



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:09 PM GMT

PDB ID : 1J0K
Title : Crystal structure of neopullulanase E357Q complex with isopanose
Authors : Hondoh, H.; Kuriki, T.; Matsuura, Y.
Deposited on : 2002-11-14
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

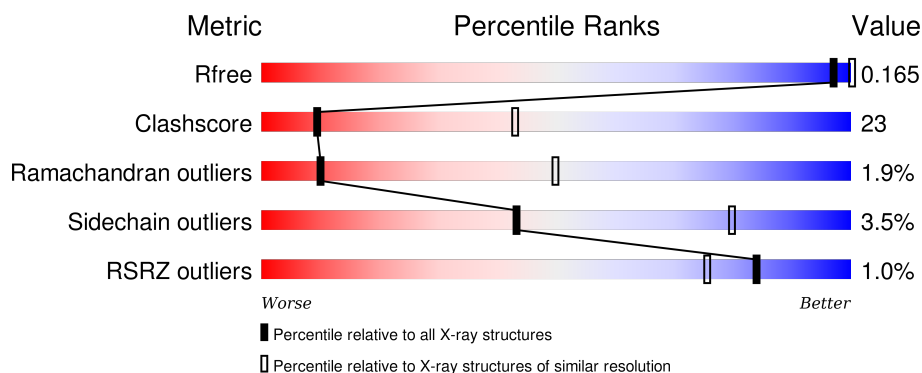
1 Overall quality at a glance

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))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	588	<div> <div></div> <div>58% 39% .</div> </div>
1	B	588	<div> <div></div> <div>54% 43% .</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9971 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 neopullulanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4889	3158	817	892	22			
1	B	588	Total	C	N	O	S	0	0	0
			4889	3158	817	892	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	ALA	ARG	SEE REMARK 999	UNP P38940
A	357	GLN	GLU	ENGINEERED	UNP P38940
B	290	ALA	ARG	SEE REMARK 999	UNP P38940
B	357	GLN	GLU	ENGINEERED	UNP P38940

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	3	Total	C	O	0	0
			34	18	16		
2	B	3	Total	C	O	0	0
			34	18	16		

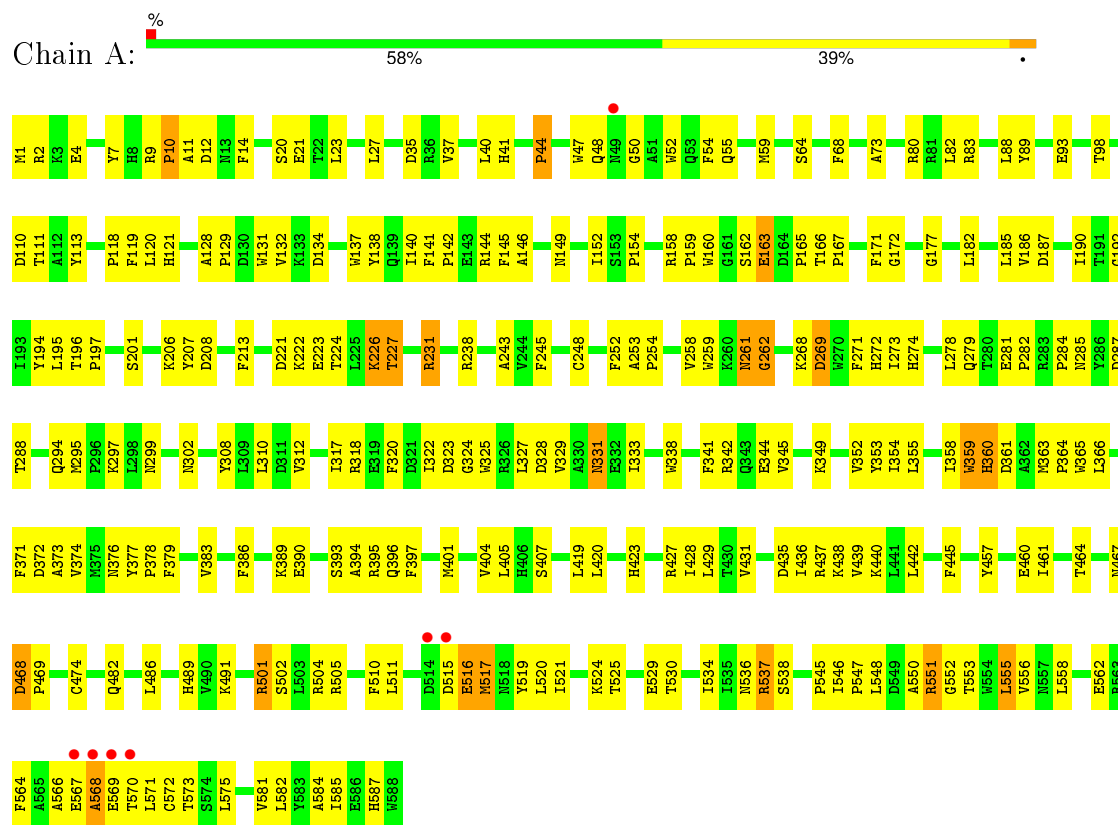
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total	O	0	0
			71	71		
3	B	54	Total	O	0	0
			54	54		

