



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2025 – 08:41 PM EDT

PDB ID : 1NBF  
Title : Crystal structure of a UBP-family deubiquitinating enzyme in isolation and in complex with ubiquitin aldehyde  
Authors : Hu, M.; Li, P.; Li, M.; Li, W.; Yao, T.; Wu, J.-W.; Gu, W.; Cohen, R.E.; Shi, Y.  
Deposited on : 2002-12-02  
Resolution : 2.30 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

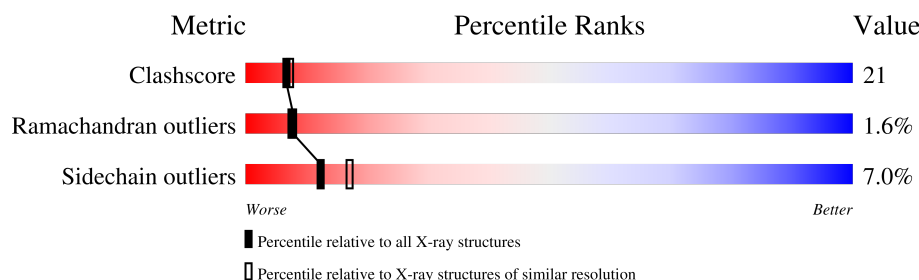
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)

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  $\geq 3$ , 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	353	 66% 27% 5% ••
1	B	353	 69% 25% ••
1	E	353	 43% 47% 6% •
2	C	76	 75% 22% •
2	D	76	 71% 26% •

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9976 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 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2820	1781	482	541	16			
1	B	347	Total	C	N	O	S	0	0	0
			2820	1781	482	541	16			
1	E	340	Total	C	N	O	S	0	0	0
			2760	1745	473	526	16			

- Molecule 2 is a protein called Ubiquitin aldehyde.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	376	GLZ	GLY	modified residue	UNP P62988
D	376	GLZ	GLY	modified residue	UNP P62988

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	139	Total	O	0	0
			139	139		
3	C	31	Total	O	0	0
			31	31		
3	D	22	Total	O	0	0
			22	22		

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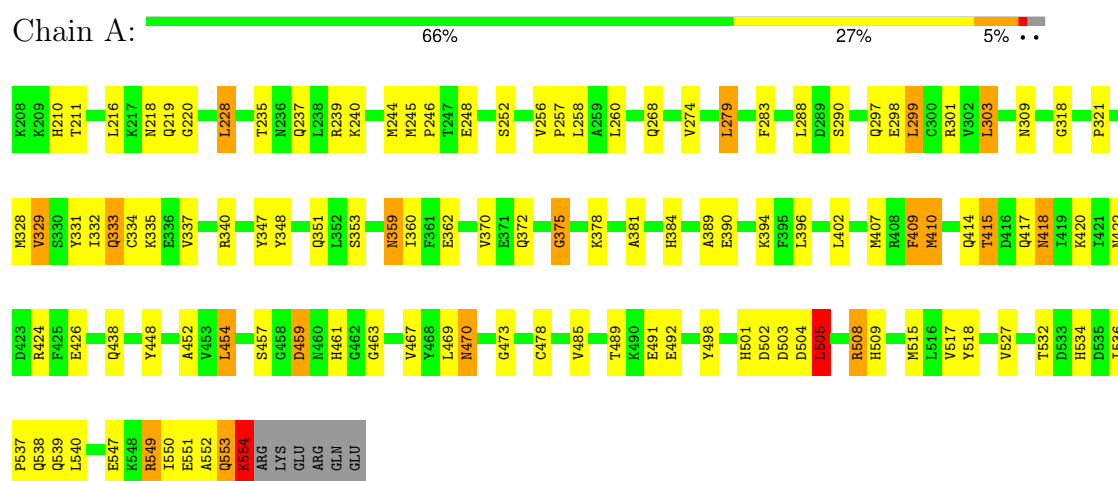
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	40	Total	O	0	0
			40	40		

### 3 Residue-property plots

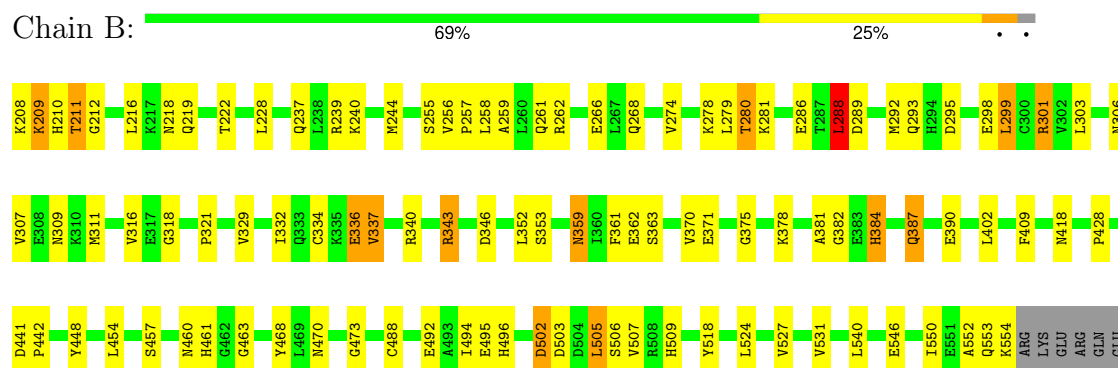
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

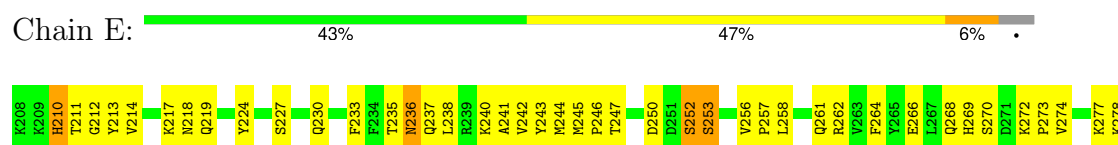
#### • Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7

