE:HG13	1:A:564:ILE:O	2.06	0.54
2:B:354:THR:O	2:B:372:LEU:HA	2.07	0.54
1:A:226:ARG:O	1:A:230:ARG:CG	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ILE:O	1:A:288:MET:HB3	2.07	0.54
1:A:868:GLY:O	1:A:870:LEU:HB2	2.08	0.54
1:A:190:ILE:CD1	1:A:213:HIS:HA	2.38	0.54
1:A:226:ARG:HH21	1:A:243:VAL:HG11	1.73	0.54
1:A:111:LYS:HE2	1:A:306:SER:N	2.23	0.54
1:A:446:TRP:CD2	1:A:465:ASN:HB2	2.42	0.54
1:A:965:SER:HA	1:A:976:GLU:HG3	1.90	0.53
1:A:38:ARG:NH2	1:A:743:ASP:OD2	2.28	0.53
1:A:1017:ASP:HB2	2:B:345:GLU:OE1	2.07	0.53
1:A:-28:MET:HA	1:A:-23:HIS:CD2	2.44	0.53
1:A:144:LEU:O	1:A:145:ASN:C	2.51	0.53
1:A:225:ILE:O	1:A:229:THR:HG23	2.08	0.53
2:B:349:ASP:H	2:B:373:ARG:NH2	2.06	0.53
1:A:65:GLU:O	1:A:67:SER:N	2.42	0.53
1:A:226:ARG:O	1:A:230:ARG:HG3	2.09	0.53
1:A:630:GLN:O	1:A:815:GLN:NE2	2.40	0.53
1:A:807:LEU:HG	1:A:846:GLY:HA3	1.89	0.53
1:A:-23:HIS:CD2	1:A:834:LEU:HD13	2.43	0.53
1:A:76:GLU:HG2	1:A:124:PRO:HD3	1.91	0.53
1:A:372:ASN:O	1:A:373:THR:C	2.52	0.53
2:B:582:MET:O	2:B:586:GLN:HG3	2.09	0.53
1:A:598:ALA:O	1:A:601:LEU:HB2	2.09	0.52
2:B:448:LYS:HB3	2:B:580:TYR:CE2	2.44	0.52
1:A:422:LEU:HD22	2:B:564:ASN:HB3	1.90	0.52
1:A:1010:MET:HE3	1:A:1013:LEU:HD12	1.91	0.52
1:A:451:GLY:HA3	1:A:1014:GLN:HG3	1.89	0.52
1:A:635:LEU:O	1:A:638:VAL:HG12	2.09	0.52
1:A:1032:GLU:O	1:A:1033:GLN:C	2.52	0.52
1:A:43:ILE:HG13	1:A:85:GLU:O	2.09	0.52
1:A:470:THR:HB	1:A:471:PRO:CD	2.39	0.52
1:A:599:MET:HE2	1:A:635:LEU:HD21	1.90	0.52
1:A:4:ARG:HG3	1:A:5:PRO:HD2	1.92	0.52
1:A:397:PRO:HD2	1:A:400:ALA:HB2	1.91	0.52
1:A:529:GLU:OE1	1:A:529:GLU:HA	2.08	0.52
1:A:42:LEU:HD22	1:A:70:PHE:CD2	2.45	0.52
1:A:193:VAL:HG23	1:A:282:MET:HG2	1.92	0.52
1:A:449:PRO:HA	2:B:467:TYR:HE2	1.75	0.52
1:A:883:ASP:OD2	1:A:884:LYS:HD3	2.10	0.51
1:A:1023:ARG:HH22	1:A:1029:ASP:CG	2.18	0.51
1:A:511:ALA:C	1:A:513:LEU:H	2.18	0.51
1:A:829:LEU:HD21	1:A:986:LYS:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:PHE:HB2	2:B:370:LEU:HD11	1.91	0.51
1:A:878:HIS:HD2	1:A:963:VAL:HA	1.75	0.51
2:B:335:TRP:HB2	2:B:338:ILE:HD11	1.92	0.51
2:B:476:GLU:O	2:B:480:LYS:HG3	2.11	0.51
1:A:28:ASN:OD1	1:A:30:MET:HE3	2.10	0.51
1:A:868:GLY:O	1:A:870:LEU:N	2.44	0.51
2:B:576:THR:HA	2:B:579:GLN:HB2	1.92	0.51
1:A:191:ILE:HG12	1:A:210:LYS:HG3	1.92	0.51
1:A:367:LEU:HD21	1:A:389:TYR:HB3	1.93	0.51
1:A:875:HIS:O	1:A:879:GLN:HG2	2.10	0.51
1:A:903:GLY:O	1:A:905:CYS:N	2.42	0.51
2:B:396:LEU:C	2:B:398:PHE:H	2.19	0.51
1:A:542:GLU:CG	2:B:380:LEU:CD2	2.88	0.51
1:A:199:SER:HA	1:A:201:ASN:HB2	1.93	0.51
1:A:692:CYS:HB3	1:A:699:LEU:HD13	1.92	0.51
2:B:328:LEU:O	2:B:334:TYR:CD2	2.63	0.51
1:A:111:LYS:HD3	1:A:306:SER:HB2	1.92	0.50
1:A:111:LYS:HZ1	1:A:305:PRO:HA	1.76	0.50
1:A:300:ASP:HB2	1:A:696:GLY:HA2	1.93	0.50
1:A:538:ASP:OD1	1:A:541:SER:HB3	2.11	0.50
1:A:567:LYS:O	1:A:570:LEU:N	2.43	0.50
1:A:1023:ARG:HH11	1:A:1023:ARG:HB3	1.75	0.50
1:A:366:PRO:HB2	1:A:575:ASN:HB3	1.93	0.50
1:A:924:LYS:NZ	1:A:928:GLN:CB	2.53	0.50
1:A:956:LEU:N	1:A:956:LEU:HD23	2.27	0.50
2:B:392:PHE:HE2	2:B:413:LEU:HD21	1.75	0.50
1:A:154:ARG:C	1:A:156:LEU:N	2.70	0.50
2:B:400:SER:OG	2:B:401:VAL:N	2.43	0.50
1:A:29:GLY:HA2	2:B:497:GLN:CD	2.36	0.50
1:A:470:THR:HB	1:A:471:PRO:HD2	1.93	0.50
1:A:749:GLN:HG2	1:A:764:LEU:H	1.76	0.50
1:A:781:LEU:HD13	1:A:783:TRP:CH2	2.47	0.50
1:A:356:VAL:HG23	1:A:383:TRP:CH2	2.47	0.50
1:A:108:ARG:CZ	1:A:111:LYS:HD2	2.41	0.50
1:A:116:GLU:O	1:A:119:PHE:N	2.45	0.50
1:A:347:ASN:HB3	1:A:350:ASP:CB	2.42	0.50
1:A:903:GLY:C	1:A:905:CYS:N	2.70	0.50
1:A:945:PHE:O	1:A:947:TYR:HD1	1.95	0.50
1:A:794:PHE:HD1	1:A:794:PHE:O	1.94	0.50
1:A:833:MET:HA	1:A:904:TYR:HE1	1.76	0.50
1:A:595:PRO:C	1:A:597:GLN:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:TRP:CH2	1:A:850:VAL:HG11	2.47	0.49
1:A:913:ILE:HD12	1:A:914:GLY:O	2.12	0.49
1:A:924:LYS:HZ1	1:A:928:GLN:CB	2.19	0.49
1:A:468:LYS:HB3	2:B:481:ARG:NH2	2.27	0.49
1:A:61:LEU:HD12	1:A:61:LEU:N	2.27	0.49
1:A:372:ASN:O	1:A:372:ASN:OD1	2.30	0.49
1:A:899:ARG:NH1	1:A:983:MET:HE1	2.27	0.49
1:A:15:LEU:HD21	1:A:738:GLN:HE22	1.77	0.49
1:A:300:ASP:C	1:A:301:CYS:SG	2.95	0.49
1:A:965:SER:C	1:A:967:GLY:H	2.14	0.49
1:A:945:PHE:CG	2:B:598:LEU:HB3	2.47	0.49
1:A:467:ASN:HD21	1:A:678:LYS:HE2	1.76	0.49
1:A:542:GLU:HG3	2:B:380:LEU:CD1	2.42	0.49