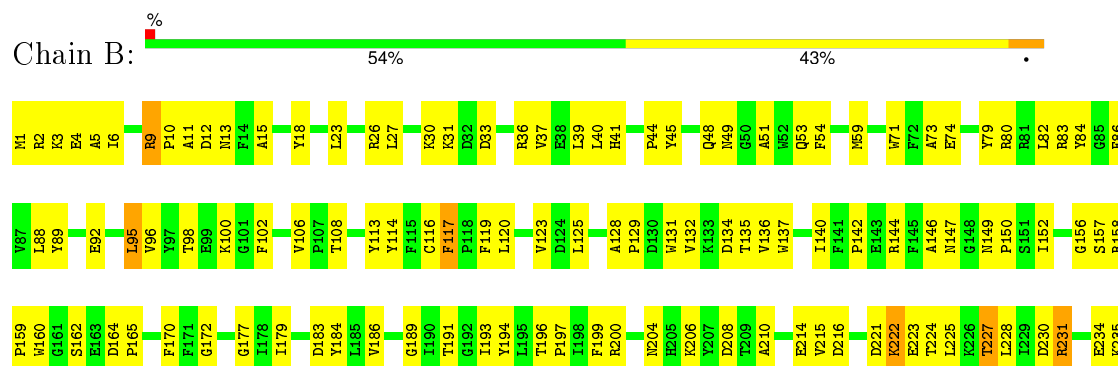
3 Residue-property plots

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

● Molecule 1: neopullulanase



● Molecule 1: neopullulanase



R504	D821	Q400	R504
R505	I322	M401	R505
G506	D323	V404	G506
E507	G324	S407	E507
L511	W325	M410	L511
D514	I327	E414	D514
D515	D328	L419	D515
I521	V329	L420	I521
K524	A330	H423	K524
T525	N331	D435	T525
D526	E332	I436	D526
G527	I333	R437	G527
D528	F337	K440	D528
E529	W338	L441	E529
I534	R339	L442	I534
I537	E340	T448	I537
K541	F341	F449	K541
P545	G262	S452	P545
I546	E263	G458	I546
P547	Q343	I461	P547
L548	E344	G466	L548
D549	E349	M467	D549
A550	K349	D468	A550
R551	Y267	N469	R551
W554	K268	E470	W554
L555	D269	C471	L555
V556	W270	R472	V556
E562	F271	K473	E562
R563	H272	C474	R563
P564	I273	M475	P564
A565	L278	D478	A565
A566	Q279	P479	A566
E567	T280	M480	E567
A568	E281	Q481	A568
E569	P282	Q482	E569
T570	R283	V488	T570
L571	P284	Q492	L571
C572	W285	R497	C572
V581	D287	Y500	V581
L582	Q294	R501	L582
Y583	W295	S502	Y583
A584	P296	L503	A584
I585	N299		I585
E586	K306		E586
H587	R307		H587
W588	Y308		W588
	L309		
	I310		
	D311		
	E315		
	W316		
	E319		
	Q396		
	N399		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.01Å 73.76Å 123.25Å 90.00° 90.15° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20 19.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-3.20) 100.0 (19.98-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.17 (at 3.22Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.174 , 0.212 0.174 , 0.165	Depositor DCC
R_{free} test set	1011 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.5	EDS
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 20298 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9971	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.43	0/5047	0.66	0/6857
1	B	0.43	0/5047	0.66	1/6857 (0.0%)
All	All	0.43	0/10094	0.66	1/13714 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	PHE	N-CA-C	-5.75	95.48	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	4889	0	4645	203	0
1	B	4889	0	4645	240	0
2	A	34	0	30	2	0
2	B	34	0	30	2	0
3	A	71	0	0	3	0
3	B	54	0	0	2	0
All	All	9971	0	9350	433	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 23.

