



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:29 PM UTC

PDB ID : 2AYO / pdb_00002ayo
Title : Structure of USP14 bound to ubiquitin aldehyde
Authors : Hu, M.; Li, P.; Jeffrey, P.D.; Shi, Y.
Deposited on : 2005-09-07
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

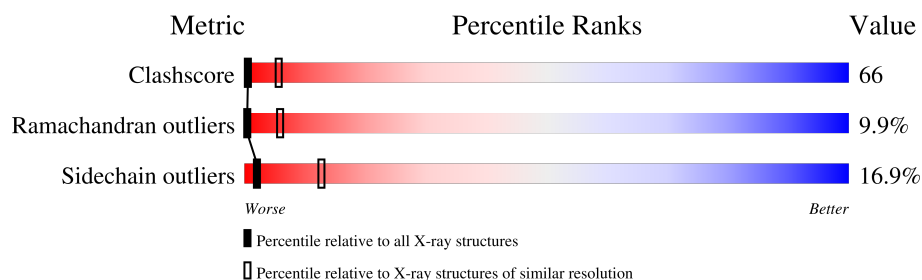
1 Overall quality at a glance

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))
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	404	
2	B	76	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLZ	B	76	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3411 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 Ubiquitin carboxyl-terminal hydrolase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2810	1782	470	538	20			

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	10	0	0
			601	378	105	117	1			

There is a discrepancy between the modelled and reference sequences:

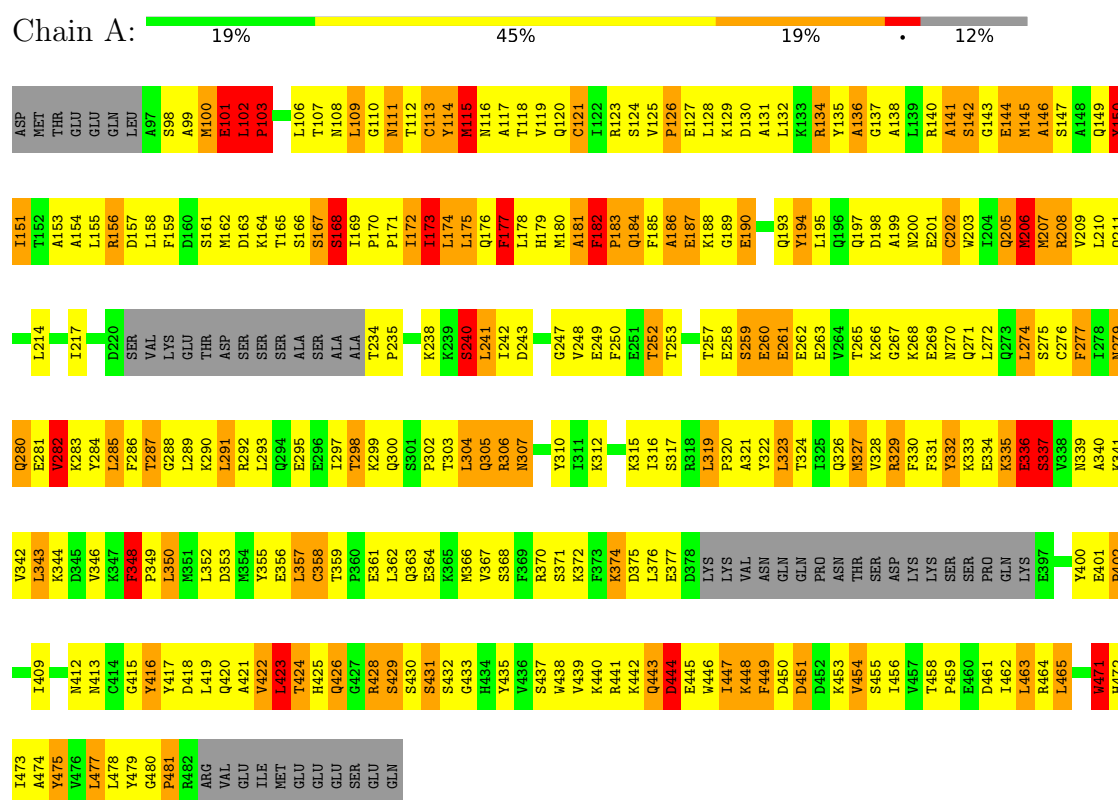
Chain	Residue	Modelled	Actual	Comment	Reference
B	76	GLZ	GLY	modified residue	UNP P62988

3 Residue-property plots

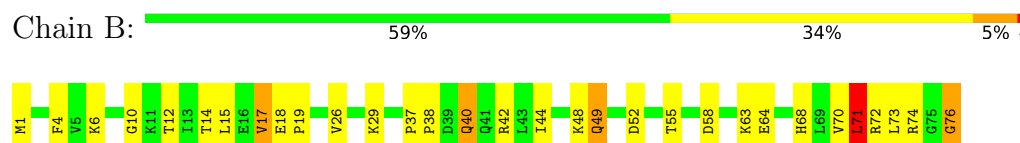
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 14



- Molecule 2: Ubiquitin



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.93Å 183.93Å 45.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (99.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.290 , 0.330	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3411	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.78	2/2860 (0.1%)	1.39	49/3852 (1.3%)
2	B	0.61	0/603	1.10	4/811 (0.5%)
All	All	0.76	2/3463 (0.1%)	1.34	53/4663 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	LEU	CA-C	6.32	1.60	1.52
1	A	422	VAL	CA-CB	-5.49	1.47	1.54