1:A:797:ASN:OD1	1:A:797:ASN:C	2.56	0.49
1:A:47:HIS:CD2	1:A:51:LYS:HE3	2.47	0.49
1:A:372:ASN:O	1:A:373:THR:O	2.29	0.49
1:A:12:GLY:O	1:A:13:ILE:C	2.55	0.49
1:A:542:GLU:HG3	2:B:380:LEU:HD13	1.94	0.49
1:A:181:ILE:HG12	1:A:278:MET:CE	2.41	0.49
1:A:945:PHE:CD2	1:A:946:GLY:N	2.81	0.49
1:A:-17:TYR:CD1	1:A:-17:TYR:C	2.91	0.48
1:A:137:GLN:HE22	1:A:140:ARG:HH11	1.60	0.48
1:A:352:ASP:CB	1:A:409:VAL:O	2.50	0.48
1:A:360:ILE:O	1:A:366:PRO:CD	2.61	0.48
1:A:728:GLN:O	1:A:729:LYS:C	2.55	0.48
1:A:1035:ALA:O	1:A:1036:LEU:C	2.56	0.48
1:A:243:VAL:O	1:A:247:GLN:NE2	2.46	0.48
1:A:572:VAL:HG21	1:A:583:MET:HG2	1.95	0.48
1:A:393:ILE:N	1:A:394:PRO:CD	2.76	0.48
1:A:532:LYS:HG3	1:A:561:ILE:HG21	1.94	0.48
1:A:724:LYS:C	1:A:724:LYS:HD2	2.37	0.48
2:B:370:LEU:HD23	2:B:381:ILE:HD12	1.95	0.48
1:A:306:SER:C	1:A:308:SER:H	2.21	0.48
1:A:452:LEU:CD1	1:A:454:ASP:HB2	2.43	0.48
1:A:633:ILE:O	1:A:634:GLN:C	2.55	0.48
1:A:934:PHE:O	1:A:935:GLY:C	2.56	0.48
1:A:540:LEU:HD11	1:A:999:ILE:HD12	1.96	0.48
1:A:583:MET:O	1:A:587:VAL:HG23	2.12	0.48
2:B:453:ASN:O	2:B:457:GLN:HG3	2.13	0.48
1:A:8:GLY:HA3	1:A:14:HIS:C	2.39	0.48
1:A:491:VAL:HG12	1:A:491:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:LYS:O	1:A:725:ASP:CB	2.59	0.48
1:A:802:LYS:HD2	1:A:805:ASP:HB2	1.96	0.48
1:A:870:LEU:O	1:A:871:GLN:CB	2.61	0.48
1:A:1021:TYR:HE1	1:A:1025:THR:HG1	1.59	0.48
1:A:-17:TYR:C	1:A:-17:TYR:HD1	2.22	0.48
1:A:114:ASN:C	1:A:114:ASN:ND2	2.71	0.48
1:A:456:LEU:O	1:A:457:ASN:HB2	2.13	0.48
1:A:218:GLU:HA	1:A:221:ILE:HD12	1.96	0.48
1:A:325:LYS:HE3	1:A:482:SER:HB2	1.95	0.48
2:B:502:GLU:HA	2:B:505:SER:OG	2.14	0.48
1:A:254:VAL:HG22	1:A:261:PHE:CE1	2.46	0.48
1:A:200:PRO:HB2	1:A:202:ASN:H	1.79	0.47
1:A:881:LEU:HD11	1:A:927:GLY:HA2	1.96	0.47
1:A:8:GLY:HA3	1:A:14:HIS:HA	1.96	0.47
1:A:172:GLU:HG3	1:A:274:ARG:HD2	1.94	0.47
1:A:939:ASP:HB3	1:A:1021:TYR:CE2	2.47	0.47
1:A:404:LEU:HD21	1:A:475:LEU:HD11	1.97	0.47
1:A:843:ASP:C	1:A:843:ASP:OD1	2.56	0.47
1:A:715:LEU:HD21	1:A:735:LEU:HD12	1.97	0.47
1:A:1001:LEU:HD22	1:A:1001:LEU:HA	1.75	0.47
1:A:8:GLY:HA2	1:A:714:ASN:ND2	2.29	0.47
1:A:627:LYS:HG3	1:A:631:TYR:HE2	1.76	0.47
1:A:672:LYS:HA	1:A:675:MET:HG2	1.96	0.47
1:A:680:VAL:O	1:A:681:SER:C	2.57	0.47
1:A:375:ARG:O	1:A:376:VAL:C	2.56	0.47
1:A:450:HIS:HD2	1:A:1011:PRO:HB3	1.78	0.47
1:A:980:PHE:O	1:A:981:GLN:C	2.57	0.47
1:A:8:GLY:HA3	1:A:14:HIS:CA	2.45	0.47
1:A:94:LEU:O	1:A:95:PHE:HB3	2.14	0.47
1:A:190:ILE:HD12	1:A:213:HIS:HA	1.97	0.47
1:A:293:LEU:C	1:A:295:SER:N	2.68	0.47
1:A:361:TYR:HA	1:A:366:PRO:HD3	1.97	0.47
2:B:552:GLN:O	2:B:553:ALA:C	2.56	0.47
2:B:567:LYS:N	2:B:568:PRO:HD2	2.30	0.47
2:B:593:LYS:C	2:B:595:ASN:H	2.23	0.47
1:A:357:ARG:HH11	1:A:371:VAL:CG1	2.28	0.46
1:A:444:ASN:HB3	1:A:465:ASN:O	2.15	0.46
1:A:1044:ASN:HA	1:A:1051:TRP:HB2	1.97	0.46
2:B:509:ILE:HD11	2:B:521:ILE:HG23	1.97	0.46
1:A:73:VAL:O	1:A:94:LEU:O	2.32	0.46
1:A:368:CYS:O	1:A:369:ASP:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:LEU:HD22	1:A:1010:MET:HE1	1.96	0.46
2:B:544:ARG:HA	2:B:547:GLU:HG2	1.97	0.46
1:A:4:ARG:HB2	1:A:76:GLU:OE1	2.14	0.46
1:A:355:TYR:HE2	1:A:371:VAL:CG1	2.23	0.46
1:A:539:PRO:O	1:A:540:LEU:C	2.58	0.46
1:A:623:LEU:HD21	1:A:628:LEU:HB2	1.97	0.46
2:B:358:ARG:HH22	2:B:380:LEU:HD21	1.81	0.46
1:A:96:GLN:OE1	1:A:97:PRO:HD3	2.16	0.46
1:A:148:LYS:O	1:A:148:LYS:HD3	2.15	0.46
1:A:837:GLY:N	1:A:849:GLU:OE2	2.36	0.46
1:A:15:LEU:HD22	1:A:718:ILE:HD13	1.97	0.46
1:A:229:THR:OG1	1:A:230:ARG:N	2.49	0.46
1:A:565:LEU:HB3	1:A:566:PRO:HD3	1.98	0.46
2:B:446:GLY:O	2:B:449:LEU:HB3	2.16	0.46
1:A:7:SER:C	1:A:8:GLY:O	2.59	0.46
1:A:65:GLU:C	1:A:67:SER:N	2.73	0.46
1:A:337:LYS:HD2	1:A:476:GLU:OE2	2.15	0.46
1:A:644:TYR:O	1:A:683:ARG:NH2	2.48	0.46
1:A:724:LYS:HA	1:A:731:GLN:NE2	2.31	0.46
1:A:825:GLN:C	1:A:827:GLN:N	2.69	0.46
1:A:1023:ARG:NH2	1:A:1029:ASP:CG	2.74	0.46
2:B:338:ILE:HD12	2:B:343:VAL:HG22	1.98	0.46
1:A:91:ASP:OD1	1:A:711:LYS:NZ	2.45	0.46
1:A:526:ASN:O	1:A:529:GLU:N	2.48	0.46
1:A:540:LEU:HD11	1:A:1019:ILE:HG22	1.97	0.46
1:A:672:LYS:O	1:A:675:MET:HB2	2.15	0.46
1:A:812:LEU:CD2	1:A:1005:MET:HG3	2.45	0.46
1:A:884:LYS:NZ	1:A:925:ASP:OD1	2.40	0.46
2:B:505:SER:C	2:B:507:GLU:H	2.24	0.46
1:A:25:LEU:N	1:A:25:LEU:HD12	2.31	0.45
