



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:25 PM UTC

PDB ID : 6NCT / pdb_00006nct
Title : Structure of p110alpha/niSH2 - vector data collection
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Deposited on : 2018-12-12
Resolution : 3.35 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
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

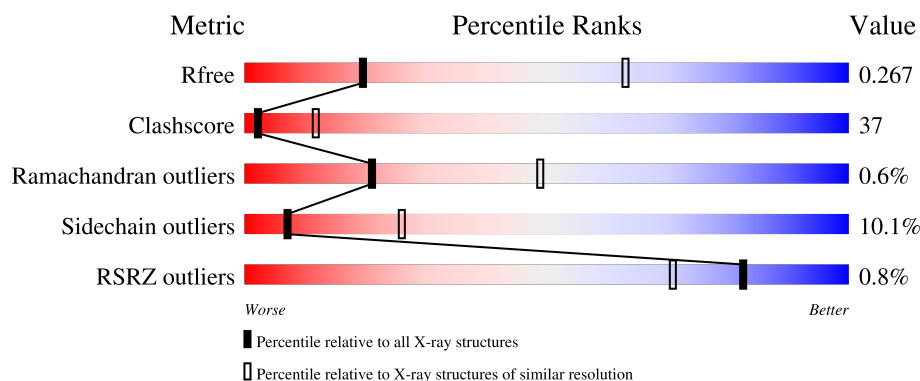
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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 4 unique types of molecules in this entry. The entry contains 10493 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	1039	Total	C	N	O	S	0	0	0
			8504	5440	1452	1543	69			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	expression tag	UNP P42336
A	-26	SER	-	expression tag	UNP P42336
A	-25	TYR	-	expression tag	UNP P42336
A	-24	TYR	-	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	HIS	-	expression tag	UNP P42336
A	-17	ASP	-	expression tag	UNP P42336
A	-16	TYR	-	expression tag	UNP P42336
A	-15	ASP	-	expression tag	UNP P42336
A	-14	ILE	-	expression tag	UNP P42336
A	-13	PRO	-	expression tag	UNP P42336
A	-12	THR	-	expression tag	UNP P42336
A	-11	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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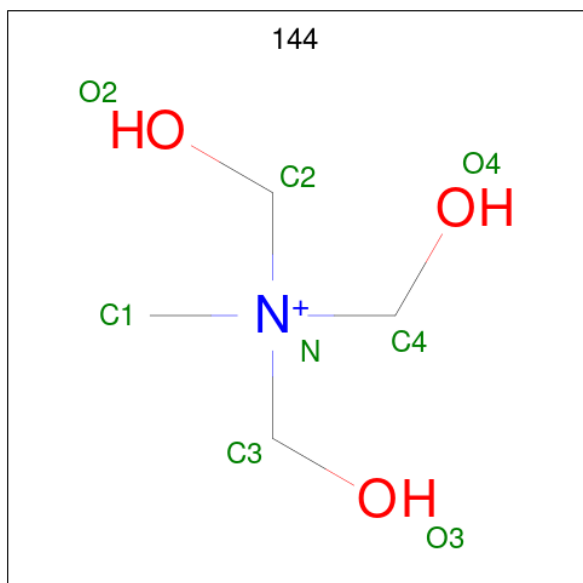
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

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

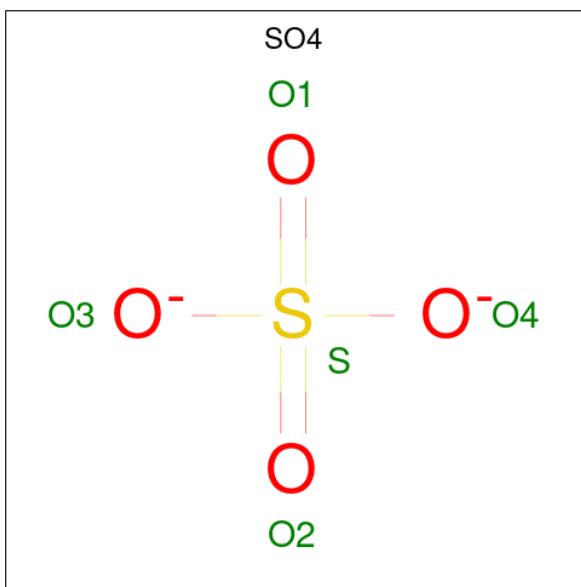
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	225	Total	C	N	O	S	0	0	0
			1958	1233	343	376	6			

- Molecule 3 is TRIS-HYDROXYMETHYL-METHYL-AMMONIUM (CCD ID: 144) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

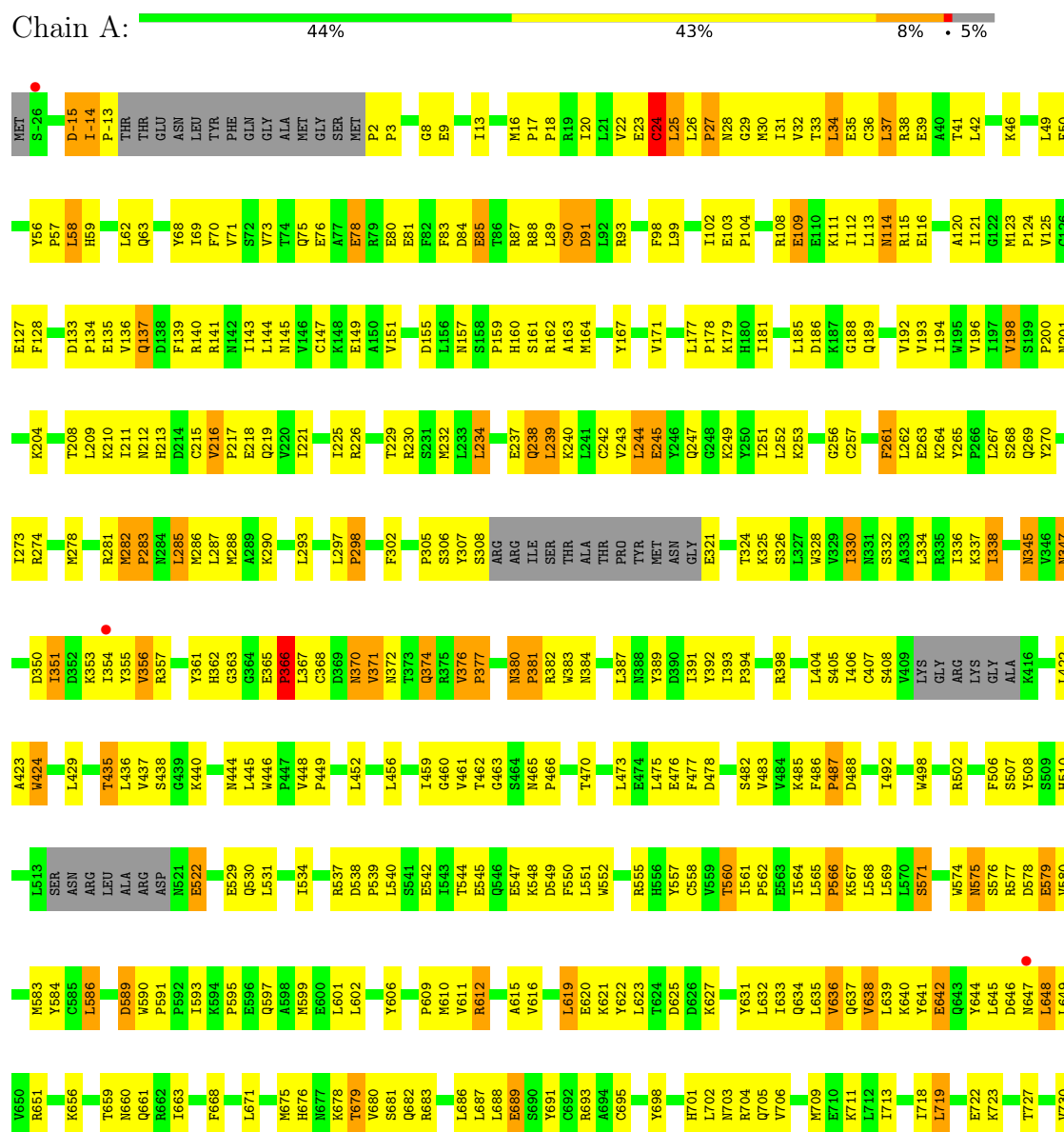


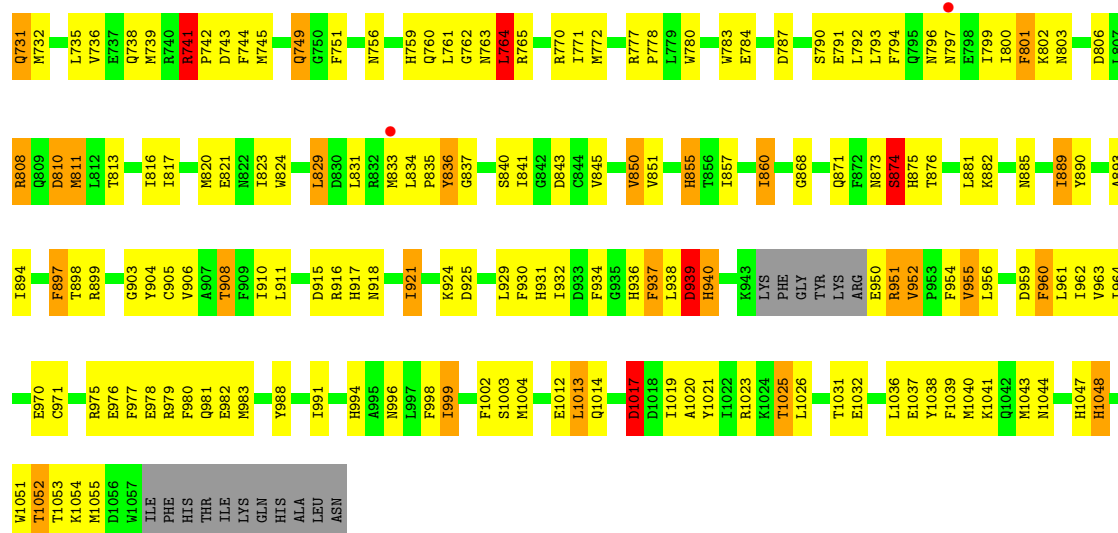
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

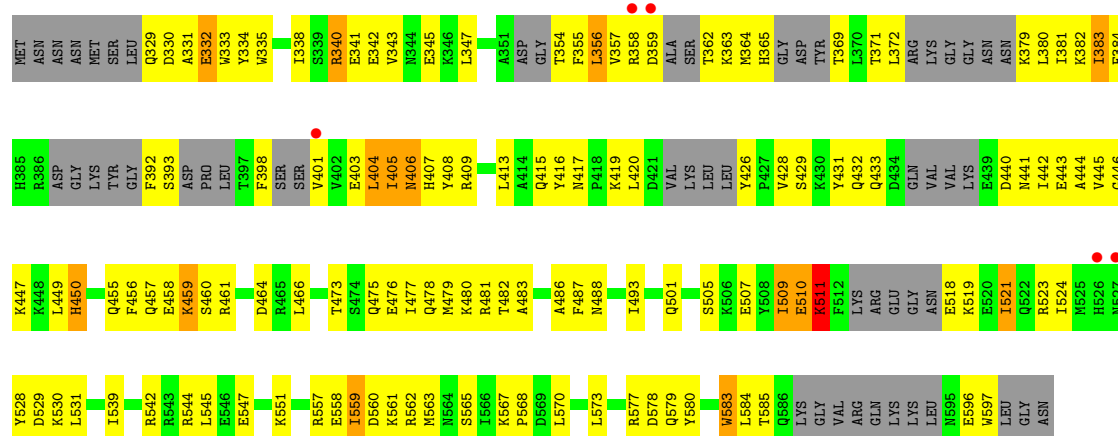
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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





● Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.36Å 117.72Å 151.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.54 – 3.35 49.54 – 3.35	Depositor EDS
% Data completeness (in resolution range)	96.4 (49.54-3.35) 96.4 (49.54-3.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.199 , 0.271 0.213 , 0.267	Depositor DCC
R_{free} test set	1462 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	113.1	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 124.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10493	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 144

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	1.18	18/8703 (0.2%)	1.62	85/11766 (0.7%)
2	B	1.02	0/1984	1.65	10/2645 (0.4%)
All	All	1.15	18/10687 (0.2%)	1.63	95/14411 (0.7%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	741	ARG	C-N	10.43	1.49	1.33
1	A	679	THR	C-O	6.86	1.31	1.24
1	A	633	ILE	C-O	-6.04	1.17	1.24
1	A	245	GLU	C-O	-5.95	1.17	1.24
1	A	283	PRO	C-O	-5.54	1.16	1.23
1	A	739	MET	C-O	-5.35	1.17	1.24
1	A	840	SER	CA-CB	-5.31	1.46	1.53
1	A	760	GLN	C-O	-5.29	1.17	1.23
1	A	718	ILE	C-O	-5.26	1.18	1.24
1	A	719	LEU	C-O	-5.15	1.18	1.24
1	A	689	GLU	C-O	-5.14	1.18	1.24
1	A	345	ASN	C-O	5.12	1.29	1.24
1	A	803	ASN	C-O	-5.11	1.18	1.24
1	A	78	GLU	C-O	-5.10	1.17	1.23
1	A	595	PRO	C-O	-5.08	1.17	1.24
1	A	745	MET	C-O	-5.06	1.18	1.24
1	A	566	PRO	C-O	-5.02	1.18	1.24
1	A	764	LEU	C-O	-5.00	1.17	1.23

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	741	ARG	CA-C-N	12.00	133.00	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	741	ARG	C-N-CA	12.00	133.00	119.32
1	A	-15	ASP	CA-C-N	8.07	125.32	120.24
1	A	-15	ASP	C-N-CA	8.07	125.32	120.24
1	A	463	GLY	CA-C-O	-7.89	116.61	122.37
1	A	647	ASN	CA-CB-CG	-7.59	105.01	112.60
1	A	380	ASN	CB-CA-C	7.54	116.56	111.20
1	A	940	HIS	CA-C-N	7.22	130.27	120.38
1	A	940	HIS	C-N-CA	7.22	130.27	120.38
2	B	482	THR	CA-CB-OG1	-6.96	99.15	109.60
1	A	1048	HIS	CB-CA-C	6.68	116.44	109.83
1	A	635	LEU	CA-C-O	-6.64	113.51	120.55
1	A	836	TYR	N-CA-C	-6.60	101.64	110.55
1	A	27	PRO	CA-C-N	6.58	129.76	120.28
1	A	27	PRO	C-N-CA	6.58	129.76	120.28
1	A	487	PRO	CB-CA-C	-6.57	102.82	111.23
1	A	282	MET	CA-C-O	6.50	124.13	119.32
1	A	801	PHE	CA-C-O	-6.40	113.51	120.36
1	A	939	ASP	CA-CB-CG	6.39	119.00	112.60
1	A	751	PHE	CA-C-O	-6.19	114.66	121.28
1	A	936	HIS	CA-C-O	-6.17	114.25	121.16
1	A	749	GLN	CB-CG-CD	6.01	122.81	112.60
1	A	575	ASN	CA-C-O	-5.98	114.54	120.82
1	A	784	GLU	CB-CG-CD	5.94	122.69	112.60
1	A	744	PHE	CA-C-O	-5.93	114.21	120.55
1	A	237	GLU	CB-CG-CD	5.91	122.64	112.60
2	B	510	GLU	N-CA-C	-5.88	107.09	114.56
1	A	238	GLN	N-CA-C	-5.86	104.80	111.07
1	A	363	GLY	CA-C-N	5.82	128.44	122.80
1	A	363	GLY	C-N-CA	5.82	128.44	122.80
1	A	200	PRO	N-CA-C	-5.81	107.09	114.35
1	A	1017	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	566	PRO	CB-CA-C	-5.73	103.95	112.55
1	A	583	MET	CA-C-O	-5.67	114.86	120.82
1	A	837	GLY	CA-C-O	-5.63	116.51	121.58
1	A	78	GLU	CB-CG-CD	5.61	122.14	112.60
1	A	960	PHE	N-CA-C	-5.59	105.27	111.36
1	A	749	GLN	CA-C-O	-5.58	114.95	120.70
2	B	511	LYS	N-CA-C	5.57	118.54	111.69
1	A	13	ILE	N-CA-CB	-5.56	104.66	111.00
1	A	229	THR	CA-CB-OG1	-5.54	101.30	109.60
1	A	642	GLU	CB-CG-CD	5.54	122.01	112.60
1	A	136	VAL	N-CA-C	-5.53	105.12	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	GLN	N-CA-C	-5.51	105.27	111.28
1	A	579	GLU	N-CA-C	-5.51	105.18	111.07
1	A	488	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	381	PRO	CA-C-O	-5.44	115.41	121.23
1	A	109	GLU	N-CA-C	-5.43	105.26	111.07
1	A	560	THR	CA-CB-OG1	-5.41	101.48	109.60
1	A	889	ILE	N-CA-C	-5.41	105.23	110.42
1	A	114	ASN	N-CA-C	-5.41	105.99	112.59
2	B	560	ASP	N-CA-C	-5.39	105.30	111.07
1	A	529	GLU	N-CA-C	-5.37	106.32	112.92
2	B	363	LYS	CA-C-N	5.36	127.46	120.28
2	B	363	LYS	C-N-CA	5.36	127.46	120.28
1	A	370	ASN	CA-CB-CG	-5.35	107.25	112.60
1	A	208	THR	CA-CB-OG1	-5.35	101.58	109.60
1	A	810	ASP	N-CA-C	-5.35	105.35	111.07
1	A	636	VAL	N-CA-CB	5.33	117.79	110.54
1	A	897	PHE	N-CA-C	-5.32	105.38	111.07
1	A	567	LYS	N-CA-C	-5.32	105.59	111.71
1	A	24	CYS	CB-CA-C	5.31	119.09	110.22
1	A	365	GLU	CA-C-N	5.31	126.48	119.84
1	A	365	GLU	C-N-CA	5.31	126.48	119.84
1	A	620	GLU	N-CA-C	-5.28	105.42	111.07
1	A	656	LYS	N-CA-C	-5.28	105.53	111.28
1	A	578	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	185	LEU	CA-C-O	-5.26	115.73	121.89
2	B	331	ALA	CA-C-N	5.25	131.57	121.54
2	B	331	ALA	C-N-CA	5.25	131.57	121.54
2	B	340	ARG	CB-CA-C	-5.20	102.72	110.88
1	A	73	VAL	CA-C-O	-5.20	114.93	121.11
2	B	539	ILE	N-CA-C	-5.19	105.33	110.62
1	A	744	PHE	CA-CB-CG	-5.17	108.63	113.80
1	A	91	ASP	N-CA-C	-5.16	106.58	112.92
1	A	102	ILE	CA-C-O	-5.14	116.54	121.63
1	A	487	PRO	CA-C-O	-5.14	115.60	121.56
1	A	998	PHE	CA-C-O	-5.12	115.44	120.82
1	A	424	TRP	CA-C-O	-5.11	115.81	121.33
1	A	925	ASP	N-CA-C	-5.10	105.72	111.28
1	A	612	ARG	CB-CA-C	-5.09	102.66	110.81
1	A	682	GLN	CA-C-O	-5.09	115.11	120.55
1	A	868	GLY	CA-C-N	5.08	129.36	122.19
1	A	868	GLY	C-N-CA	5.08	129.36	122.19
1	A	937	PHE	CA-C-N	-5.08	116.22	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	937	PHE	C-N-CA	-5.08	116.22	123.03
1	A	366	PRO	CA-N-CD	-5.06	104.91	112.00
1	A	836	TYR	CA-C-O	-5.06	115.84	121.81
1	A	749	GLN	N-CA-C	-5.04	105.70	111.14
1	A	625	ASP	N-CA-C	-5.03	105.79	111.28
1	A	816	ILE	N-CA-C	-5.03	105.59	110.42
1	A	578	ASP	CB-CA-C	-5.03	102.76	110.81
1	A	208	THR	CA-C-O	-5.02	115.93	120.95
1	A	347	ASN	CA-C-N	5.02	126.88	120.56
1	A	347	ASN	C-N-CA	5.02	126.88	120.56

There are no chirality outliers.

There are no planarity outliers.

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	8504	0	8471	602	0
2	B	1958	0	1908	186	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
4	A	15	0	0	0	0
All	All	10493	0	10403	766	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 37.