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	LEU	N-CA-C	11.43	135.07	109.81
1	A	101	GLU	N-CA-C	11.42	127.36	110.46
2	B	52	ASP	N-CA-C	10.20	124.81	111.75
1	A	102	LEU	CA-C-N	10.11	132.48	119.84
1	A	102	LEU	C-N-CA	10.11	132.48	119.84
1	A	350	LEU	N-CA-C	-9.49	101.84	113.41
1	A	182	PHE	CA-C-N	8.74	128.47	119.56
1	A	182	PHE	C-N-CA	8.74	128.47	119.56
1	A	177	PHE	N-CA-C	-8.51	101.22	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	PRO	N-CA-C	8.38	129.74	112.47
1	A	423	LEU	N-CA-C	-8.12	96.23	108.99
1	A	150	TYR	N-CA-C	7.87	119.64	111.14
1	A	475	TYR	N-CA-C	-7.79	105.75	114.62
1	A	277	PHE	N-CA-C	7.68	120.49	110.43
1	A	402	PRO	N-CA-CB	7.39	111.01	103.25
1	A	279	ASN	N-CA-C	-7.37	97.38	109.40
1	A	183	PRO	N-CA-C	7.06	123.02	113.84
1	A	447	ILE	N-CA-C	6.94	119.42	108.87
1	A	348	PHE	CA-C-N	6.88	126.84	120.03
1	A	348	PHE	C-N-CA	6.88	126.84	120.03
1	A	136	ALA	N-CA-C	6.86	119.60	109.24
1	A	121	CYS	N-CA-C	-6.79	103.49	111.03
1	A	336	GLU	N-CA-C	6.61	119.23	108.26
1	A	113	CYS	N-CA-C	-6.52	104.21	111.71
1	A	465	LEU	N-CA-C	-6.37	105.47	113.18
1	A	480	GLY	CA-C-N	6.31	127.73	119.84
1	A	480	GLY	C-N-CA	6.31	127.73	119.84
2	B	49	GLN	N-CA-C	-6.31	99.36	109.96
1	A	402	PRO	N-CA-C	-6.27	99.56	112.47
1	A	448	LYS	N-CA-C	6.13	117.82	109.11
1	A	282	VAL	CB-CA-C	-5.87	103.52	111.15
1	A	300	GLN	N-CA-C	-5.84	101.00	109.59
1	A	176	GLN	N-CA-C	-5.79	105.71	112.89
1	A	334	GLU	N-CA-C	5.79	118.19	108.23
1	A	100	MET	N-CA-C	-5.78	100.56	109.52
1	A	206	MET	N-CA-C	-5.76	105.00	111.28
1	A	477	LEU	N-CA-C	-5.69	101.32	110.14
1	A	400	TYR	N-CA-C	5.63	119.73	112.41
1	A	115	MET	N-CA-C	-5.60	105.07	111.07
1	A	424	THR	N-CA-C	5.58	116.56	107.23
1	A	433	GLY	N-CA-C	5.53	118.65	110.63
1	A	265	THR	N-CA-C	5.49	117.17	108.67
1	A	447	ILE	CB-CA-C	-5.40	103.81	111.21
2	B	71	LEU	CB-CA-C	-5.37	109.34	117.07
1	A	319	LEU	N-CA-C	5.34	117.33	110.39
1	A	335	LYS	N-CA-C	-5.32	99.47	110.80
1	A	343	LEU	N-CA-C	5.31	119.45	111.81
1	A	305	GLN	N-CA-C	5.22	117.02	110.91
1	A	374	LYS	N-CA-C	-5.21	106.42	112.89
1	A	180	MET	N-CA-C	-5.15	105.36	110.97
2	B	17	VAL	N-CA-C	5.06	115.98	108.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	ARG	N-CA-C	5.05	114.70	108.19
1	A	141	ALA	N-CA-C	5.04	116.73	108.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2810	0	2766	433	0
2	B	601	0	630	61	0
All	All	3411	0	3396	446	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 66.