1:A:114:ASN:HA	1:A:117:ILE:HG13	1.98	0.45
1:A:622:TYR:N	1:A:622:TYR:CD1	2.84	0.45
1:A:530:GLN:O	1:A:533:ALA:HB3	2.17	0.45
1:A:121:ILE:CG2	1:A:688:LEU:HD13	2.47	0.45
2:B:439:GLU:O	2:B:445:VAL:CG2	2.54	0.45
1:A:5:PRO:C	1:A:7:SER:N	2.74	0.45
1:A:885:ASN:HB3	1:A:889:ILE:HG22	1.98	0.45
1:A:956:LEU:N	1:A:1047:HIS:CE1	2.71	0.45
1:A:106:GLY:O	1:A:108:ARG:N	2.50	0.45
1:A:200:PRO:CG	1:A:201:ASN:HA	2.46	0.45
1:A:939:ASP:O	1:A:942:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PRO:C	1:A:7:SER:H	2.23	0.45
1:A:267:LEU:HD13	1:A:273:ILE:HG13	1.99	0.45
1:A:921:ILE:HG12	1:A:931:HIS:CE1	2.52	0.45
2:B:435:GLN:C	2:B:437:VAL:N	2.75	0.45
1:A:164:MET:HE1	1:A:263:GLU:HB3	1.99	0.45
1:A:260:TYR:N	1:A:260:TYR:CD1	2.85	0.45
1:A:509:SER:HB2	1:A:513:LEU:HB3	1.98	0.45
1:A:749:GLN:HG2	1:A:763:ASN:HA	1.97	0.45
1:A:789:MET:O	1:A:790:SER:C	2.59	0.45
1:A:151:VAL:HG11	1:A:302:PHE:HB2	1.98	0.45
2:B:567:LYS:N	2:B:568:PRO:CD	2.80	0.45
1:A:-19:HIS:NE2	1:A:926:ASP:HB2	2.32	0.45
1:A:299:MET:O	1:A:697:MET:HE3	2.17	0.45
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.52	0.45
1:A:622:TYR:N	1:A:622:TYR:HD1	2.15	0.45
1:A:802:LYS:HD3	1:A:805:ASP:OD2	2.17	0.45
1:A:807:LEU:HD11	1:A:848:ILE:HD11	1.99	0.45
1:A:114:ASN:HD22	1:A:115:ARG:N	2.15	0.44
1:A:172:GLU:HG2	1:A:271:LYS:HG2	2.00	0.44
1:A:372:ASN:HB2	1:A:385:GLU:CD	2.42	0.44
1:A:735:LEU:O	1:A:735:LEU:HG	2.14	0.44
1:A:53:ALA:C	1:A:55:LYS:N	2.76	0.44
1:A:843:ASP:O	1:A:844:CYS:HB2	2.16	0.44
1:A:352:ASP:O	1:A:353:LYS:HD2	2.17	0.44
1:A:373:THR:C	1:A:375:ARG:H	2.26	0.44
1:A:457:ASN:OD1	1:A:459:ILE:HG22	2.17	0.44
2:B:343:VAL:HG21	2:B:358:ARG:HG3	1.99	0.44
1:A:196:VAL:HG22	1:A:287:LEU:HB2	2.00	0.44
1:A:584:TYR:CE1	1:A:610:MET:HG3	2.53	0.44
1:A:256:GLY:O	1:A:793:LEU:HD23	2.18	0.44
1:A:562:PRO:C	1:A:564:ILE:H	2.26	0.44
1:A:741:ARG:HB3	1:A:743:ASP:OD1	2.17	0.44
1:A:799:ILE:HD12	1:A:799:ILE:C	2.42	0.44
1:A:916:ARG:HB3	1:A:921:ILE:HD11	1.99	0.44
1:A:939:ASP:HB3	1:A:1021:TYR:HE2	1.82	0.44
2:B:441:ASN:C	2:B:443:GLU:H	2.25	0.44
1:A:543:ILE:HD11	1:A:567:LYS:HD3	1.98	0.44
1:A:938:LEU:O	1:A:939:ASP:C	2.61	0.44
2:B:554:ALA:HA	2:B:557:ARG:NH1	2.33	0.44
1:A:409:VAL:C	1:A:418:GLU:HB2	2.42	0.44
1:A:560:THR:O	1:A:562:PRO:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:LEU:O	2:B:373:ARG:HB2	2.17	0.44
1:A:732:MET:HE3	1:A:732:MET:HB3	1.51	0.44
1:A:885:ASN:HB3	1:A:889:ILE:O	2.17	0.44
1:A:970:GLU:OE2	1:A:970:GLU:HA	2.18	0.44
2:B:570:LEU:O	2:B:570:LEU:HG	2.18	0.44
1:A:433:THR:O	1:A:434:ASP:CB	2.66	0.43
1:A:201:ASN:C	1:A:203:ASP:H	2.25	0.43
1:A:370:ASN:C	1:A:370:ASN:OD1	2.61	0.43
1:A:961:LEU:HD22	1:A:977:PHE:CE2	2.50	0.43
1:A:-24:HIS:CD2	1:A:852:ARG:HD3	2.53	0.43
1:A:647:ASN:ND2	1:A:650:VAL:H	2.16	0.43
1:A:65:GLU:O	1:A:66:SER:C	2.60	0.43
1:A:595:PRO:C	1:A:597:GLN:N	2.77	0.43
1:A:853:ASN:ND2	1:A:925:ASP:OD2	2.51	0.43
1:A:936:HIS:CD2	1:A:1012:GLU:CD	2.96	0.43
1:A:961:LEU:CD2	1:A:977:PHE:HE2	2.31	0.43
1:A:969:GLN:O	1:A:970:GLU:HB2	2.19	0.43
1:A:77:ALA:HB2	2:B:486:ALA:HB2	2.00	0.43
1:A:800:ILE:HD11	1:A:850:VAL:HG22	2.00	0.43
2:B:426:TYR:O	2:B:428:VAL:HG23	2.18	0.43
1:A:154:ARG:O	1:A:156:LEU:N	2.50	0.43
1:A:453:GLU:HB2	2:B:348:ARG:HH22	1.83	0.43
1:A:520:ASP:HB3	1:A:521:ASN:H	1.46	0.43
1:A:13:ILE:HG21	1:A:17:PRO:HD3	2.00	0.43
1:A:204:LYS:O	1:A:205:GLN:NE2	2.51	0.43
1:A:788:ILE:H	1:A:788:ILE:HG13	1.61	0.43
1:A:910:ILE:HD13	1:A:1026:LEU:HD21	2.01	0.43
1:A:1023:ARG:HA	1:A:1028:LEU:HD12	2.00	0.43
2:B:520:GLU:O	2:B:521:ILE:C	2.61	0.43
1:A:393:ILE:N	1:A:394:PRO:HD2	2.34	0.43
1:A:859:GLN:O	1:A:863:LYS:N	2.43	0.43
1:A:859:GLN:HA	1:A:862:CYS:HB2	2.01	0.43
1:A:10:LEU:HD13	1:A:16:MET:HE2	2.01	0.43
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.84	0.43
1:A:121:ILE:HG23	1:A:688:LEU:HD13	2.00	0.43
1:A:154:ARG:HD2	1:A:658:LEU:O	2.18	0.43
1:A:619:LEU:O	1:A:620:GLU:C	2.62	0.43
1:A:119:PHE:CE2	1:A:707:GLU:HG3	2.54	0.43
1:A:200:PRO:HB2	1:A:202:ASN:N	2.34	0.43
1:A:322:THR:C	1:A:324:THR:H	2.27	0.43
1:A:334:LEU:HD21	1:A:336:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:PRO:HA	2:B:467:TYR:CE2	2.54	0.43
1:A:756:ASN:OD1	1:A:756:ASN:C	2.62	0.43
1:A:873:ASN:ND2	1:A:876:THR:HG23	2.33	0.42
1:A:994:HIS:O	1:A:995:ALA:C	2.60	0.42
