



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:05 PM UTC

PDB ID : 1JF5 / pdb_00001jf5
Title : CRYSTAL STRUCTURE OF THERMOACTINOMYCES VULGARIS R-47
ALPHA-AMYLASE 2 MUTANT F286A
Authors : Ohtaki, A.; Kondo, S.; Shimura, Y.; Tonozuka, T.; Sakano, Y.; Kamitori, S.
Deposited on : 2001-06-20
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

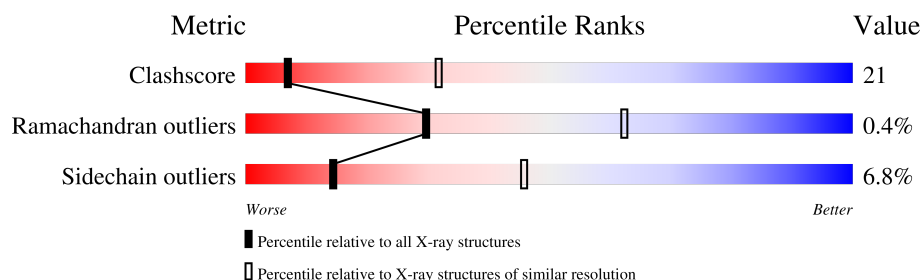
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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	585	
1	B	585	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9542 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 ALPHA AMYLASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4770	3050	831	874	15			
1	B	585	Total	C	N	O	S	0	0	0
			4770	3050	831	874	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ALA	PHE	engineered mutation	UNP Q08751
B	286	ALA	PHE	engineered mutation	UNP Q08751

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

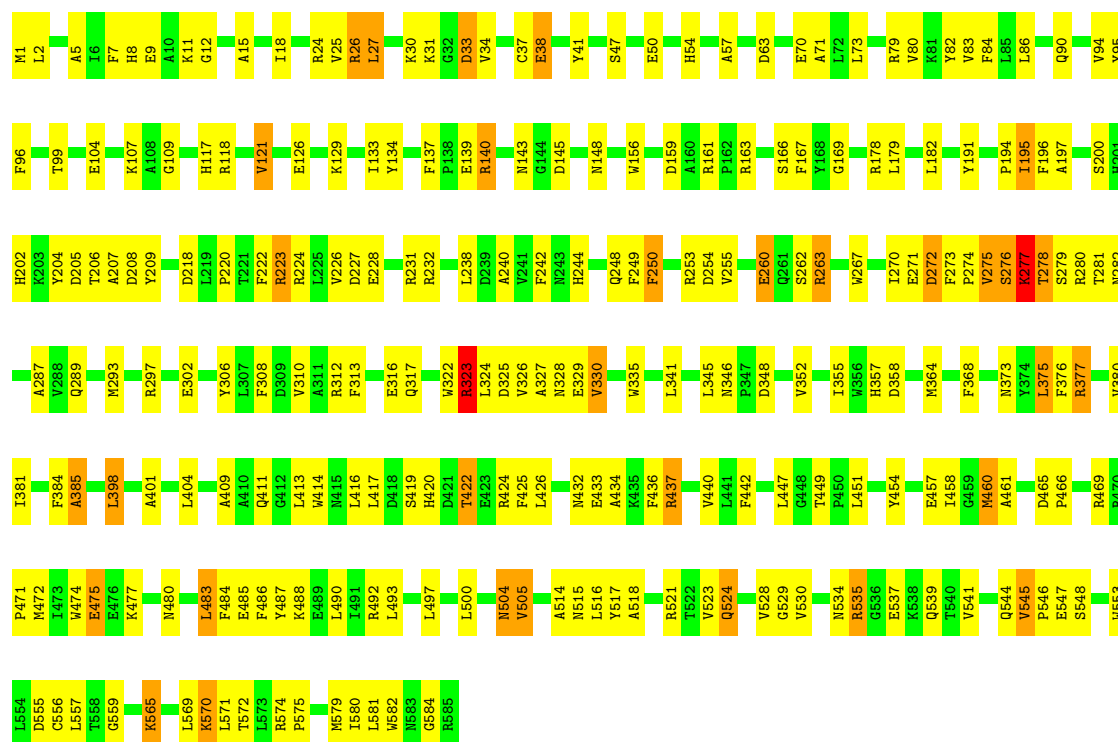
3 Residue-property plots

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. 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.

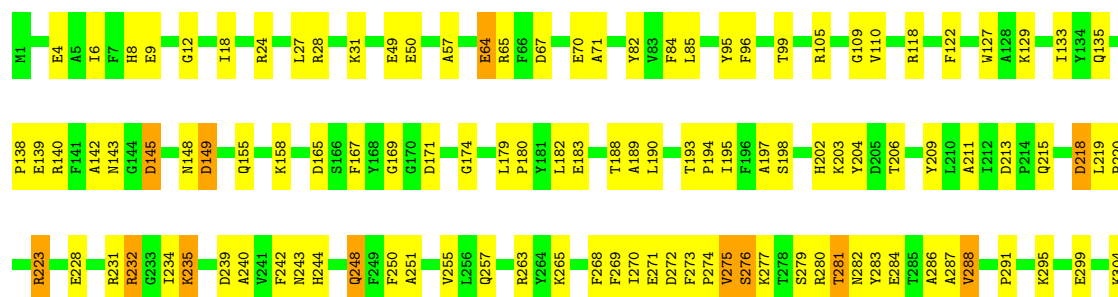
• Molecule 1: ALPHA AMYLASE II

Chain A: 



• Molecule 1: ALPHA AMYLASE II

Chain B: 