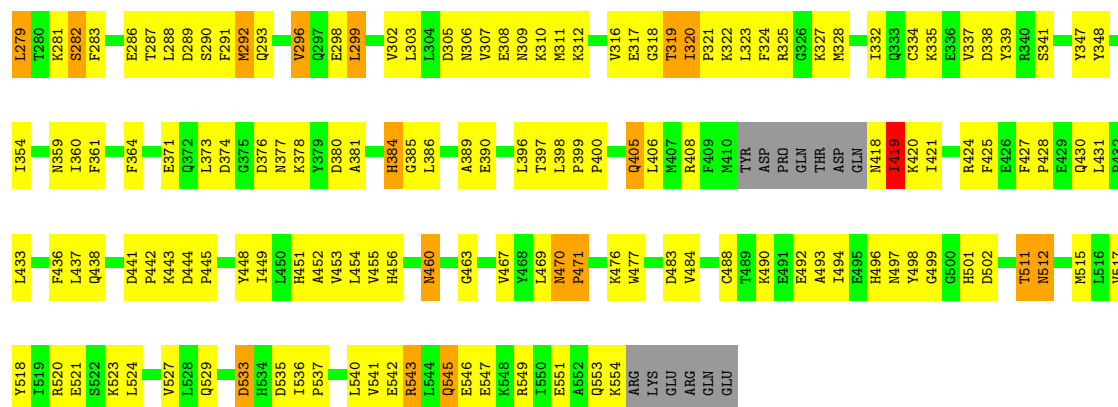


#### • Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7



#### • Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7





- Molecule 2: Ubiquitin aldehyde



- Molecule 2: Ubiquitin aldehyde



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.73Å 101.17Å 141.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.218 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9976	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	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	0.42	0/2880	0.71	4/3885 (0.1%)
1	B	0.42	0/2880	0.70	4/3885 (0.1%)
1	E	0.34	0/2817	0.61	2/3796 (0.1%)
2	C	0.39	0/603	0.67	0/811
2	D	0.37	0/603	0.67	0/811
All	All	0.39	0/9783	0.67	10/13188 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	554	LYS	N-CA-C	-8.61	87.74	111.00
1	B	384	HIS	N-CA-C	-7.53	90.67	111.00
1	A	505	LEU	CA-CB-CG	6.55	130.37	115.30
1	B	382	GLY	N-CA-C	-6.51	96.83	113.10
1	E	419	ILE	N-CA-C	5.99	127.17	111.00
1	A	235	THR	N-CA-C	-5.88	95.13	111.00
1	B	506	SER	N-CA-C	-5.77	95.42	111.00
1	E	335	LYS	N-CA-C	5.70	126.40	111.00
1	B	288	LEU	CA-CB-CG	5.45	127.83	115.30
1	A	470	ASN	N-CA-C	-5.23	96.87	111.00

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	2820	0	2753	104	0
1	B	2820	0	2753	83	0
1	E	2760	0	2706	202	0
2	C	601	0	626	15	0
2	D	601	0	626	16	0
3	A	142	0	0	7	0
3	B	139	0	0	8	0
3	C	31	0	0	2	0
3	D	22	0	0	2	0
3	E	40	0	0	13	0
All	All	9976	0	9464	402	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 21.