1:A:18:PRO:HA	1:A:38:ARG:HB2	2.01	0.42
1:A:702:LEU:HD23	1:A:702:LEU:HA	1.91	0.42
2:B:506:LYS:HA	2:B:509:ILE:HG22	2.00	0.42
1:A:360:ILE:O	1:A:366:PRO:HD2	2.19	0.42
1:A:453:GLU:HB2	2:B:348:ARG:NH2	2.34	0.42
1:A:712:LEU:HD11	1:A:781:LEU:HD11	2.01	0.42
2:B:491:ILE:O	2:B:492:LYS:C	2.60	0.42
2:B:552:GLN:C	2:B:554:ALA:N	2.76	0.42
1:A:69:ILE:HD12	1:A:69:ILE:HA	1.70	0.42
1:A:540:LEU:HG	1:A:999:ILE:HG21	2.02	0.42
1:A:787:ASP:O	1:A:790:SER:OG	2.33	0.42
1:A:945:PHE:CG	1:A:946:GLY:N	2.87	0.42
2:B:484:ILE:HG13	2:B:545:LEU:HD23	2.00	0.42
1:A:53:ALA:O	1:A:55:LYS:N	2.52	0.42
2:B:417:ASN:HA	2:B:418:PRO:HD2	1.91	0.42
2:B:430:LYS:O	2:B:432:GLN:N	2.53	0.42
2:B:473:THR:HG23	2:B:552:GLN:NE2	2.33	0.42
1:A:340:CYS:HB2	1:A:382:ARG:HG3	2.01	0.42
1:A:627:LYS:CG	1:A:631:TYR:HE2	2.33	0.42
2:B:362:THR:OG1	2:B:365:HIS:HD2	2.03	0.42
2:B:473:THR:O	2:B:474:SER:C	2.61	0.42
1:A:448:VAL:HA	1:A:449:PRO:HD3	1.83	0.42
1:A:830:ASP:O	1:A:899:ARG:HD3	2.20	0.42
2:B:459:LYS:HB3	2:B:570:LEU:CD1	2.49	0.42
2:B:362:THR:OG1	2:B:365:HIS:CD2	2.73	0.42
1:A:480:PHE:C	1:A:482:SER:H	2.28	0.42
1:A:523:LEU:O	1:A:523:LEU:CD2	2.54	0.42
1:A:649:LEU:O	1:A:650:VAL:C	2.62	0.42
1:A:1031:THR:O	1:A:1034:GLU:N	2.53	0.42
2:B:335:TRP:HB2	2:B:338:ILE:CD1	2.50	0.42
2:B:501:GLN:OE1	2:B:527:ASN:ND2	2.53	0.42
2:B:509:ILE:C	2:B:511:LYS:N	2.76	0.42
2:B:519:LYS:O	2:B:520:GLU:C	2.63	0.42
1:A:5:PRO:HG2	2:B:479:MET:SD	2.59	0.42
1:A:293:LEU:O	1:A:295:SER:N	2.53	0.42
1:A:744:PHE:CD2	1:A:748:LEU:HD12	2.55	0.42
2:B:467:TYR:HD1	2:B:467:TYR:O	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:VAL:HG11	1:A:99:LEU:HD22	2.02	0.41
1:A:367:LEU:HD12	1:A:368:CYS:C	2.45	0.41
1:A:736:VAL:O	1:A:737:GLU:C	2.63	0.41
1:A:945:PHE:HB2	2:B:598:LEU:HD13	2.02	0.41
1:A:989:LEU:HD21	1:A:1036:LEU:HG	2.02	0.41
2:B:544:ARG:O	2:B:547:GLU:CG	2.68	0.41
2:B:567:LYS:H	2:B:568:PRO:HD2	1.85	0.41
1:A:25:LEU:HB2	1:A:100:LYS:HG3	2.01	0.41
1:A:880:TRP:O	1:A:884:LYS:HG2	2.20	0.41
2:B:578:ASP:OD1	2:B:581:LEU:HD23	2.19	0.41
1:A:-23:HIS:CG	1:A:834:LEU:HD13	2.56	0.41
1:A:361:TYR:CD2	1:A:365:GLU:N	2.88	0.41
1:A:367:LEU:HD22	1:A:389:TYR:HB3	2.02	0.41
1:A:446:TRP:CH2	1:A:465:ASN:HA	2.55	0.41
2:B:408:TYR:CD1	2:B:413:LEU:HG	2.55	0.41
1:A:491:VAL:O	1:A:491:VAL:CG1	2.68	0.41
1:A:525:GLU:OE2	1:A:525:GLU:N	2.54	0.41
1:A:526:ASN:OD1	1:A:526:ASN:N	2.53	0.41
1:A:942:LYS:HB2	1:A:946:GLY:HA3	2.00	0.41
1:A:190:ILE:HD11	1:A:213:HIS:HA	2.03	0.41
1:A:740:ARG:O	1:A:741:ARG:C	2.62	0.41
1:A:4:ARG:NH1	2:B:482:THR:OG1	2.54	0.41
1:A:772:MET:CE	1:A:772:MET:CA	2.88	0.41
1:A:878:HIS:CD2	1:A:963:VAL:HA	2.54	0.41
1:A:995:ALA:O	1:A:996:ASN:C	2.64	0.41
2:B:566:ILE:O	2:B:566:ILE:HG23	2.21	0.41
1:A:221:ILE:HG13	1:A:221:ILE:H	1.71	0.41
1:A:985:TYR:CZ	1:A:1040:MET:HG2	2.56	0.41
2:B:348:ARG:O	2:B:349:ASP:HB2	2.20	0.41
2:B:437:VAL:O	2:B:439:GLU:HG3	2.20	0.41
2:B:480:LYS:HD3	2:B:545:LEU:HD11	2.03	0.41
2:B:554:ALA:HA	2:B:557:ARG:NH2	2.36	0.41
1:A:180:HIS:HE1	1:A:825:GLN:HG2	1.85	0.41
1:A:355:TYR:CE2	1:A:371:VAL:CG1	3.00	0.41
1:A:661:GLN:OE1	1:A:698:TYR:HB2	2.20	0.41
1:A:745:MET:HA	1:A:745:MET:CE	2.38	0.41
1:A:937:PHE:C	1:A:937:PHE:CD1	2.99	0.41
2:B:427:PRO:O	2:B:428:VAL:C	2.64	0.41
2:B:555:GLU:O	2:B:559:ILE:HG12	2.21	0.41
1:A:614:PHE:O	1:A:615:ALA:C	2.63	0.41
1:A:661:GLN:O	1:A:661:GLN:CG	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:PHE:O	1:A:794:PHE:CD1	2.73	0.41
1:A:1010:MET:HA	1:A:1011:PRO:HD3	1.87	0.41
2:B:518:GLU:O	2:B:521:ILE:HB	2.21	0.41
1:A:92:LEU:O	1:A:93:ARG:HB2	2.20	0.40
1:A:263:GLU:OE2	1:A:265:TYR:HE2	2.03	0.40
1:A:888:GLU:C	1:A:890:TYR:N	2.77	0.40
2:B:394:ASP:N	2:B:395:PRO:HD2	2.37	0.40
2:B:489:GLU:O	2:B:493:ILE:HG13	2.22	0.40
2:B:569:ASP:O	2:B:571:ILE:N	2.55	0.40
1:A:537:ARG:HD3	2:B:365:HIS:HE1	1.86	0.40
1:A:722:GLU:O	1:A:723:LYS:HG2	2.21	0.40
1:A:53:ALA:C	1:A:55:LYS:H	2.29	0.40
1:A:175:PRO:CD	1:A:176:GLU:H	2.34	0.40
1:A:661:GLN:O	1:A:661:GLN:HG2	2.22	0.40
1:A:88:ARG:O	1:A:89:LEU:C	2.63	0.40
1:A:292:SER:O	1:A:296:GLN:HG3	2.22	0.40
1:A:456:LEU:HD12	1:A:456:LEU:HA	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1032/1096 (94%)	797 (77%)	161 (16%)	74 (7%)	1	9
2	B	225/279 (81%)	168 (75%)	33 (15%)	24 (11%)	0	5
All	All	1257/1375 (91%)	965 (77%)	194 (15%)	98 (8%)	1	8