L580	F486	L404	E505
L581			
L582	L490	Q408	F308
L583			D309
L584	S499	Q411	V310
L585	N504	W414	A311
	V505	L415	R312
	N515	L417	
	L516	D418	Q317
	F519		
	V520	T422	D320
	R521	E423	R323
	T522	R424	L324
	V523	F425	A327
		L426	N328
	Q526	T427	E329
	H527	F436	V330
			D331
V530		L441	R332
R531		F442	A333
N533		Q443	F334
N534		M444	W335
R535			
R536		L447	A349
E537			
R538		L451	V352
Q539		L452	G353
		Y453	E354
			L355
		D456	W356
		F457	H357
L542		I458	D358
V545		G459	
P546		M460	N364
E547		A461	
		G462	M372
G550		A463	N373
K551		T464	Y374
T552		D465	L375
W553		P466	F376
L554		D467	R377
D555		D468	
		C468	L381
G564		R469	R382
K565		R470	F383
		P471	
		M472	T386
		I473	G387
		W474	E388
		E475	
T572		E476	A391
L573		R477	E392
R574		E478	R393
P575		Q479	F394
Y576		N480	
Y577			L398
G578			
N579		L482	A401

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, α , β , γ	112.60Å 118.05Å 113.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.39 – 3.20	Depositor
% Data completeness (in resolution range)	99.7 (38.39-3.20)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9542	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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:
CA

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	0.66	0/4899	1.04	14/6632 (0.2%)
1	B	0.66	0/4899	1.03	16/6632 (0.2%)
All	All	0.66	0/9798	1.04	30/13264 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ILE	N-CA-C	-8.06	105.33	113.47
1	A	161	ARG	CA-C-N	7.96	128.01	119.89
1	A	161	ARG	C-N-CA	7.96	128.01	119.89
1	B	276	SER	N-CA-C	7.31	117.52	107.73
1	A	145	ASP	CA-C-N	6.44	126.13	119.56
1	A	145	ASP	C-N-CA	6.44	126.13	119.56
1	A	33	ASP	N-CA-C	6.42	119.09	111.71
1	A	323	ARG	N-CA-C	-6.38	98.02	108.41
1	B	18	ILE	N-CA-C	-6.21	107.08	113.10
1	A	524	GLN	CB-CA-C	-6.15	109.46	116.54
1	A	275	VAL	N-CA-C	6.12	116.51	107.15
1	A	385	ALA	N-CA-C	6.02	119.00	111.24
1	A	417	LEU	N-CA-C	-5.74	106.44	113.50
1	B	248	GLN	N-CA-C	-5.42	106.72	113.38
1	B	394	PHE	N-CA-C	-5.34	105.36	111.07
1	A	7	PHE	N-CA-C	5.29	117.42	109.23
1	B	145	ASP	CA-C-N	5.27	124.88	119.56
1	B	145	ASP	C-N-CA	5.27	124.88	119.56
1	B	427	THR	N-CA-C	-5.22	105.67	111.36
1	B	520	VAL	N-CA-C	5.20	115.39	108.11
1	A	287	ALA	CB-CA-C	-5.19	110.57	116.54
1	B	287	ALA	CB-CA-C	-5.16	110.61	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	532	LEU	N-CA-C	5.16	117.11	107.99
1	B	317	GLN	N-CA-C	-5.13	106.99	113.20
1	B	288	VAL	N-CA-C	5.09	115.23	108.11
1	B	417	LEU	N-CA-C	-5.08	107.64	113.88
1	B	211	ALA	N-CA-C	5.06	117.65	109.06
1	A	80	VAL	N-CA-C	5.04	115.00	108.35
1	B	323	ARG	N-CA-C	-5.04	99.08	107.99
1	B	539	GLN	N-CA-C	5.01	117.42	109.50