All (433) 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:2:ARG:HH21	1:B:4:GLU:HB2	1.19	1.02
1:B:253:ALA:HB3	1:B:254:PRO:HD3	1.49	0.94
1:B:545:PRO:HA	1:B:572:CYS:HB2	1.55	0.89
1:A:23:LEU:HD23	1:A:120:LEU:HD21	1.55	0.88
1:A:2:ARG:NH2	1:B:4:GLU:HB2	1.91	0.86
1:A:393:SER:OG	1:A:396:GLN:HG3	1.76	0.84
1:A:159:PRO:HG2	1:A:162:SER:HB2	1.59	0.84
1:A:429:LEU:HD23	1:A:464:THR:HG22	1.59	0.84
1:A:41:HIS:HB2	1:A:82:LEU:HD11	1.61	0.82
1:B:147:ASN:HD21	1:B:150:PRO:HG3	1.46	0.81
1:A:201:SER:HB3	1:A:206:LYS:HG3	1.61	0.80
1:A:44:PRO:HG3	1:A:83:ARG:HG2	1.62	0.80
1:A:501:ARG:HD2	1:A:505:ARG:HD2	1.64	0.78
1:B:41:HIS:HB2	1:B:82:LEU:HD11	1.67	0.77
1:A:511:LEU:HD23	1:A:547:PRO:HG2	1.66	0.77
1:B:149:ASN:OD1	1:B:152:ILE:HG12	1.86	0.76
1:B:400:GLN:O	1:B:404:VAL:HG13	1.85	0.76
1:A:2:ARG:HH21	1:B:4:GLU:CB	1.98	0.75
1:B:3:LYS:HA	1:B:6:ILE:HD12	1.69	0.75
1:B:222:LYS:HG3	1:B:320:PHE:HZ	1.52	0.74
1:A:389:LYS:HE2	1:A:431:VAL:HG13	1.69	0.74
1:A:429:LEU:HD23	1:A:464:THR:CG2	2.18	0.73
1:B:328:ASP:HA	1:B:357:GLN:HB3	1.71	0.73
1:A:558:LEU:HD21	1:A:584:ALA:HB2	1.70	0.72
1:B:326:ARG:HE	1:B:375:MET:CE	2.03	0.72
1:B:326:ARG:HE	1:B:375:MET:HE3	1.54	0.72
1:A:47:TRP:HZ2	1:A:111:THR:HG23	1.54	0.72
1:B:389:LYS:HB3	1:B:391:GLU:HG3	1.73	0.71
1:B:310:LEU:HD13	1:B:344:GLU:OE2	1.91	0.70
1:A:440:LYS:HG2	1:A:489:HIS:CE1	2.27	0.69
1:A:349:LYS:O	1:A:352:VAL:HG23	1.92	0.69
1:A:299:ASN:ND2	1:A:302:ASN:HB2	2.07	0.69
1:B:420:LEU:HD13	1:B:442:LEU:HB3	1.75	0.69
1:A:359:TRP:HA	1:A:377:TYR:HD1	1.57	0.69
1:B:551:ARG:HE	1:B:551:ARG:HA	1.59	0.68
1:B:331:ASN:HD22	1:B:331:ASN:N	1.91	0.68
1:B:567:GLU:C	1:B:569:GLU:H	1.96	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ARG:NH1	1:B:328:ASP:HB3	2.10	0.67
1:A:59:MET:HG2	1:A:73:ALA:HB2	1.76	0.67
1:B:511:LEU:HB2	1:B:521:ILE:HG22	1.75	0.67
1:B:12:ASP:HB3	1:B:363:MET:SD	2.34	0.67
1:B:315:TYR:CE1	1:B:319:GLU:HG3	2.29	0.67
1:B:247:HIS:CD2	1:B:295:MET:HB3	2.30	0.66
1:A:279:GLN:O	1:A:284:PRO:HA	1.94	0.66
1:A:390:GLU:HG2	1:A:537:ARG:HD3	1.78	0.66
1:A:331:ASN:HD22	1:A:331:ASN:N	1.93	0.66
1:A:551:ARG:HA	1:A:551:ARG:HE	1.61	0.66
1:A:144:ARG:HH21	1:A:165:PRO:HB2	1.61	0.66
1:B:1:MET:HA	1:B:33:ASP:OD2	1.95	0.66
1:B:88:LEU:N	1:B:88:LEU:HD12	2.11	0.65
1:B:221:ASP:OD1	1:B:223:GLU:HB3	1.96	0.65
1:B:282:PRO:HG2	1:B:283:ARG:H	1.61	0.65
1:A:129:PRO:O	1:A:132:VAL:HG22	1.96	0.65
1:B:525:THR:HG22	1:B:527:GLY:H	1.61	0.65
1:A:435:ASP:OD1	1:A:437:ARG:HB2	1.97	0.65
1:B:160:TRP:CE2	1:B:474:CYS:HB3	2.33	0.64
1:B:1:MET:HG2	1:B:95:LEU:HD12	1.79	0.64
1:A:272:HIS:HB2	1:A:287:ASP:HB2	1.80	0.64
1:A:47:TRP:CZ2	1:A:52:TRP:HB2	2.32	0.64
1:B:39:LEU:HD11	1:B:84:TYR:HB2	1.80	0.63
1:A:226:LYS:HA	1:A:226:LYS:HE2	1.79	0.63
1:A:525:THR:HG22	1:A:530:THR:HG23	1.81	0.63
1:B:563:ARG:NH2	1:B:586:GLU:OE1	2.32	0.63
1:B:357:GLN:OE1	2:B:606:GLC:H62	1.99	0.63
1:A:359:TRP:HA	1:A:377:TYR:CD1	2.33	0.63
1:B:23:LEU:HB3	1:B:120:LEU:HD21	1.80	0.63
1:A:546:ILE:O	1:A:570:THR:HB	1.99	0.62
1:A:427:ARG:O	1:A:431:VAL:HG23	1.99	0.62
1:A:327:LEU:HD11	1:A:341:PHE:CZ	2.34	0.62
1:B:96:VAL:O	1:B:102:PHE:HA	1.99	0.62
1:B:329:VAL:HG22	2:B:606:GLC:H61	1.80	0.62
1:B:521:ILE:HG12	1:B:534:ILE:HG12	1.80	0.62
1:A:132:VAL:HG11	1:A:353:TYR:CD1	2.35	0.62
1:B:511:LEU:HD23	1:B:547:PRO:HG2	1.81	0.62
1:A:253:ALA:HB3	1:A:254:PRO:HD3	1.82	0.62
1:A:166:THR:HB	1:A:167:PRO:HD2	1.81	0.62
1:A:299:ASN:HD22	1:A:302:ASN:HB2	1.66	0.61
1:B:326:ARG:NH1	1:B:328:ASP:OD2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PHE:CD2	1:A:121:HIS:CE1	2.89	0.60
1:B:339:ARG:HG3	1:B:339:ARG:HH11	1.66	0.60
1:B:502:SER:HB3	1:B:529:GLU:HG3	1.82	0.60
1:A:269:ASP:HB3	1:A:302:ASN:ND2	2.17	0.60
1:B:547:PRO:O	1:B:548:LEU:HD12	2.02	0.60
1:B:74:GLU:O	1:B:74:GLU:HG3	2.01	0.60
1:B:254:PRO:O	1:B:258:VAL:HG23	2.02	0.60
1:A:515:ASP:C	1:A:517:MET:H	2.05	0.60
1:A:243:ALA:HB2	1:A:325:TRP:CE3	2.36	0.60
1:B:333:ILE:HD12	1:B:338:TRP:CZ2	2.37	0.59
1:A:461:ILE:HB	1:A:482:GLN:HB2	1.84	0.59
1:A:555:LEU:HD22	1:A:555:LEU:N	2.17	0.59
1:A:47:TRP:CZ2	1:A:111:THR:HG23	2.37	0.59
1:B:147:ASN:ND2	1:B:150:PRO:HG3	2.15	0.59
1:A:317:ILE:HA	1:A:322:ILE:HG12	1.84	0.59
1:A:226:LYS:HE3	1:A:320:PHE:HA	1.85	0.59
1:A:331:ASN:HD22	1:A:331:ASN:H	1.50	0.58
1:B:197:PRO:HB2	1:B:206:LYS:HB2	1.86	0.58
1:A:269:ASP:HB3	1:A:302:ASN:HD22	1.68	0.58
1:B:223:GLU:O	1:B:227:THR:HG22	2.03	0.58
1:A:223:GLU:O	1:A:227:THR:HG22	2.04	0.58
1:B:222:LYS:HG3	1:B:320:PHE:CZ	2.36	0.58
1:A:376:ASN:O	1:A:379:PHE:HB3	2.04	0.58
1:B:123:VAL:HG13	3:B:1082:HOH:O	2.02	0.58
1:B:306:LYS:HG3	1:B:337:PHE:HD2	1.69	0.58
1:A:502:SER:HB3	1:A:529:GLU:HB3	1.85	0.58
1:B:134:ASP:CG	1:B:505:ARG:HH21	2.07	0.57
1:A:331:ASN:HB3	1:A:358:ILE:HG12	1.86	0.57
1:A:390:GLU:OE1	1:A:438:LYS:HE3	2.04	0.57