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	SER

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Mol	Chain	Res	Type
1	A	14	HIS
1	A	66	SER
1	A	107	ASN
1	A	114	ASN
1	A	200	PRO
1	A	222	ALA
1	A	298	PRO
1	A	369	ASP
1	A	375	ARG
1	A	450	HIS
1	A	535	SER
1	A	722	GLU
1	A	723	LYS
1	A	808	ARG
1	A	826	ASN
1	A	829	LEU
1	A	866	LEU
1	A	867	LYS
1	A	869	ALA
1	A	871	GLN
1	A	949	ARG
1	A	966	LYS
2	B	331	ALA
2	B	338	ILE
2	B	372	LEU
2	B	430	LYS
2	B	431	TYR
2	B	434	ASP
2	B	438	LYS
2	B	442	ILE
1	A	-27	SER
1	A	13	ILE
1	A	38	ARG
1	A	54	ARG
1	A	235	SER
1	A	373	THR
1	A	434	ASP
1	A	451	GLY
1	A	725	ASP
1	A	791	GLU
1	A	868	GLY
1	A	904	TYR

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Mol	Chain	Res	Type
1	A	939	ASP
1	A	946	GLY
2	B	340	ARG
2	B	428	VAL
2	B	519	LYS
1	A	-14	PRO
1	A	9	GLU
1	A	230	ARG
1	A	247	GLN
1	A	294	TYR
1	A	339	LEU
1	A	378	CYS
1	A	526	ASN
1	A	561	ILE
1	A	563	GLU
1	A	918	ASN
1	A	970	GLU
1	A	1016	PHE
2	B	349	ASP
2	B	398	PHE
2	B	416	TYR
2	B	429	SER
2	B	432	GLN
2	B	484	ILE
2	B	506	LYS
2	B	521	ILE
2	B	594	LEU
1	A	95	PHE
1	A	109	GLU
1	A	307	TYR
1	A	371	VAL
1	A	507	SER
1	A	513	LEU
1	A	596	GLU
1	A	678	LYS
1	A	945	PHE
1	A	980	PHE
1	A	116	GLU
1	A	155	ASP
1	A	245	GLU
1	A	368	CYS
1	A	376	VAL

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Mol	Chain	Res	Type
1	A	728	GLN
1	A	825	GLN
2	B	520	GLU
2	B	570	LEU
1	A	8	GLY
1	A	75	GLN
2	B	437	VAL
1	A	491	VAL
1	A	117	ILE
1	A	366	PRO
1	A	391	ILE
1	A	967	GLY
2	B	436	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	955/999 (96%)	782 (82%)	173 (18%)	2	10
2	B	227/259 (88%)	189 (83%)	38 (17%)	2	13
All	All	1182/1258 (94%)	971 (82%)	211 (18%)	2	10

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-20	HIS
1	A	-15	ILE
1	A	-13	THR
1	A	-12	THR
1	A	4	ARG
1	A	13	ILE
1	A	14	HIS
1	A	15	LEU
1	A	20	ILE
1	A	25	LEU

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Mol	Chain	Res	Type
1	A	31	ILE
1	A	32	VAL
1	A	35	GLU
1	A	39	GLU
1	A	43	ILE
1	A	44	THR
1	A	52	GLU
1	A	61	LEU
1	A	62	LEU
1	A	65	GLU
1	A	69	ILE
1	A	73	VAL
1	A	75	GLN
1	A	76	GLU
1	A	93	ARG
1	A	96	GLN
1	A	99	LEU
1	A	107	ASN
1	A	109	GLU
1	A	111	LYS
1	A	112	ILE
1	A	113	LEU
1	A	114	ASN
1	A	121	ILE
1	A	123	MET
1	A	125	VAL
1	A	130	MET
1	A	132	LYS
1	A	135	GLU
1	A	136	VAL
1	A	146	VAL
1	A	153	LEU
1	A	156	LEU
1	A	158	SER
1	A	171	VAL
1	A	173	SER
1	A	177	LEU
1	A	190	ILE
1	A	197	ILE
1	A	198	VAL
1	A	202	ASN
1	A	205	GLN

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Mol	Chain	Res	Type
1	A	208	THR
1	A	209	LEU
1	A	212	ASN
1	A	216	VAL
1	A	221	ILE
1	A	230	ARG
1	A	231	SER
1	A	234	LEU
1	A	246	TYR
1	A	251	ILE
1	A	267	LEU
1	A	278	MET
1	A	282	MET
1	A	287	LEU
1	A	292	SER
1	A	295	SER
1	A	297	LEU
1	A	303	THR
1	A	322	THR
1	A	323	SER
1	A	327	LEU
1	A	339	LEU
1	A	343	TYR
1	A	347	ASN
1	A	351	ILE
1	A	353	LYS
1	A	360	ILE
1	A	365	GLU
1	A	368	CYS
1	A	373	THR
1	A	393	ILE
1	A	404	LEU
1	A	406	ILE
1	A	427	ILE
1	A	433	THR
1	A	436	LEU
1	A	445	LEU
1	A	452	LEU
1	A	456	LEU
1	A	459	ILE
1	A	462	THR
1	A	464	SER