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	4770	0	4603	209	0
1	B	4770	0	4603	195	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	9542	0	9206	396	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 (396) 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:275:VAL:HA	1:A:282:ASN:HD21	1.22	1.05
1:B:545:VAL:HG21	1:B:569:LEU:HD13	1.39	1.04
1:A:328:ASN:HB3	1:A:355:ILE:HD12	1.40	1.02
1:B:535:ARG:HD3	1:B:539:GLN:HE22	1.30	0.96
1:A:514:ALA:HB1	1:A:539:GLN:HE22	1.31	0.94
1:A:223:ARG:HB3	1:A:223:ARG:NH1	1.88	0.89
1:A:579:MET:HE2	1:A:581:LEU:HD21	1.55	0.88
1:B:243:ASN:HD21	1:B:295:LYS:NZ	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ILE:HD11	1:B:460:MET:HG3	1.61	0.82
1:B:535:ARG:HD3	1:B:539:GLN:NE2	1.95	0.81
1:A:433:GLU:HG2	1:A:437:ARG:HD2	1.63	0.80
1:A:255:VAL:HG22	1:A:262:SER:OG	1.81	0.80
1:B:223:ARG:HB3	1:B:223:ARG:NH2	1.98	0.78
1:A:254:ASP:OD2	1:A:262:SER:HB2	1.84	0.78
1:A:416:LEU:H	1:A:416:LEU:HD23	1.49	0.78
1:B:547:GLU:HG2	1:B:551:LYS:HZ2	1.50	0.77
1:B:183:GLU:OE2	1:B:232:ARG:HG3	1.84	0.77
1:A:277:LYS:HB2	1:A:277:LYS:NZ	2.02	0.74
1:B:416:LEU:HD23	1:B:416:LEU:H	1.52	0.74
1:A:275:VAL:O	1:A:276:SER:HB2	1.87	0.73
1:B:545:VAL:HG21	1:B:569:LEU:CD1	2.18	0.73
1:B:190:LEU:HD13	1:B:234:ILE:HG21	1.70	0.72
1:A:223:ARG:HB3	1:A:223:ARG:HH11	1.53	0.72
1:B:243:ASN:HD21	1:B:295:LYS:HZ1	1.36	0.72
1:B:401:ALA:O	1:B:404:LEU:HB2	1.90	0.72
1:B:135:GLN:HB2	1:B:451:LEU:HD21	1.70	0.71
1:A:197:ALA:HB3	1:A:208:ASP:HB3	1.73	0.70
1:A:582:TRP:CE2	1:A:584:GLY:HA2	2.26	0.70
1:A:485:GLU:HA	1:A:488:LYS:HD3	1.73	0.70
1:A:275:VAL:HA	1:A:282:ASN:ND2	2.03	0.69
1:B:219:LEU:HD11	1:B:317:GLN:OE1	1.92	0.69
1:B:190:LEU:HD13	1:B:234:ILE:CG2	2.22	0.69
1:B:386:THR:OG1	1:B:388:GLU:HG3	1.93	0.69
1:B:467:ASP:OD2	1:B:470:ARG:NH1	2.26	0.68
1:B:542:LEU:HD21	1:B:568:GLN:NE2	2.08	0.68
1:A:398:LEU:HD21	1:A:442:PHE:CZ	2.29	0.68
1:A:401:ALA:HA	1:A:404:LEU:HD13	1.76	0.68
1:B:133:ILE:CD1	1:B:189:ALA:HB3	2.24	0.67
1:B:309:ASP:OD2	1:B:312:ARG:NH2	2.27	0.67
1:A:515:ASN:ND2	1:A:534:ASN:HB3	2.11	0.66
1:A:514:ALA:HB1	1:A:539:GLN:NE2	2.08	0.66
1:A:514:ALA:CB	1:A:539:GLN:HE22	2.07	0.66
1:B:328:ASN:HB3	1:B:355:ILE:HG12	1.77	0.66
1:B:320:ASP:O	1:B:349:ALA:HA	1.96	0.66
1:B:198:SER:HB3	1:B:203:LYS:HG3	1.79	0.65
1:A:306:TYR:O	1:A:310:VAL:HG23	1.97	0.65
1:B:219:LEU:HB3	1:B:220:PRO:HD3	1.78	0.64
1:B:240:ALA:HB1	1:B:242:PHE:CE1	2.32	0.64
1:A:47:SER:HB3	1:A:50:GLU:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:LEU:HD23	1:B:28:ARG:N	2.13	0.64
1:A:133:ILE:HD12	1:A:449:THR:HG21	1.79	0.64
1:A:523:VAL:HG22	1:A:524:GLN:HG2	1.80	0.64
1:B:328:ASN:N	1:B:328:ASN:HD22	1.95	0.63
1:A:398:LEU:HD21	1:A:442:PHE:HZ	1.64	0.63
1:B:458:ILE:HG12	1:B:472:MET:HE1	1.81	0.63
1:B:27:LEU:HD12	1:B:84:PHE:CD2	2.33	0.62
1:B:331:ASP:OD2	1:B:333:ALA:HB3	1.99	0.62
1:A:84:PHE:HB2	1:A:96:PHE:HB3	1.81	0.62
1:B:255:VAL:O	1:B:275:VAL:HG21	1.99	0.62
1:B:273:PHE:HA	1:B:274:PRO:C	2.25	0.62
1:A:224:ARG:HE	1:A:224:ARG:HA	1.63	0.62
1:B:458:ILE:C	1:B:458:ILE:HD12	2.24	0.61
1:B:271:GLU:HB2	1:B:282:ASN:O	2.00	0.61
1:A:475:GLU:OE1	1:A:477:LYS:HB2	2.01	0.61
1:A:544:GLN:O	1:A:545:VAL:HG13	2.01	0.60
1:B:516:LEU:C	1:B:516:LEU:HD23	2.27	0.60
1:A:218:ASP:OD1	1:A:220:PRO:HD2	2.02	0.60
1:A:118:ARG:O	1:A:121:VAL:HG23	2.01	0.60
1:A:12:GLY:HA2	1:A:364:MET:HE1	1.83	0.60
1:B:84:PHE:HB2	1:B:96:PHE:HB3	1.83	0.60
1:B:228:GLU:OE2	1:B:231:ARG:NH1	2.35	0.60
1:A:224:ARG:HA	1:A:224:ARG:NE	2.17	0.60
1:A:133:ILE:HD12	1:A:449:THR:CG2	2.32	0.60
1:A:409:ALA:O	1:A:413:LEU:HD13	2.02	0.60