All (766) 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:602:LEU:HA	1:A:612:ARG:NH1	1.46	1.25
1:A:764:LEU:HD12	1:A:783:TRP:CD1	1.75	1.20
1:A:761:LEU:HD21	1:A:797:ASN:ND2	1.63	1.14
1:A:761:LEU:CD2	1:A:797:ASN:HD22	1.61	1.12
2:B:379:LYS:CE	2:B:419:LYS:HE2	1.79	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:MET:HE1	1:A:89:LEU:HD22	1.29	1.09
2:B:379:LYS:HZ1	2:B:419:LYS:HE3	1.17	1.08
1:A:988:TYR:CD2	1:A:1039:PHE:CD2	2.44	1.06
1:A:772:MET:HE2	1:A:772:MET:HA	1.36	1.06
1:A:761:LEU:HD21	1:A:797:ASN:HD22	0.89	1.06
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.35	1.05
1:A:910:ILE:HA	1:A:1025:THR:HG21	1.39	1.04
1:A:645:LEU:CD2	1:A:683:ARG:HG2	1.87	1.04
1:A:764:LEU:CD1	1:A:783:TRP:NE1	2.21	1.03
2:B:379:LYS:NZ	2:B:419:LYS:CE	2.24	0.99
1:A:988:TYR:CE2	1:A:1039:PHE:CD2	2.50	0.98
1:A:16:MET:SD	1:A:90:CYS:HB3	2.04	0.97
1:A:988:TYR:CE2	1:A:1039:PHE:HD2	1.82	0.97
1:A:108:ARG:O	1:A:112:ILE:HG12	1.64	0.96
1:A:24:CYS:SG	1:A:49:LEU:HD13	2.06	0.96
2:B:379:LYS:HE2	2:B:419:LYS:HE2	1.48	0.95
2:B:358:ARG:HG2	2:B:359:ASP:H	1.31	0.95
2:B:431:TYR:CE1	2:B:433:GLN:HB2	2.02	0.94
1:A:57:PRO:HB3	2:B:524:ILE:CD1	1.96	0.94
2:B:501:GLN:OE1	2:B:528:TYR:HD1	1.48	0.94
1:A:2:PRO:HG2	1:A:3:PRO:HD2	1.50	0.93
1:A:610:MET:HE2	1:A:610:MET:HA	1.50	0.91
1:A:834:LEU:HD22	1:A:924:LYS:CE	2.01	0.91
2:B:379:LYS:NZ	2:B:419:LYS:HE3	1.85	0.90
2:B:379:LYS:CE	2:B:419:LYS:CE	2.50	0.90
1:A:408:SER:HB3	1:A:422:LEU:HD11	1.54	0.90
1:A:602:LEU:HA	1:A:612:ARG:HH11	1.12	0.89
1:A:353:LYS:HA	1:A:377:PRO:HB3	1.55	0.89
2:B:511:LYS:N	2:B:511:LYS:HE2	1.87	0.89
1:A:764:LEU:HD12	1:A:783:TRP:NE1	1.84	0.88
2:B:519:LYS:HB3	2:B:523:ARG:HH12	1.38	0.88
2:B:379:LYS:NZ	2:B:419:LYS:HE2	1.88	0.88
1:A:764:LEU:CD1	1:A:783:TRP:CD1	2.56	0.87
2:B:379:LYS:HE2	2:B:419:LYS:CE	2.03	0.87
1:A:988:TYR:CD2	1:A:1039:PHE:CE2	2.62	0.87
1:A:351:ILE:HG21	1:A:408:SER:HB2	1.57	0.87
1:A:885:ASN:ND2	1:A:893:ALA:CB	2.38	0.86
1:A:1043:MET:SD	1:A:1047:HIS:HE1	1.99	0.86
2:B:343:VAL:CG1	2:B:356:LEU:HD11	2.04	0.86
1:A:910:ILE:HA	1:A:1025:THR:CG2	2.06	0.86
1:A:24:CYS:SG	1:A:49:LEU:CD1	2.64	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:PHE:CD1	1:A:487:PRO:HD2	2.11	0.85
1:A:540:LEU:HD11	1:A:1019:ILE:HG22	1.58	0.85
2:B:333:TRP:HA	2:B:429:SER:OG	1.77	0.84
1:A:30:MET:SD	1:A:57:PRO:O	2.35	0.84
1:A:709:MET:O	1:A:713:ILE:HG13	1.77	0.83
2:B:563:MET:O	2:B:567:LYS:HB2	1.78	0.83
2:B:413:LEU:HG	2:B:420:LEU:CD1	2.08	0.82
2:B:333:TRP:HH2	2:B:405:ILE:HG13	1.42	0.82
1:A:2:PRO:CG	1:A:3:PRO:HD2	2.10	0.82
1:A:128:PHE:HB3	1:A:140:ARG:NH1	1.93	0.82
2:B:511:LYS:HG2	2:B:518:GLU:N	1.95	0.81
2:B:392:PHE:CE1	2:B:416:TYR:CD2	2.68	0.81
1:A:648:LEU:H	1:A:648:LEU:HD12	1.43	0.81
1:A:59:HIS:O	1:A:62:LEU:HG	1.81	0.81
1:A:602:LEU:HA	1:A:612:ARG:HH12	1.43	0.81
1:A:904:TYR:CD1	1:A:931:HIS:HD2	1.99	0.80
1:A:251:ILE:HG21	1:A:262:LEU:CD2	2.11	0.80
2:B:343:VAL:HG13	2:B:356:LEU:HD11	1.61	0.80
1:A:602:LEU:CA	1:A:612:ARG:NH1	2.39	0.79
1:A:209:LEU:HD12	1:A:209:LEU:C	2.08	0.79
2:B:333:TRP:CH2	2:B:405:ILE:HG13	2.17	0.79
1:A:57:PRO:HB3	2:B:524:ILE:HD11	1.65	0.79
2:B:333:TRP:CZ2	2:B:405:ILE:HG21	2.17	0.78
2:B:330:ASP:O	2:B:334:TYR:HB3	1.84	0.78
1:A:128:PHE:HB3	1:A:140:ARG:HH11	1.49	0.78
1:A:328:TRP:CE2	1:A:577:ARG:HD2	2.18	0.78
1:A:702:LEU:O	1:A:706:VAL:HG23	1.84	0.78
1:A:538:ASP:HA	1:A:996:ASN:HD21	1.48	0.77
1:A:24:CYS:SG	1:A:49:LEU:HD22	2.23	0.77
1:A:885:ASN:HD22	1:A:893:ALA:CB	1.96	0.77
2:B:356:LEU:HD13	2:B:356:LEU:C	2.09	0.77
1:A:545:GLU:OE2	2:B:379:LYS:HB3	1.84	0.77
1:A:167:TYR:HE1	1:A:297:LEU:HD21	1.51	0.76
1:A:367:LEU:HD22	1:A:391:ILE:CG2	2.16	0.76
1:A:135:GLU:OE1	1:A:644:TYR:HB3	1.86	0.76
1:A:851:VAL:HG11	1:A:924:LYS:HZ3	1.51	0.76
1:A:164:MET:HE1	1:A:263:GLU:HB2	1.66	0.75
1:A:764:LEU:HD13	1:A:783:TRP:NE1	2.00	0.75
1:A:823:ILE:HD13	1:A:994:HIS:CG	2.21	0.75
2:B:431:TYR:HE1	2:B:433:GLN:HB2	1.49	0.75
1:A:506:PHE:HB3	1:A:508:TYR:HE1	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:413:LEU:HG	2:B:420:LEU:CB	2.16	0.75
1:A:905:CYS:SG	1:A:1043:MET:HE1	2.26	0.74
1:A:841:ILE:HD12	1:A:841:ILE:O	1.88	0.73
1:A:602:LEU:HD22	1:A:612:ARG:CD	2.18	0.73
1:A:2:PRO:HB2	1:A:3:PRO:CD	2.17	0.73
1:A:590:TRP:CD1	1:A:591:PRO:HD2	2.22	0.73
1:A:508:TYR:CE2	1:A:510:HIS:CD2	2.77	0.73
2:B:521:ILE:HD13	2:B:521:ILE:H	1.52	0.73
1:A:645:LEU:HD21	1:A:683:ARG:HG2	1.69	0.73
1:A:834:LEU:CD2	1:A:924:LYS:CE	2.66	0.73
1:A:959:ASP:O	1:A:962:ILE:HG12	1.89	0.73
1:A:285:LEU:N	1:A:285:LEU:HD23	2.04	0.72
1:A:24:CYS:SG	1:A:49:LEU:CD2	2.77	0.72
1:A:540:LEU:HD11	1:A:1019:ILE:CG2	2.18	0.72
1:A:874:SER:HB3	1:A:959:ASP:OD1	1.89	0.72
1:A:545:GLU:HA	1:A:548:LYS:HD2	1.70	0.72
2:B:343:VAL:HG12	2:B:347:LEU:HD12	1.71	0.72
1:A:57:PRO:HB3	2:B:524:ILE:HD13	1.72	0.71
1:A:440:LYS:HA	1:A:475:LEU:O	1.89	0.71
1:A:35:GLU:O	1:A:35:GLU:HG3	1.91	0.71
1:A:539:PRO:HD3	1:A:996:ASN:HD22	1.56	0.71
1:A:834:LEU:HD22	1:A:924:LYS:HE2	1.71	0.71
1:A:904:TYR:CG	1:A:931:HIS:HD2	2.09	0.71
1:A:351:ILE:CD1	1:A:408:SER:OG	2.39	0.70
1:A:851:VAL:HG11	1:A:924:LYS:NZ	2.06	0.70
1:A:57:PRO:CG	2:B:524:ILE:HG12	2.22	0.70
1:A:1052:THR:OG1	1:A:1053:THR:HG23	1.91	0.70
2:B:358:ARG:HG2	2:B:359:ASP:N	2.04	0.70
1:A:29:GLY:HA3	2:B:501:GLN:HB2	1.73	0.70
1:A:508:TYR:CD2	1:A:510:HIS:HD2	2.10	0.70
1:A:89:LEU:C	1:A:89:LEU:HD23	2.17	0.70
2:B:457:GLN:O	2:B:461:ARG:HG3	1.92	0.70
1:A:719:LEU:HA	1:A:723:LYS:HB2	1.74	0.69
2:B:338:ILE:HB	2:B:342:GLU:CD	2.16	0.69
1:A:336:ILE:HD12	1:A:389:TYR:CZ	2.27	0.69
1:A:823:ILE:HD13	1:A:994:HIS:CD2	2.28	0.69
2:B:333:TRP:CH2	2:B:405:ILE:HG21	2.26	0.69
1:A:749:GLN:O	1:A:762:GLY:HA2	1.93	0.69
2:B:404:LEU:O	2:B:404:LEU:HD12	1.94	0.68
2:B:501:GLN:CD	2:B:528:TYR:HD1	2.01	0.68
1:A:178:PRO:HG2	1:A:181:ILE:HD12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ASP:HA	1:A:996:ASN:ND2	2.07	0.68
1:A:437:VAL:HG13	1:A:477:PHE:CD2	2.29	0.68
2:B:443:GLU:O	2:B:447:LYS:N	2.24	0.68
1:A:885:ASN:ND2	1:A:893:ALA:HB2	2.08	0.68
1:A:929:LEU:C	1:A:929:LEU:HD23	2.19	0.68
1:A:334:LEU:HA	1:A:393:ILE:HD11	1.75	0.67
1:A:910:ILE:CA	1:A:1025:THR:HG21	2.18	0.67
1:A:16:MET:CE	1:A:89:LEU:HD22	2.16	0.67
1:A:68:TYR:HB3	1:A:103:GLU:CG	2.25	0.67
2:B:456:PHE:CE1	2:B:460:SER:HB3	2.28	0.67
1:A:120:ALA:HB2	1:A:703:ASN:OD1	1.95	0.67
1:A:121:ILE:HD11	1:A:689:GLU:HA	1.76	0.67
1:A:2:PRO:CB	1:A:3:PRO:CD	2.72	0.67
1:A:610:MET:HE2	1:A:610:MET:CA	2.22	0.67
1:A:508:TYR:CD2	1:A:510:HIS:CD2	2.83	0.67
1:A:836:TYR:CE1	1:A:932:ILE:HG22	2.30	0.67
2:B:358:ARG:CG	2:B:359:ASP:H	2.08	0.67
2:B:392:PHE:HE1	2:B:416:TYR:CD2	2.12	0.67
1:A:2:PRO:HB2	1:A:3:PRO:HD3	1.76	0.67
1:A:436:LEU:C	1:A:436:LEU:HD13	2.20	0.67
2:B:413:LEU:HG	2:B:420:LEU:HB3	1.76	0.67
1:A:772:MET:HE2	1:A:772:MET:CA	2.21	0.66
1:A:791:GLU:OE1	1:A:791:GLU:N	2.24	0.66
1:A:602:LEU:HD22	1:A:612:ARG:HD3	1.78	0.66
1:A:602:LEU:O	1:A:638:VAL:HG22	1.96	0.66
2:B:558:GLU:OE2	2:B:562:ARG:HG3	1.96	0.66
2:B:510:GLU:HB2	2:B:511:LYS:NZ	2.10	0.66
1:A:218:GLU:HB2	1:A:264:LYS:HE2	1.77	0.66
1:A:534:ILE:HA	1:A:537:ARG:CD	2.25	0.66
1:A:1025:THR:HG22	1:A:1026:LEU:HD23	1.78	0.66
1:A:351:ILE:HG12	1:A:408:SER:OG	1.96	0.66
1:A:177:LEU:CD2	1:A:274:ARG:CZ	2.73	0.66
2:B:501:GLN:OE1	2:B:528:TYR:CD1	2.40	0.65
1:A:251:ILE:HG21	1:A:262:LEU:HD21	1.78	0.65
2:B:507:GLU:O	2:B:507:GLU:HG2	1.95	0.65
1:A:506:PHE:HB3	1:A:508:TYR:CE1	2.31	0.65
1:A:16:MET:HG3	1:A:38:ARG:HG3	1.77	0.65
1:A:834:LEU:CD2	1:A:924:LYS:NZ	2.59	0.65
1:A:885:ASN:HB3	1:A:889:ILE:HG22	1.78	0.65
1:A:16:MET:SD	1:A:90:CYS:CB	2.83	0.65
1:A:671:LEU:HB2	1:A:688:LEU:HD21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:TRP:HA	2:B:429:SER:CB	2.27	0.65
2:B:483:ALA:O	2:B:486:ALA:HB3	1.97	0.65
1:A:139:PHE:CD2	1:A:645:LEU:HB3	2.32	0.65
1:A:263:GLU:HG2	1:A:265:TYR:CE2	2.32	0.64
1:A:32:VAL:HG23	1:A:56:TYR:CE2	2.32	0.64
1:A:885:ASN:ND2	1:A:893:ALA:HB1	2.10	0.64
1:A:345:ASN:HD22	2:B:557:ARG:HG2	1.63	0.64
2:B:413:LEU:CG	2:B:420:LEU:HB3	2.28	0.64
1:A:245:GLU:O	1:A:249:LYS:HE3	1.97	0.64
1:A:904:TYR:CG	1:A:931:HIS:CD2	2.85	0.64
1:A:337:LYS:HB3	1:A:476:GLU:HB3	1.80	0.64
1:A:405:SER:HB2	1:A:423:ALA:O	1.97	0.64
1:A:602:LEU:HD22	1:A:612:ARG:HD2	1.80	0.64
1:A:57:PRO:HG3	2:B:524:ILE:HG12	1.81	0.63
1:A:367:LEU:HD22	1:A:391:ILE:HG21	1.79	0.63
1:A:584:TYR:CD2	1:A:610:MET:HG3	2.34	0.63
1:A:873:ASN:O	1:A:876:THR:HG23	1.98	0.63
1:A:988:TYR:HD2	1:A:1039:PHE:CE2	2.13	0.63
1:A:793:LEU:HG	1:A:794:PHE:CD2	2.33	0.63
1:A:561:ILE:O	1:A:564:ILE:HG22	1.99	0.62
1:A:908:THR:HG21	1:A:954:PHE:HB2	1.81	0.62