All (402) 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:E:332:ILE:HB	1:E:341:SER:HB3	1.38	1.05
1:E:451:HIS:HA	1:E:470:ASN:HD21	1.27	0.96
1:A:417:GLN:HE22	1:A:461:HIS:CE1	1.83	0.95
1:E:449:ILE:HD12	1:E:524:LEU:HD11	1.45	0.95
1:A:552:ALA:C	1:A:554:LYS:H	1.70	0.94
1:A:459:ASP:OD1	1:A:461:HIS:HB2	1.68	0.93
1:A:409:PHE:HB3	1:A:418:ASN:HD21	1.34	0.93
1:E:424:ARG:HA	1:E:499:GLY:HA2	1.50	0.92
1:E:308:GLU:HB2	1:E:320:ILE:HD12	1.53	0.91
1:A:415:THR:HG23	1:A:417:GLN:H	1.37	0.89
1:B:553:GLN:HB2	3:B:614:HOH:O	1.73	0.88
1:E:321:PRO:O	1:E:325:ARG:HB3	1.76	0.86
1:E:419:ILE:HD12	1:E:419:ILE:H	1.42	0.84
1:E:396:LEU:HG	3:E:563:HOH:O	1.75	0.84
1:E:454:LEU:HB2	1:E:515:MET:HB3	1.59	0.84
1:A:502:ASP:C	1:A:504:ASP:H	1.81	0.83
1:A:409:PHE:HB3	1:A:418:ASN:ND2	1.92	0.83
1:E:354:ILE:CD1	1:E:406:LEU:HB3	2.11	0.81
1:B:286:GLU:HG2	1:E:337:VAL:HG22	1.63	0.79
1:E:281:LYS:HG2	1:E:286:GLU:OE2	1.83	0.79
1:E:328:MET:HA	3:E:563:HOH:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:424:ARG:HA	1:E:499:GLY:CA	2.12	0.79
1:A:378:LYS:HE2	3:A:697:HOH:O	1.84	0.78
1:A:552:ALA:C	1:A:554:LYS:N	2.36	0.78
1:A:417:GLN:NE2	1:A:461:HIS:CE1	2.52	0.77
1:E:470:ASN:HD22	1:E:470:ASN:H	1.33	0.77
1:E:320:ILE:HB	1:E:321:PRO:HD3	1.67	0.76
1:A:329:VAL:HG22	1:A:396:LEU:HG	1.68	0.76
1:E:492:GLU:HA	1:E:496:HIS:HB2	1.67	0.76
1:E:287:THR:OG1	1:E:290:SER:HB3	1.86	0.76
1:E:537:PRO:O	1:E:541:VAL:HG23	1.89	0.73
1:E:541:VAL:O	1:E:545:GLN:HB2	1.89	0.72
2:C:301:MET:HE1	2:C:319:PRO:HG3	1.71	0.72
1:E:279:LEU:HD22	1:E:283:PHE:HE1	1.55	0.71
1:E:238:LEU:O	1:E:242:VAL:HG23	1.91	0.71
1:E:520:ARG:O	1:E:524:LEU:HG	1.90	0.71
1:E:354:ILE:HD12	1:E:406:LEU:HB3	1.73	0.71
1:B:244:MET:HG3	3:B:684:HOH:O	1.91	0.70
1:E:419:ILE:HG22	1:E:420:LYS:H	1.55	0.70
1:A:211:THR:HG21	1:A:485:VAL:HG12	1.73	0.69
1:E:269:HIS:HE1	1:E:533:ASP:OD1	1.74	0.69
1:E:488:CYS:HB2	1:E:492:GLU:CD	2.12	0.69
1:E:262:ARG:HD2	3:E:587:HOH:O	1.93	0.69
1:E:455:VAL:HG11	1:E:511:THR:HG23	1.73	0.69
1:E:442:PRO:O	1:E:443:LYS:HB2	1.94	0.68
1:B:209:LYS:HG2	1:B:210:HIS:H	1.58	0.68
2:D:306:LYS:HE3	2:D:310:GLY:O	1.92	0.67
1:B:387:GLN:HA	1:B:387:GLN:HE21	1.59	0.67
1:E:306:ASN:O	1:E:310:LYS:HB2	1.94	0.67
1:E:242:VAL:HG21	1:E:264:PHE:HE2	1.57	0.67
1:E:448:TYR:HB3	1:E:518:TYR:HB3	1.75	0.67
1:B:461:HIS:HE1	3:B:677:HOH:O	1.78	0.66
1:B:289:ASP:HA	1:B:292:MET:CE	2.24	0.66
1:E:256:VAL:HB	1:E:257:PRO:HD3	1.76	0.66
1:A:381:ALA:HB3	1:A:384:HIS:HB2	1.79	0.65
1:E:257:PRO:HG2	1:E:310:LYS:HG3	1.77	0.65
1:E:419:ILE:HD12	1:E:419:ILE:N	2.11	0.65
1:A:502:ASP:C	1:A:504:ASP:N	2.49	0.65
1:A:359:ASN:C	1:A:359:ASN:HD22	1.99	0.65
1:B:210:HIS:CG	1:B:211:THR:H	2.15	0.64
1:E:243:TYR:HA	1:E:261:GLN:HE21	1.62	0.64
1:B:218:ASN:HD21	1:B:222:THR:H	1.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:ALA:C	1:B:554:LYS:H	2.00	0.63
1:A:359:ASN:ND2	1:A:362:GLU:H	1.96	0.63
1:A:410:MET:O	1:A:410:MET:HG3	1.97	0.63
1:B:457:SER:O	1:B:463:GLY:HA3	1.97	0.63
1:E:233:PHE:HZ	1:E:268:GLN:HB2	1.64	0.63
1:A:491:GLU:CD	1:A:491:GLU:H	2.02	0.63
1:B:448:TYR:HB3	1:B:518:TYR:HB3	1.79	0.63
1:E:418:ASN:O	1:E:460:ASN:OD1	2.17	0.63
1:E:298:GLU:O	1:E:302:VAL:HG23	1.98	0.63
1:E:334:CYS:HA	1:E:389:ALA:HA	1.80	0.62
1:A:394:LYS:HE3	3:A:683:HOH:O	2.00	0.62
1:B:228:LEU:HD23	1:B:299:LEU:HD13	1.80	0.62
2:C:301:MET:CE	2:C:319:PRO:HG3	2.29	0.62
1:E:444:ASP:HB3	3:E:586:HOH:O	1.99	0.62
1:B:292:MET:HG2	3:B:649:HOH:O	1.99	0.61
1:E:243:TYR:CD1	1:E:536:ILE:HG12	2.35	0.61
1:B:289:ASP:HA	1:B:292:MET:HE3	1.82	0.61
1:E:380:ASP:HA	1:E:385:GLY:O	2.00	0.61
1:E:324:PHE:O	1:E:348:TYR:HA	1.99	0.61