All (446) 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:319:LEU:O	1:A:412:ASN:HB3	1.37	1.24
1:A:203:TRP:NE1	1:A:207:MET:HE2	1.59	1.17
1:A:424:THR:HG21	1:A:472:HIS:HB3	1.24	1.17
1:A:292:ARG:NH2	2:B:68:HIS:CE1	2.19	1.11
1:A:282:VAL:HG13	1:A:287:THR:HB	1.25	1.10
1:A:238:LYS:NZ	1:A:412:ASN:HD21	1.50	1.09
1:A:203:TRP:HE1	1:A:207:MET:CE	1.64	1.08
1:A:165:THR:HG22	1:A:166:SER:N	1.66	1.07
1:A:165:THR:CG2	1:A:166:SER:H	1.68	1.06
1:A:165:THR:HG22	1:A:166:SER:H	0.93	1.03
2:B:15:LEU:HD11	2:B:29:LYS:HB3	1.40	1.02
1:A:115:MET:HE1	1:A:174:LEU:HD11	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:TRP:HE1	1:A:207:MET:HE2	0.81	0.98
1:A:280:GLN:HE22	1:A:344:LYS:HD3	1.28	0.98
1:A:359:THR:O	1:A:363:GLN:HG3	1.65	0.96
1:A:292:ARG:HG3	2:B:6:LYS:NZ	1.81	0.96
1:A:443:GLN:O	1:A:444:ASP:HB2	1.65	0.96
1:A:113:CYS:SG	2:B:76:GLZ:C	2.55	0.94
1:A:199:ALA:HB2	1:A:435:TYR:CE1	2.02	0.94
1:A:292:ARG:HH22	2:B:68:HIS:CE1	1.83	0.91
1:A:292:ARG:NE	2:B:6:LYS:HZ3	1.68	0.91
1:A:307:ASN:HD22	1:A:307:ASN:H	1.14	0.91
1:A:114:TYR:CD2	1:A:115:MET:N	2.40	0.89
1:A:115:MET:HE1	1:A:174:LEU:CD1	2.02	0.89
1:A:367:VAL:O	1:A:371:SER:HB2	1.73	0.88
1:A:292:ARG:NH2	2:B:68:HIS:ND1	2.21	0.88
1:A:424:THR:CG2	1:A:472:HIS:HB3	2.03	0.88
1:A:292:ARG:HE	2:B:6:LYS:NZ	1.71	0.88
1:A:426:GLN:HB3	1:A:472:HIS:ND1	1.89	0.87
1:A:165:THR:HG22	1:A:167:SER:H	1.39	0.87
1:A:292:ARG:HG3	2:B:6:LYS:HZ1	1.39	0.87
1:A:131:ALA:HB1	1:A:214:LEU:HD22	1.55	0.87
1:A:277:PHE:HE1	1:A:292:ARG:HD2	1.39	0.86
1:A:175:LEU:HD12	1:A:175:LEU:O	1.76	0.86
1:A:292:ARG:HE	2:B:6:LYS:HZ3	0.85	0.85
1:A:277:PHE:CE1	1:A:292:ARG:HD2	2.12	0.85
1:A:292:ARG:HG3	2:B:6:LYS:CE	2.07	0.84
1:A:442:LYS:HD3	1:A:445:GLU:OE1	1.76	0.84
1:A:298:THR:O	2:B:14:THR:HG21	1.77	0.83
1:A:352:LEU:HB3	1:A:417:TYR:HB2	1.61	0.82
1:A:316:ILE:HG21	1:A:319:LEU:HD21	1.62	0.81
1:A:275:SER:HB2	1:A:292:ARG:HH11	1.45	0.81
1:A:124:SER:O	1:A:126:PRO:HD3	1.80	0.81
1:A:238:LYS:NZ	1:A:412:ASN:ND2	2.29	0.81
1:A:154:ALA:HB2	1:A:177:PHE:HD1	1.46	0.80
1:A:115:MET:CE	1:A:174:LEU:HD11	2.11	0.80
2:B:15:LEU:HD11	2:B:29:LYS:CB	2.12	0.80
1:A:430:SER:O	1:A:431:SER:HB2	1.78	0.80
1:A:101:GLU:C	1:A:102:LEU:HG	2.07	0.80
1:A:238:LYS:HZ2	1:A:412:ASN:HD21	1.29	0.79
1:A:102:LEU:CD1	1:A:103:PRO:HD3	2.13	0.79
1:A:441:ARG:O	1:A:442:LYS:HG3	1.83	0.79
1:A:123:ARG:HH21	1:A:162:MET:HB3	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:O	1:A:174:LEU:HD22	1.85	0.77
1:A:283:LYS:HA	1:A:283:LYS:HE2	1.65	0.77
1:A:425:HIS:HB2	1:A:435:TYR:CE2	2.20	0.76
1:A:173:ILE:HG13	1:A:174:LEU:H	1.50	0.76
1:A:293:LEU:HD11	1:A:357:LEU:HD21	1.65	0.76
1:A:250:PHE:O	1:A:268:LYS:HG2	1.86	0.76
1:A:114:TYR:HD2	1:A:115:MET:N	1.82	0.75
1:A:154:ALA:HB2	1:A:177:PHE:CD1	2.21	0.75
1:A:259:SER:O	1:A:261:GLU:N	2.19	0.75
1:A:316:ILE:HG21	1:A:319:LEU:CD2	2.15	0.75
1:A:103:PRO:HB3	1:A:454:VAL:HG11	1.66	0.75
1:A:165:THR:HG22	1:A:167:SER:N	2.02	0.74
1:A:292:ARG:HG3	2:B:6:LYS:HE2	1.69	0.73
1:A:292:ARG:HH21	2:B:68:HIS:CE1	2.02	0.73
1:A:350:LEU:HD21	1:A:463:LEU:HD11	1.70	0.73
1:A:292:ARG:CG	2:B:6:LYS:NZ	2.52	0.73
1:A:319:LEU:O	1:A:412:ASN:CB	2.30	0.73
1:A:197:GLN:NE2	2:B:74:ARG:HH12	1.86	0.72
1:A:199:ALA:HB2	1:A:435:TYR:CD1	2.24	0.72
1:A:238:LYS:HZ1	1:A:412:ASN:HD21	1.36	0.72
1:A:307:ASN:H	1:A:307:ASN:ND2	1.86	0.72
1:A:199:ALA:CB	1:A:435:TYR:CE1	2.72	0.72
1:A:292:ARG:CG	2:B:6:LYS:HZ1	2.03	0.72
1:A:350:LEU:HD11	1:A:463:LEU:HD11	1.72	0.71
1:A:111:ASN:CA	2:B:76:GLZ:HA1	2.20	0.71
1:A:422:VAL:HG12	1:A:423:LEU:N	2.05	0.71
1:A:115:MET:O	1:A:119:VAL:HG23	1.92	0.70
1:A:200:ASN:HB2	1:A:475:TYR:HE2	1.55	0.70
1:A:343:LEU:O	1:A:343:LEU:HG	1.91	0.69
1:A:352:LEU:HD23	1:A:417:TYR:HD1	1.58	0.69
1:A:193:GLN:O	1:A:194:TYR:HB2	1.92	0.69
1:A:425:HIS:CD2	1:A:435:TYR:HE2	2.11	0.69
1:A:448:LYS:HG2	1:A:448:LYS:O	1.91	0.69
1:A:426:GLN:HG2	1:A:472:HIS:CE1	2.28	0.68
1:A:275:SER:HB2	1:A:292:ARG:NH1	2.08	0.68
1:A:330:PHE:N	1:A:342:VAL:HG23	2.07	0.68
1:A:127:GLU:HG2	1:A:322:TYR:OH	1.92	0.68
1:A:331:PHE:O	1:A:340:ALA:HB3	1.94	0.68
1:A:158:LEU:HD12	1:A:173:ILE:HD11	1.76	0.68
1:A:363:GLN:O	1:A:367:VAL:HG23	1.93	0.68
1:A:234:THR:HB	1:A:235:PRO:HD3	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:CYS:HA	1:A:116:ASN:HD22	1.61	0.66
1:A:111:ASN:HA	2:B:76:GLZ:HA1	1.75	0.66
1:A:290:LYS:C	1:A:292:ARG:H	2.04	0.66
1:A:242:ILE:CG2	1:A:272:LEU:HD21	2.26	0.66
1:A:326:GLN:HG2	1:A:326:GLN:O	1.94	0.65
1:A:446:TRP:CD1	1:A:462:ILE:HD11	2.31	0.65
1:A:295:GLU:OE2	1:A:312:LYS:HD2	1.97	0.65
1:A:120:GLN:CD	1:A:449:PHE:HD2	2.04	0.65
1:A:286:PHE:CZ	1:A:357:LEU:HD12	2.32	0.65
1:A:317:SER:O	1:A:362:LEU:HD12	1.96	0.65
1:A:249:GLU:O	1:A:250:PHE:HD2	1.79	0.64
1:A:102:LEU:HD13	1:A:103:PRO:HD3	1.78	0.64
1:A:140:ARG:HB2	1:A:149:GLN:NE2	2.13	0.64
1:A:366:MET:HE2	1:A:415:GLY:H	1.62	0.64
1:A:183:PRO:O	1:A:185:PHE:N	2.31	0.63
1:A:286:PHE:HA	1:A:289:LEU:HD12	1.78	0.63