2:B:342:GLU:HA	2:B:345:GLU:HG2	1.81	0.62
1:A:39:GLU:H	1:A:39:GLU:CD	2.06	0.62
1:A:39:GLU:N	1:A:39:GLU:OE1	2.33	0.62
1:A:68:TYR:HB3	1:A:103:GLU:HG2	1.80	0.62
1:A:62:LEU:HD12	1:A:62:LEU:O	1.99	0.62
1:A:599:MET:HB3	1:A:1004:MET:CE	2.29	0.62
1:A:108:ARG:HD3	1:A:111:LYS:HD2	1.81	0.62
1:A:833:MET:O	1:A:835:PRO:HD3	1.98	0.62
1:A:851:VAL:CG1	1:A:924:LYS:NZ	2.62	0.62
1:A:610:MET:HA	1:A:610:MET:CE	2.24	0.62
1:A:834:LEU:CD2	1:A:924:LYS:HE2	2.29	0.62
2:B:413:LEU:HG	2:B:420:LEU:HD13	1.80	0.62
2:B:355:PHE:HD2	2:B:426:TYR:O	1.82	0.62
1:A:508:TYR:HE2	1:A:510:HIS:CD2	2.17	0.61
1:A:508:TYR:HD2	1:A:510:HIS:HD2	1.48	0.61
2:B:432:GLN:OE1	2:B:432:GLN:HA	1.99	0.61
1:A:140:ARG:O	1:A:144:LEU:HD11	1.99	0.61
1:A:904:TYR:HB3	1:A:931:HIS:NE2	2.16	0.61
1:A:599:MET:O	1:A:1004:MET:HE3	2.00	0.61
1:A:719:LEU:HD13	1:A:771:ILE:CD1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:ILE:HG23	1:A:1026:LEU:HD21	1.82	0.61
1:A:356:VAL:HB	1:A:372:ASN:HD21	1.65	0.61
1:A:177:LEU:HD11	1:A:268:SER:CB	2.30	0.61
2:B:347:LEU:CD1	2:B:371:THR:HG21	2.31	0.61
1:A:764:LEU:CD1	1:A:783:TRP:CE2	2.84	0.60
2:B:406:ASN:HA	2:B:409:ARG:HD3	1.81	0.60
1:A:139:PHE:HD2	1:A:645:LEU:HB3	1.66	0.60
1:A:217:PRO:HB3	1:A:252:LEU:HD12	1.82	0.60
2:B:441:ASN:OD1	2:B:444:ALA:HB2	2.01	0.60
1:A:962:ILE:HG13	1:A:963:VAL:N	2.16	0.60
1:A:542:GLU:HG2	2:B:340:ARG:HD3	1.82	0.60
1:A:764:LEU:HD12	1:A:783:TRP:CG	2.33	0.60
1:A:383:TRP:O	1:A:383:TRP:CD1	2.54	0.60
1:A:950:GLU:HG2	1:A:1038:TYR:OH	2.01	0.60
2:B:333:TRP:HE3	2:B:333:TRP:O	1.84	0.60
1:A:939:ASP:CG	1:A:939:ASP:O	2.44	0.60
1:A:46:LYS:HG2	1:A:50:PHE:CE2	2.35	0.60
2:B:473:THR:O	2:B:477:ILE:HG13	2.01	0.60
1:A:157:ASN:HB3	1:A:161:SER:HB2	1.83	0.60
1:A:698:TYR:CD1	1:A:701:HIS:HB2	2.37	0.60
1:A:143:ILE:HG13	1:A:143:ILE:O	2.01	0.60
1:A:189:GLN:HB3	1:A:210:LYS:HE3	1.83	0.60
2:B:343:VAL:HG11	2:B:356:LEU:HD11	1.80	0.60
2:B:567:LYS:HB3	2:B:568:PRO:HD3	1.84	0.59
1:A:128:PHE:CD1	1:A:686:LEU:HD21	2.37	0.59
1:A:338:ILE:HD13	1:A:338:ILE:N	2.18	0.59
2:B:559:ILE:HD13	2:B:559:ILE:N	2.17	0.59
1:A:345:ASN:ND2	2:B:557:ARG:HG2	2.17	0.59
1:A:602:LEU:O	1:A:638:VAL:CG2	2.51	0.59
1:A:904:TYR:CD1	1:A:931:HIS:CD2	2.87	0.59
2:B:392:PHE:CE1	2:B:416:TYR:CE2	2.90	0.59
1:A:78:GLU:HG3	1:A:124:PRO:HG3	1.84	0.59
1:A:192:VAL:HG13	1:A:283:PRO:HB2	1.85	0.59
1:A:144:LEU:HD21	1:A:305:PRO:HG3	1.84	0.59
1:A:668:PHE:CE2	1:A:702:LEU:HD22	2.38	0.59
1:A:764:LEU:HD13	1:A:783:TRP:HE1	1.66	0.59
1:A:961:LEU:HD22	1:A:977:PHE:HE2	1.68	0.59
1:A:632:LEU:HD12	1:A:632:LEU:O	2.02	0.59
1:A:84:ASP:HB3	1:A:87:ARG:HG3	1.85	0.58
2:B:510:GLU:C	2:B:511:LYS:HE2	2.28	0.58
1:A:698:TYR:O	1:A:701:HIS:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:LEU:HD13	1:A:771:ILE:HD11	1.83	0.58
2:B:519:LYS:HB3	2:B:523:ARG:NH1	2.16	0.58
1:A:263:GLU:CG	1:A:265:TYR:CE2	2.86	0.58
1:A:602:LEU:HD13	1:A:649:LEU:HD22	1.85	0.58
1:A:1043:MET:SD	1:A:1047:HIS:CE1	2.89	0.58
2:B:369:THR:HG23	2:B:382:LYS:HA	1.84	0.58
1:A:177:LEU:HD11	1:A:268:SER:HB2	1.85	0.58
1:A:534:ILE:HA	1:A:537:ARG:HD3	1.85	0.58
1:A:606:TYR:O	1:A:612:ARG:NH2	2.37	0.58
1:A:599:MET:HB3	1:A:1004:MET:HE1	1.84	0.58
1:A:709:MET:HE2	1:A:841:ILE:HG12	1.86	0.58
2:B:404:LEU:HD12	2:B:404:LEU:C	2.29	0.58
2:B:529:ASP:O	2:B:530:LYS:C	2.47	0.58
1:A:956:LEU:HD11	1:A:980:PHE:CZ	2.39	0.57
2:B:449:LEU:CD2	2:B:580:TYR:HB3	2.34	0.57
1:A:159:PRO:O	1:A:160:HIS:C	2.46	0.57
1:A:177:LEU:HD23	1:A:274:ARG:CZ	2.35	0.57
1:A:209:LEU:HD13	1:A:211:ILE:HG13	1.86	0.57
1:A:268:SER:HA	1:A:273:ILE:HG21	1.86	0.57
1:A:268:SER:HA	1:A:273:ILE:CG2	2.35	0.57
2:B:333:TRP:HB3	2:B:429:SER:HB3	1.85	0.57
2:B:510:GLU:HB2	2:B:511:LYS:HE2	1.87	0.57
1:A:599:MET:HE1	1:A:631:TYR:CB	2.35	0.57
1:A:619:LEU:N	1:A:619:LEU:HD23	2.20	0.57
2:B:405:ILE:N	2:B:405:ILE:HD13	2.19	0.57
1:A:9:GLU:OE2	1:A:16:MET:HG2	2.04	0.57
1:A:163:ALA:HA	1:A:297:LEU:HD11	1.86	0.57
1:A:2:PRO:CB	1:A:3:PRO:HD2	2.34	0.56
1:A:806:ASP:OD2	1:A:808:ARG:NH1	2.37	0.56
2:B:442:ILE:HG23	2:B:584:LEU:HD21	1.87	0.56
2:B:501:GLN:O	2:B:505:SER:N	2.36	0.56
1:A:85:GLU:OE2	1:A:85:GLU:HA	2.04	0.56
1:A:325:LYS:HD2	1:A:330:ILE:HD11	1.87	0.56
1:A:576:SER:O	1:A:580:VAL:HG23	2.05	0.56
2:B:379:LYS:CD	2:B:419:LYS:HE2	2.36	0.56
1:A:16:MET:CG	1:A:38:ARG:HG3	2.35	0.56
1:A:544:THR:OG1	1:A:547:GLU:HG2	2.06	0.56
1:A:351:ILE:HD13	1:A:408:SER:OG	2.05	0.56
1:A:459:ILE:HG23	1:A:641:TYR:OH	2.06	0.56
1:A:1044:ASN:HB2	1:A:1051:TRP:HB2	1.87	0.56
2:B:442:ILE:HG23	2:B:584:LEU:CD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LYS:HD2	1:A:330:ILE:CD1	2.36	0.56
1:A:-15:ASP:CG	1:A:-13:PRO:HD2	2.31	0.56
2:B:343:VAL:HG13	2:B:356:LEU:CD1	2.35	0.56
1:A:351:ILE:CG1	1:A:408:SER:OG	2.54	0.56
1:A:367:LEU:CD2	1:A:391:ILE:HG21	2.36	0.56
1:A:1012:GLU:OE1	1:A:1012:GLU:N	2.31	0.55
1:A:31:ILE:HD11	2:B:531:LEU:CD1	2.24	0.55
1:A:347:ASN:ND2	2:B:561:LYS:HG2	2.21	0.55
1:A:800:ILE:HG13	1:A:850:VAL:HG23	1.88	0.55
1:A:438:SER:HA	1:A:477:PHE:HB3	1.87	0.55
1:A:141:ARG:O	1:A:144:LEU:CD1	2.55	0.55
1:A:16:MET:HE1	1:A:89:LEU:CD2	2.20	0.55
1:A:590:TRP:CD1	1:A:591:PRO:CD	2.90	0.55
2:B:413:LEU:O	2:B:420:LEU:HB2	2.06	0.55
1:A:534:ILE:O	1:A:537:ARG:HB2	2.07	0.55
1:A:540:LEU:CD1	1:A:1019:ILE:HG22	2.35	0.55
1:A:759:HIS:CD2	1:A:794:PHE:CZ	2.94	0.55
2:B:413:LEU:CD2	2:B:420:LEU:HD13	2.37	0.55
1:A:58:LEU:N	1:A:58:LEU:CD1	2.69	0.55
1:A:831:LEU:HD22	1:A:903:GLY:CA	2.37	0.55
1:A:937:PHE:CD1	1:A:938:LEU:HG	2.42	0.55
2:B:356:LEU:HD13	2:B:356:LEU:O	2.07	0.55
1:A:140:ARG:O	1:A:144:LEU:CD1	2.55	0.55
1:A:181:ILE:HG12	1:A:278:MET:SD	2.46	0.55
1:A:660:ASN:OD1	1:A:660:ASN:C	2.50	0.55
1:A:668:PHE:CD2	1:A:702:LEU:HD22	2.42	0.55
2:B:369:THR:HA	2:B:383:ILE:HG13	1.89	0.55
2:B:413:LEU:HB3	2:B:420:LEU:HB3	1.88	0.55
1:A:593:ILE:HD12	1:A:597:GLN:HB3	1.89	0.54
1:A:602:LEU:HB3	1:A:638:VAL:HG11	1.88	0.54
2:B:563:MET:O	2:B:567:LYS:CB	2.53	0.54
1:A:243:VAL:O	1:A:247:GLN:HB2	2.07	0.54
1:A:336:ILE:HD12	1:A:389:TYR:CE1	2.41	0.54
2:B:510:GLU:HB2	2:B:511:LYS:CE	2.37	0.54
1:A:215:CYS:SG	1:A:219:GLN:HB2	2.47	0.54
1:A:281:ARG:HH11	1:A:282:MET:H	1.54	0.54
1:A:565:LEU:N	1:A:566:PRO:CD	2.71	0.54
1:A:792:LEU:HD22	1:A:792:LEU:N	2.23	0.54
2:B:456:PHE:HE1	2:B:460:SER:HB3	1.71	0.54
2:B:501:GLN:CD	2:B:528:TYR:CD1	2.85	0.54
1:A:557:TYR:O	1:A:560:THR:OG1	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:LEU:O	1:A:937:PHE:O	2.24	0.54
1:A:141:ARG:O	1:A:144:LEU:HD12	2.08	0.54
1:A:370:ASN:C	1:A:370:ASN:OD1	2.51	0.54
1:A:772:MET:HA	1:A:772:MET:CE	2.23	0.54
1:A:128:PHE:CE1	1:A:686:LEU:CD2	2.91	0.54
1:A:243:VAL:HG12	1:A:247:GLN:HE21	1.73	0.54
1:A:356:VAL:CG2	1:A:406:ILE:HG12	2.37	0.54
1:A:551:LEU:HD21	1:A:564:ILE:HD11	1.90	0.54
1:A:636:VAL:O	1:A:639:LEU:HB2	2.08	0.54
1:A:16:MET:SD	1:A:38:ARG:HG3	2.48	0.54
1:A:17:PRO:O	1:A:38:ARG:HB2	2.07	0.54
1:A:115:ARG:O	1:A:115:ARG:HG2	2.08	0.54
1:A:461:VAL:HG11	1:A:679:THR:HB	1.90	0.54
1:A:83:PHE:HD2	1:A:113:LEU:HD13	1.73	0.53
1:A:293:LEU:HD12	1:A:293:LEU:O	2.09	0.53
1:A:1017:ASP:O	1:A:1020:ALA:HB3	2.08	0.53
1:A:83:PHE:CD2	1:A:113:LEU:HD13	2.44	0.53
1:A:238:GLN:OE1	1:A:238:GLN:HA	2.08	0.53
1:A:580:VAL:HG12	1:A:584:TYR:CE1	2.43	0.53
2:B:333:TRP:CE3	2:B:333:TRP:C	2.87	0.53
2:B:449:LEU:HB3	2:B:580:TYR:HB3	1.91	0.53
1:A:355:TYR:HB3	1:A:374:GLN:HA	1.89	0.53
1:A:1013:LEU:N	1:A:1013:LEU:HD23	2.24	0.53
1:A:1054:LYS:O	1:A:1055:MET:HG3	2.09	0.53
1:A:719:LEU:CD1	1:A:771:ILE:HD11	2.39	0.53
1:A:1002:PHE:HB3	1:A:1019:ILE:HG12	1.90	0.53
1:A:398:ARG:HH11	1:A:398:ARG:HG3	1.73	0.52
1:A:905:CYS:SG	1:A:1043:MET:CE	2.97	0.52
1:A:976:GLU:O	1:A:979:ARG:HB2	2.09	0.52
1:A:765:ARG:NH1	1:A:796:ASN:HD21	2.06	0.52
2:B:456:PHE:CD2	2:B:577:ARG:NH1	2.77	0.52
1:A:28:ASN:HB2	1:A:30:MET:HE2	1.90	0.52
1:A:63:GLN:HB2	1:A:68:TYR:HE2	1.73	0.52
1:A:404:LEU:HD12	1:A:404:LEU:C	2.34	0.52
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.45	0.52
1:A:602:LEU:HD21	1:A:615:ALA:HB3	1.91	0.52
1:A:568:LEU:O	1:A:568:LEU:HG	2.10	0.52
2:B:413:LEU:CG	2:B:420:LEU:HD13	2.38	0.52
1:A:545:GLU:OE2	2:B:379:LYS:CB	2.55	0.52
2:B:413:LEU:HG	2:B:420:LEU:HD12	1.89	0.52
1:A:602:LEU:CD2	1:A:612:ARG:HD3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:GLN:HG2	2:B:505:SER:HB3	1.92	0.52
1:A:-14:ILE:N	1:A:-13:PRO:HD2	2.25	0.52
2:B:356:LEU:CD1	2:B:371:THR:HB	2.40	0.52
2:B:407:HIS:C	2:B:407:HIS:CD2	2.88	0.52
1:A:251:ILE:HD13	1:A:262:LEU:HD22	1.90	0.51
1:A:31:ILE:O	1:A:31:ILE:HG22	2.09	0.51
1:A:601:LEU:HA	1:A:606:TYR:CD2	2.46	0.51
2:B:335:TRP:HB2	2:B:338:ILE:HG12	1.91	0.51