1:A:38:GLU:OE1	1:A:54:HIS:HB3	2.02	0.59
1:B:573:LEU:HD13	1:B:579:MET:HE3	1.82	0.59
1:B:129:LYS:HA	1:B:411:GLN:OE1	2.02	0.59
1:B:269:PHE:HB2	1:B:284:GLU:HB3	1.84	0.59
1:A:535:ARG:NH2	1:A:537:GLU:HB2	2.17	0.59
1:B:582:TRP:CE2	1:B:584:GLY:HA2	2.38	0.59
1:B:545:VAL:HG23	1:B:545:VAL:O	2.02	0.59
1:A:297:ARG:HH12	1:B:118:ARG:HH22	1.49	0.58
1:B:547:GLU:HG2	1:B:551:LYS:NZ	2.18	0.58
1:B:401:ALA:HA	1:B:404:LEU:HD13	1.84	0.58
1:B:582:TRP:CZ2	1:B:584:GLY:HA2	2.39	0.58
1:A:2:LEU:HD12	1:A:2:LEU:H	1.68	0.58
1:B:545:VAL:CG2	1:B:569:LEU:HD13	2.25	0.58
1:B:330:VAL:HB	1:B:335:TRP:NE1	2.19	0.58
1:B:24:ARG:HD2	1:B:70:GLU:HG2	1.86	0.58
1:A:263:ARG:HD2	1:A:263:ARG:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ASN:ND2	1:A:348:ASP:H	2.02	0.57
1:B:133:ILE:HD12	1:B:189:ALA:HB3	1.86	0.57
1:B:145:ASP:HB3	1:B:148:ASN:ND2	2.18	0.57
1:A:117:HIS:HB3	1:B:299:GLU:CD	2.30	0.57
1:A:516:LEU:HD13	1:A:541:VAL:HG11	1.86	0.57
1:A:324:LEU:HD13	1:A:335:TRP:CZ3	2.40	0.57
1:B:357:HIS:O	1:B:358:ASP:C	2.48	0.57
1:A:79:ARG:HH22	1:B:288:VAL:HG22	1.69	0.56
1:A:277:LYS:HB2	1:A:277:LYS:HZ2	1.69	0.56
1:A:324:LEU:HD13	1:A:335:TRP:CH2	2.40	0.56
1:A:381:ILE:O	1:A:385:ALA:HB3	2.06	0.56
1:A:24:ARG:HD2	1:A:70:GLU:CD	2.30	0.56
1:B:223:ARG:HB3	1:B:223:ARG:CZ	2.35	0.56
1:A:195:ILE:O	1:A:196:PHE:HD2	1.89	0.56
1:A:31:LYS:HE3	1:A:63:ASP:O	2.05	0.55
1:A:223:ARG:HB3	1:A:223:ARG:CZ	2.36	0.55
1:B:139:GLU:OE2	1:B:140:ARG:NH1	2.39	0.55
1:A:202:HIS:CE1	1:A:205:ASP:OD1	2.59	0.55
1:A:228:GLU:OE1	1:A:231:ARG:NH1	2.37	0.55
1:B:243:ASN:HD21	1:B:295:LYS:HZ2	1.49	0.55
1:A:276:SER:O	1:A:277:LYS:HB2	2.05	0.55
1:A:223:ARG:HH22	1:A:227:ASP:CG	2.15	0.55
1:B:143:ASN:ND2	1:B:169:GLY:O	2.39	0.55
1:A:419:SER:OG	1:A:422:THR:HG23	2.07	0.55
1:B:276:SER:OG	1:B:277:LYS:N	2.40	0.55
1:A:270:ILE:HD13	1:A:275:VAL:HG21	1.88	0.55
1:B:425:PHE:HB3	1:B:436:PHE:HE1	1.70	0.54
1:B:197:ALA:HA	1:B:213:ASP:HB2	1.89	0.54
1:A:289:GLN:HE21	1:A:289:GLN:HA	1.71	0.54
1:B:142:ALA:O	1:B:174:GLY:HA3	2.08	0.54
1:B:232:ARG:HG3	1:B:232:ARG:HH11	1.73	0.54
1:B:193:THR:HB	1:B:194:PRO:HD2	1.90	0.54
1:A:518:ALA:HA	1:A:530:VAL:O	2.08	0.54
1:B:145:ASP:HB3	1:B:148:ASN:HD21	1.73	0.54
1:A:376:PHE:O	1:A:380:VAL:HG23	2.07	0.53
1:B:281:THR:HG23	1:B:291:PRO:HB3	1.91	0.53
1:A:281:THR:OG1	1:A:289:GLN:NE2	2.41	0.53
1:A:416:LEU:H	1:A:416:LEU:CD2	2.21	0.53
1:A:41:TYR:HB3	1:A:82:TYR:HB3	1.91	0.53
1:A:195:ILE:O	1:A:195:ILE:HG13	2.09	0.53
1:B:323:ARG:HD2	1:B:323:ARG:C	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ILE:HG22	1:B:357:HIS:H	1.74	0.53
1:A:84:PHE:O	1:A:95:TYR:HA	2.08	0.53
1:A:126:GLU:OE1	1:A:129:LYS:HE3	2.09	0.53
1:A:267:TRP:CZ2	1:A:302:GLU:HB3	2.44	0.53
1:B:383:PHE:CE1	1:B:391:ALA:HA	2.44	0.52
1:A:289:GLN:HE21	1:A:289:GLN:CA	2.23	0.52
1:B:441:LEU:HD13	1:B:578:GLY:HA3	1.89	0.52
1:A:134:TYR:CZ	1:A:454:TYR:HA	2.45	0.52
1:A:202:HIS:HE1	1:A:205:ASP:OD1	1.92	0.52
1:A:99:THR:OG1	1:A:109:GLY:HA3	2.09	0.52
1:A:504:ASN:N	1:A:504:ASN:HD22	2.07	0.52
1:B:180:PRO:HG3	1:B:232:ARG:HH22	1.75	0.52
1:A:1:MET:HE3	1:A:94:VAL:HG12	1.92	0.51
1:A:486:PHE:CZ	1:A:490:LEU:HD11	2.44	0.51
1:B:6:ILE:HG23	1:B:27:LEU:HD21	1.91	0.51
1:B:138:PRO:HG3	1:B:195:ILE:CG2	2.40	0.51
1:A:289:GLN:HA	1:A:289:GLN:NE2	2.25	0.51
1:B:133:ILE:HD13	1:B:189:ALA:HB3	1.92	0.51
1:B:8:HIS:CG	1:B:9:GLU:N	2.79	0.51
1:B:149:ASP:N	1:B:149:ASP:OD2	2.43	0.50
1:B:193:THR:HB	1:B:194:PRO:CD	2.42	0.50
1:B:504:ASN:C	1:B:504:ASN:HD22	2.19	0.50
1:A:297:ARG:NH1	1:B:118:ARG:HH12	2.10	0.50
1:A:535:ARG:HG3	1:A:539:GLN:OE1	2.11	0.50
1:A:117:HIS:HB3	1:B:299:GLU:OE2	2.11	0.50