1:A:556:VAL:HB	1:A:584:ALA:HB3	1.86	0.57
1:B:554:TRP:CD2	1:B:565:ALA:HB2	2.40	0.57
1:A:64:SER:HB2	1:A:68:PHE:O	2.04	0.57
1:A:207:TYR:HB3	2:A:602:GLC:O6	2.05	0.57
1:B:349:LYS:HG2	1:B:352:VAL:HG23	1.87	0.57
1:A:536:ASN:O	1:A:538:SER:N	2.37	0.57
1:A:383:VAL:HG12	1:A:442:LEU:HD22	1.87	0.56
1:B:479:PRO:HA	1:B:482:GLN:HG2	1.87	0.56
1:B:419:LEU:HD23	1:B:419:LEU:H	1.70	0.56
1:B:488:GLN:O	1:B:492:GLN:HB2	2.05	0.56
1:B:449:PHE:O	1:B:497:ARG:NH2	2.37	0.56
1:B:383:VAL:HG12	1:B:442:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:VAL:HG13	1:A:405:LEU:N	2.21	0.56
1:A:2:ARG:NH1	1:B:2:ARG:HE	2.03	0.56
1:B:383:VAL:HG12	1:B:442:LEU:CD2	2.35	0.56
1:A:342:ARG:NH2	1:A:372:ASP:OD1	2.39	0.56
1:B:196:THR:HB	1:B:197:PRO:HD2	1.88	0.55
1:A:345:VAL:HG11	1:A:354:ILE:HD11	1.87	0.55
1:A:355:LEU:HD12	1:A:373:ALA:O	2.07	0.55
1:B:448:THR:HG22	1:B:503:LEU:HD22	1.89	0.55
1:A:333:ILE:HD12	1:A:338:TRP:CZ2	2.42	0.55
1:B:140:ILE:O	1:B:142:PRO:HD3	2.07	0.55
1:A:23:LEU:HD12	1:A:23:LEU:C	2.28	0.55
1:A:366:LEU:HD21	1:A:374:VAL:HG13	1.88	0.55
1:B:327:LEU:HD22	1:B:338:TRP:CH2	2.42	0.55
1:B:410:ASN:O	1:B:414:GLU:HG3	2.07	0.55
1:A:297:LYS:HE2	1:B:119:PHE:CZ	2.41	0.54
1:B:279:GLN:N	1:B:285:ASN:OD1	2.34	0.54
1:B:48:GLN:HG2	1:B:53:GLN:CD	2.28	0.54
1:A:395:ARG:HB2	1:A:516:GLU:HG3	1.89	0.54
1:B:258:VAL:HA	1:B:265:SER:CB	2.37	0.54
1:B:545:PRO:CA	1:B:572:CYS:HB2	2.33	0.54
1:B:461:ILE:HB	1:B:482:GLN:HB2	1.90	0.54
1:B:278:LEU:HA	1:B:285:ASN:HD21	1.72	0.54
1:A:149:ASN:ND2	1:A:152:ILE:HG12	2.22	0.54
1:A:521:ILE:HG23	1:A:534:ILE:HG12	1.89	0.54
1:B:326:ARG:HH12	1:B:328:ASP:HB3	1.72	0.54
1:A:227:THR:O	1:A:231:ARG:HB2	2.08	0.54
1:B:306:LYS:HG3	1:B:337:PHE:CD2	2.42	0.54
1:A:359:TRP:O	1:A:360:HIS:HB3	2.08	0.54
1:A:140:ILE:HB	1:A:195:LEU:HD23	1.90	0.54
1:B:253:ALA:HB3	1:B:254:PRO:CD	2.32	0.54
1:B:44:PRO:HG3	1:B:83:ARG:HG2	1.89	0.54
1:A:460:GLU:HG2	1:A:461:ILE:HG23	1.90	0.54
1:B:146:ALA:O	1:B:177:GLY:HA3	2.07	0.54
1:A:2:ARG:CZ	1:B:2:ARG:HE	2.21	0.53
1:B:555:LEU:HD12	1:B:564:PHE:CZ	2.44	0.53
1:A:341:PHE:CE2	1:A:354:ILE:HD13	2.43	0.53
1:A:273:ILE:HD13	1:A:278:LEU:HD11	1.89	0.53
1:B:546:ILE:O	1:B:546:ILE:HG13	2.07	0.53
1:A:278:LEU:O	1:A:279:GLN:HG2	2.09	0.53
1:A:327:LEU:HD22	1:A:338:TRP:CZ3	2.43	0.53
1:A:137:TRP:HA	1:A:192:GLY:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:LEU:HD22	1:B:585:ILE:HD12	1.90	0.53
1:A:354:ILE:HG22	1:A:371:PHE:HD1	1.74	0.53
1:A:308:TYR:O	1:A:312:VAL:HG23	2.09	0.53
1:A:23:LEU:HD12	1:A:23:LEU:O	2.08	0.52
1:B:554:TRP:CE3	1:B:565:ALA:HB2	2.44	0.52
1:A:243:ALA:HB2	1:A:325:TRP:CZ3	2.44	0.52
1:A:35:ASP:HB2	1:A:89:TYR:O	2.09	0.52
1:B:134:ASP:OD2	1:B:505:ARG:NH2	2.42	0.52
1:A:138:TYR:CZ	1:A:457:TYR:HA	2.45	0.52
1:B:273:ILE:HD13	1:B:278:LEU:HD11	1.91	0.52
1:A:467:ASN:O	1:A:468:ASP:C	2.48	0.52
1:A:468:ASP:OD2	1:A:469:PRO:HA	2.10	0.52
1:B:244:VAL:HG22	1:B:328:ASP:OD1	2.09	0.52
1:A:138:TYR:HB2	1:A:190:ILE:HD12	1.91	0.52
1:A:328:ASP:OD2	1:A:329:VAL:HG23	2.10	0.52
1:B:159:PRO:HB2	1:B:162:SER:HB2	1.91	0.52
1:A:568:ALA:HB3	1:A:569:GLU:OE2	2.11	0.51
1:A:324:GLY:HA2	1:A:352:VAL:HG13	1.92	0.51
1:A:134:ASP:OD1	1:A:504:ARG:HD2	2.10	0.51
1:B:258:VAL:HA	1:B:265:SER:HB2	1.92	0.51
1:B:225:LEU:O	1:B:228:LEU:HB3	2.10	0.51
1:B:562:GLU:HG2	1:B:563:ARG:N	2.26	0.51
1:B:501:ARG:NH1	1:B:505:ARG:HD2	2.25	0.51
1:A:567:GLU:OE2	1:A:571:LEU:HD21	2.10	0.51
1:A:2:ARG:NH1	1:A:4:GLU:HG3	2.24	0.51
1:B:100:LYS:HG3	1:B:113:TYR:HA	1.92	0.51
1:B:197:PRO:HD3	1:B:242:ASP:OD1	2.11	0.51
1:B:227:THR:O	1:B:231:ARG:HB2	2.10	0.51
1:B:243:ALA:HB2	1:B:325:TRP:CE3	2.45	0.51
1:B:546:ILE:HG12	1:B:571:LEU:O	2.11	0.51
1:A:460:GLU:OE2	1:A:460:GLU:N	2.37	0.51
1:B:507:GLU:O	1:B:524:LYS:HA	2.11	0.51
1:B:379:PHE:O	1:B:383:VAL:HG23	2.11	0.50
1:A:419:LEU:H	1:A:419:LEU:HD23	1.75	0.50
1:B:253:ALA:CB	1:B:254:PRO:HD3	2.31	0.50
1:A:259:TRP:CD1	1:A:259:TRP:O	2.64	0.50
1:B:31:LYS:NZ	1:B:395:ARG:NH1	2.60	0.50
1:B:571:LEU:HD22	1:B:571:LEU:N	2.27	0.50
1:B:339:ARG:HG3	1:B:339:ARG:NH1	2.27	0.50
1:A:502:SER:HB3	1:A:529:GLU:CB	2.41	0.49
1:A:310:LEU:HD22	1:A:344:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:VAL:HG13	1:A:405:LEU:H	1.76	0.49
1:B:550:ALA:HB1	1:B:566:ALA:O	2.13	0.49
1:A:149:ASN:HD22	1:A:152:ILE:HG12	1.76	0.49
1:A:27:LEU:HD23	1:A:37:VAL:HG11	1.94	0.49
1:B:10:PRO:HA	1:B:15:ALA:HB3	1.95	0.49
1:B:386:PHE:CZ	1:B:537:ARG:HD3	2.48	0.49
1:A:238:ARG:HA	1:A:323:ASP:OD1	2.12	0.49
1:A:515:ASP:HB3	1:A:519:TYR:CD1	2.48	0.49
1:B:200:ARG:O	1:B:210:ALA:HB3	2.13	0.49
1:B:230:ASP:O	1:B:234:GLU:HG2	2.13	0.49
1:A:397:PHE:O	1:A:401:MET:HG2	2.12	0.49
1:A:510:PHE:CD2	1:A:520:LEU:HD11	2.48	0.49
1:A:2:ARG:NH1	1:A:4:GLU:CG	2.76	0.48
1:A:279:GLN:HB2	1:A:285:ASN:ND2	2.28	0.48
1:A:171:PHE:CD2	1:A:474:CYS:SG	3.06	0.48