1:A:475:TYR:CE1	2:B:73:LEU:HD12	2.33	0.63
1:A:307:ASN:HD22	1:A:307:ASN:N	1.91	0.63
1:A:143:GLY:O	1:A:144:GLU:HB2	1.99	0.63
1:A:435:TYR:OH	2:B:73:LEU:O	2.13	0.63
1:A:475:TYR:CD1	2:B:73:LEU:HD12	2.32	0.63
1:A:113:CYS:N	2:B:76:GLZ:O	2.30	0.63
1:A:206:MET:O	1:A:209:VAL:HG23	1.99	0.63
1:A:140:ARG:HB2	1:A:149:GLN:HE21	1.64	0.63
1:A:207:MET:HG3	1:A:242:ILE:HD13	1.79	0.63
1:A:114:TYR:HA	1:A:435:TYR:HD1	1.63	0.62
1:A:138:ALA:C	1:A:140:ARG:H	2.05	0.62
1:A:280:GLN:HE22	1:A:344:LYS:CD	2.07	0.62
1:A:286:PHE:O	1:A:289:LEU:HB2	1.98	0.62
1:A:123:ARG:HG2	1:A:123:ARG:HH11	1.65	0.62
1:A:329:ARG:HG2	1:A:342:VAL:O	1.99	0.62
1:A:330:PHE:CE2	2:B:70:VAL:HG13	2.35	0.62
1:A:366:MET:O	1:A:370:ARG:HB3	2.00	0.62
1:A:153:ALA:HA	1:A:156:ARG:HE	1.64	0.62
1:A:238:LYS:HZ2	1:A:412:ASN:ND2	1.95	0.62
1:A:185:PHE:O	1:A:186:ALA:HB2	1.99	0.61
1:A:279:ASN:C	1:A:281:GLU:H	2.08	0.61
1:A:353:ASP:CG	1:A:370:ARG:HH21	2.08	0.61
1:A:199:ALA:N	1:A:435:TYR:HE1	1.99	0.61
1:A:339:ASN:OD1	2:B:40:GLN:NE2	2.34	0.61
1:A:258:GLU:O	1:A:260:GLU:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ILE:CG1	1:A:174:LEU:H	2.14	0.61
1:A:165:THR:CG2	1:A:167:SER:H	2.09	0.60
1:A:280:GLN:NE2	1:A:344:LYS:HD3	2.09	0.60
1:A:307:ASN:ND2	1:A:307:ASN:N	2.47	0.60
1:A:440:LYS:HD2	1:A:446:TRP:CZ3	2.36	0.60
1:A:339:ASN:O	1:A:429:SER:HB3	2.02	0.59
1:A:173:ILE:O	1:A:177:PHE:HB2	2.03	0.59
1:A:141:ALA:O	1:A:142:SER:HB3	2.02	0.59
1:A:422:VAL:HG12	1:A:423:LEU:H	1.66	0.59
1:A:175:LEU:HD12	1:A:175:LEU:C	2.27	0.59
1:A:370:ARG:O	1:A:374:LYS:HB2	2.01	0.59
1:A:175:LEU:CD1	1:A:179:HIS:ND1	2.66	0.59
1:A:168:SER:O	1:A:170:PRO:HD3	2.03	0.59
1:A:199:ALA:H	1:A:435:TYR:HE1	1.48	0.58
1:A:113:CYS:SG	2:B:76:GLZ:CA	2.91	0.58
1:A:174:LEU:HD22	1:A:174:LEU:C	2.28	0.58
1:A:291:LEU:N	1:A:291:LEU:HD12	2.17	0.58
1:A:179:HIS:CD2	1:A:185:PHE:O	2.55	0.58
1:A:275:SER:CB	1:A:292:ARG:NH1	2.66	0.58
1:A:128:LEU:O	1:A:131:ALA:HB3	2.02	0.58
1:A:118:THR:HG21	1:A:202:CYS:SG	2.44	0.58
1:A:303:THR:O	1:A:304:LEU:HG	2.04	0.58
1:A:198:ASP:CB	2:B:72:ARG:HG2	2.33	0.57
1:A:108:ASN:OD1	1:A:108:ASN:C	2.47	0.57
1:A:329:ARG:HG2	1:A:329:ARG:NH1	2.18	0.57
2:B:17:VAL:HG12	2:B:29:LYS:HE3	1.85	0.57
1:A:299:LYS:HD2	1:A:310:TYR:CD2	2.40	0.57
1:A:329:ARG:NH1	1:A:342:VAL:O	2.37	0.57
1:A:208:ARG:HG2	2:B:48:LYS:CD	2.34	0.57
1:A:165:THR:HG21	1:A:167:SER:OG	2.05	0.57
1:A:428:ARG:O	1:A:429:SER:C	2.48	0.57
1:A:458:THR:O	1:A:461:ASP:HB2	2.03	0.57
1:A:446:TRP:CD1	1:A:462:ILE:CD1	2.87	0.57
1:A:419:LEU:HD12	1:A:420:GLN:H	1.70	0.57
1:A:178:LEU:O	1:A:181:ALA:HB3	2.04	0.56
1:A:183:PRO:O	1:A:184:GLN:C	2.48	0.56
1:A:199:ALA:HB2	1:A:435:TYR:HE1	1.64	0.56
1:A:282:VAL:HG11	1:A:288:GLY:N	2.20	0.56
1:A:359:THR:C	1:A:363:GLN:HE21	2.13	0.56
1:A:438:TRP:CD1	1:A:438:TRP:N	2.73	0.56
1:A:447:ILE:HG21	1:A:449:PHE:HE1	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:PRO:O	1:A:417:TYR:OH	2.18	0.56
1:A:183:PRO:C	1:A:185:PHE:N	2.63	0.56
1:A:329:ARG:HG2	1:A:329:ARG:HH11	1.70	0.56
1:A:425:HIS:ND1	1:A:425:HIS:C	2.64	0.56
1:A:150:TYR:HD1	1:A:151:ILE:N	2.04	0.56
1:A:203:TRP:CD1	1:A:207:MET:HE2	2.40	0.56
1:A:422:VAL:CG1	1:A:423:LEU:N	2.69	0.56
1:A:121:CYS:SG	1:A:423:LEU:HD23	2.45	0.56
1:A:287:THR:O	1:A:291:LEU:HD13	2.06	0.56
1:A:362:LEU:HD23	1:A:362:LEU:C	2.31	0.56
1:A:368:SER:O	1:A:372:LYS:CB	2.54	0.55
1:A:420:GLN:OE1	1:A:478:LEU:HD23	2.06	0.55
1:A:150:TYR:HB2	1:A:177:PHE:CZ	2.41	0.55
1:A:282:VAL:O	1:A:283:LYS:CE	2.54	0.55
1:A:121:CYS:O	1:A:124:SER:OG	2.17	0.55
1:A:174:LEU:O	1:A:178:LEU:N	2.39	0.55
1:A:442:LYS:HB2	1:A:445:GLU:HB2	1.87	0.55
1:A:259:SER:O	1:A:260:GLU:C	2.50	0.55
1:A:329:ARG:HA	1:A:342:VAL:HB	1.88	0.55
1:A:162:MET:HA	1:A:169:ILE:CD1	2.37	0.55
1:A:364:GLU:HA	1:A:367:VAL:HG23	1.89	0.55
1:A:366:MET:CE	1:A:415:GLY:O	2.55	0.55
1:A:450:ASP:O	1:A:451:ASP:C	2.50	0.55
1:A:115:MET:HE3	1:A:178:LEU:CD2	2.37	0.54
1:A:153:ALA:O	1:A:156:ARG:N	2.41	0.54
1:A:248:VAL:HG12	1:A:320:PRO:HD3	1.89	0.54
1:A:257:THR:O	1:A:257:THR:HG22	2.08	0.54
1:A:252:THR:O	1:A:267:GLY:N	2.41	0.54
1:A:282:VAL:HG11	1:A:288:GLY:H	1.73	0.54
1:A:425:HIS:CD2	1:A:435:TYR:CE2	2.94	0.54
1:A:252:THR:O	1:A:266:LYS:HA	2.07	0.54
1:A:425:HIS:HD2	1:A:435:TYR:HE2	1.52	0.54
1:A:116:ASN:O	1:A:120:GLN:HG3	2.07	0.54
1:A:282:VAL:O	1:A:283:LYS:HE2	2.08	0.54
1:A:299:LYS:HD2	1:A:310:TYR:CE2	2.42	0.54
1:A:114:TYR:HE1	1:A:197:GLN:H	1.54	0.54
1:A:290:LYS:O	1:A:292:ARG:N	2.41	0.54
1:A:447:ILE:HG21	1:A:449:PHE:CE1	2.43	0.54
1:A:471:TRP:CG	1:A:472:HIS:H	2.26	0.54
1:A:102:LEU:HB2	1:A:103:PRO:HD3	1.89	0.54
1:A:103:PRO:HB3	1:A:454:VAL:CG1	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:HIS:NE2	1:A:185:PHE:O	2.41	0.54
1:A:343:LEU:H	1:A:343:LEU:HD23	1.73	0.54
1:A:442:LYS:O	1:A:444:ASP:N	2.40	0.54
1:A:240:SER:OG	1:A:243:ASP:HB2	2.08	0.53
1:A:364:GLU:O	1:A:367:VAL:HB	2.09	0.53
1:A:205:GLN:O	1:A:209:VAL:HG22	2.08	0.53