1:B:281:LYS:HE3	1:E:338:ASP:HB2	1.82	0.61
1:B:301:ARG:HA	1:B:301:ARG:NE	2.16	0.61
1:B:209:LYS:NZ	1:B:209:LYS:HB3	2.15	0.61
1:E:308:GLU:CB	1:E:320:ILE:HD12	2.28	0.60
1:B:237:GLN:HE21	1:B:527:VAL:HA	1.66	0.60
1:E:224:TYR:HE1	1:E:299:LEU:HD12	1.66	0.60
1:B:262:ARG:O	1:B:266:GLU:HG2	2.01	0.60
1:A:211:THR:HG21	1:A:485:VAL:CG1	2.32	0.60
1:E:380:ASP:HB3	1:E:386:LEU:HD23	1.84	0.60
1:B:262:ARG:CZ	1:B:278:LYS:HD3	2.31	0.60
1:B:218:ASN:ND2	1:B:222:THR:H	1.99	0.59
1:E:262:ARG:NH1	1:E:278:LYS:HG2	2.17	0.59
1:A:415:THR:HG23	1:A:417:GLN:N	2.13	0.59
1:A:211:THR:HG23	1:A:478:CYS:SG	2.42	0.59
1:E:354:ILE:HD11	1:E:406:LEU:HB3	1.82	0.59
1:B:210:HIS:CG	1:B:211:THR:N	2.71	0.58
1:E:266:GLU:HB3	1:E:274:VAL:HG22	1.85	0.58
1:E:245:MET:SD	1:E:257:PRO:HB3	2.43	0.58
1:E:289:ASP:HA	1:E:292:MET:SD	2.43	0.58
1:A:554:LYS:HG3	1:A:554:LYS:O	2.02	0.58
1:A:378:LYS:NZ	1:E:325:ARG:HH22	2.01	0.58
1:E:289:ASP:O	1:E:293:GLN:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:452:ALA:HB3	1:E:517:VAL:HB	1.85	0.58
1:A:420:LYS:HE2	1:A:422:ASN:OD1	2.04	0.58
1:E:307:VAL:O	1:E:311:MET:HG3	2.03	0.58
1:E:546:GLU:HA	1:E:549:ARG:HD2	1.85	0.57
1:E:242:VAL:O	1:E:245:MET:HE2	2.04	0.57
1:E:318:GLY:C	1:E:320:ILE:H	2.08	0.57
1:E:456:HIS:CE1	1:E:463:GLY:HA3	2.39	0.57
1:A:333:GLN:HG3	1:A:340:ARG:HG3	1.85	0.57
1:E:269:HIS:CE1	1:E:533:ASP:OD1	2.57	0.57
1:E:219:GLN:OE1	1:E:277:LYS:HB2	2.05	0.56
1:E:374:ASP:O	1:E:378:LYS:HG3	2.05	0.56
1:E:242:VAL:HG13	1:E:245:MET:HE2	1.86	0.56
2:D:325:ASN:O	2:D:328:ALA:HB3	2.05	0.56
1:E:224:TYR:CE1	1:E:299:LEU:HD12	2.39	0.56
1:A:415:THR:HG23	1:A:417:GLN:HB2	1.88	0.56
1:E:431:LEU:HG	1:E:433:LEU:HG	1.87	0.56
1:E:453:VAL:O	1:E:455:VAL:HG23	2.06	0.56
1:E:252:SER:HB2	1:E:543:ARG:HH12	1.71	0.56
1:E:252:SER:HB2	1:E:543:ARG:NH1	2.21	0.56
1:E:354:ILE:HD11	1:E:406:LEU:HD13	1.86	0.56
1:E:235:THR:O	1:E:235:THR:HG22	2.06	0.56
1:B:359:ASN:ND2	1:B:362:GLU:H	2.04	0.55
1:A:248:GLU:HG3	1:A:539:GLN:CD	2.26	0.55
1:B:546:GLU:OE1	1:B:550:ILE:HG13	2.07	0.55
1:E:529:GLN:N	3:E:581:HOH:O	2.39	0.55
1:E:279:LEU:O	1:E:282:SER:HB3	2.06	0.55
1:E:364:PHE:HB3	1:E:436:PHE:CE2	2.41	0.55
1:E:233:PHE:CZ	1:E:268:GLN:HB2	2.41	0.55
1:E:376:ASP:OD1	1:E:376:ASP:O	2.25	0.55
1:E:347:TYR:OH	1:E:399:PRO:HD3	2.07	0.55
1:E:227:SER:HB3	1:E:467:VAL:HB	1.88	0.55
1:E:408:ARG:HD2	1:E:421:ILE:O	2.07	0.55
1:A:424:ARG:NH1	1:A:426:GLU:OE2	2.40	0.54
1:A:549:ARG:O	1:A:552:ALA:N	2.35	0.54
1:E:237:GLN:NE2	1:E:323:LEU:HD21	2.23	0.54
1:A:375:GLY:HA2	1:A:378:LYS:HE3	1.88	0.54
1:B:334:CYS:HB3	1:B:337:VAL:HG13	1.89	0.54
1:E:327:LYS:HB2	1:E:397:THR:HG22	1.87	0.54
1:E:444:ASP:OD1	1:E:520:ARG:NH1	2.39	0.54
1:E:460:ASN:C	1:E:460:ASN:HD22	2.11	0.54
2:D:308:LEU:HD21	2:D:371:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:THR:HG22	3:A:648:HOH:O	2.06	0.54
1:E:360:ILE:HG22	3:E:577:HOH:O	2.06	0.54
1:A:549:ARG:NH2	1:A:553:GLN:NE2	2.56	0.54
1:E:477:TRP:CD1	1:E:490:LYS:HG2	2.42	0.54
1:E:523:LYS:O	1:E:527:VAL:HG23	2.07	0.54
1:B:554:LYS:HE3	3:B:614:HOH:O	2.08	0.53
1:B:288:LEU:HD23	1:B:289:ASP:N	2.22	0.53
1:A:448:TYR:HB3	1:A:518:TYR:HB3	1.90	0.53
1:E:332:ILE:HA	1:E:390:GLU:O	2.09	0.53
1:E:337:VAL:HG12	1:E:339:TYR:H	1.74	0.53
1:E:501:HIS:HD2	1:E:502:ASP:O	1.92	0.53
1:E:476:LYS:HE3	3:E:575:HOH:O	2.08	0.53
1:B:209:LYS:HG2	1:B:210:HIS:N	2.23	0.52
1:E:247:THR:HA	1:E:250:ASP:OD1	2.10	0.52
1:E:488:CYS:HB2	1:E:492:GLU:OE2	2.08	0.52
1:E:553:GLN:O	1:E:554:LYS:CG	2.57	0.52
1:A:348:TYR:CD1	2:D:347:GLY:HA3	2.43	0.52
1:B:219:GLN:HE22	1:B:280:THR:HB	1.74	0.52
1:B:289:ASP:HA	1:B:292:MET:HE1	1.91	0.52