1:A:182:LEU:O	1:A:186:VAL:HG23	2.13	0.48
1:B:80:ARG:O	1:B:119:PHE:HA	2.13	0.48
1:A:224:THR:O	1:A:227:THR:HG23	2.13	0.48
1:A:146:ALA:O	1:A:177:GLY:HA3	2.13	0.48
1:A:389:LYS:HE2	1:A:431:VAL:CG1	2.41	0.48
1:B:196:THR:HB	1:B:197:PRO:CD	2.44	0.48
1:A:144:ARG:HH21	1:A:165:PRO:CB	2.26	0.48
1:A:420:LEU:HD13	1:A:442:LEU:HB3	1.95	0.48
1:B:158:ARG:NE	1:B:158:ARG:HA	2.28	0.48
1:A:185:LEU:HD22	1:A:190:ILE:HG13	1.95	0.48
1:B:466:GLY:H	1:B:470:GLU:CG	2.27	0.48
1:B:326:ARG:NE	1:B:375:MET:CE	2.75	0.48
1:B:551:ARG:HH12	1:B:568:ALA:HA	1.79	0.48
1:B:354:ILE:HG22	1:B:371:PHE:HD1	1.79	0.48
1:B:128:ALA:O	1:B:129:PRO:C	2.51	0.48
1:A:281:GLU:HA	1:A:282:PRO:C	2.34	0.48
1:B:45:TYR:N	1:B:45:TYR:CD1	2.81	0.48
1:A:98:THR:HB	1:A:113:TYR:O	2.13	0.48
1:B:567:GLU:C	1:B:569:GLU:N	2.66	0.47
1:B:281:GLU:HA	1:B:282:PRO:C	2.34	0.47
1:A:187:ASP:O	1:A:491:LYS:NZ	2.46	0.47
1:B:556:VAL:O	1:B:583:TYR:HA	2.13	0.47
1:A:440:LYS:HG2	1:A:489:HIS:NE2	2.29	0.47
1:A:272:HIS:CD2	1:A:297:LYS:HD3	2.49	0.47
1:B:554:TRP:C	1:B:555:LEU:HD23	2.35	0.47
1:A:47:TRP:CE2	1:A:52:TRP:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:TYR:N	1:B:378:PRO:CD	2.78	0.47
1:A:154:PRO:HD2	1:A:172:GLY:HA2	1.95	0.47
1:B:467:ASN:O	1:B:468:ASP:C	2.53	0.47
1:B:199:PHE:HA	1:B:214:GLU:O	2.15	0.47
1:B:135:THR:CG2	1:B:136:VAL:N	2.77	0.47
1:A:10:PRO:O	1:A:11:ALA:HB2	2.15	0.47
1:B:129:PRO:O	1:B:132:VAL:HG22	2.15	0.47
1:B:268:LYS:HD3	1:B:269:ASP:N	2.29	0.47
1:B:98:THR:HB	1:B:113:TYR:O	2.15	0.47
1:A:145:PHE:HB3	3:A:1107:HOH:O	2.14	0.47
1:A:110:ASP:OD1	1:A:111:THR:N	2.48	0.47
1:B:376:ASN:OD1	1:B:378:PRO:HD2	2.15	0.47
1:B:331:ASN:ND2	1:B:331:ASN:N	2.62	0.47
1:B:563:ARG:O	1:B:564:PHE:HB3	2.14	0.47
1:B:461:ILE:HB	1:B:482:GLN:CB	2.45	0.47
1:A:40:LEU:HG	1:A:54:PHE:CD2	2.50	0.47
1:B:165:PRO:HG3	1:B:473:LYS:HA	1.97	0.47
1:B:82:LEU:HG	1:B:83:ARG:N	2.30	0.47
1:B:247:HIS:HD2	1:B:295:MET:HB3	1.78	0.47
1:A:365:TRP:HB3	1:A:371:PHE:HD2	1.80	0.47
1:B:545:PRO:HA	1:B:572:CYS:CB	2.37	0.46
1:B:221:ASP:OD1	1:B:224:THR:N	2.43	0.46
1:B:339:ARG:O	1:B:343:GLN:HG3	2.15	0.46
1:B:395:ARG:HD2	1:B:399:ASN:ND2	2.30	0.46
1:A:158:ARG:NH1	1:A:163:GLU:OE2	2.48	0.46
1:A:429:LEU:HA	1:A:439:VAL:CG2	2.46	0.46
1:A:272:HIS:HB3	1:A:287:ASP:OD2	2.15	0.46
1:A:555:LEU:CD1	1:A:585:ILE:HD12	2.45	0.46
1:A:329:VAL:O	1:A:329:VAL:HG12	2.15	0.46
1:A:288:THR:HB	1:A:295:MET:O	2.14	0.46
1:B:10:PRO:O	1:B:11:ALA:HB2	2.16	0.46
1:B:272:HIS:HE2	1:B:299:ASN:HA	1.81	0.46
1:B:13:ASN:HB3	1:B:407:SER:O	2.16	0.46
1:B:478:ASP:OD2	1:B:481:GLN:NE2	2.48	0.46
1:A:4:GLU:HB2	1:B:5:ALA:HB2	1.97	0.46
1:A:7:TYR:O	1:A:27:LEU:HD12	2.16	0.46
1:B:423:HIS:O	1:B:471:CYS:SG	2.74	0.46
1:B:331:ASN:ND2	1:B:332:GLU:HG3	2.31	0.46
1:B:555:LEU:HD22	1:B:585:ILE:CD1	2.46	0.45
1:A:327:LEU:HD22	1:A:338:TRP:CH2	2.52	0.45
1:B:9:ARG:HA	1:B:10:PRO:HD3	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ASN:ND2	1:B:379:PHE:HB2	2.32	0.45
1:A:252:PHE:CD2	1:A:254:PRO:HD2	2.51	0.45
1:B:324:GLY:HA2	1:B:352:VAL:HG13	1.97	0.45
1:B:349:LYS:CG	1:B:352:VAL:HG23	2.46	0.45
1:A:196:THR:HB	1:A:197:PRO:HD2	1.98	0.45
1:B:259:TRP:HA	1:B:278:LEU:HD22	1.98	0.45
1:B:294:GLN:H	1:B:294:GLN:CD	2.20	0.45
1:A:274:HIS:CD2	3:A:1036:HOH:O	2.69	0.45
1:B:554:TRP:CE2	1:B:565:ALA:HB2	2.51	0.45
1:B:365:TRP:HB3	1:B:371:PHE:HD2	1.82	0.45
1:B:401:MET:O	1:B:404:VAL:HG22	2.16	0.45
1:B:534:ILE:CD1	1:B:546:ILE:HG22	2.47	0.45
1:A:11:ALA:O	1:A:12:ASP:C	2.54	0.45
1:B:165:PRO:CG	1:B:473:LYS:HA	2.47	0.45
1:B:144:ARG:HH11	1:B:144:ARG:HG3	1.82	0.45
1:A:9:ARG:O	1:A:14:PHE:HB2	2.16	0.45
1:B:2:ARG:HG2	1:B:2:ARG:HH11	1.82	0.45
1:A:360:HIS:O	1:A:361:ASP:C	2.54	0.45
1:B:135:THR:HG22	1:B:136:VAL:N	2.30	0.45
1:A:552:GLY:O	1:A:587:HIS:HA	2.17	0.45
1:B:259:TRP:HH2	1:B:280:THR:HG23	1.82	0.45
1:A:196:THR:HB	1:A:197:PRO:CD	2.47	0.45
1:B:259:TRP:HD1	1:B:260:LYS:HD2	1.82	0.44
1:A:428:ILE:HD12	1:A:439:VAL:HG13	1.99	0.44
1:B:359:TRP:HA	1:B:377:TYR:HD1	1.82	0.44
1:B:193:ILE:HG13	1:B:237:ILE:HG21	1.98	0.44
1:A:2:ARG:HH12	1:A:4:GLU:HG3	1.81	0.44
1:B:551:ARG:HE	1:B:551:ARG:CA	2.28	0.44
1:A:548:LEU:HD23	1:A:553:THR:HG21	1.99	0.44
1:A:582:LEU:HD12	1:A:582:LEU:N	2.33	0.44
1:B:1:MET:CA	1:B:33:ASP:OD2	2.65	0.44
1:A:207:TYR:OH	1:A:423:HIS:NE2	2.50	0.44
1:B:129:PRO:HB2	1:B:131:TRP:NE1	2.32	0.44
1:A:501:ARG:HD2	1:A:505:ARG:CD	2.43	0.44
1:A:141:PHE:HD2	1:A:144:ARG:HG2	1.82	0.44
1:A:80:ARG:O	1:A:119:PHE:HA	2.17	0.44
1:A:261:ASN:O	1:A:262:GLY:C	2.56	0.44
1:B:2:ARG:HD3	1:B:30:LYS:CD	2.48	0.44
1:B:333:ILE:HD12	1:B:338:TRP:HZ2	1.83	0.44
1:A:502:SER:CB	1:A:529:GLU:HB3	2.48	0.44
1:B:27:LEU:HD23	1:B:37:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ARG:NE	1:A:551:ARG:HA	2.31	0.43
1:A:386:PHE:CE1	1:A:394:ALA:HA	2.53	0.43
1:A:128:ALA:O	1:A:129:PRO:C	2.55	0.43