1:A:338:ILE:HD11	1:A:387:LEU:HD12	1.93	0.51
1:A:780:TRP:CD1	1:A:780:TRP:C	2.89	0.51
2:B:509:ILE:HG22	2:B:509:ILE:O	2.09	0.51
1:A:376:VAL:HB	1:A:381:PRO:HA	1.91	0.51
1:A:23:GLU:HG2	1:A:33:THR:HG23	1.91	0.51
1:A:937:PHE:HD1	1:A:938:LEU:HG	1.75	0.51
1:A:834:LEU:CD2	1:A:924:LYS:HZ3	2.23	0.51
2:B:340:ARG:HB2	2:B:340:ARG:CZ	2.41	0.51
1:A:424:TRP:CZ3	1:A:460:GLY:HA3	2.45	0.51
1:A:114:ASN:OD1	1:A:114:ASN:C	2.54	0.51
1:A:209:LEU:HD12	1:A:209:LEU:O	2.10	0.51
1:A:645:LEU:HD22	1:A:683:ARG:HG2	1.83	0.51
2:B:583:TRP:CZ3	2:B:584:LEU:HB2	2.46	0.51
1:A:22:VAL:N	1:A:34:LEU:O	2.42	0.50
1:A:602:LEU:CA	1:A:612:ARG:HH12	2.14	0.50
1:A:834:LEU:HD21	1:A:924:LYS:NZ	2.26	0.50
2:B:456:PHE:HD2	2:B:577:ARG:NH1	2.09	0.50
1:A:209:LEU:CD1	1:A:211:ILE:HG13	2.41	0.50
2:B:379:LYS:HZ3	2:B:419:LYS:CE	2.21	0.50
2:B:398:PHE:HE1	2:B:407:HIS:ND1	2.10	0.50
1:A:240:LYS:O	1:A:244:LEU:HD13	2.11	0.50
1:A:446:TRP:CD2	1:A:465:ASN:HB2	2.47	0.50
1:A:821:GLU:OE1	1:A:833:MET:O	2.29	0.50
1:A:211:ILE:HG22	1:A:212:ASN:O	2.11	0.50
1:A:435:THR:OG1	1:A:485:LYS:HE2	2.11	0.50
1:A:452:LEU:HD12	1:A:452:LEU:O	2.11	0.50
1:A:778:PRO:HB3	1:A:802:LYS:HG3	1.93	0.50
1:A:772:MET:HB2	1:A:778:PRO:HG2	1.94	0.50
1:A:929:LEU:HD23	1:A:930:PHE:N	2.25	0.50
2:B:449:LEU:HD22	2:B:580:TYR:HB3	1.92	0.50
1:A:98:PHE:CD1	1:A:98:PHE:C	2.89	0.50
1:A:193:VAL:CG2	1:A:282:MET:HE3	2.41	0.50
1:A:921:ILE:HD11	1:A:931:HIS:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:TYR:O	1:A:1021:TYR:HD1	1.94	0.50
1:A:539:PRO:HD3	1:A:996:ASN:ND2	2.25	0.50
1:A:552:TRP:HA	1:A:552:TRP:CE3	2.47	0.50
1:A:124:PRO:HG2	1:A:127:GLU:HB2	1.92	0.50
1:A:834:LEU:HD22	1:A:924:LYS:HE3	1.88	0.50
1:A:194:ILE:HD12	1:A:194:ILE:N	2.27	0.49
1:A:906:VAL:O	1:A:910:ILE:HG13	2.12	0.49
1:A:392:TYR:HB3	1:A:394:PRO:HD2	1.95	0.49
1:A:-15:ASP:OD1	1:A:-14:ILE:N	2.43	0.49
1:A:209:LEU:C	1:A:209:LEU:CD1	2.81	0.49
1:A:934:PHE:CD1	1:A:934:PHE:N	2.80	0.49
1:A:1014:GLN:OE1	1:A:1014:GLN:HA	2.13	0.49
1:A:542:GLU:OE2	1:A:542:GLU:HA	2.12	0.49
1:A:874:SER:HA	1:A:959:ASP:OD1	2.11	0.49
2:B:457:GLN:O	2:B:461:ARG:CG	2.58	0.49
2:B:584:LEU:HD12	2:B:585:THR:H	1.78	0.49
1:A:39:GLU:HG3	1:A:742:PRO:HG3	1.94	0.49
1:A:89:LEU:C	1:A:89:LEU:CD2	2.85	0.49
1:A:910:ILE:CG2	1:A:1026:LEU:HD21	2.43	0.49
2:B:356:LEU:HD12	2:B:371:THR:HB	1.94	0.49
1:A:28:ASN:CB	1:A:30:MET:HE2	2.42	0.49
1:A:855:HIS:N	1:A:855:HIS:CD2	2.81	0.49
1:A:962:ILE:HG13	1:A:963:VAL:H	1.78	0.49
2:B:357:VAL:HG23	2:B:357:VAL:O	2.11	0.49
1:A:977:PHE:HE1	1:A:981:GLN:HE21	1.59	0.49
2:B:476:GLU:HB3	2:B:480:LYS:NZ	2.27	0.49
2:B:510:GLU:HB2	2:B:511:LYS:HZ1	1.78	0.49
1:A:955:VAL:O	1:A:955:VAL:HG12	2.12	0.49
2:B:487:PHE:O	2:B:488:ASN:C	2.56	0.49
1:A:253:LYS:HD2	1:A:288:MET:HE3	1.95	0.49
1:A:881:LEU:C	1:A:881:LEU:HD23	2.38	0.49
1:A:894:ILE:O	1:A:898:THR:OG1	2.23	0.49
1:A:921:ILE:HD11	1:A:931:HIS:CE1	2.47	0.49
1:A:63:GLN:HB2	1:A:68:TYR:CE2	2.48	0.48
1:A:461:VAL:O	1:A:461:VAL:HG13	2.13	0.48
2:B:332:GLU:OE1	2:B:429:SER:O	2.30	0.48
2:B:358:ARG:O	2:B:359:ASP:HB2	2.12	0.48
1:A:58:LEU:N	1:A:58:LEU:HD12	2.29	0.48
1:A:179:LYS:N	1:A:179:LYS:HD3	2.28	0.48
1:A:242:CYS:O	1:A:243:VAL:C	2.55	0.48
1:A:251:ILE:CG2	1:A:262:LEU:CD2	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:PRO:HB3	1:A:693:ARG:HD3	1.96	0.48
1:A:817:ILE:HD13	1:A:904:TYR:HE1	1.78	0.48
2:B:446:GLY:HA2	2:B:449:LEU:HG	1.94	0.48
1:A:561:ILE:O	1:A:562:PRO:C	2.56	0.48
1:A:574:TRP:CZ3	1:A:580:VAL:HG13	2.48	0.48
1:A:705:GLN:O	1:A:709:MET:HG2	2.13	0.48
1:A:26:LEU:HB3	1:A:27:PRO:HD2	1.95	0.48
2:B:528:TYR:O	2:B:531:LEU:HB3	2.13	0.48
1:A:367:LEU:HD22	1:A:391:ILE:HG22	1.96	0.48
1:A:975:ARG:CZ	1:A:979:ARG:HH21	2.27	0.48
2:B:401:VAL:O	2:B:404:LEU:HB3	2.14	0.48
2:B:479:MET:HE2	2:B:479:MET:HB3	1.83	0.48
1:A:380:ASN:N	1:A:381:PRO:HD3	2.29	0.48
1:A:568:LEU:O	1:A:568:LEU:CG	2.62	0.48
1:A:841:ILE:HD12	1:A:841:ILE:C	2.39	0.48
1:A:435:THR:OG1	1:A:485:LYS:HG2	2.13	0.48
1:A:937:PHE:CE1	1:A:1002:PHE:HE1	2.32	0.48
1:A:534:ILE:HD11	1:A:547:GLU:OE1	2.13	0.47
1:A:634:GLN:OE1	1:A:634:GLN:N	2.45	0.47
1:A:639:LEU:HD23	1:A:639:LEU:HA	1.67	0.47
2:B:584:LEU:HG	2:B:585:THR:N	2.29	0.47
1:A:28:ASN:ND2	1:A:30:MET:HE2	2.29	0.47
1:A:128:PHE:CB	1:A:140:ARG:NH1	2.71	0.47
1:A:133:ASP:OD1	1:A:134:PRO:HD2	2.15	0.47
1:A:759:HIS:CD2	1:A:794:PHE:HZ	2.32	0.47
1:A:960:PHE:N	1:A:960:PHE:CD1	2.82	0.47
1:A:367:LEU:HD12	1:A:368:CYS:O	2.14	0.47
1:A:456:LEU:HD12	1:A:456:LEU:HA	1.72	0.47
1:A:609:PRO:O	1:A:612:ARG:HB3	2.14	0.47
1:A:659:THR:O	1:A:659:THR:HG22	2.13	0.47
2:B:449:LEU:HB3	2:B:580:TYR:CD2	2.49	0.47
1:A:177:LEU:HD21	1:A:274:ARG:NH2	2.30	0.47
1:A:762:GLY:O	1:A:763:ASN:C	2.57	0.47
1:A:71:VAL:HG23	1:A:80:GLU:C	2.40	0.47
2:B:356:LEU:C	2:B:356:LEU:CD1	2.83	0.47
1:A:25:LEU:CD1	1:A:25:LEU:N	2.77	0.47
1:A:362:HIS:CE1	1:A:574:TRP:CD2	3.03	0.47
1:A:791:GLU:H	1:A:791:GLU:CD	2.19	0.47
1:A:1044:ASN:CB	1:A:1051:TRP:HB2	2.44	0.47
2:B:413:LEU:HB3	2:B:420:LEU:O	2.14	0.47
2:B:426:TYR:HB3	2:B:428:VAL:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:HB3	1:A:111:LYS:HB2	1.97	0.47
1:A:831:LEU:HD23	1:A:899:ARG:O	2.15	0.47
1:A:874:SER:CB	1:A:959:ASP:OD1	2.61	0.47
1:A:1021:TYR:CD1	1:A:1021:TYR:C	2.92	0.47
1:A:1040:MET:HE1	1:A:1052:THR:C	2.39	0.47
2:B:329:GLN:C	2:B:329:GLN:CD	2.83	0.47
1:A:16:MET:SD	1:A:90:CYS:CA	3.03	0.47
1:A:68:TYR:HB3	1:A:103:GLU:HA	1.96	0.47
1:A:162:ARG:HH21	1:A:298:PRO:C	2.22	0.47
1:A:831:LEU:HD22	1:A:903:GLY:HA2	1.97	0.47
1:A:915:ASP:OD1	1:A:951:ARG:NH1	2.48	0.47
2:B:329:GLN:CD	2:B:329:GLN:O	2.58	0.47
1:A:186:ASP:OD1	1:A:189:GLN:HB2	2.15	0.46
1:A:321:GLU:N	1:A:321:GLU:OE1	2.48	0.46
1:A:28:ASN:HD22	1:A:30:MET:HE2	1.80	0.46
1:A:251:ILE:HG22	1:A:252:LEU:N	2.29	0.46
1:A:257:CYS:HA	1:A:787:ASP:OD2	2.15	0.46
1:A:534:ILE:O	1:A:537:ARG:CB	2.63	0.46
1:A:590:TRP:CG	1:A:591:PRO:CD	2.99	0.46
1:A:770:ARG:HG3	1:A:772:MET:CE	2.46	0.46
1:A:904:TYR:CE2	1:A:930:PHE:HA	2.50	0.46
2:B:478:GLN:HA	2:B:481:ARG:HB2	1.97	0.46
1:A:817:ILE:HG22	1:A:835:PRO:HB3	1.97	0.46
2:B:413:LEU:CB	2:B:420:LEU:HB3	2.45	0.46
1:A:63:GLN:N	1:A:68:TYR:OH	2.48	0.46
1:A:226:ARG:O	1:A:230:ARG:HG3	2.15	0.46
1:A:28:ASN:HD22	1:A:30:MET:CE	2.29	0.46
1:A:356:VAL:HB	1:A:372:ASN:ND2	2.30	0.46
1:A:383:TRP:O	1:A:383:TRP:HD1	1.97	0.46
1:A:642:GLU:HB3	1:A:683:ARG:HH22	1.81	0.46
2:B:416:TYR:CD1	2:B:416:TYR:O	2.68	0.46
1:A:116:GLU:HB3	1:A:703:ASN:HD21	1.80	0.46
1:A:522:GLU:O	1:A:522:GLU:OE1	2.33	0.46
1:A:177:LEU:CD2	1:A:274:ARG:NH2	2.79	0.46
1:A:552:TRP:HA	1:A:552:TRP:HE3	1.78	0.46
1:A:645:LEU:HD23	1:A:683:ARG:HG2	1.87	0.46
1:A:908:THR:HG21	1:A:954:PHE:CB	2.46	0.46
2:B:416:TYR:CD1	2:B:416:TYR:C	2.90	0.46
2:B:456:PHE:CD1	2:B:456:PHE:C	2.92	0.46
1:A:57:PRO:CB	2:B:524:ILE:CD1	2.83	0.46
1:A:256:GLY:HA2	1:A:787:ASP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:TYR:O	1:A:1021:TYR:CD1	2.69	0.46
1:A:32:VAL:HG23	1:A:56:TYR:CZ	2.51	0.46
1:A:144:LEU:HD12	1:A:144:LEU:H	1.80	0.46
1:A:612:ARG:HD3	1:A:612:ARG:HA	1.79	0.46
1:A:639:LEU:O	1:A:683:ARG:NH2	2.49	0.46
1:A:114:ASN:OD1	1:A:114:ASN:O	2.34	0.46
1:A:508:TYR:O	1:A:508:TYR:CD1	2.69	0.46
1:A:558:CYS:HB3	1:A:564:ILE:CG2	2.46	0.46
1:A:857:ILE:O	1:A:860:ILE:HB	2.16	0.46
1:A:623:LEU:HA	1:A:623:LEU:HD12	1.64	0.45
2:B:333:TRP:HE3	2:B:333:TRP:C	2.24	0.45
2:B:392:PHE:HE1	2:B:416:TYR:CG	2.33	0.45
1:A:24:CYS:SG	1:A:49:LEU:HD11	2.55	0.45
1:A:32:VAL:HG11	1:A:49:LEU:HD11	1.99	0.45
1:A:39:GLU:CD	1:A:39:GLU:N	2.73	0.45
1:A:234:LEU:HD12	1:A:239:LEU:HA	1.99	0.45
2:B:347:LEU:CD1	2:B:371:THR:CG2	2.94	0.45
1:A:465:ASN:HD21	1:A:470:THR:HG21	1.80	0.45
1:A:544:THR:O	1:A:548:LYS:HG3	2.15	0.45
2:B:483:ALA:HB3	2:B:545:LEU:HD21	1.98	0.45
1:A:678:LYS:NZ	2:B:478:GLN:HE22	2.13	0.45
1:A:735:LEU:HD22	1:A:771:ILE:HG13	1.98	0.45
1:A:976:GLU:OE1	1:A:979:ARG:NH1	2.49	0.45
1:A:1043:MET:O	1:A:1047:HIS:ND1	2.38	0.45
1:A:62:LEU:HD12	1:A:62:LEU:C	2.41	0.45
1:A:128:PHE:CD1	1:A:686:LEU:CD2	2.99	0.45
2:B:408:TYR:CE1	2:B:413:LEU:HA	2.50	0.45
2:B:431:TYR:CZ	2:B:433:GLN:HB2	2.49	0.45
1:A:17:PRO:HG2	1:A:20:ILE:HB	1.99	0.45
1:A:952:VAL:HG12	1:A:955:VAL:HG23	1.98	0.45
2:B:544:ARG:O	2:B:547:GLU:HG2	2.16	0.45
1:A:209:LEU:HD11	1:A:211:ILE:CD1	2.47	0.45
1:A:89:LEU:HD23	1:A:89:LEU:O	2.17	0.45
1:A:251:ILE:CD1	1:A:290:LYS:HG2	2.47	0.45
1:A:353:LYS:HA	1:A:377:PRO:CB	2.37	0.45
1:A:979:ARG:O	1:A:982:GLU:HB2	2.17	0.45
1:A:71:VAL:HG23	1:A:81:GLU:HA	1.98	0.45
1:A:637:GLN:C	1:A:639:LEU:N	2.74	0.45
2:B:426:TYR:HB3	2:B:428:VAL:CG2	2.47	0.45
1:A:88:ARG:HD2	1:A:743:ASP:HB3	1.98	0.45