1:A:211:GLN:N	1:A:242:ILE:HD12	2.23	0.53
1:A:366:MET:O	1:A:370:ARG:CB	2.57	0.53
2:B:63:LYS:O	2:B:64:GLU:HB2	2.09	0.53
1:A:119:VAL:HG12	1:A:119:VAL:O	2.09	0.53
1:A:331:PHE:CD2	1:A:342:VAL:HG22	2.43	0.53
1:A:199:ALA:CB	1:A:435:TYR:HE1	2.19	0.53
1:A:120:GLN:NE2	1:A:449:PHE:CD2	2.77	0.53
1:A:242:ILE:HG22	1:A:272:LEU:HD21	1.90	0.53
1:A:422:VAL:CG1	1:A:423:LEU:H	2.22	0.53
1:A:450:ASP:HB3	1:A:453:LYS:HB2	1.91	0.53
1:A:102:LEU:CB	1:A:103:PRO:HD3	2.39	0.52
1:A:290:LYS:C	1:A:292:ARG:N	2.68	0.52
1:A:348:PHE:N	1:A:348:PHE:CD1	2.78	0.52
1:A:297:ILE:HD11	1:A:312:LYS:HE3	1.92	0.52
1:A:123:ARG:HH21	1:A:162:MET:CB	2.22	0.52
1:A:275:SER:OG	1:A:292:ARG:NH1	2.43	0.52
1:A:284:TYR:O	1:A:285:LEU:C	2.51	0.52
1:A:114:TYR:CD2	1:A:114:TYR:C	2.87	0.51
1:A:210:LEU:HD22	1:A:214:LEU:HD11	1.92	0.51
1:A:189:GLY:O	1:A:190:GLU:C	2.53	0.51
1:A:439:VAL:HG12	1:A:440:LYS:N	2.24	0.51
1:A:366:MET:CE	1:A:415:GLY:H	2.23	0.51
1:A:355:TYR:CE1	1:A:363:GLN:HB3	2.45	0.51
1:A:366:MET:O	1:A:370:ARG:N	2.43	0.51
1:A:115:MET:HE3	1:A:178:LEU:HD22	1.92	0.51
1:A:137:GLY:N	1:A:156:ARG:HH22	2.09	0.51
2:B:42:ARG:HB2	2:B:70:VAL:O	2.11	0.51
1:A:352:LEU:HB3	1:A:417:TYR:CB	2.37	0.51
1:A:353:ASP:OD2	1:A:370:ARG:NH2	2.44	0.51
1:A:425:HIS:C	1:A:425:HIS:HD1	2.19	0.51
1:A:240:SER:O	1:A:241:LEU:C	2.53	0.51
1:A:258:GLU:O	1:A:260:GLU:HB3	2.11	0.51
2:B:42:ARG:HD2	2:B:49:GLN:OE1	2.11	0.51
1:A:102:LEU:HD12	1:A:103:PRO:HD3	1.90	0.50
1:A:249:GLU:HG2	1:A:270:ASN:OD1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASP:O	1:A:134:ARG:HG2	2.11	0.50
1:A:475:TYR:CE1	2:B:73:LEU:CD1	2.95	0.50
1:A:125:VAL:O	1:A:128:LEU:HB3	2.11	0.50
1:A:320:PRO:HG2	1:A:323:LEU:HD12	1.93	0.50
1:A:198:ASP:OD1	1:A:198:ASP:C	2.54	0.50
1:A:108:ASN:OD1	1:A:109:LEU:N	2.44	0.50
1:A:279:ASN:C	1:A:281:GLU:N	2.68	0.50
1:A:279:ASN:O	1:A:281:GLU:N	2.45	0.50
1:A:330:PHE:N	1:A:342:VAL:CG2	2.74	0.50
1:A:153:ALA:CA	1:A:156:ARG:HE	2.24	0.49
1:A:172:ILE:HG13	1:A:173:ILE:H	1.77	0.49
1:A:117:ALA:O	1:A:118:THR:C	2.55	0.49
1:A:185:PHE:N	1:A:185:PHE:CD2	2.79	0.49
1:A:260:GLU:O	1:A:261:GLU:CB	2.61	0.49
1:A:290:LYS:HA	1:A:293:LEU:CD1	2.43	0.49
1:A:252:THR:CG2	1:A:267:GLY:O	2.61	0.49
1:A:315:LYS:HD3	1:A:358:CYS:O	2.12	0.49
1:A:336:GLU:O	1:A:337:SER:HB2	2.12	0.49
1:A:137:GLY:CA	1:A:140:ARG:HD2	2.43	0.49
1:A:252:THR:HG22	1:A:267:GLY:O	2.13	0.49
1:A:253:THR:HG22	1:A:266:LYS:HD3	1.94	0.49
1:A:299:LYS:O	1:A:307:ASN:HA	2.13	0.49
1:A:329:ARG:CA	1:A:342:VAL:HB	2.43	0.49
1:A:138:ALA:C	1:A:140:ARG:N	2.70	0.49
1:A:182:PHE:CE1	1:A:205:GLN:HG2	2.47	0.49
1:A:137:GLY:HA3	1:A:140:ARG:HD2	1.95	0.48
1:A:198:ASP:HB3	2:B:72:ARG:HG2	1.94	0.48
1:A:291:LEU:H	1:A:291:LEU:CD1	2.26	0.48
1:A:419:LEU:HA	1:A:479:TYR:CD2	2.48	0.48
1:A:326:GLN:HE22	2:B:70:VAL:HG21	1.78	0.48
1:A:108:ASN:OD1	1:A:110:GLY:N	2.31	0.48
1:A:277:PHE:CE2	2:B:10:GLY:HA2	2.48	0.48
1:A:141:ALA:O	1:A:142:SER:CB	2.61	0.48
1:A:247:GLY:O	1:A:320:PRO:HG3	2.13	0.48
1:A:366:MET:HE1	1:A:415:GLY:O	2.13	0.48
1:A:199:ALA:O	1:A:202:CYS:HB3	2.14	0.48
1:A:181:ALA:O	1:A:183:PRO:HD3	2.13	0.48
1:A:208:ARG:HG2	2:B:48:LYS:HD3	1.95	0.48
1:A:368:SER:O	1:A:372:LYS:HB3	2.13	0.48
1:A:145:MET:O	1:A:146:ALA:HB2	2.12	0.48
1:A:201:GLU:OE2	2:B:72:ARG:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:HD22	1:A:323:LEU:HD21	1.96	0.48
1:A:285:LEU:O	1:A:286:PHE:C	2.57	0.48
1:A:290:LYS:HA	1:A:293:LEU:HD12	1.95	0.48
1:A:298:THR:CG2	1:A:307:ASN:HB3	2.44	0.48
1:A:425:HIS:HD2	1:A:435:TYR:CE2	2.30	0.47
1:A:426:GLN:HB3	1:A:472:HIS:HA	1.96	0.47
1:A:106:LEU:HD21	1:A:162:MET:SD	2.54	0.47
1:A:353:ASP:OD1	1:A:370:ARG:NH2	2.47	0.47
1:A:364:GLU:HA	1:A:367:VAL:CG2	2.44	0.47
1:A:120:GLN:CD	1:A:449:PHE:CD2	2.89	0.47
1:A:291:LEU:N	1:A:291:LEU:CD1	2.76	0.47
1:A:103:PRO:CB	1:A:454:VAL:HG11	2.41	0.47
1:A:287:THR:HG22	1:A:291:LEU:HD11	1.95	0.47
1:A:321:ALA:HA	1:A:413:ASN:HB2	1.95	0.47
1:A:114:TYR:HA	1:A:435:TYR:CD1	2.47	0.47
1:A:163:ASP:C	1:A:164:LYS:HG3	2.40	0.47
1:A:329:ARG:HB3	1:A:342:VAL:H	1.80	0.47
1:A:332:TYR:CD1	1:A:332:TYR:C	2.93	0.47
1:A:447:ILE:HG22	1:A:448:LYS:N	2.29	0.47
2:B:15:LEU:CD2	2:B:26:VAL:HG13	2.44	0.47
1:A:171:PRO:HB3	1:A:174:LEU:HD12	1.96	0.47
1:A:170:PRO:O	1:A:172:ILE:HG12	2.15	0.47
1:A:462:ILE:C	1:A:464:ARG:H	2.23	0.47
1:A:471:TRP:CG	1:A:472:HIS:N	2.81	0.47
1:A:112:THR:O	1:A:116:ASN:ND2	2.47	0.47
1:A:361:GLU:O	1:A:364:GLU:HB2	2.14	0.47
1:A:416:TYR:CD1	1:A:416:TYR:N	2.82	0.47
1:A:143:GLY:O	1:A:144:GLU:CB	2.61	0.46
1:A:249:GLU:C	1:A:317:SER:HB3	2.41	0.46
1:A:280:GLN:NE2	1:A:344:LYS:CD	2.75	0.46
1:A:282:VAL:O	1:A:283:LYS:HE3	2.14	0.46
1:A:316:ILE:HG21	1:A:319:LEU:HD23	1.94	0.46
1:A:242:ILE:CG2	1:A:272:LEU:CD2	2.94	0.46
1:A:141:ALA:CB	1:A:150:TYR:HD2	2.29	0.46
1:A:197:GLN:NE2	2:B:74:ARG:NH1	2.62	0.46
1:A:368:SER:O	1:A:372:LYS:HB2	2.15	0.46
1:A:474:ALA:HB1	1:A:477:LEU:HD21	1.98	0.46
1:A:174:LEU:O	1:A:178:LEU:CB	2.64	0.46