1:A:9:ARG:NE	1:B:361:ASP:OD1	2.41	0.43
1:B:44:PRO:HB2	1:B:45:TYR:CE1	2.52	0.43
1:B:395:ARG:HD2	1:B:399:ASN:HD21	1.83	0.43
1:B:18:TYR:O	1:B:125:LEU:HD11	2.19	0.43
1:A:226:LYS:HA	1:A:226:LYS:CE	2.46	0.43
1:A:252:PHE:CG	1:A:254:PRO:HD2	2.52	0.43
1:A:213:PHE:HE1	1:A:308:TYR:CE2	2.35	0.43
1:B:27:LEU:HD22	1:B:86:PHE:CD1	2.54	0.43
1:B:189:GLY:O	1:B:191:THR:HG23	2.18	0.43
1:A:55:GLN:HE21	1:A:55:GLN:HB2	1.63	0.43
1:A:429:LEU:HA	1:A:439:VAL:HG21	2.01	0.43
1:B:79:TYR:HB3	3:B:1113:HOH:O	2.19	0.43
1:B:436:ILE:O	1:B:440:LYS:HG3	2.18	0.43
1:B:320:PHE:O	1:B:321:ASP:CB	2.66	0.43
1:B:88:LEU:N	1:B:88:LEU:CD1	2.81	0.43
1:B:461:ILE:HD11	1:B:475:MET:SD	2.58	0.43
1:B:137:TRP:NE1	1:B:452:SER:OG	2.51	0.43
1:A:4:GLU:H	1:A:4:GLU:CD	2.22	0.43
1:B:326:ARG:HG2	1:B:355:LEU:HD23	2.00	0.43
1:A:149:ASN:HD21	1:A:152:ILE:HG23	1.84	0.43
1:B:435:ASP:OD1	1:B:437:ARG:HB2	2.19	0.43
1:B:186:VAL:HG21	1:B:235:LYS:HD3	2.00	0.43
1:B:389:LYS:O	1:B:390:GLU:HB2	2.18	0.43
1:A:397:PHE:HZ	1:A:445:PHE:CE2	2.36	0.43
1:A:318:ARG:HH11	1:A:318:ARG:HG2	1.83	0.43
1:B:242:ASP:OD2	1:B:326:ARG:HD2	2.18	0.43
1:A:457:TYR:O	1:A:457:TYR:CG	2.72	0.43
1:A:524:LYS:NZ	3:A:1058:HOH:O	2.52	0.43
1:B:84:TYR:O	1:B:114:TYR:HB3	2.18	0.42
1:B:466:GLY:H	1:B:470:GLU:CD	2.22	0.42
1:A:208:ASP:OD1	1:A:208:ASP:N	2.52	0.42
1:B:265:SER:C	1:B:267:TYR:H	2.21	0.42
1:B:106:VAL:O	1:B:108:THR:HG23	2.19	0.42
1:B:567:GLU:OE1	1:B:571:LEU:HD21	2.20	0.42
1:B:500:TYR:HB3	1:B:529:GLU:OE2	2.19	0.42
1:B:340:GLU:O	1:B:341:PHE:C	2.56	0.42
1:B:31:LYS:HZ1	1:B:395:ARG:NH1	2.18	0.42
1:A:221:ASP:O	1:A:222:LYS:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:MET:HG2	1:B:73:ALA:HB2	2.01	0.42
1:B:563:ARG:HG2	1:B:564:PHE:N	2.35	0.42
1:A:555:LEU:CD2	1:A:555:LEU:N	2.83	0.42
1:A:294:GLN:CD	1:A:294:GLN:H	2.23	0.42
1:B:83:ARG:NE	1:B:116:CYS:HB2	2.35	0.42
1:B:376:ASN:O	1:B:379:PHE:HB3	2.20	0.42
1:B:420:LEU:CD1	1:B:442:LEU:HB3	2.47	0.42
1:B:40:LEU:O	1:B:84:TYR:HA	2.20	0.42
1:B:79:TYR:O	1:B:80:ARG:HB2	2.18	0.42
1:A:515:ASP:HB3	1:A:519:TYR:CE1	2.55	0.42
1:A:40:LEU:HD23	1:A:40:LEU:C	2.41	0.42
1:A:429:LEU:HD11	1:A:436:ILE:HD13	2.02	0.42
1:B:272:HIS:HB2	1:B:287:ASP:HB2	2.02	0.42
1:B:36:ARG:NH1	1:B:89:TYR:CD1	2.88	0.42
1:A:248:CYS:SG	1:A:271:PHE:HE1	2.43	0.42
1:A:407:SER:HB2	1:B:9:ARG:NH2	2.34	0.41
1:A:131:TRP:CZ3	1:A:238:ARG:HG3	2.55	0.41
1:B:199:PHE:CE1	1:B:316:TRP:CZ2	3.08	0.41
1:B:147:ASN:OD1	1:B:172:GLY:O	2.38	0.41
1:A:379:PHE:O	1:A:383:VAL:HG23	2.20	0.41
1:B:255:PHE:HA	1:B:271:PHE:CE2	2.54	0.41
1:B:286:TYR:CE2	1:B:296:PRO:HB3	2.54	0.41
1:A:1:MET:CE	1:A:93:GLU:HG2	2.50	0.41
1:B:156:GLY:O	1:B:157:SER:C	2.57	0.41
1:A:550:ALA:HB1	1:A:566:ALA:O	2.20	0.41
1:B:215:VAL:O	1:B:216:ASP:C	2.59	0.41
1:B:479:PRO:HA	1:B:482:GLN:CG	2.49	0.41
1:B:419:LEU:CD2	1:B:419:LEU:H	2.33	0.41
1:A:48:GLN:C	1:A:50:GLY:N	2.74	0.41
1:A:258:VAL:HG11	1:A:273:ILE:CD1	2.51	0.41
1:A:501:ARG:HG3	1:A:501:ARG:HH11	1.85	0.41
1:A:331:ASN:ND2	1:A:331:ASN:H	2.17	0.41
1:A:243:ALA:HB1	1:A:245:PHE:CE1	2.56	0.41
1:B:458:GLY:HA2	1:B:461:ILE:HG12	2.03	0.41
1:B:208:ASP:N	1:B:208:ASP:OD1	2.53	0.41
1:B:572:CYS:SG	1:B:572:CYS:O	2.78	0.41
1:B:40:LEU:HG	1:B:54:PHE:CD2	2.56	0.41
1:B:419:LEU:HD23	1:B:419:LEU:O	2.19	0.41
1:A:567:GLU:O	1:A:568:ALA:C	2.59	0.41
1:B:396:GLN:O	1:B:399:ASN:HB2	2.21	0.41
1:A:295:MET:HE1	2:A:601:GLC:O5	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LEU:HD22	1:B:117:PHE:CD2	2.56	0.41
1:A:555:LEU:HD23	1:A:564:PHE:CE1	2.55	0.41
1:B:278:LEU:N	1:B:278:LEU:CD1	2.84	0.41
1:A:88:LEU:N	1:A:88:LEU:HD12	2.36	0.41
1:A:573:THR:HG22	1:A:575:LEU:HG	2.03	0.41
1:B:49:ASN:C	1:B:51:ALA:N	2.74	0.41
1:A:486:LEU:O	1:A:489:HIS:HB3	2.21	0.41
1:B:221:ASP:O	1:B:224:THR:N	2.54	0.41
1:B:179:ILE:HG12	1:B:228:LEU:HA	2.03	0.41
1:B:26:ARG:HA	1:B:71:TRP:O	2.21	0.41
1:A:545:PRO:HA	1:A:572:CYS:HA	2.03	0.40
1:A:363:MET:HB3	1:A:364:PRO:HD3	2.03	0.40
1:B:265:SER:C	1:B:267:TYR:N	2.75	0.40
1:A:383:VAL:HG12	1:A:442:LEU:CD2	2.50	0.40
1:B:341:PHE:CE2	1:B:354:ILE:HD13	2.56	0.40
1:B:183:ASP:O	1:B:184:TYR:C	2.58	0.40
1:B:137:TRP:CD1	1:B:452:SER:OG	2.75	0.40
1:B:241:LEU:HG	1:B:322:ILE:HG21	2.04	0.40
1:B:551:ARG:NE	1:B:551:ARG:CA	2.85	0.40
1:B:354:ILE:HG22	1:B:354:ILE:O	2.21	0.40
1:A:2:ARG:HH21	1:B:4:GLU:CG	2.35	0.40
1:B:258:VAL:O	1:B:262:GLY:N	2.50	0.40
1:B:327:LEU:HD22	1:B:338:TRP:HH2	1.84	0.40
1:B:581:VAL:HG21	1:B:583:TYR:CZ	2.55	0.40
1:A:581:VAL:HG22	1:A:582:LEU:N	2.36	0.40
1:B:170:PHE:CE1	1:B:204:ASN:HB3	2.56	0.40
1:B:308:TYR:O	1:B:311:ASP:HB2	2.21	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	586/588 (100%)	522 (89%)	51 (9%)	13 (2%)	8	45
1	B	586/588 (100%)	521 (89%)	56 (10%)	9 (2%)	13	55
All	All	1172/1176 (100%)	1043 (89%)	107 (9%)	22 (2%)	10	50