1:B:554:LEU:O	1:B:581:LEU:HA	2.12	0.50
1:A:57:ALA:HB2	1:A:71:ALA:HB2	1.94	0.50
1:A:424:ARG:HD2	1:A:461:ALA:C	2.37	0.49
1:B:143:ASN:ND2	1:B:169:GLY:HA3	2.26	0.49
1:B:138:PRO:HG3	1:B:195:ILE:HG22	1.93	0.49
1:A:178:ARG:HG3	1:A:474:TRP:CZ2	2.48	0.49
1:A:457:GLU:HA	1:A:487:TYR:CE1	2.47	0.49
1:B:82:TYR:C	1:B:110:VAL:HG23	2.37	0.49
1:B:308:PHE:O	1:B:311:ALA:HB3	2.12	0.49
1:A:579:MET:CE	1:A:581:LEU:HD21	2.34	0.49
1:B:444:MET:HG3	1:B:490:LEU:HB3	1.92	0.49
1:A:326:VAL:HG12	1:A:326:VAL:O	2.13	0.49
1:A:163:ARG:HB2	1:A:163:ARG:NH1	2.28	0.49
1:A:278:THR:C	1:A:280:ARG:H	2.21	0.49
1:B:99:THR:OG1	1:B:109:GLY:HA3	2.13	0.49
1:A:2:LEU:HD12	1:A:2:LEU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LEU:HD23	1:A:341:LEU:C	2.38	0.48
1:A:324:LEU:HB2	1:A:327:ALA:HB2	1.94	0.48
1:B:179:LEU:N	1:B:180:PRO:CD	2.76	0.48
1:A:352:VAL:HG21	1:A:414:TRP:CZ2	2.48	0.48
1:A:432:ASN:OD1	1:A:434:ALA:N	2.46	0.48
1:B:465:ASP:OD1	1:B:469:ARG:NH2	2.46	0.48
1:A:197:ALA:O	1:A:207:ALA:HB3	2.14	0.48
1:B:206:THR:HG21	1:B:209:TYR:CG	2.49	0.48
1:B:424:ARG:HD2	1:B:461:ALA:C	2.39	0.48
1:A:380:VAL:HG12	1:A:425:PHE:CZ	2.49	0.48
1:B:255:VAL:HG12	1:B:275:VAL:CG1	2.44	0.48
1:B:533:ASN:ND2	1:B:574:ARG:O	2.47	0.48
1:B:324:LEU:HD13	1:B:335:TRP:CH2	2.49	0.48
1:A:411:GLN:HA	1:A:447:LEU:HD11	1.96	0.48
1:B:244:HIS:CD2	1:B:286:ALA:HB2	2.48	0.48
1:A:504:ASN:C	1:A:504:ASN:ND2	2.72	0.47
1:B:328:ASN:N	1:B:328:ASN:ND2	2.62	0.47
1:A:1:MET:HE1	1:A:86:LEU:C	2.39	0.47
1:A:297:ARG:HH11	1:B:118:ARG:HH12	1.62	0.47
1:B:65:ARG:HH11	1:B:65:ARG:HG2	1.78	0.47
1:B:232:ARG:HH11	1:B:232:ARG:CG	2.27	0.47
1:B:281:THR:HG22	1:B:283:TYR:CE2	2.49	0.47
1:A:297:ARG:HH12	1:B:118:ARG:NH2	2.11	0.47
1:A:436:PHE:O	1:A:440:VAL:HG23	2.14	0.47
1:B:422:THR:OG1	1:B:423:GLU:N	2.46	0.47
1:B:323:ARG:NH2	1:B:372:MET:HE3	2.30	0.47
1:B:447:LEU:HB2	1:B:505:VAL:CG2	2.45	0.47
1:A:24:ARG:HD2	1:A:70:GLU:CG	2.44	0.47
1:B:27:LEU:HD23	1:B:27:LEU:C	2.39	0.47
1:B:143:ASN:HA	1:B:171:ASP:OD2	2.15	0.47
1:A:565:LYS:O	1:A:565:LYS:HG2	2.14	0.47
1:B:223:ARG:HB3	1:B:223:ARG:HH21	1.77	0.47
1:A:493:LEU:HD11	1:A:556:CYS:HB3	1.97	0.47
1:B:475:GLU:OE2	1:B:475:GLU:HA	2.14	0.47
1:A:133:ILE:CD1	1:A:449:THR:HG21	2.45	0.47
1:B:324:LEU:HD13	1:B:335:TRP:CZ3	2.49	0.47
1:A:271:GLU:HG3	1:A:272:ASP:CG	2.41	0.46
1:A:582:TRP:CD1	1:A:584:GLY:H	2.33	0.46
1:B:542:LEU:HD21	1:B:568:GLN:CD	2.40	0.46
1:B:480:ASN:ND2	1:B:483:LEU:HB2	2.30	0.46
1:B:504:ASN:HD22	1:B:504:ASN:N	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:LEU:HD12	1:A:368:PHE:CE2	2.50	0.46
1:A:377:ARG:HG2	1:A:377:ARG:HH11	1.80	0.46
1:A:194:PRO:HG2	1:A:204:TYR:CE1	2.51	0.46
1:B:377:ARG:CZ	1:B:381:ILE:HD11	2.46	0.46
1:A:1:MET:HE1	1:A:86:LEU:O	2.15	0.46
1:A:346:ASN:HD22	1:A:346:ASN:C	2.23	0.46
1:B:206:THR:HG21	1:B:209:TYR:CD1	2.51	0.46
1:B:442:PHE:O	1:B:443:GLN:C	2.58	0.46
1:B:453:TYR:HB3	1:B:456:ASP:OD2	2.15	0.46
1:A:250:PHE:CD1	1:A:250:PHE:C	2.94	0.46
1:B:582:TRP:CH2	1:B:584:GLY:HA2	2.51	0.46
1:A:330:VAL:HG22	1:A:335:TRP:NE1	2.31	0.46
1:B:427:THR:OG1	1:B:462:GLY:O	2.29	0.46
1:B:65:ARG:HG2	1:B:65:ARG:NH1	2.31	0.45
1:B:555:ASP:C	1:B:555:ASP:OD2	2.60	0.45
1:B:582:TRP:CE2	1:B:584:GLY:CA	3.00	0.45
1:A:8:HIS:HD2	1:A:26:ARG:O	1.98	0.45
1:B:31:LYS:HG3	1:B:67:ASP:OD1	2.17	0.45
1:B:193:THR:O	1:B:194:PRO:C	2.60	0.45
1:A:83:VAL:HG22	1:A:84:PHE:N	2.31	0.45
1:B:475:GLU:O	1:B:476:GLU:C	2.59	0.45
1:B:564:GLY:HA3	1:B:569:LEU:HD12	1.99	0.45
1:A:27:LEU:HD13	1:A:84:PHE:CD2	2.52	0.45
1:A:497:LEU:HD12	1:A:500:LEU:CD1	2.47	0.45
1:A:545:VAL:HG21	1:A:569:LEU:HB2	1.97	0.45