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Mol	Chain	Res	Type
1	A	470	THR
1	A	472	CYS
1	A	481	SER
1	A	492	ILE
1	A	494	GLU
1	A	508	TYR
1	A	520	ASP
1	A	522	GLU
1	A	523	LEU
1	A	525	GLU
1	A	526	ASN
1	A	529	GLU
1	A	531	LEU
1	A	532	LYS
1	A	535	SER
1	A	541	SER
1	A	545	GLU
1	A	561	ILE
1	A	563	GLU
1	A	564	ILE
1	A	625	ASP
1	A	627	LYS
1	A	633	ILE
1	A	648	LEU
1	A	675	MET
1	A	679	THR
1	A	681	SER
1	A	697	MET
1	A	716	THR
1	A	718	ILE
1	A	722	GLU
1	A	724	LYS
1	A	725	ASP
1	A	726	GLU
1	A	735	LEU
1	A	746	ASP
1	A	756	ASN
1	A	767	GLU
1	A	770	ARG
1	A	772	MET
1	A	776	LYS
1	A	788	ILE

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Mol	Chain	Res	Type
1	A	790	SER
1	A	798	GLU
1	A	807	LEU
1	A	829	LEU
1	A	834	LEU
1	A	856	THR
1	A	860	ILE
1	A	863	LYS
1	A	866	LEU
1	A	870	LEU
1	A	889	ILE
1	A	908	THR
1	A	924	LYS
1	A	929	LEU
1	A	933	ASP
1	A	937	PHE
1	A	942	LYS
1	A	943	LYS
1	A	944	LYS
1	A	951	ARG
1	A	952	VAL
1	A	956	LEU
1	A	959	ASP
1	A	965	SER
1	A	966	LYS
1	A	972	THR
1	A	973	LYS
1	A	976	GLU
1	A	989	LEU
1	A	997	LEU
1	A	1001	LEU
1	A	1018	ASP
1	A	1022	ILE
1	A	1023	ARG
1	A	1025	THR
1	A	1036	LEU
1	A	1053	THR
2	B	328	LEU
2	B	342	GLU
2	B	345	GLU
2	B	355	PHE
2	B	356	LEU

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Mol	Chain	Res	Type
2	B	368	TYR
2	B	371	THR
2	B	373	ARG
2	B	381	ILE
2	B	396	LEU
2	B	405	ILE
2	B	409	ARG
2	B	415	GLN
2	B	416	TYR
2	B	417	ASN
2	B	428	VAL
2	B	431	TYR
2	B	441	ASN
2	B	448	LYS
2	B	454	THR
2	B	459	LYS
2	B	477	ILE
2	B	485	GLU
2	B	493	ILE
2	B	498	CYS
2	B	500	THR
2	B	511	LYS
2	B	518	GLU
2	B	527	ASN
2	B	542	ARG
2	B	549	LEU
2	B	550	LYS
2	B	566	ILE
2	B	567	LYS
2	B	573	LEU
2	B	574	ARG
2	B	579	GLN
2	B	585	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-24	HIS
1	A	-20	HIS
1	A	107	ASN
1	A	114	ASN
1	A	137	GLN

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Mol	Chain	Res	Type
1	A	142	ASN
1	A	180	HIS
1	A	205	GLN
1	A	345	ASN
1	A	372	ASN
1	A	374	GLN
1	A	450	HIS
1	A	467	ASN
1	A	497	ASN
1	A	510	HIS
1	A	605	ASN
1	A	647	ASN
1	A	661	GLN
1	A	759	HIS
1	A	785	ASN
1	A	825	GLN
1	A	853	ASN
1	A	873	ASN
1	A	920	ASN
1	A	931	HIS
1	A	936	HIS
1	A	940	HIS
1	A	981	GLN
1	A	996	ASN
1	A	1014	GLN
1	A	1042	GLN
1	A	1047	HIS
2	B	365	HIS
2	B	406	ASN
2	B	415	GLN
2	B	475	GLN
2	B	478	GLN
2	B	527	ASN
2	B	564	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
4	PO4	A	1102	-	4,4,4	1.36	1 (25%)	6,6,6	0.50	0
3	PBU	A	1101	-	39,39,39	1.78	6 (15%)	54,57,57	1.72	12 (22%)
3	PBU	B	2001	-	39,39,39	1.98	9 (23%)	54,57,57	1.43	9 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PBU	A	1101	-	-	8/36/60/60	0/1/1/1
3	PBU	B	2001	-	-	14/36/60/60	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	PBU	O1'-C11	6.11	1.51	1.33
3	A	1101	PBU	O1'-C11	5.54	1.49	1.33
3	A	1101	PBU	O2'-C7	4.96	1.48	1.34
3	B	2001	PBU	O2'-C7	4.57	1.47	1.34
3	B	2001	PBU	P4-O4	4.35	1.67	1.59
3	B	2001	PBU	P5-O5	4.12	1.66	1.59
3	A	1101	PBU	P5-O5	4.05	1.66	1.59
3	A	1101	PBU	P4-O4	3.49	1.65	1.59
3	B	2001	PBU	P1-O1	2.88	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	PBU	C1'-C2'	2.76	1.59	1.50
4	A	1102	PO4	P-O1	2.58	1.56	1.50
3	B	2001	PBU	C5-C4	2.27	1.56	1.52
3	A	1101	PBU	C3'-C2'	2.26	1.57	1.50
3	B	2001	PBU	C3-C4	2.24	1.58	1.52
3	B	2001	PBU	P1-OP1	2.04	1.67	1.59
3	B	2001	PBU	P4-O41	2.00	1.56	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	PBU	O2'-C7-C8	5.44	123.26	111.48
3	A	1101	PBU	O1'-C11-C12	4.04	124.17	111.83
3	A	1101	PBU	O1-C1-C6	-4.03	100.19	108.73
3	B	2001	PBU	O2'-C7-C8	3.97	120.06	111.48
3	B	2001	PBU	O5-C5-C4	3.77	116.77	108.76
3	A	1101	PBU	O1'-C1'-C2'	3.40	118.21	108.40
3	A	1101	PBU	O5-C5-C4	3.06	115.27	108.76
3	A	1101	PBU	C6-C5-C4	-2.89	105.21	111.72
3	B	2001	PBU	C2-C3-C4	2.89	116.24	109.68
3	A	1101	PBU	O2'-C7-O7	-2.73	117.33	123.70
3	B	2001	PBU	O2'-C7-O7	-2.59	117.65	123.70
3	B	2001	PBU	O1'-C1'-C2'	2.39	115.30	108.40
3	A	1101	PBU	C3-C2-C1	2.38	115.08	109.68
3	B	2001	PBU	O1-C1-C6	2.36	113.74	108.73
3	A	1101	PBU	O53-P5-O52	2.31	116.47	107.80
3	B	2001	PBU	C1'-O1'-C11	2.30	125.53	117.12
3	B	2001	PBU	O53-P5-O52	2.27	116.32	107.80
3	A	1101	PBU	O1'-C11-O11	-2.23	118.05	123.63
3	B	2001	PBU	O1'-C11-C12	2.23	118.63	111.83
3	A	1101	PBU	O4-C4-C5	2.18	113.39	108.76
3	A	1101	PBU	C6-C1-C2	2.08	113.75	110.86

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	PBU	C1-O1-P1-OP1
3	A	1101	PBU	C2-C1-O1-P1
3	A	1101	PBU	C6-C1-O1-P1
3	B	2001	PBU	C1-O1-P1-OP1
3	B	2001	PBU	C1-O1-P1-OP2