1:A:243:VAL:HG12	1:A:247:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:ASP:C	1:A:806:ASP:OD1	2.59	0.45
1:A:960:PHE:N	1:A:960:PHE:HD1	2.15	0.44
1:A:961:LEU:HD22	1:A:977:PHE:CE2	2.50	0.44
2:B:392:PHE:CD1	2:B:416:TYR:CE2	3.05	0.44
1:A:977:PHE:HE1	1:A:981:GLN:NE2	2.15	0.44
1:A:988:TYR:CD1	1:A:988:TYR:C	2.94	0.44
1:A:1037:GLU:O	1:A:1041:LYS:HG3	2.17	0.44
2:B:573:LEU:N	2:B:573:LEU:HD23	2.33	0.44
1:A:756:ASN:C	1:A:756:ASN:OD1	2.58	0.44
2:B:413:LEU:HD21	2:B:420:LEU:HD13	1.98	0.44
1:A:139:PHE:CD1	1:A:139:PHE:C	2.96	0.44
1:A:357:ARG:HG3	1:A:371:VAL:HG12	2.00	0.44
1:A:569:LEU:HD13	1:A:611:VAL:HG21	1.98	0.44
2:B:333:TRP:CB	2:B:429:SER:HB3	2.47	0.44
1:A:57:PRO:CB	2:B:524:ILE:HD13	2.43	0.44
1:A:691:TYR:CE1	1:A:695:CYS:HB3	2.53	0.44
2:B:334:TYR:HA	2:B:357:VAL:CG2	2.48	0.44
1:A:540:LEU:CB	1:A:1023:ARG:HD2	2.47	0.44
1:A:575:ASN:OD1	1:A:576:SER:N	2.50	0.44
1:A:808:ARG:HA	1:A:811:MET:HB2	1.98	0.44
2:B:392:PHE:CD1	2:B:393:SER:N	2.85	0.44
1:A:251:ILE:CG2	1:A:252:LEU:N	2.80	0.44
1:A:498:TRP:CH2	1:A:502:ARG:HD2	2.53	0.44
1:A:552:TRP:CZ3	1:A:555:ARG:HD3	2.52	0.44
1:A:1003:SER:HA	1:A:1019:ILE:CD1	2.47	0.44
2:B:362:THR:HB	2:B:365:HIS:HB2	2.00	0.44
2:B:372:LEU:HD12	2:B:379:LYS:HB2	2.00	0.44
2:B:333:TRP:CZ2	2:B:405:ILE:CG2	2.97	0.44
1:A:376:VAL:N	1:A:377:PRO:CD	2.80	0.44
1:A:376:VAL:HG11	1:A:380:ASN:O	2.18	0.44
1:A:465:ASN:HA	1:A:466:PRO:HD3	1.92	0.44
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.85	0.43
1:A:568:LEU:HA	1:A:571:SER:OG	2.18	0.43
1:A:627:LYS:HD2	1:A:627:LYS:HA	1.82	0.43
2:B:343:VAL:CG1	2:B:356:LEU:CD1	2.89	0.43
1:A:215:CYS:SG	1:A:219:GLN:CB	3.05	0.43
1:A:354:ILE:HG12	1:A:408:SER:CB	2.48	0.43
1:A:882:LYS:O	1:A:885:ASN:O	2.36	0.43
1:A:123:MET:CE	1:A:675:MET:CE	2.96	0.43
1:A:302:PHE:CD1	1:A:302:PHE:C	2.95	0.43
1:A:806:ASP:OD1	1:A:808:ARG:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:PHE:HE1	2:B:407:HIS:CG	2.35	0.43
2:B:413:LEU:C	2:B:420:LEU:HB2	2.43	0.43
1:A:162:ARG:NH2	1:A:298:PRO:C	2.77	0.43
2:B:384:PHE:CD1	2:B:392:PHE:HA	2.53	0.43
2:B:445:VAL:CG1	2:B:583:TRP:CZ3	3.01	0.43
2:B:458:GLU:C	2:B:458:GLU:CD	2.85	0.43
1:A:449:PRO:HG2	1:A:452:LEU:HG	2.01	0.43
1:A:939:ASP:HB3	1:A:1021:TYR:CD2	2.54	0.43
1:A:68:TYR:HB3	1:A:103:GLU:HG3	1.99	0.43
1:A:405:SER:HA	1:A:424:TRP:HA	2.01	0.43
1:A:897:PHE:C	1:A:897:PHE:CD1	2.97	0.43
1:A:8:GLY:O	1:A:75:GLN:NE2	2.52	0.43
1:A:70:PHE:CD1	1:A:99:LEU:HB3	2.53	0.43
1:A:350:ASP:OD2	2:B:565:SER:HB3	2.19	0.43
1:A:461:VAL:HB	1:A:640:LYS:HE3	2.00	0.43
1:A:565:LEU:N	1:A:566:PRO:HD2	2.33	0.43
1:A:823:ILE:CG2	1:A:994:HIS:CD2	3.01	0.43
1:A:121:ILE:HD11	1:A:689:GLU:CA	2.46	0.43
1:A:133:ASP:OD1	1:A:133:ASP:C	2.62	0.43
1:A:361:TYR:HA	1:A:366:PRO:HD3	2.00	0.43
1:A:899:ARG:NH1	1:A:983:MET:HE1	2.34	0.43
1:A:910:ILE:O	1:A:1025:THR:HG21	2.19	0.43
1:A:1003:SER:HA	1:A:1019:ILE:HD11	2.00	0.43
1:A:534:ILE:O	1:A:537:ARG:CG	2.67	0.43
1:A:929:LEU:C	1:A:929:LEU:CD2	2.89	0.43
2:B:379:LYS:HZ3	2:B:419:LYS:HE2	1.78	0.43
1:A:18:PRO:O	1:A:38:ARG:N	2.47	0.43
1:A:178:PRO:CG	1:A:181:ILE:HD12	2.48	0.43
1:A:251:ILE:CG2	1:A:262:LEU:HD23	2.48	0.43
1:A:542:GLU:CG	2:B:340:ARG:HD3	2.49	0.43
1:A:881:LEU:HD23	1:A:881:LEU:O	2.18	0.43
1:A:977:PHE:O	1:A:980:PHE:HB3	2.19	0.43
2:B:445:VAL:HG11	2:B:583:TRP:CH2	2.54	0.43
1:A:91:ASP:OD1	1:A:711:LYS:NZ	2.51	0.42
1:A:328:TRP:CZ2	1:A:577:ARG:HD2	2.54	0.42
1:A:382:ARG:O	1:A:384:ASN:ND2	2.52	0.42
2:B:362:THR:HB	2:B:365:HIS:CB	2.49	0.42
2:B:596:GLU:HG2	2:B:597:TRP:CD2	2.54	0.42
1:A:562:PRO:HB2	1:A:593:ILE:HG22	2.00	0.42
1:A:934:PHE:H	1:A:934:PHE:HD1	1.63	0.42
1:A:147:CYS:O	1:A:151:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:TRP:HZ2	1:A:579:GLU:HG2	1.84	0.42
1:A:820:MET:O	1:A:821:GLU:C	2.62	0.42
1:A:956:LEU:N	1:A:956:LEU:HD23	2.35	0.42
1:A:961:LEU:HA	1:A:964:ILE:HD12	2.02	0.42
2:B:456:PHE:CD1	2:B:570:LEU:HD11	2.55	0.42
2:B:466:LEU:HD23	2:B:466:LEU:N	2.34	0.42
1:A:307:TYR:O	1:A:308:SER:C	2.62	0.42
1:A:713:ILE:HG12	1:A:801:PHE:HZ	1.85	0.42
1:A:836:TYR:CZ	1:A:932:ILE:HG22	2.53	0.42
1:A:69:ILE:HD11	1:A:83:PHE:HA	2.01	0.42
1:A:145:ASN:O	1:A:149:GLU:HG3	2.18	0.42
1:A:239:LEU:O	1:A:239:LEU:HD22	2.19	0.42
1:A:324:THR:OG1	1:A:482:SER:HB3	2.20	0.42
1:A:621:LYS:HE2	1:A:622:TYR:HE1	1.84	0.42
1:A:791:GLU:N	1:A:791:GLU:CD	2.78	0.42
1:A:1017:ASP:O	1:A:1020:ALA:CB	2.68	0.42
2:B:450:HIS:CD2	2:B:450:HIS:C	2.97	0.42
1:A:256:GLY:C	1:A:787:ASP:OD2	2.63	0.42
1:A:841:ILE:HD11	1:A:845:VAL:HG12	2.02	0.42
1:A:1047:HIS:O	1:A:1048:HIS:HB3	2.20	0.42
2:B:382:LYS:O	2:B:392:PHE:HB3	2.19	0.42
1:A:68:TYR:HA	1:A:104:PRO:HD3	2.01	0.42
1:A:76:GLU:O	1:A:78:GLU:N	2.50	0.42
1:A:217:PRO:O	1:A:218:GLU:C	2.63	0.42
1:A:534:ILE:O	1:A:537:ARG:HG3	2.19	0.42
1:A:764:LEU:HD12	1:A:783:TRP:CE2	2.50	0.42
1:A:171:VAL:HG22	1:A:269:GLN:HG2	2.00	0.42
1:A:586:LEU:HD23	1:A:586:LEU:N	2.35	0.42
1:A:632:LEU:HD12	1:A:632:LEU:C	2.45	0.42
1:A:648:LEU:H	1:A:648:LEU:CD1	2.14	0.42
2:B:510:GLU:OE1	2:B:511:LYS:NZ	2.52	0.42
1:A:354:ILE:HG12	1:A:408:SER:HB2	2.02	0.42
1:A:446:TRP:CH2	1:A:465:ASN:HA	2.55	0.42
1:A:540:LEU:HD12	1:A:999:ILE:HD12	2.02	0.42
1:A:676:HIS:CD2	1:A:843:ASP:HB2	2.55	0.42
1:A:829:LEU:HG	1:A:831:LEU:HD12	2.02	0.42
2:B:441:ASN:HB3	2:B:444:ALA:HB3	2.02	0.42
1:A:163:ALA:CA	1:A:297:LEU:HD11	2.47	0.41
1:A:177:LEU:HD21	1:A:274:ARG:CZ	2.49	0.41
1:A:216:VAL:HB	1:A:217:PRO:CD	2.50	0.41
1:A:507:SER:OG	1:A:508:TYR:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:LEU:HD21	1:A:550:PHE:HE1	1.84	0.41
1:A:646:ASP:OD2	1:A:651:ARG:NH2	2.47	0.41
2:B:542:ARG:O	2:B:545:LEU:HB3	2.20	0.41
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.89	0.41
1:A:904:TYR:HB3	1:A:931:HIS:CD2	2.55	0.41
1:A:193:VAL:C	1:A:194:ILE:HD12	2.45	0.41
1:A:370:ASN:OD1	1:A:387:LEU:HD22	2.21	0.41
1:A:875:HIS:HA	1:A:962:ILE:HD12	2.02	0.41
1:A:951:ARG:HG2	1:A:952:VAL:N	2.34	0.41
2:B:417:ASN:HB3	2:B:420:LEU:HD11	2.03	0.41
1:A:32:VAL:CG2	1:A:56:TYR:CE2	3.02	0.41
1:A:351:ILE:CG2	1:A:408:SER:HB2	2.39	0.41
1:A:565:LEU:HD23	1:A:590:TRP:CH2	2.55	0.41
1:A:69:ILE:HG12	1:A:70:PHE:H	1.86	0.41
1:A:599:MET:HE1	1:A:631:TYR:HB2	2.03	0.41
1:A:939:ASP:HB3	1:A:1021:TYR:CE2	2.56	0.41
1:A:253:LYS:HD3	1:A:286:MET:HE2	2.01	0.41
1:A:345:ASN:HD22	2:B:557:ARG:CG	2.30	0.41
1:A:465:ASN:ND2	1:A:470:THR:HG21	2.34	0.41
1:A:637:GLN:C	1:A:639:LEU:H	2.29	0.41
1:A:824:TRP:HZ3	1:A:833:MET:SD	2.43	0.41
2:B:406:ASN:HA	2:B:409:ARG:HB2	2.03	0.41
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.56	0.41
1:A:356:VAL:HG23	1:A:383:TRP:HZ2	1.86	0.41
1:A:777:ARG:N	1:A:778:PRO:CD	2.84	0.41
1:A:1052:THR:OG1	1:A:1053:THR:N	2.53	0.41
1:A:16:MET:SD	1:A:90:CYS:HA	2.61	0.41
1:A:83:PHE:CZ	1:A:112:ILE:HG22	2.56	0.41
1:A:188:GLY:HA2	1:A:213:HIS:HD2	1.86	0.41
1:A:436:LEU:C	1:A:436:LEU:CD1	2.92	0.41
1:A:549:ASP:O	1:A:550:PHE:C	2.63	0.41
1:A:732:MET:HE1	1:A:770:ARG:HA	2.02	0.41
1:A:738:GLN:HE22	1:A:741:ARG:HE	1.67	0.41
1:A:890:TYR:CD1	1:A:890:TYR:C	2.98	0.41
1:A:916:ARG:HE	1:A:916:ARG:HA	1.85	0.41
1:A:221:ILE:O	1:A:225:ILE:HG12	2.21	0.41
1:A:374:GLN:H	1:A:374:GLN:HG2	1.57	0.41
1:A:602:LEU:C	1:A:612:ARG:HH12	2.28	0.41
1:A:810:ASP:O	1:A:811:MET:C	2.63	0.41
1:A:959:ASP:O	1:A:962:ILE:CG1	2.64	0.41
2:B:335:TRP:CD1	2:B:335:TRP:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:455:GLN:HE21	2:B:573:LEU:HD13	1.86	0.41
1:A:128:PHE:CE1	1:A:686:LEU:HD21	2.55	0.40
1:A:508:TYR:HD2	1:A:510:HIS:CD2	2.28	0.40
1:A:293:LEU:HD12	1:A:293:LEU:C	2.47	0.40
1:A:445:LEU:HD23	1:A:445:LEU:N	2.36	0.40
1:A:542:GLU:HB3	2:B:380:LEU:HD22	2.02	0.40
1:A:589:ASP:OD1	1:A:589:ASP:N	2.53	0.40
1:A:956:LEU:HD11	1:A:980:PHE:HZ	1.84	0.40
1:A:550:PHE:C	1:A:550:PHE:CD1	3.00	0.40
1:A:565:LEU:HD23	1:A:590:TRP:CZ2	2.55	0.40
1:A:602:LEU:N	1:A:602:LEU:HD23	2.37	0.40
1:A:808:ARG:HA	1:A:811:MET:CB	2.52	0.40
2:B:464:ASP:OD1	2:B:464:ASP:C	2.63	0.40
2:B:455:GLN:O	2:B:459:LYS:N	2.38	0.40
1:A:37:LEU:HD22	1:A:37:LEU:HA	1.92	0.40
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.88	0.40
1:A:356:VAL:HG23	1:A:406:ILE:HG12	2.04	0.40
1:A:610:MET:CA	1:A:610:MET:CE	2.93	0.40
1:A:680:VAL:O	1:A:681:SER:C	2.65	0.40
1:A:719:LEU:HB3	1:A:731:GLN:HE21	1.86	0.40
1:A:1002:PHE:C	1:A:1019:ILE:HD11	2.47	0.40
1:A:1023:ARG:NH1	2:B:341:GLU:OE2	2.53	0.40
1:A:1032:GLU:O	1:A:1036:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1027/1096 (94%)	955 (93%)	65 (6%)	7 (1%)	18 46
2	B	201/279 (72%)	186 (92%)	15 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1228/1375 (89%)	1141 (93%)	80 (6%)	7 (1%)	21	49