1:A:355:TYR:O	1:A:357:LEU:N	2.43	0.46
1:A:113:CYS:O	1:A:117:ALA:N	2.32	0.46
1:A:444:ASP:O	1:A:459:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:PRO:O	1:A:462:ILE:N	2.48	0.46
1:A:173:ILE:HG13	1:A:174:LEU:N	2.23	0.46
1:A:292:ARG:NH2	2:B:68:HIS:HD1	2.09	0.46
1:A:150:TYR:O	1:A:153:ALA:N	2.46	0.45
1:A:440:LYS:HD2	1:A:446:TRP:CH2	2.51	0.45
1:A:107:THR:CB	1:A:170:PRO:HG3	2.46	0.45
1:A:117:ALA:HA	1:A:437:SER:HB2	1.98	0.45
1:A:185:PHE:O	1:A:186:ALA:CB	2.64	0.45
1:A:162:MET:HA	1:A:169:ILE:HD11	1.97	0.45
1:A:353:ASP:CG	1:A:370:ARG:NH2	2.73	0.45
1:A:422:VAL:HG11	1:A:465:LEU:HD13	1.98	0.45
1:A:129:LYS:O	1:A:132:LEU:N	2.48	0.45
1:A:167:SER:OG	1:A:168:SER:N	2.48	0.45
1:A:206:MET:O	1:A:209:VAL:CG2	2.64	0.45
1:A:107:THR:HB	1:A:170:PRO:HG3	1.97	0.45
1:A:298:THR:O	2:B:14:THR:CG2	2.59	0.45
1:A:150:TYR:HD1	1:A:151:ILE:H	1.64	0.45
1:A:162:MET:HA	1:A:169:ILE:HD12	1.98	0.45
1:A:262:GLU:O	1:A:263:GLU:C	2.59	0.45
1:A:280:GLN:NE2	1:A:344:LYS:NZ	2.64	0.45
1:A:328:VAL:HG12	1:A:328:VAL:O	2.16	0.45
1:A:173:ILE:O	1:A:177:PHE:N	2.45	0.45
1:A:120:GLN:HA	1:A:123:ARG:HB2	1.99	0.45
1:A:208:ARG:HG2	2:B:48:LYS:HZ3	1.82	0.45
1:A:355:TYR:C	1:A:357:LEU:H	2.24	0.44
1:A:359:THR:HG22	1:A:361:GLU:H	1.82	0.44
1:A:161:SER:OG	1:A:169:ILE:HD13	2.17	0.44
1:A:200:ASN:HB2	1:A:475:TYR:CE2	2.45	0.44
1:A:111:ASN:HA	2:B:76:GLZ:CA	2.44	0.44
1:A:330:PHE:HE2	2:B:70:VAL:HG13	1.80	0.44
1:A:425:HIS:HB2	1:A:435:TYR:HE2	1.77	0.44
1:A:282:VAL:CG1	1:A:288:GLY:N	2.80	0.44
1:A:352:LEU:HD23	1:A:417:TYR:CD1	2.45	0.44
1:A:366:MET:HE2	1:A:415:GLY:N	2.31	0.44
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.82	0.44
1:A:428:ARG:O	1:A:429:SER:O	2.36	0.43
1:A:118:THR:HG22	1:A:206:MET:HE2	2.00	0.43
1:A:183:PRO:C	1:A:185:PHE:H	2.25	0.43
1:A:332:TYR:C	1:A:332:TYR:HD1	2.26	0.43
1:A:198:ASP:HB2	2:B:72:ARG:HG2	2.00	0.43
1:A:426:GLN:CB	1:A:472:HIS:HA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LYS:NZ	1:A:473:ILE:HD12	2.34	0.43
1:A:277:PHE:CD2	2:B:10:GLY:HA2	2.54	0.43
1:A:439:VAL:CG1	1:A:440:LYS:N	2.82	0.43
1:A:198:ASP:OD1	1:A:200:ASN:N	2.52	0.43
1:A:286:PHE:C	1:A:286:PHE:CD2	2.97	0.43
1:A:241:LEU:HD13	1:A:241:LEU:O	2.19	0.42
2:B:4:PHE:HB3	2:B:12:THR:CG2	2.49	0.42
1:A:162:MET:C	1:A:164:LYS:H	2.27	0.42
1:A:349:PRO:HG2	1:A:352:LEU:HD12	2.01	0.42
1:A:425:HIS:HB2	1:A:435:TYR:CD2	2.54	0.42
1:A:437:SER:C	1:A:438:TRP:CD1	2.96	0.42
1:A:110:GLY:O	1:A:111:ASN:ND2	2.51	0.42
1:A:165:THR:CG2	1:A:166:SER:N	2.39	0.42
1:A:201:GLU:HG3	2:B:49:GLN:OE1	2.19	0.42
2:B:37:PRO:HA	2:B:38:PRO:HD3	1.90	0.42
1:A:111:ASN:C	2:B:76:GLZ:HA1	2.44	0.42
1:A:362:LEU:C	1:A:364:GLU:N	2.75	0.42
1:A:170:PRO:HA	1:A:171:PRO:HD3	1.91	0.42
1:A:252:THR:HG23	1:A:267:GLY:C	2.45	0.42
1:A:106:LEU:HD22	1:A:171:PRO:HG3	2.02	0.42
1:A:107:THR:OG1	1:A:170:PRO:HG3	2.19	0.42
1:A:136:ALA:C	1:A:156:ARG:HH22	2.28	0.42
1:A:315:LYS:HB3	1:A:358:CYS:O	2.19	0.42
1:A:113:CYS:CB	2:B:76:GLZ:O	2.67	0.42
1:A:123:ARG:HH11	1:A:123:ARG:CG	2.32	0.42
1:A:276:CYS:O	1:A:276:CYS:SG	2.77	0.42
1:A:370:ARG:O	1:A:374:LYS:CB	2.67	0.42
1:A:110:GLY:C	1:A:111:ASN:ND2	2.78	0.42
1:A:111:ASN:HA	2:B:76:GLZ:C	2.50	0.42
1:A:177:PHE:HD2	1:A:177:PHE:HA	1.71	0.42
1:A:242:ILE:O	1:A:243:ASP:C	2.63	0.42
2:B:44:ILE:HD13	2:B:49:GLN:HA	2.02	0.42
1:A:292:ARG:NH2	2:B:68:HIS:HE1	2.05	0.41
1:A:420:GLN:HB3	1:A:421:ALA:H	1.66	0.41
1:A:119:VAL:O	1:A:119:VAL:CG1	2.68	0.41
1:A:421:ALA:HB3	1:A:478:LEU:HB3	2.02	0.41
1:A:329:ARG:C	1:A:342:VAL:HG23	2.45	0.41
2:B:1:MET:HE3	2:B:19:PRO:HG3	2.02	0.41
1:A:181:ALA:HB1	1:A:182:PHE:CE2	2.56	0.41
1:A:187:GLU:HB2	1:A:195:LEU:HD12	2.01	0.41
1:A:362:LEU:C	1:A:364:GLU:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LYS:CB	1:A:445:GLU:HB2	2.50	0.41
1:A:130:ASP:OD2	1:A:130:ASP:N	2.49	0.41
1:A:151:ILE:HD11	1:A:181:ALA:CB	2.51	0.41
1:A:250:PHE:HB2	1:A:269:GLU:O	2.21	0.41
1:A:135:TYR:CD1	1:A:136:ALA:N	2.87	0.41
1:A:260:GLU:C	1:A:260:GLU:CD	2.88	0.41
1:A:321:ALA:O	1:A:481:PRO:HD3	2.21	0.41
1:A:159:PHE:C	1:A:161:SER:H	2.28	0.41
1:A:302:PRO:C	1:A:304:LEU:H	2.28	0.41
1:A:471:TRP:HA	1:A:471:TRP:CE3	2.56	0.41
1:A:210:LEU:HD22	1:A:214:LEU:CD1	2.51	0.41
1:A:260:GLU:O	1:A:261:GLU:HB3	2.21	0.41
1:A:330:PHE:HB3	2:B:71:LEU:HD22	2.03	0.41
2:B:71:LEU:HB3	2:B:72:ARG:H	1.55	0.41
1:A:258:GLU:O	1:A:259:SER:C	2.64	0.41
1:A:292:ARG:HH21	2:B:68:HIS:HE1	1.61	0.41
1:A:156:ARG:HD2	1:A:157:ASP:N	2.36	0.40
1:A:268:LYS:C	1:A:269:GLU:HG3	2.46	0.40
1:A:375:ASP:O	1:A:377:GLU:N	2.53	0.40
2:B:55:THR:O	2:B:58:ASP:HB2	2.21	0.40
1:A:159:PHE:C	1:A:161:SER:N	2.79	0.40
1:A:305:GLN:O	1:A:306:ARG:HB3	2.22	0.40
1:A:330:PHE:CA	1:A:342:VAL:HG23	2.51	0.40
1:A:182:PHE:CD1	1:A:205:GLN:HG2	2.57	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	349/404 (86%)	240 (69%)	67 (19%)	42 (12%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
All	All	423/480 (88%)	311 (74%)	70 (16%)	42 (10%)	0	6