1:E:470:ASN:H	1:E:470:ASN:ND2	2.04	0.52
1:E:291:PHE:HB2	3:E:564:HOH:O	2.09	0.52
1:E:456:HIS:HE1	1:E:463:GLY:HA3	1.72	0.52
1:E:449:ILE:HD11	1:E:521:GLU:HG3	1.92	0.52
1:A:228:LEU:HD12	1:A:299:LEU:HD13	1.91	0.52
1:B:257:PRO:O	1:B:261:GLN:HG3	2.10	0.52
1:E:460:ASN:C	1:E:460:ASN:ND2	2.62	0.52
1:A:417:GLN:NE2	1:A:461:HIS:NE2	2.48	0.52
1:E:354:ILE:HD11	1:E:406:LEU:HD22	1.92	0.52
1:A:552:ALA:O	1:A:554:LYS:N	2.42	0.51
1:B:208:LYS:HB2	1:B:208:LYS:NZ	2.25	0.51
1:B:219:GLN:HB2	1:B:222:THR:CG2	2.40	0.51
1:A:415:THR:CG2	3:A:648:HOH:O	2.58	0.51
1:E:311:MET:O	1:E:317:GLU:HB2	2.10	0.51
1:E:444:ASP:N	1:E:445:PRO:HD3	2.26	0.51
1:B:216:LEU:HD23	1:B:274:VAL:HB	1.92	0.51
1:E:258:LEU:HD13	1:E:258:LEU:O	2.10	0.51
1:E:398:LEU:HG	1:E:437:LEU:HD21	1.93	0.51
1:A:375:GLY:O	1:A:378:LYS:HG3	2.11	0.51
1:E:549:ARG:O	1:E:553:GLN:HG3	2.11	0.51
1:E:398:LEU:HB3	1:E:448:TYR:OH	2.10	0.50
1:E:419:ILE:N	1:E:419:ILE:CD1	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:THR:CG2	1:A:417:GLN:HB2	2.41	0.50
1:B:210:HIS:CD2	1:B:211:THR:HG23	2.45	0.50
1:E:454:LEU:CB	1:E:515:MET:HB3	2.37	0.50
1:A:239:ARG:HH11	1:A:268:GLN:NE2	2.09	0.50
1:E:237:GLN:HE22	1:E:323:LEU:HD21	1.75	0.50
1:E:241:ALA:HB1	1:E:316:VAL:HG21	1.93	0.50
1:E:359:ASN:HD22	1:E:361:PHE:HB3	1.75	0.50
1:B:210:HIS:O	1:B:212:GLY:N	2.44	0.50
1:B:281:LYS:HE3	1:E:338:ASP:CB	2.41	0.50
1:E:469:LEU:C	1:E:471:PRO:HD3	2.33	0.49
1:E:441:ASP:HB2	3:E:586:HOH:O	2.11	0.49
1:B:219:GLN:HB2	1:B:222:THR:HG21	1.94	0.49
3:A:667:HOH:O	2:D:347:GLY:HA2	2.12	0.49
1:A:489:THR:OG1	1:A:492:GLU:HG3	2.11	0.49
1:A:547:GLU:HA	3:A:693:HOH:O	2.12	0.49
1:A:329:VAL:HG22	1:A:396:LEU:CG	2.40	0.49
1:A:381:ALA:CB	1:A:384:HIS:HB2	2.42	0.49
1:E:247:THR:HB	1:E:258:LEU:HD23	1.93	0.49
1:E:252:SER:O	1:E:253:SER:HB2	2.13	0.49
1:A:550:ILE:HB	3:A:693:HOH:O	2.13	0.49
1:E:242:VAL:HG13	1:E:245:MET:CE	2.43	0.49
1:B:418:ASN:HB3	1:B:460:ASN:ND2	2.28	0.48
3:B:654:HOH:O	2:C:347:GLY:HA2	2.13	0.48
1:E:316:VAL:O	1:E:316:VAL:HG22	2.13	0.48
1:E:451:HIS:CA	1:E:470:ASN:HD21	2.14	0.48
1:E:542:GLU:HA	1:E:545:GLN:HE21	1.78	0.48
1:A:549:ARG:HH21	1:A:553:GLN:NE2	2.11	0.48
1:E:230:GLN:HE21	1:E:230:GLN:HA	1.78	0.48
1:E:242:VAL:HG21	1:E:264:PHE:CE2	2.43	0.48
1:E:244:MET:HE1	1:E:537:PRO:HG3	1.95	0.48
1:E:291:PHE:C	1:E:293:GLN:H	2.17	0.48
1:A:553:GLN:O	1:A:554:LYS:HB3	2.12	0.48
2:C:363:LYS:O	2:C:364:GLU:HB2	2.14	0.48
1:E:529:GLN:HG3	3:E:581:HOH:O	2.12	0.48
1:E:553:GLN:O	1:E:554:LYS:CD	2.61	0.48
2:C:318:GLU:N	2:C:321:ASP:OD2	2.33	0.48
2:C:336:ILE:HD12	2:C:369:LEU:HD21	1.95	0.48
1:E:378:LYS:CB	1:E:386:LEU:HB3	2.43	0.48
1:E:256:VAL:HA	1:E:282:SER:OG	2.14	0.47
1:E:452:ALA:HB2	1:E:469:LEU:CD2	2.44	0.47
1:E:497:ASN:OD1	1:E:511:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ASN:HB2	3:B:605:HOH:O	2.14	0.47
1:E:546:GLU:O	1:E:549:ARG:HB2	2.15	0.47
1:B:298:GLU:OE2	2:C:372:ARG:HD3	2.15	0.47
1:E:373:LEU:HB3	1:E:377:ASN:O	2.14	0.47
1:A:454:LEU:HD22	1:A:467:VAL:HG23	1.97	0.47
1:E:281:LYS:HA	1:E:286:GLU:CD	2.35	0.47
1:E:374:ASP:O	1:E:378:LYS:N	2.48	0.47
1:B:387:GLN:HE21	1:B:387:GLN:CA	2.24	0.47
1:A:370:VAL:CG1	1:A:390:GLU:HB3	2.45	0.47
1:A:459:ASP:C	1:A:461:HIS:H	2.17	0.47
1:E:547:GLU:C	1:E:549:ARG:H	2.17	0.47
2:C:301:MET:HE1	3:C:384:HOH:O	2.15	0.47
1:B:256:VAL:N	1:B:257:PRO:CD	2.78	0.46
1:B:256:VAL:HB	1:B:257:PRO:HD3	1.97	0.46
1:B:502:ASP:HA	1:B:509:HIS:ND1	2.30	0.46
1:B:336:GLU:C	1:B:337:VAL:HG12	2.35	0.46
1:A:237:GLN:HE21	1:A:527:VAL:HA	1.80	0.46
1:A:470:ASN:OD1	1:A:473:GLY:HA2	2.16	0.46
1:E:241:ALA:CB	1:E:316:VAL:HG21	2.45	0.46
1:A:245:MET:HA	1:A:246:PRO:HD3	1.75	0.46