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	918	ASN
1	A	530	GLN
1	A	874	SER
1	A	198	VAL
1	A	298	PRO
1	A	377	PRO

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	953/999 (95%)	859 (90%)	94 (10%)	7	27
2	B	215/259 (83%)	191 (89%)	24 (11%)	6	21
All	All	1168/1258 (93%)	1050 (90%)	118 (10%)	7	26

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-14	ILE
1	A	24	CYS
1	A	25	LEU
1	A	34	LEU
1	A	36	CYS
1	A	37	LEU
1	A	41	THR
1	A	58	LEU
1	A	85	GLU
1	A	90	CYS
1	A	93	ARG

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Mol	Chain	Res	Type
1	A	109	GLU
1	A	125	VAL
1	A	137	GLN
1	A	155	ASP
1	A	196	VAL
1	A	198	VAL
1	A	204	LYS
1	A	216	VAL
1	A	232	MET
1	A	234	LEU
1	A	239	LEU
1	A	244	LEU
1	A	261	PHE
1	A	267	LEU
1	A	285	LEU
1	A	306	SER
1	A	326	SER
1	A	330	ILE
1	A	332	SER
1	A	338	ILE
1	A	351	ILE
1	A	356	VAL
1	A	366	PRO
1	A	371	VAL
1	A	374	GLN
1	A	376	VAL
1	A	407	CYS
1	A	435	THR
1	A	444	ASN
1	A	448	VAL
1	A	462	THR
1	A	473	LEU
1	A	478	ASP
1	A	483	VAL
1	A	492	ILE
1	A	522	GLU
1	A	571	SER
1	A	586	LEU
1	A	589	ASP
1	A	616	VAL
1	A	619	LEU
1	A	638	VAL