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ALA
1	A	167	SER
1	A	168	SER
1	A	181	ALA
1	A	190	GLU
1	A	259	SER
1	A	260	GLU
1	A	261	GLU
1	A	337	SER
1	A	356	GLU
1	A	376	LEU
1	A	402	PRO
1	A	409	ILE
1	A	449	PHE
1	A	451	ASP
1	A	142	SER
1	A	144	GLU
1	A	145	MET
1	A	173	ILE
1	A	184	GLN
1	A	186	ALA
1	A	280	GLN
1	A	291	LEU
1	A	327	MET
1	A	429	SER
1	A	431	SER
1	A	443	GLN
1	A	444	ASP
1	A	463	LEU
1	A	481	PRO
1	A	102	LEU
1	A	103	PRO
1	A	187	GLU
1	A	304	LEU
1	A	335	LYS
1	A	240	SER

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Mol	Chain	Res	Type
1	A	285	LEU
1	A	306	ARG
1	A	471	TRP
1	A	194	TYR
1	A	99	ALA
1	A	401	GLU

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	305/363 (84%)	245 (80%)	60 (20%)	1	8
2	B	68/68 (100%)	65 (96%)	3 (4%)	25	51
All	All	373/431 (86%)	310 (83%)	63 (17%)	2	13

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	SER
1	A	100	MET
1	A	101	GLU
1	A	102	LEU
1	A	103	PRO
1	A	109	LEU
1	A	111	ASN
1	A	114	TYR
1	A	115	MET
1	A	126	PRO
1	A	134	ARG
1	A	147	SER
1	A	151	ILE
1	A	155	LEU
1	A	156	ARG
1	A	168	SER
1	A	172	ILE