1:B:240:LYS:HE3	1:B:531:VAL:HG22	1.98	0.46
1:A:328:MET:HG3	1:A:347:TYR:CD1	2.50	0.46
1:E:224:TYR:HB2	1:E:296:VAL:HG13	1.98	0.46
1:E:455:VAL:HG11	1:E:511:THR:CG2	2.43	0.46
1:B:552:ALA:C	1:B:554:LYS:N	2.69	0.46
1:E:419:ILE:HG22	1:E:420:LYS:N	2.27	0.46
1:A:309:ASN:HB3	3:C:403:HOH:O	2.16	0.46
1:E:483:ASP:OD1	1:E:484:VAL:HG23	2.16	0.46
1:E:452:ALA:HB2	1:E:469:LEU:HD21	1.98	0.45
1:E:470:ASN:HD22	1:E:470:ASN:N	1.99	0.45
1:E:427:PHE:CE1	1:E:494:ILE:HG23	2.52	0.45
1:A:318:GLY:O	1:A:321:PRO:HD2	2.16	0.45
1:A:332:ILE:HD11	2:D:304:PHE:CE1	2.52	0.45
1:A:550:ILE:O	1:A:550:ILE:HG22	2.16	0.45
1:B:359:ASN:C	1:B:359:ASN:HD22	2.19	0.45
1:B:505:LEU:HD22	1:B:505:LEU:HA	1.74	0.45
1:E:241:ALA:HB1	1:E:311:MET:HE2	1.98	0.45
1:E:262:ARG:NH1	1:E:278:LYS:CG	2.79	0.45
1:E:339:TYR:CD1	1:E:339:TYR:C	2.89	0.45
1:B:378:LYS:NZ	3:B:647:HOH:O	2.40	0.45
1:E:266:GLU:OE2	1:E:270:SER:HB3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:355:THR:O	2:D:358:ASP:HB2	2.16	0.45
1:E:322:LYS:O	1:E:400:PRO:HG2	2.16	0.45
1:E:373:LEU:HD22	1:E:377:ASN:HB3	1.98	0.45
1:E:551:GLU:C	1:E:553:GLN:N	2.69	0.45
1:A:297:GLN:HE22	2:D:344:ILE:HD13	1.82	0.45
1:A:426:GLU:HG2	1:A:498:TYR:CD1	2.52	0.45
1:A:501:HIS:HD2	1:A:508:ARG:NH1	2.14	0.45
1:E:227:SER:CB	1:E:467:VAL:HB	2.47	0.45
1:A:256:VAL:HB	1:A:257:PRO:HD3	1.97	0.45
1:B:553:GLN:O	1:B:554:LYS:HG3	2.16	0.45
1:E:470:ASN:ND2	1:E:470:ASN:N	2.64	0.45
1:B:259:ALA:HB1	1:B:279:LEU:HA	1.98	0.45
1:E:316:VAL:HG22	1:E:319:THR:OG1	2.17	0.45
1:E:511:THR:HG22	3:E:566:HOH:O	2.17	0.45
2:D:307:THR:HB	3:D:396:HOH:O	2.17	0.45
1:B:359:ASN:HD22	1:B:361:PHE:N	2.14	0.44
1:B:255:SER:HB3	1:B:258:LEU:HB3	1.99	0.44
1:E:245:MET:CE	1:E:261:GLN:HG3	2.47	0.44
1:E:258:LEU:HD13	1:E:258:LEU:C	2.38	0.44
1:E:477:TRP:HD1	1:E:490:LYS:HG2	1.79	0.44
1:A:505:LEU:O	1:A:505:LEU:HD22	2.18	0.44
2:D:363:LYS:O	2:D:364:GLU:HB2	2.17	0.44
1:A:359:ASN:C	1:A:359:ASN:ND2	2.70	0.44
1:B:258:LEU:CD1	1:B:262:ARG:NH2	2.81	0.44
2:D:342:ARG:HB2	2:D:370:VAL:HG23	1.99	0.44
1:A:218:ASN:ND2	1:A:220:GLY:H	2.14	0.44
1:A:299:LEU:O	1:A:303:LEU:HB2	2.16	0.44
1:E:242:VAL:O	1:E:245:MET:HG3	2.17	0.44
1:E:299:LEU:O	1:E:303:LEU:HG	2.18	0.44
1:E:451:HIS:HA	1:E:470:ASN:ND2	2.12	0.44
1:A:426:GLU:HG2	1:A:498:TYR:CE1	2.52	0.44
1:A:501:HIS:CD2	1:A:508:ARG:NH1	2.85	0.44
1:B:343:ARG:HH11	1:B:343:ARG:HG2	1.82	0.44
1:E:243:TYR:CE1	1:E:536:ILE:HG12	2.53	0.44
1:A:298:GLU:OE2	2:D:372:ARG:HD3	2.17	0.44
1:A:279:LEU:HD22	1:A:283:PHE:CZ	2.52	0.44
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.85	0.44
1:E:236:ASN:ND2	1:E:529:GLN:O	2.49	0.44
1:A:359:ASN:ND2	1:A:362:GLU:HG3	2.33	0.43
1:E:210:HIS:CD2	1:E:210:HIS:N	2.84	0.43
1:E:378:LYS:HB2	1:E:386:LEU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:427:PHE:HA	1:E:428:PRO:HD3	1.76	0.43
1:E:308:GLU:CA	1:E:320:ILE:HD12	2.48	0.43
1:A:415:THR:HG23	1:A:417:GLN:CB	2.49	0.43
1:A:318:GLY:C	1:A:321:PRO:HD2	2.38	0.43
1:E:455:VAL:HG13	1:E:512:ASN:C	2.39	0.43
1:A:256:VAL:N	1:A:257:PRO:CD	2.82	0.43
1:E:305:ASP:O	1:E:309:ASN:HB2	2.19	0.43
1:A:219:GLN:NE2	1:A:290:SER:OG	2.52	0.43
1:A:554:LYS:O	1:A:554:LYS:CG	2.67	0.43
1:B:332:ILE:O	1:B:340:ARG:HA	2.18	0.43
1:A:547:GLU:O	1:A:551:GLU:HG3	2.19	0.43
1:B:293:GLN:HB3	2:C:375:GLY:C	2.39	0.43
1:E:233:PHE:HE2	1:E:264:PHE:O	2.01	0.43
1:B:307:VAL:O	1:B:311:MET:HG3	2.19	0.42
1:B:346:ASP:O	2:C:346:ALA:HA	2.18	0.42
1:B:381:ALA:HB3	1:B:384:HIS:HB2	2.00	0.42
1:B:301:ARG:HG2	2:C:344:ILE:HD12	2.01	0.42
1:E:218:ASN:OD1	1:E:218:ASN:O	2.37	0.42
1:E:398:LEU:CB	1:E:448:TYR:OH	2.67	0.42
1:B:352:LEU:HB3	1:B:363:SER:OG	2.19	0.42
