



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:02 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

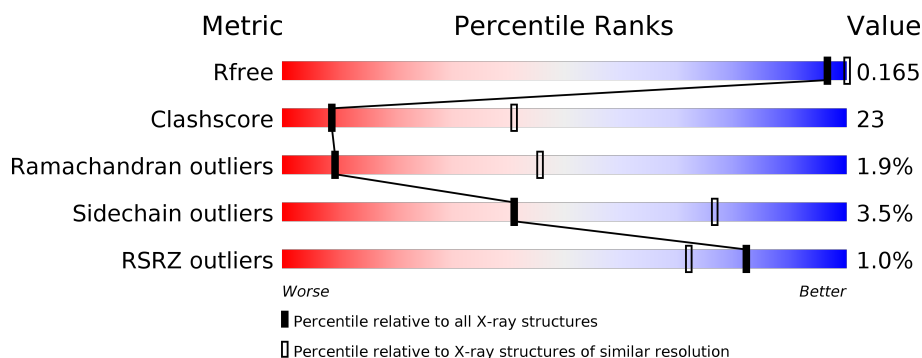
1 Overall quality at a glance

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}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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> <div></div> <div>58%</div> <div>39%</div> <div>.</div> </div> </div>
1	B	588	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>43%</div> <div>.</div> </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		

R504	R505	G506	E507	L511	D514	D515	I521	K524	T525	D526	G527	D528	E529	L534	R537	K541	P545	I546	P547	L548	D549	A550	R551	W554	L555	V556	E562	R563	F564	A565	A566	E567	A568	E569	T570	L571	C572	V581	L582	Y583	A584	I585	E586	H587	W588			
Q400	M401	V404	S407	N410	E414	L419	L420	H423	D435	I436	R437	K440	L441	L442	T448	F449	S452	G458	I461	G466	N467	D468	P469	E470	C471	K472	C473	C474	M475	D478	P479	M480	Q481	Q482	Q488	Q492	R497	Y500	R501	S502	L503							
D321	I322	G323	W325	R326	L327	D328	V329	A330	N331	E332	I333	F337	W338	R339	E340	F341	G342	Q343	E344	K349	V352	Y353	I354	L355	G356	Q357	I358	W359	R360	D361	A362	M363	P364	W365	F371	M375	N376	Y377	P378	F379	V383	F386	K389	E390	E391	R395	Q396	N399
K236	L237	L241	D242	A243	V244	H247	A253	P254	F255	W258	W259	K260	N261	G262	E263	S264	S265	K266	Y267	K268	D269	W270	F271	H272	L273	L278	Q279	T280	E281	P282	R283	P284	N285	Y286	D287	Q294	W295	P296	N299	K306	R307	Y308	L309	D311	Y315	W316	E319	F320

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
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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 [i](#)

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:A:59:MET:HG2	1:A:73:ALA:HB2	1.76	0.67
1:B:326:ARG:NH1	1:B:328:ASP:HB3	2.10	0.67
1:B:12:ASP:HB3	1:B:363:MET:SD	2.34	0.67
1:B:511:LEU:HB2	1:B:521:ILE:HG22	1.75	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:144:ARG:HH21	1:A:165:PRO:HB2	1.61	0.66
1:A:551:ARG:HA	1:A:551:ARG:HE	1.61	0.66
1:B:1:MET:HA	1:B:33:ASP:OD2	1.95	0.66
1:B:221:ASP:OD1	1:B:223:GLU:HB3	1.96	0.65
1:B:88:LEU:N	1:B:88:LEU:HD12	2.11	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:A:272:HIS:HB2	1:A:287:ASP:HB2	1.80	0.64
1:B:1:MET:HG2	1:B:95:LEU:HD12	1.79	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: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:B:357:GLN:OE1	2:B:606:GLC:H62	1.99	0.63
1:A:546:ILE:O	1:A:570:THR:HB	1.99	0.62
1:A:327:LEU:HD11	1:A:341:PHE:CZ	2.34	0.62
1:A:427:ARG:O	1:A:431:VAL:HG23	1.99	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:166:THR:HB	1:A:167:PRO:HD2	1.81	0.62
1:A:253:ALA:HB3	1:A:254:PRO:HD3	1.82	0.62
1:A:299:ASN:HD22	1:A:302:ASN:HB2	1.66	0.61
1:A:119:PHE:CD2	1:A:121:HIS:CE1	2.89	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ARG:NH1	1:B:328:ASP:OD2	2.34	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:A:515:ASP:C	1:A:517:MET:H	2.05	0.60
1:B:254:PRO:O	1:B:258:VAL:HG23	2.02	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:A:223:GLU:O	1:A:227:THR:HG22	2.04	0.58
1:B:223:GLU:O	1:B:227:THR:HG22	2.03	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:B:222:LYS:HG3	1:B:320:PHE:CZ	2.36	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:A:404:VAL:HG13	1:A:405:LEU:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:VAL:HG12	1:B:442:LEU:HD22	1.88	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: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:196:THR:HB	1:B:197:PRO:HD2	1.88	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:A:395:ARG:HB2	1:A:516:GLU:HG3	1.89	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:B:258:VAL:HA	1:B:265:SER:CB	2.37	0.54
1:A:149:ASN:ND2	1:A:152:ILE:HG12	2.22	0.54
1:B:278:LEU:HA	1:B:285:ASN:HD21	1.72	0.54
1:B:461:ILE:HB	1:B:482:GLN:HB2	1.90	0.54
1:B:545:PRO:CA	1:B:572:CYS:HB2	2.33	0.54
1:A:521:ILE:HG23	1:A:534:ILE:HG12	1.89	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:B:326:ARG:HH12	1:B:328:ASP:HB3	1.72	0.54
1:A:140:ILE:HB	1:A:195:LEU:HD23	1.90	0.54
1:A:359:TRP:O	1:A:360:HIS:HB3	2.08	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:137:TRP:HA	1:A:192:GLY:O	2.08	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