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Mol	Chain	Res	Type
1	A	173	ILE
1	A	174	LEU
1	A	175	LEU
1	A	177	PHE
1	A	182	PHE
1	A	188	LYS
1	A	202	CYS
1	A	205	GLN
1	A	206	MET
1	A	207	MET
1	A	208	ARG
1	A	217	ILE
1	A	240	SER
1	A	241	LEU
1	A	252	THR
1	A	271	GLN
1	A	274	LEU
1	A	282	VAL
1	A	287	THR
1	A	298	THR
1	A	307	ASN
1	A	323	LEU
1	A	324	THR
1	A	327	MET
1	A	329	ARG
1	A	332	TYR
1	A	333	LYS
1	A	336	GLU
1	A	337	SER
1	A	346	VAL
1	A	348	PHE
1	A	357	LEU
1	A	358	CYS
1	A	416	TYR
1	A	418	ASP
1	A	423	LEU
1	A	426	GLN
1	A	432	SER
1	A	444	ASP
1	A	454	VAL
1	A	455	SER
1	A	456	ILE

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Mol	Chain	Res	Type
1	A	471	TRP
2	B	18	GLU
2	B	40	GLN
2	B	71	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	116	ASN
1	A	176	GLN
1	A	197	GLN
1	A	205	GLN
1	A	244	GLN
1	A	280	GLN
1	A	307	ASN
1	A	326	GLN
1	A	339	ASN
1	A	363	GLN
1	A	412	ASN
1	A	426	GLN
1	A	443	GLN
2	B	25	ASN
2	B	31	GLN
2	B	40	GLN
2	B	60	ASN
2	B	68	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLZ	B	76	2	3,3,3	2.42	1 (33%)	1,2,2	0.52	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
2	GLZ	B	76	2	-	0/0/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	76	GLZ	O-C	4.13	1.43	1.20

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	76	GLZ	9	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.