1:B:495:GLU:CD	1:B:495:GLU:H	2.22	0.42
1:E:240:LYS:HE3	1:E:535:ASP:CG	2.38	0.42
1:E:430:GLN:HE21	1:E:430:GLN:HB3	1.58	0.42
1:A:240:LYS:O	1:A:244:MET:HG2	2.20	0.42
1:A:418:ASN:HB2	2:D:371:LEU:HD23	2.01	0.42
1:A:457:SER:O	1:A:463:GLY:HA2	2.20	0.42
1:B:418:ASN:HD21	2:C:340:GLN:NE2	2.16	0.42
1:E:272:LYS:HG2	1:E:273:PRO:HD2	2.02	0.42
1:E:318:GLY:O	1:E:320:ILE:N	2.51	0.42
1:E:405:GLN:HE21	1:E:405:GLN:HB2	1.56	0.42
1:A:216:LEU:HD23	1:A:274:VAL:HB	2.01	0.42
1:A:549:ARG:O	1:A:552:ALA:HB3	2.20	0.42
1:B:441:ASP:HA	1:B:442:PRO:HD3	1.91	0.42
1:E:454:LEU:N	1:E:454:LEU:HD22	2.35	0.42
1:A:501:HIS:O	1:A:504:ASP:HB2	2.18	0.42
1:B:239:ARG:HH11	1:B:268:GLN:NE2	2.18	0.42
1:B:293:GLN:HB3	2:C:375:GLY:O	2.20	0.42
1:A:335:LYS:HE3	1:A:372:GLN:OE1	2.20	0.42
1:A:549:ARG:HH21	1:A:553:GLN:HE21	1.68	0.42
1:E:288:LEU:HG	1:E:289:ASP:N	2.35	0.42
1:E:310:LYS:O	1:E:310:LYS:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:327:LYS:O	1:E:396:LEU:HB2	2.19	0.42
1:E:420:LYS:NZ	1:E:512:ASN:HD21	2.18	0.42
1:E:511:THR:CG2	3:E:566:HOH:O	2.68	0.41
1:B:209:LYS:HB3	1:B:209:LYS:HZ2	1.82	0.41
1:B:318:GLY:O	1:B:321:PRO:HD2	2.20	0.41
1:E:245:MET:HA	1:E:246:PRO:HD3	1.84	0.41
1:E:262:ARG:HH12	1:E:278:LYS:HD3	1.85	0.41
1:A:491:GLU:CD	1:A:491:GLU:N	2.73	0.41
1:A:501:HIS:C	1:A:509:HIS:ND1	2.74	0.41
1:E:477:TRP:CE3	1:E:493:ALA:HB1	2.54	0.41
1:B:370:VAL:CG1	1:B:390:GLU:HB2	2.50	0.41
1:E:303:LEU:O	1:E:307:VAL:HG23	2.20	0.41
1:A:532:THR:OG1	1:A:534:HIS:HB3	2.21	0.41
2:D:308:LEU:HB2	3:D:396:HOH:O	2.19	0.41
1:A:333:GLN:O	1:A:389:ALA:HB1	2.21	0.41
1:A:489:THR:HB	1:A:491:GLU:OE2	2.21	0.41
1:A:550:ILE:O	1:A:550:ILE:CG2	2.68	0.41
1:B:295:ASP:HB2	2:C:372:ARG:HG2	2.02	0.41
1:E:217:LYS:HG3	1:E:274:VAL:O	2.20	0.41
1:E:396:LEU:N	3:E:563:HOH:O	2.52	0.41
1:E:460:ASN:ND2	1:E:460:ASN:O	2.49	0.41
1:A:378:LYS:NZ	1:E:325:ARG:NH2	2.68	0.41
1:A:452:ALA:HB3	1:A:517:VAL:HB	2.03	0.41
1:B:288:LEU:O	1:B:292:MET:HE3	2.21	0.41
1:B:329:VAL:O	1:B:329:VAL:HG13	2.21	0.41
1:B:492:GLU:O	1:B:496:HIS:HB3	2.21	0.41
1:E:241:ALA:HB1	1:E:311:MET:CE	2.51	0.41
1:E:262:ARG:HH11	1:E:278:LYS:HG2	1.84	0.41
1:E:268:GLN:HG2	1:E:268:GLN:O	2.20	0.41
1:E:384:HIS:ND1	1:E:384:HIS:N	2.69	0.41
1:E:540:LEU:HD13	1:E:540:LEU:C	2.41	0.41
1:A:301:ARG:HA	1:A:301:ARG:NE	2.36	0.41
1:A:359:ASN:HD21	1:A:362:GLU:H	1.66	0.41
1:A:414:GLN:O	1:A:415:THR:HB	2.20	0.41
2:D:361:ILE:HD13	2:D:367:LEU:HD21	2.03	0.41
1:B:468:TYR:HD2	1:B:488:CYS:HG	1.70	0.40
1:E:312:LYS:HA	1:E:317:GLU:HG3	2.02	0.40
1:E:371:GLU:O	1:E:390:GLU:HA	2.21	0.40
1:E:455:VAL:HG13	1:E:512:ASN:O	2.21	0.40
1:A:334:CYS:HB2	1:A:337:VAL:O	2.20	0.40
1:A:454:LEU:HB2	1:A:515:MET:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ASP:CG	1:A:503:ASP:H	2.24	0.40
1:A:536:ILE:HA	1:A:537:PRO:HD3	1.85	0.40
1:B:288:LEU:HD23	1:B:292:MET:HE1	2.03	0.40
2:C:322:THR:O	2:C:326:VAL:HG23	2.21	0.40
1:E:449:ILE:HD11	1:E:521:GLU:CG	2.50	0.40
1:B:470:ASN:OD1	1:B:473:GLY:HA2	2.20	0.40
1:E:354:ILE:HG12	1:E:425:PHE:CE2	2.56	0.40
1:A:331:TYR:OH	1:A:438:GLN:NE2	2.51	0.40
1:B:309:ASN:OD1	2:D:360:ASN:OD1	2.40	0.40
1:B:371:GLU:O	1:B:390:GLU:HA	2.20	0.40
1:B:502:ASP:HB3	1:B:509:HIS:HE1	1.86	0.40
1:E:244:MET:CE	1:E:537:PRO:HG3	2.51	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	345/353 (98%)	323 (94%)	18 (5%)	4 (1%)	11	12
1	B	345/353 (98%)	322 (93%)	20 (6%)	3 (1%)	14	17
1	E	336/353 (95%)	278 (83%)	46 (14%)	12 (4%)	3	1
2	C	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
2	D	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
All	All	1174/1211 (97%)	1068 (91%)	87 (7%)	19 (2%)	8	7