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	515	ASP
1	A	501	ARG
1	A	21	GLU
1	A	262	GLY
1	A	516	GLU
1	B	569	GLU
1	B	570	THR
1	A	142	PRO
1	A	160	TRP
1	A	360	HIS
1	A	537	ARG
1	A	468	ASP
1	A	568	ALA
1	B	263	GLU
1	B	468	ASP
1	B	568	ALA
1	A	118	PRO
1	B	321	ASP
1	A	44	PRO
1	B	282	PRO
1	B	329	VAL
1	A	10	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	521/521 (100%)	505 (97%)	16 (3%)	47	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	521/521 (100%)	501 (96%)	20 (4%)	40	78
All	All	1042/1042 (100%)	1006 (96%)	36 (4%)	43	80

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	163	GLU
1	A	194	TYR
1	A	226	LYS
1	A	227	THR
1	A	231	ARG
1	A	261	ASN
1	A	268	LYS
1	A	269	ASP
1	A	331	ASN
1	A	359	TRP
1	A	378	PRO
1	A	517	MET
1	A	551	ARG
1	A	555	LEU
1	A	562	GLU
1	B	9	ARG
1	B	92	GLU
1	B	95	LEU
1	B	164	ASP
1	B	194	TYR
1	B	222	LYS
1	B	227	THR
1	B	231	ARG
1	B	260	LYS
1	B	268	LYS
1	B	278	LEU
1	B	328	ASP
1	B	331	ASN
1	B	339	ARG
1	B	359	TRP
1	B	375	MET
1	B	541	LYS
1	B	551	ARG
1	B	555	LEU
1	B	572	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	49	ASN
1	A	55	GLN
1	A	139	GLN
1	A	149	ASN
1	A	274	HIS
1	A	299	ASN
1	A	331	ASN
1	A	370	GLN
1	A	418	ASN
1	A	446	GLN
1	A	482	GLN
1	A	488	GLN
1	A	492	GLN
1	B	48	GLN
1	B	55	GLN
1	B	139	GLN
1	B	147	ASN
1	B	176	GLN
1	B	331	ASN
1	B	370	GLN
1	B	399	ASN
1	B	400	GLN
1	B	418	ASN
1	B	446	GLN
1	B	482	GLN
1	B	492	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