1:A:569:LEU:HG	1:A:571:LEU:HD13	1.99	0.45
1:A:420:HIS:ND1	1:A:420:HIS:N	2.65	0.45
1:B:357:HIS:HA	1:B:374:TYR:OH	2.16	0.45
1:A:313:PHE:O	1:A:317:GLN:HG2	2.17	0.45
1:A:140:ARG:HG2	1:A:469:ARG:O	2.17	0.45
1:A:249:PHE:O	1:A:250:PHE:C	2.59	0.45
1:A:312:ARG:O	1:A:316:GLU:HG3	2.17	0.45
1:A:27:LEU:HD22	1:A:37:CYS:SG	2.57	0.45
1:A:271:GLU:HG2	1:A:282:ASN:O	2.17	0.45
1:B:218:ASP:HB2	1:B:220:PRO:HD2	1.99	0.45
1:A:30:LYS:HB3	1:A:33:ASP:HB2	1.97	0.45
1:A:574:ARG:O	1:A:575:PRO:C	2.59	0.45
1:A:523:VAL:O	1:A:523:VAL:HG13	2.17	0.44
1:A:454:TYR:O	1:A:454:TYR:CG	2.70	0.44
1:B:271:GLU:OE2	1:B:283:TYR:HA	2.17	0.44
1:A:380:VAL:HG13	1:A:384:PHE:HD1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:PHE:CE1	1:A:488:LYS:HD2	2.52	0.44
1:B:64:GLU:HG3	1:B:393:ARG:NH2	2.33	0.44
1:B:416:LEU:H	1:B:416:LEU:CD2	2.25	0.44
1:A:260:GLU:H	1:A:260:GLU:HG2	1.40	0.44
1:B:122:PHE:HB3	1:B:408:GLN:CD	2.43	0.44
1:B:499:SER:HA	1:B:523:VAL:HG12	1.99	0.44
1:A:206:THR:HG21	1:A:209:TYR:CZ	2.53	0.44
1:A:483:LEU:O	1:A:486:PHE:HB3	2.17	0.44
1:B:27:LEU:HD23	1:B:28:ARG:O	2.18	0.44
1:B:458:ILE:C	1:B:458:ILE:CD1	2.91	0.44
1:B:263:ARG:O	1:B:263:ARG:HG3	2.18	0.44
1:A:12:GLY:H	1:A:364:MET:HE1	1.82	0.44
1:A:263:ARG:HH12	1:A:302:GLU:CD	2.25	0.44
1:B:451:LEU:HD23	1:B:451:LEU:C	2.42	0.44
1:A:218:ASP:CG	1:A:220:PRO:HD2	2.41	0.44
1:A:401:ALA:O	1:A:404:LEU:HB2	2.17	0.44
1:A:465:ASP:HA	1:A:466:PRO:HA	1.78	0.43
1:A:516:LEU:HD23	1:A:517:TYR:N	2.32	0.43
1:A:12:GLY:HA2	1:A:364:MET:CE	2.48	0.43
1:A:12:GLY:CA	1:A:364:MET:HE1	2.47	0.43
1:A:179:LEU:HB3	1:A:232:ARG:HD2	2.00	0.43
1:B:255:VAL:HG11	1:B:270:ILE:HD11	2.01	0.43
1:B:354:GLU:C	1:B:355:ILE:HG13	2.42	0.43
1:A:432:ASN:OD1	1:A:432:ASN:C	2.61	0.43
1:B:197:ALA:HA	1:B:213:ASP:CB	2.47	0.43
1:B:426:LEU:HD23	1:B:461:ALA:HB2	2.00	0.43
1:B:499:SER:OG	1:B:523:VAL:HG12	2.19	0.43
1:A:375:LEU:HD12	1:A:375:LEU:HA	1.83	0.43
1:A:460:MET:HE1	1:A:472:MET:HA	1.99	0.43
1:A:579:MET:HE2	1:A:579:MET:HB3	1.78	0.43
1:B:57:ALA:HB2	1:B:71:ALA:HB2	1.99	0.43
1:B:158:LYS:CD	1:B:478:GLU:HB3	2.49	0.43
1:B:305:GLU:OE2	1:B:305:GLU:HA	2.19	0.43
1:B:376:PHE:CE1	1:B:415:ASN:HB3	2.54	0.43
1:A:191:TYR:CE1	1:A:323:ARG:HG3	2.53	0.43
1:A:137:PHE:CE1	1:A:469:ARG:HD3	2.54	0.43
1:A:222:PHE:O	1:A:226:VAL:HG23	2.19	0.43
1:A:240:ALA:HB2	1:A:322:TRP:CE3	2.54	0.43
1:A:352:VAL:HG21	1:A:414:TRP:CE2	2.54	0.43
1:B:95:TYR:CE2	1:B:105:ARG:HB2	2.54	0.43
1:B:158:LYS:HD2	1:B:478:GLU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:PHE:CG	1:B:251:ALA:N	2.87	0.43
1:B:425:PHE:HB3	1:B:436:PHE:CE1	2.51	0.43
1:B:526:GLN:C	1:B:527:HIS:HD2	2.27	0.43
1:A:244:HIS:ND1	1:A:293:MET:HB3	2.33	0.43
1:A:497:LEU:HD12	1:A:500:LEU:HD11	2.00	0.43
1:B:268:PHE:N	1:B:268:PHE:CD1	2.86	0.43
1:B:277:LYS:HG3	1:B:280:ARG:HB3	2.01	0.43
1:A:528:VAL:HA	1:A:581:LEU:O	2.19	0.43
1:A:148:ASN:OD1	1:A:148:ASN:C	2.62	0.42
1:A:200:SER:OG	1:A:202:HIS:CE1	2.72	0.42
1:B:182:LEU:HD13	1:B:190:LEU:HD11	2.01	0.42
1:B:240:ALA:HB1	1:B:242:PHE:CZ	2.54	0.42
1:A:275:VAL:O	1:A:276:SER:CB	2.58	0.42
1:A:41:TYR:CB	1:A:82:TYR:HB3	2.49	0.42
1:A:156:TRP:CE2	1:A:471:PRO:HB2	2.54	0.42
1:A:222:PHE:CZ	1:A:238:LEU:HD11	2.54	0.42
1:B:441:LEU:HD23	1:B:441:LEU:C	2.44	0.42
1:A:73:LEU:N	1:A:73:LEU:CD1	2.83	0.42
1:A:143:ASN:CG	1:A:169:GLY:O	2.63	0.42
1:B:202:HIS:O	1:B:203:LYS:HB2	2.19	0.42
1:B:255:VAL:HG12	1:B:275:VAL:HG11	2.00	0.42
1:A:134:TYR:OH	1:A:454:TYR:HA	2.18	0.42
1:A:232:ARG:HH21	1:A:232:ARG:HG3	1.84	0.42
1:A:557:LEU:HG	1:A:580:ILE:HD12	2.02	0.42
1:A:426:LEU:C	1:A:426:LEU:HD23	2.44	0.42
1:A:447:LEU:HB2	1:A:505:VAL:CG2	2.48	0.42