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	GLY
1	A	415	THR

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Mol	Chain	Res	Type
1	B	211	THR
1	E	252	SER
1	B	375	GLY
1	E	236	ASN
1	E	253	SER
1	A	252	SER
1	A	407	MET
1	E	213	TYR
1	E	319	THR
1	E	381	ALA
1	E	320	ILE
1	E	498	TYR
1	E	282	SER
1	E	471	PRO
1	E	214	VAL
1	B	494	ILE
1	E	212	GLY

### 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	314/320 (98%)	287 (91%)	27 (9%)	8	11
1	B	314/320 (98%)	290 (92%)	24 (8%)	11	14
1	E	307/320 (96%)	290 (94%)	17 (6%)	18	26
2	C	68/68 (100%)	64 (94%)	4 (6%)	16	23
2	D	68/68 (100%)	65 (96%)	3 (4%)	24	35
All	All	1071/1096 (98%)	996 (93%)	75 (7%)	12	17

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	HIS
1	A	228	LEU

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Mol	Chain	Res	Type
1	A	258	LEU
1	A	279	LEU
1	A	288	LEU
1	A	299	LEU
1	A	303	LEU
1	A	329	VAL
1	A	333	GLN
1	A	351	GLN
1	A	353	SER
1	A	359	ASN
1	A	360	ILE
1	A	402	LEU
1	A	409	PHE
1	A	410	MET
1	A	418	ASN
1	A	454	LEU
1	A	459	ASP
1	A	469	LEU
1	A	505	LEU
1	A	508	ARG
1	A	538	GLN
1	A	540	LEU
1	A	549	ARG
1	A	553	GLN
1	A	554	LYS
1	B	209	LYS
1	B	280	THR
1	B	288	LEU
1	B	299	LEU
1	B	301	ARG
1	B	303	LEU
1	B	306	ASN
1	B	316	VAL
1	B	336	GLU
1	B	337	VAL
1	B	343	ARG
1	B	353	SER
1	B	359	ASN
1	B	387	GLN
1	B	402	LEU
1	B	409	PHE
1	B	428	PRO

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Mol	Chain	Res	Type
1	B	454	LEU
1	B	502	ASP
1	B	503	ASP
1	B	505	LEU
1	B	507	VAL
1	B	524	LEU
1	B	540	LEU
2	C	318	GLU
2	C	340	GLN
2	C	360	ASN
2	C	371	LEU
2	D	308	LEU
2	D	318	GLU
2	D	371	LEU
1	E	210	HIS
1	E	211	THR
1	E	279	LEU
1	E	292	MET
1	E	296	VAL
1	E	299	LEU
1	E	384	HIS
1	E	405	GLN
1	E	419	ILE
1	E	438	GLN
1	E	460	ASN
1	E	470	ASN
1	E	511	THR
1	E	512	ASN
1	E	533	ASP
1	E	543	ARG
1	E	545	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	219	GLN
1	A	237	GLN
1	A	261	GLN
1	A	268	GLN
1	A	294	HIS
1	A	351	GLN

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Mol	Chain	Res	Type
1	A	359	ASN
1	A	405	GLN
1	A	417	GLN
1	A	438	GLN
1	A	501	HIS
1	A	538	GLN
1	A	539	GLN
1	A	545	GLN
1	A	553	GLN
1	B	218	ASN
1	B	230	GLN
1	B	237	GLN
1	B	268	GLN
1	B	306	ASN
1	B	309	ASN
1	B	359	ASN
1	B	387	GLN
1	B	447	ASN
1	B	529	GLN
1	B	545	GLN
2	C	340	GLN
2	C	360	ASN
2	D	340	GLN
2	D	362	GLN
1	E	218	ASN
1	E	226	ASN
1	E	237	GLN
1	E	268	GLN
1	E	269	HIS
1	E	293	GLN
1	E	294	HIS
1	E	306	ASN
1	E	309	ASN
1	E	372	GLN
1	E	405	GLN
1	E	430	GLN
1	E	451	HIS
1	E	456	HIS
1	E	460	ASN
1	E	470	ASN
1	E	501	HIS
1	E	512	ASN

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Mol	Chain	Res	Type
1	E	539	GLN
1	E	545	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GLZ	C	376	2,1	3,3,3	2.33	1 (33%)	1,2,2	1.23	0
2	GLZ	D	376	2,1	3,3,3	2.43	1 (33%)	1,2,2	0.82	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	C	376	2,1	-	0/0/1/1	-
2	GLZ	D	376	2,1	-	0/0/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	376	GLZ	O-C	4.17	1.43	1.20
2	C	376	GLZ	O-C	4.02	1.42	1.20

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.

## 5.5 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 [i](#)

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.