6 carbohydrates 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	GLC	A	601	2	11,11,12	0.60	0	14,15,17	0.47	0
2	GLC	A	602	2	11,11,12	0.35	0	14,15,17	1.13	2 (14%)
2	GLC	A	603	2	12,12,12	0.51	0	17,17,17	0.68	0
2	GLC	B	604	2	11,11,12	0.47	0	14,15,17	0.86	1 (7%)
2	GLC	B	605	2	11,11,12	0.42	0	14,15,17	0.83	1 (7%)
2	GLC	B	606	2	12,12,12	0.49	0	17,17,17	0.82	1 (5%)

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	GLC	A	601	2	-	0/2/19/22	0/1/1/1
2	GLC	A	602	2	-	0/2/19/22	0/1/1/1
2	GLC	A	603	2	-	0/2/22/22	0/1/1/1
2	GLC	B	604	2	-	0/2/19/22	0/1/1/1
2	GLC	B	605	2	-	0/2/19/22	0/1/1/1
2	GLC	B	606	2	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	GLC	C1-C2-C3	-2.10	107.06	109.54
2	B	606	GLC	C1-C2-C3	2.31	113.86	110.43
2	B	604	GLC	C1-O5-C5	2.40	115.30	112.25
2	B	605	GLC	C1-O5-C5	2.55	115.48	112.25
2	A	602	GLC	C1-O5-C5	2.58	115.52	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GLC	1	0
2	A	602	GLC	1	0
2	B	606	GLC	2	0

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	588/588 (100%)	-0.59	7 (1%) 81 69	1, 14, 34, 73	0
1	B	588/588 (100%)	-0.60	5 (0%) 85 78	1, 14, 39, 69	0
All	All	1176/1176 (100%)	-0.59	12 (1%) 84 75	1, 14, 36, 73	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	568	ALA	5.8
1	A	568	ALA	5.0
1	B	569	GLU	4.3
1	B	570	THR	3.9
1	A	569	GLU	3.7
1	A	514	ASP	3.6
1	B	567	GLU	3.3
1	B	514	ASP	3.1
1	A	49	ASN	2.7
1	A	570	THR	2.7
1	A	515	ASP	2.2
1	A	567	GLU	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GLC	A	603	12/12	0.93	0.18	0.44	12,21,23,24	0
2	GLC	B	605	11/12	0.98	0.15	0.13	12,12,16,19	0
2	GLC	A	601	11/12	0.97	0.15	-0.02	1,5,7,12	0
2	GLC	B	604	11/12	0.96	0.16	-0.22	7,10,12,14	0
2	GLC	A	602	11/12	0.97	0.14	-0.68	5,6,9,10	0
2	GLC	B	606	12/12	0.96	0.11	-1.23	15,19,20,21	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.