1:B:6:ILE:CG2	1:B:27:LEU:HD21	2.49	0.42
1:B:12:GLY:HA2	1:B:364:MET:HE2	2.02	0.42
1:B:327:ALA:C	1:B:329:GLU:H	2.28	0.42
1:B:515:ASN:HD21	1:B:534:ASN:ND2	2.18	0.42
1:B:257:GLN:HE21	1:B:257:GLN:HB2	1.65	0.42
1:B:573:LEU:HA	1:B:577:GLN:OE1	2.20	0.42
1:A:206:THR:HG21	1:A:209:TYR:CE2	2.54	0.42
1:A:553:TRP:CD1	1:A:581:LEU:HB3	2.55	0.42
1:A:57:ALA:CB	1:A:71:ALA:HB2	2.48	0.42
1:B:82:TYR:N	1:B:110:VAL:HG22	2.35	0.42
1:B:263:ARG:HG3	1:B:263:ARG:HH21	1.85	0.42
1:A:277:LYS:HB2	1:A:277:LYS:HZ3	1.83	0.42
1:A:373:ASN:ND2	1:A:413:LEU:HD23	2.35	0.42
1:A:570:LYS:O	1:A:571:LEU:HD12	2.20	0.42
1:B:519:PHE:CE1	1:B:530:VAL:HB	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:ASN:O	1:B:576:TYR:HA	2.19	0.42
1:A:5:ALA:HB1	1:B:4:GLU:HB3	2.01	0.41
1:A:11:LYS:N	1:A:15:ALA:HB3	2.35	0.41
1:A:324:LEU:CB	1:A:327:ALA:HB2	2.50	0.41
1:A:324:LEU:CD1	1:A:368:PHE:CE2	3.03	0.41
1:B:377:ARG:HE	1:B:418:ASP:HA	1.85	0.41
1:A:555:ASP:O	1:A:559:GLY:N	2.41	0.41
1:B:194:PRO:HD3	1:B:239:ASP:OD1	2.19	0.41
1:B:460:MET:HG2	1:B:473:ILE:HD12	2.02	0.41
1:B:555:ASP:OD1	1:B:579:MET:HG2	2.20	0.41
1:A:555:ASP:OD1	1:A:579:MET:HG2	2.20	0.41
1:B:127:TRP:CE3	1:B:235:LYS:HD3	2.56	0.41
1:A:240:ALA:HB1	1:A:242:PHE:CE1	2.55	0.41
1:A:357:HIS:O	1:A:358:ASP:C	2.63	0.41
1:A:458:ILE:HD11	1:A:472:MET:SD	2.60	0.41
1:A:504:ASN:O	1:A:521:ARG:HA	2.20	0.41
1:A:529:GLY:N	1:A:581:LEU:O	2.46	0.41
1:B:228:GLU:O	1:B:232:ARG:HD3	2.20	0.41
1:B:243:ASN:ND2	1:B:295:LYS:HZ1	2.10	0.41
1:B:464:THR:OG1	1:B:465:ASP:N	2.53	0.41
1:B:504:ASN:C	1:B:504:ASN:ND2	2.76	0.41
1:A:104:GLU:OE1	1:A:107:LYS:HD3	2.21	0.41
1:B:24:ARG:HD2	1:B:70:GLU:CG	2.50	0.41
1:B:165:ASP:OD2	1:B:165:ASP:N	2.50	0.41
1:B:574:ARG:HB3	1:B:575:PRO:CD	2.51	0.41
1:A:8:HIS:CG	1:A:9:GLU:N	2.88	0.41
1:A:454:TYR:O	1:A:454:TYR:CD1	2.73	0.41
1:B:232:ARG:CG	1:B:232:ARG:NH1	2.83	0.41
1:B:352:VAL:HG21	1:B:414:TRP:CZ2	2.55	0.41
1:A:1:MET:SD	1:A:34:VAL:HG22	2.60	0.41
1:A:325:ASP:O	1:A:326:VAL:C	2.63	0.41
1:B:582:TRP:CD2	1:B:584:GLY:HA2	2.56	0.41
1:A:273:PHE:CD1	1:A:275:VAL:HG23	2.55	0.41
1:A:326:VAL:HG12	1:A:329:GLU:HB2	2.02	0.41
1:A:515:ASN:HD22	1:A:534:ASN:HB3	1.83	0.41
1:B:202:HIS:ND1	1:B:204:TYR:HB2	2.36	0.41
1:A:12:GLY:HA2	1:A:364:MET:SD	2.61	0.41
1:A:57:ALA:HA	1:A:71:ALA:HB2	2.03	0.41
1:A:195:ILE:O	1:A:195:ILE:CG1	2.66	0.41
1:A:278:THR:O	1:A:279:SER:HB2	2.21	0.41
1:A:325:ASP:OD1	1:A:326:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:LYS:O	1:A:492:ARG:HG3	2.20	0.41
1:A:546:PRO:O	1:A:548:SER:N	2.54	0.41
1:B:304:LYS:HB2	1:B:304:LYS:HE3	1.92	0.41
1:B:377:ARG:NE	1:B:417:LEU:O	2.53	0.41
1:A:416:LEU:HB3	1:A:451:LEU:HD23	2.03	0.41
1:B:499:SER:HA	1:B:523:VAL:CG1	2.51	0.41
1:A:516:LEU:HD23	1:A:516:LEU:C	2.46	0.40
1:B:564:GLY:CA	1:B:569:LEU:HD12	2.52	0.40
1:A:273:PHE:HA	1:A:274:PRO:C	2.45	0.40
1:A:308:PHE:HB3	1:A:341:LEU:CD1	2.51	0.40
1:B:49:GLU:H	1:B:49:GLU:HG3	1.61	0.40
1:A:426:LEU:HA	1:A:436:PHE:HD1	1.85	0.40
1:A:248:GLN:HA	1:A:253:ARG:HD3	2.03	0.40
1:A:480:ASN:OD1	1:A:483:LEU:HB2	2.21	0.40
1:B:158:LYS:NZ	1:B:478:GLU:O	2.52	0.40
1:B:335:TRP:HA	1:B:335:TRP:CE3	2.57	0.40
1:B:483:LEU:O	1:B:486:PHE:HB3	2.21	0.40
1:B:550:GLY:HA2	1:B:585:ARG:NH2	2.36	0.40
1:B:572:THR:C	1:B:573:LEU:HD22	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	583/585 (100%)	556 (95%)	23 (4%)	4 (1%)	18	52
1	B	583/585 (100%)	548 (94%)	34 (6%)	1 (0%)	43	73
All	All	1166/1170 (100%)	1104 (95%)	57 (5%)	5 (0%)	30	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	547	GLU
1	A	276	SER
1	A	277	LYS
1	B	328	ASN
1	A	195	ILE