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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:308:TYR:O	1:A:312:VAL:HG23	2.09	0.53
1:A:354:ILE:HG22	1:A:371:PHE:HD1	1.74	0.53
1:A:23:LEU:HD12	1:A:23:LEU:O	2.08	0.52
1:A:243:ALA:HB2	1:A:325:TRP:CZ3	2.44	0.52
1:B:554:TRP:CE3	1:B:565:ALA:HB2	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:A:467:ASN:O	1:A:468:ASP:C	2.48	0.52
1:B:273:ILE:HD13	1:B:278:LEU:HD11	1.91	0.52
1:A:468:ASP:OD2	1:A:469:PRO:HA	2.10	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:B:244:VAL:HG22	1:B:328:ASP:OD1	2.09	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:225:LEU:O	1:B:228:LEU:HB3	2.10	0.51
1:B:258:VAL:HA	1:B:265:SER:HB2	1.92	0.51
1:A:567:GLU:OE2	1:A:571:LEU:HD21	2.10	0.51
1:B:501:ARG:NH1	1:B:505:ARG:HD2	2.25	0.51
1:B:562:GLU:HG2	1:B:563:ARG:N	2.26	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:A:460:GLU:N	1:A:460:GLU:OE2	2.37	0.51
1:B:507:GLU:O	1:B:524:LYS:HA	2.11	0.51
1:B:546:ILE:HG12	1:B:571:LEU:O	2.11	0.51
1:A:419:LEU:HD23	1:A:419:LEU:H	1.75	0.50
1:B:379:PHE:O	1:B:383:VAL:HG23	2.11	0.50
1:A:259:TRP:O	1:A:259:TRP:CD1	2.64	0.50
1:B:253:ALA:CB	1:B:254:PRO:HD3	2.31	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:310:LEU:HD22	1:A:344:GLU:HG3	1.94	0.49
1:A:502:SER:HB3	1:A:529:GLU:CB	2.41	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:238:ARG:HA	1:A:323:ASP:OD1	2.12	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: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:171:PHE:CD2	1:A:474:CYS:SG	3.06	0.48
1:A:279:GLN:HB2	1:A:285:ASN:ND2	2.28	0.48
1:A:2:ARG:NH1	1:A:4:GLU:CG	2.76	0.48
1:A:182:LEU:O	1:A:186:VAL:HG23	2.13	0.48
1:A:146:ALA:O	1:A:177:GLY:HA3	2.13	0.48
1:A:224:THR:O	1:A:227:THR:HG23	2.13	0.48
1:B:80:ARG:O	1:B:119:PHE:HA	2.13	0.48
1:A:389:LYS:HE2	1:A:431:VAL:CG1	2.41	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:B:196:THR:HB	1:B:197:PRO:CD	2.44	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:128:ALA:O	1:B:129:PRO:C	2.51	0.48
1:B:326:ARG:NE	1:B:375:MET:CE	2.75	0.48
1:B:354:ILE:HG22	1:B:371:PHE:HD1	1.79	0.48
1:B:551:ARG:HH12	1:B:568:ALA:HA	1.79	0.48
1:A:281:GLU:HA	1:A:282:PRO:C	2.34	0.48
1:A:98:THR:HB	1:A:113:TYR:O	2.13	0.48
1:B:45:TYR:N	1:B:45:TYR:CD1	2.81	0.48
1:A:187:ASP:O	1:A:491:LYS:NZ	2.46	0.47