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Mol	Chain	Res	Type
1	A	648	LEU
1	A	661	GLN
1	A	663	ILE
1	A	687	LEU
1	A	704	ARG
1	A	722	GLU
1	A	727	THR
1	A	730	VAL
1	A	731	GLN
1	A	736	VAL
1	A	741	ARG
1	A	764	LEU
1	A	790	SER
1	A	799	ILE
1	A	808	ARG
1	A	811	MET
1	A	813	THR
1	A	829	LEU
1	A	850	VAL
1	A	855	HIS
1	A	860	ILE
1	A	871	GLN
1	A	874	SER
1	A	908	THR
1	A	917	HIS
1	A	921	ILE
1	A	939	ASP
1	A	940	HIS
1	A	951	ARG
1	A	952	VAL
1	A	955	VAL
1	A	970	GLU
1	A	971	CYS
1	A	978	GLU
1	A	991	ILE
1	A	999	ILE
1	A	1013	LEU
1	A	1017	ASP
1	A	1025	THR
1	A	1031	THR
1	A	1052	THR
2	B	332	GLU

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Mol	Chain	Res	Type
2	B	354	THR
2	B	356	LEU
2	B	364	MET
2	B	381	ILE
2	B	383	ILE
2	B	403	GLU
2	B	404	LEU
2	B	405	ILE
2	B	406	ASN
2	B	415	GLN
2	B	440	ASP
2	B	450	HIS
2	B	459	LYS
2	B	475	GLN
2	B	493	ILE
2	B	509	ILE
2	B	511	LYS
2	B	521	ILE
2	B	551	LYS
2	B	559	ILE
2	B	578	ASP
2	B	579	GLN
2	B	583	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-21	HIS
1	A	28	ASN
1	A	47	HIS
1	A	75	GLN
1	A	201	ASN
1	A	202	ASN
1	A	213	HIS
1	A	247	GLN
1	A	284	ASN
1	A	347	ASN
1	A	362	HIS
1	A	372	ASN
1	A	384	ASN
1	A	444	ASN
1	A	510	HIS

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Mol	Chain	Res	Type
1	A	630	GLN
1	A	670	HIS
1	A	676	HIS
1	A	731	GLN
1	A	738	GLN
1	A	759	HIS
1	A	760	GLN
1	A	797	ASN
1	A	809	GLN
1	A	827	GLN
1	A	855	HIS
1	A	885	ASN
1	A	931	HIS
1	A	994	HIS
1	A	996	ASN
1	A	1042	GLN
1	A	1047	HIS
2	B	365	HIS
2	B	455	GLN
2	B	564	ASN

5.3.3 RNA [i](#)

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](#)

5 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	SO4	A	1302	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	A	1303	-	4,4,4	0.34	0	6,6,6	0.13	0
3	144	A	1301	-	1,7,7	0.06	0	3,9,9	1.06	0
4	SO4	A	1304	-	4,4,4	0.33	0	6,6,6	0.13	0
3	144	B	1201	-	1,7,7	0.05	0	3,9,9	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	144	A	1301	-	-	0/0/9/9	-
3	144	B	1201	-	-	0/0/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1039/1096 (94%)	-0.42	5 (0%) 87 78	59, 114, 187, 257	0
2	B	225/279 (80%)	-0.07	5 (2%) 62 46	30, 190, 250, 283	0
All	All	1264/1375 (91%)	-0.36	10 (0%) 82 71	30, 123, 218, 283	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	359	ASP	5.0
2	B	358	ARG	4.4
2	B	527	ASN	3.4
1	A	-26	SER	2.9
1	A	647	ASN	2.7
1	A	833	MET	2.6
1	A	797	ASN	2.5
2	B	401	VAL	2.5
2	B	526	HIS	2.3
1	A	354	ILE	2.2

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

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
4	SO4	A	1302	5/5	0.51	0.08	215,217,224,233	0
3	144	A	1301	8/8	0.59	0.11	139,163,171,175	0
3	144	B	1201	8/8	0.62	0.09	139,171,184,186	0
4	SO4	A	1304	5/5	0.74	0.13	184,189,211,213	0
4	SO4	A	1303	5/5	0.81	0.08	203,205,223,246	0

6.5 Other polymers

There are no such residues in this entry.