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	492/492 (100%)	455 (92%)	37 (8%)	12	42
1	B	492/492 (100%)	462 (94%)	30 (6%)	17	49
All	All	984/984 (100%)	917 (93%)	67 (7%)	14	46

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	26	ARG
1	A	27	LEU
1	A	38	GLU
1	A	90	GLN
1	A	121	VAL
1	A	139	GLU
1	A	140	ARG
1	A	159	ASP
1	A	166	SER
1	A	167	PHE
1	A	182	LEU
1	A	223	ARG
1	A	250	PHE
1	A	260	GLU
1	A	263	ARG
1	A	272	ASP
1	A	277	LYS
1	A	278	THR

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Mol	Chain	Res	Type
1	A	323	ARG
1	A	330	VAL
1	A	345	LEU
1	A	375	LEU
1	A	377	ARG
1	A	398	LEU
1	A	422	THR
1	A	437	ARG
1	A	460	MET
1	A	475	GLU
1	A	483	LEU
1	A	504	ASN
1	A	505	VAL
1	A	535	ARG
1	A	545	VAL
1	A	565	LYS
1	A	570	LYS
1	A	572	THR
1	B	50	GLU
1	B	64	GLU
1	B	85	LEU
1	B	149	ASP
1	B	155	GLN
1	B	167	PHE
1	B	188	THR
1	B	215	GLN
1	B	218	ASP
1	B	223	ARG
1	B	232	ARG
1	B	235	LYS
1	B	248	GLN
1	B	265	LYS
1	B	272	ASP
1	B	275	VAL
1	B	279	SER
1	B	281	THR
1	B	323	ARG
1	B	328	ASN
1	B	364	MET
1	B	382	ARG
1	B	398	LEU
1	B	467	ASP

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Mol	Chain	Res	Type
1	B	504	ASN
1	B	522	THR
1	B	537	GLU
1	B	552	THR
1	B	565	LYS
1	B	583	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	22	GLN
1	A	90	GLN
1	A	112	GLN
1	A	135	GLN
1	A	155	GLN
1	A	289	GLN
1	A	332	HIS
1	A	346	ASN
1	A	390	HIS
1	A	504	ASN
1	A	526	GLN
1	A	539	GLN
1	A	544	GLN
1	A	568	GLN
1	B	135	GLN
1	B	155	GLN
1	B	243	ASN
1	B	244	HIS
1	B	248	GLN
1	B	257	GLN
1	B	328	ASN
1	B	332	HIS
1	B	357	HIS
1	B	504	ASN
1	B	515	ASN
1	B	527	HIS
1	B	544	GLN
1	B	563	HIS
1	B	566	GLN
1	B	568	GLN

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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.