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Mol	Chain	Res	Type	Atoms
3	B	2001	PBU	C3'-OP1-P1-OP2
3	B	2001	PBU	C8-C7-O2'-C2'
3	B	2001	PBU	O7-C7-O2'-C2'
3	A	1101	PBU	C8-C7-O2'-C2'
3	A	1101	PBU	O7-C7-O2'-C2'
3	B	2001	PBU	C5-O5-P5-O51
3	B	2001	PBU	C11-C12-C13-C14
3	A	1101	PBU	C7-C8-C9-C10
3	B	2001	PBU	C2'-C3'-OP1-P1
3	B	2001	PBU	C6-C1-O1-P1
3	A	1101	PBU	C1-O1-P1-OP3
3	B	2001	PBU	C1-O1-P1-OP3
3	B	2001	PBU	C4-O4-P4-O43
3	B	2001	PBU	C5-O5-P5-O52
3	B	2001	PBU	O1'-C11-C12-C13
3	A	1101	PBU	C4-O4-P4-O41
3	B	2001	PBU	O11-C11-C12-C13

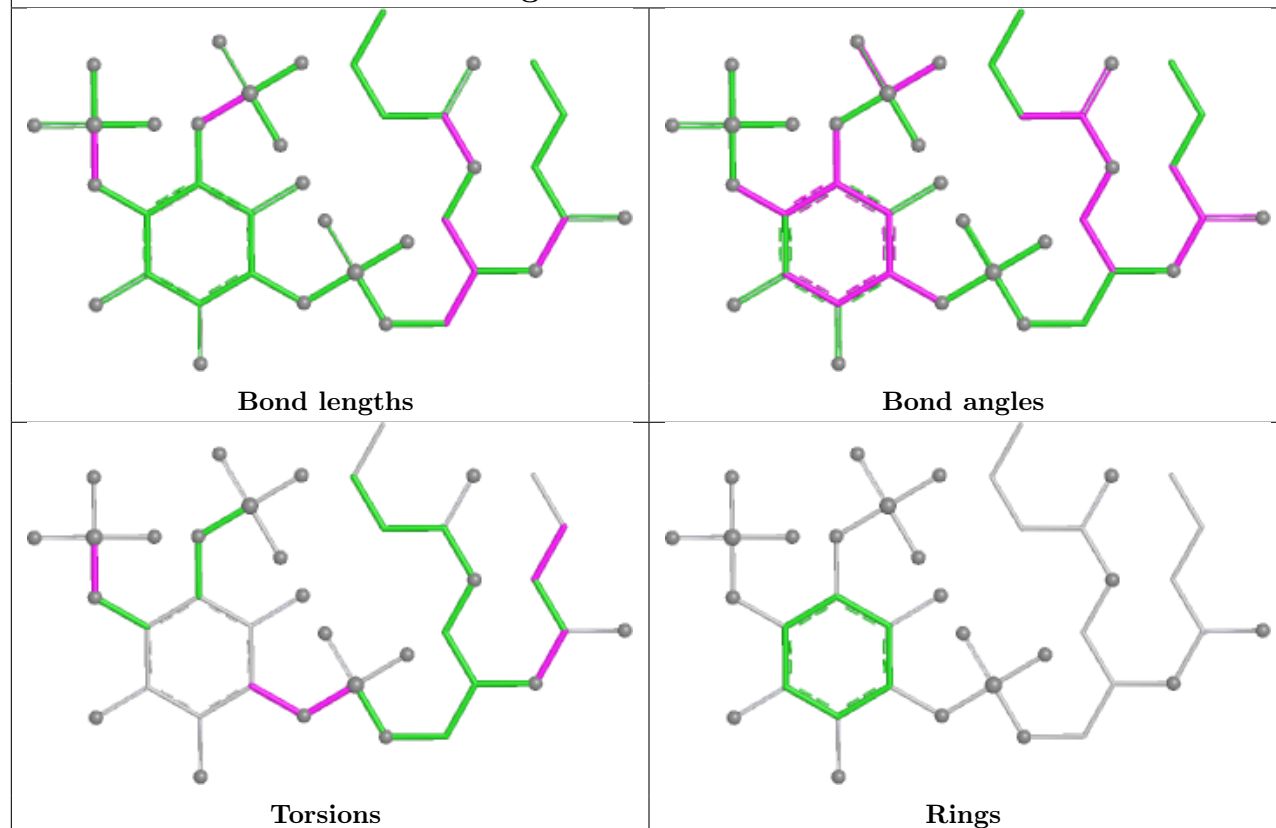
There are no ring outliers.

1 monomer is involved in 1 short contact:

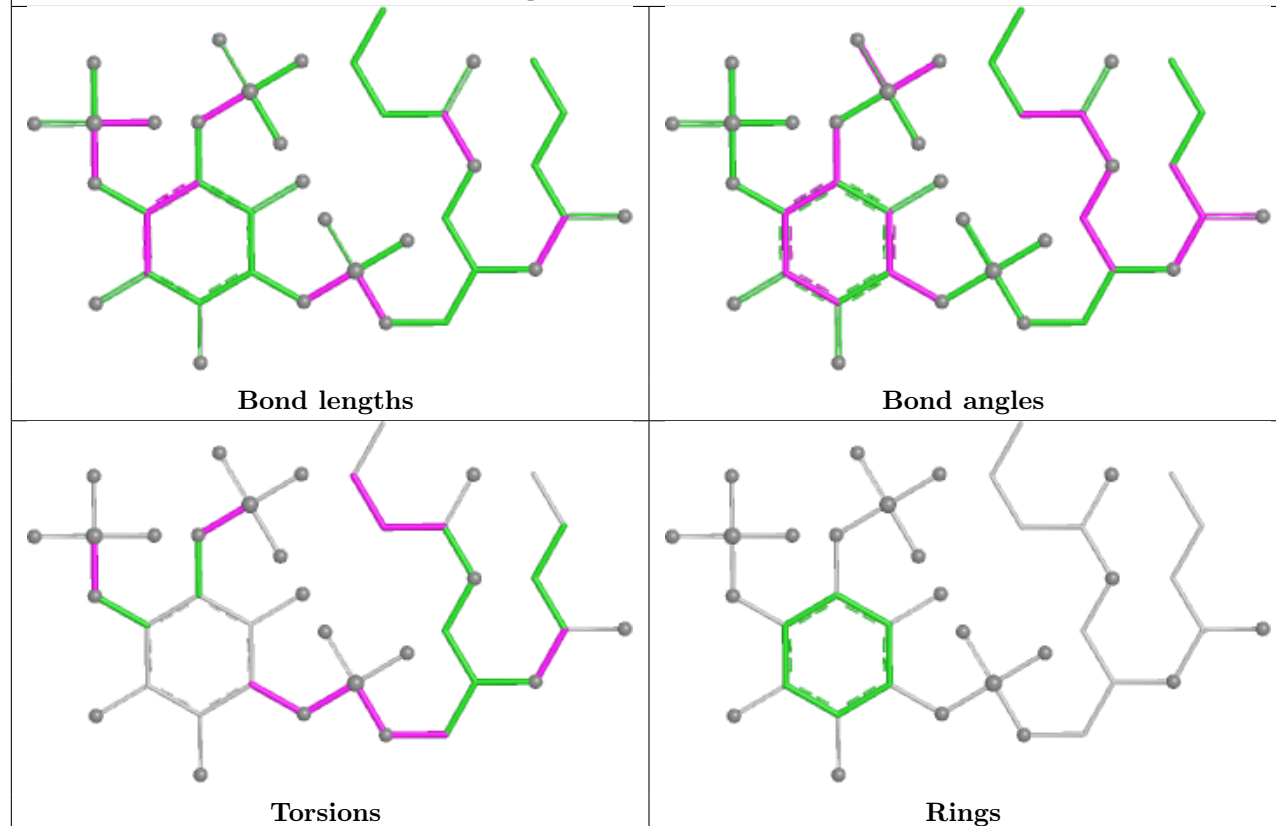
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	PBU	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

Ligand PBU A 1101



Ligand PBU B 2001



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	1042/1096 (95%)	-0.39	3 (0%)	90 76	66, 83, 107, 127	0
2	B	241/279 (86%)	0.05	2 (0%)	82 60	108, 130, 154, 163	0
All	All	1283/1375 (93%)	-0.30	5 (0%)	88 72	66, 87, 139, 163	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	335	TRP	2.6
2	B	588	GLY	2.5
1	A	301	CYS	2.4
1	A	322	THR	2.3
1	A	947	TYR	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](#)

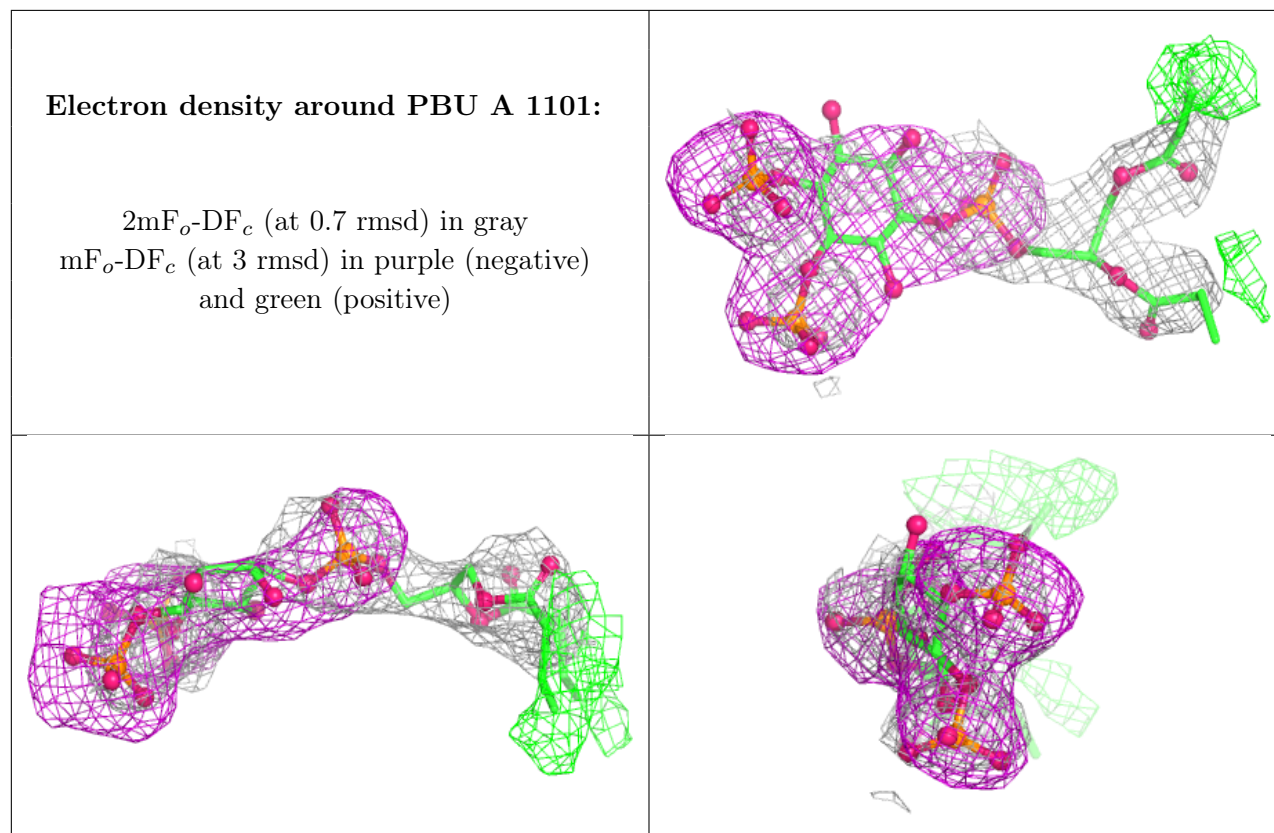
There are no oligosaccharides in this entry.

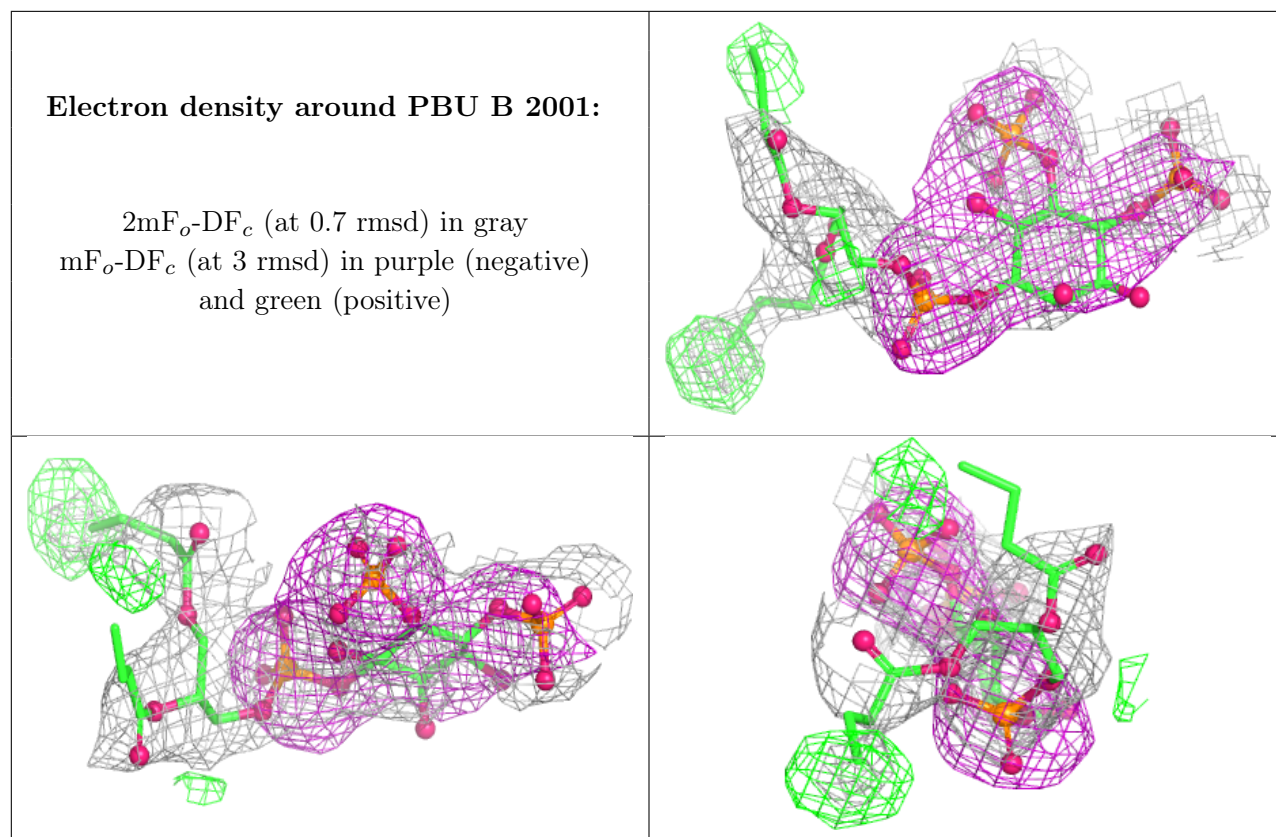
6.4 Ligands [i](#)

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
3	PBU	A	1101	39/39	0.26	0.20	111,115,121,124	0
3	PBU	B	2001	39/39	0.50	0.18	109,113,117,118	0
4	PO4	A	1102	5/5	0.80	0.14	90,90,90,90	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 [i](#)

There are no such residues in this entry.