1:B:281:GLU:HA	1:B:282:PRO:C	2.34	0.47
1:B:556:VAL:O	1:B:583:TYR:HA	2.13	0.47
1:B:567:GLU:C	1:B:569:GLU:N	2.66	0.47
1:A:272:HIS:CD2	1:A:297:LYS:HD3	2.49	0.47
1:A:440:LYS:HG2	1:A:489:HIS:NE2	2.29	0.47
1:B:554:TRP:C	1:B:555:LEU:HD23	2.35	0.47
1:A:154:PRO:HD2	1:A:172:GLY:HA2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:TRP:CE2	1:A:52:TRP:HB2	2.49	0.47
1:B:377:TYR:N	1:B:378:PRO:CD	2.78	0.47
1:A:10:PRO:O	1:A:11:ALA:HB2	2.15	0.47
1:B:135:THR:CG2	1:B:136:VAL:N	2.77	0.47
1:B:199:PHE:HA	1:B:214:GLU:O	2.15	0.47
1:B:467:ASN:O	1:B:468:ASP:C	2.53	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:A:145:PHE:HB3	3:A:1107:HOH:O	2.14	0.47
1:B:98:THR:HB	1:B:113:TYR:O	2.15	0.47
1:A:110:ASP:OD1	1:A:111:THR:N	2.48	0.47
1:A:40:LEU:HG	1:A:54:PHE:CD2	2.50	0.47
1:B:331:ASN:ND2	1:B:331:ASN:N	2.62	0.47
1:B:376:ASN:OD1	1:B:378:PRO:HD2	2.15	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:B:165:PRO:HG3	1:B:473:LYS:HA	1.97	0.47
1:B:247:HIS:HD2	1:B:295:MET:HB3	1.78	0.47
1:B:82:LEU:HG	1:B:83:ARG:N	2.30	0.47
1:A:365:TRP:HB3	1:A:371:PHE:HD2	1.80	0.47
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:B:545:PRO:HA	1:B:572:CYS:CB	2.37	0.46
1:A:158:ARG:NH1	1:A:163:GLU:OE2	2.48	0.46
1:A:272:HIS:HB3	1:A:287:ASP:OD2	2.15	0.46
1:A:288:THR:HB	1:A:295:MET:O	2.14	0.46
1:A:329:VAL:O	1:A:329:VAL:HG12	2.15	0.46
1:A:429:LEU:HA	1:A:439:VAL:CG2	2.46	0.46
1:A:555:LEU:CD1	1:A:585:ILE:HD12	2.45	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: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:A:4:GLU:HB2	1:B:5:ALA:HB2	1.97	0.46
1:B:331:ASN:ND2	1:B:332:GLU:HG3	2.31	0.46
1:A:327:LEU:HD22	1:A:338:TRP:CH2	2.52	0.45
1:B:555:LEU:HD22	1:B:585:ILE:CD1	2.46	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:A:196:THR:HB	1:A:197:PRO:HD2	1.98	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:B:376:ASN:ND2	1:B:379:PHE:HB2	2.32	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:365:TRP:HB3	1:B:371:PHE:HD2	1.82	0.45
1:B:554:TRP:CE2	1:B:565:ALA:HB2	2.51	0.45
1:A:11:ALA:O	1:A:12:ASP:C	2.54	0.45
1:A:9:ARG:O	1:A:14:PHE:HB2	2.16	0.45
1:B:144:ARG:HH11	1:B:144:ARG:HG3	1.82	0.45
1:B:401:MET:O	1:B:404:VAL:HG22	2.16	0.45
1:B:165:PRO:CG	1:B:473:LYS:HA	2.47	0.45
1:B:534:ILE:CD1	1:B:546:ILE:HG22	2.47	0.45
1:A:360:HIS:O	1:A:361:ASP:C	2.54	0.45
1:A:552:GLY:O	1:A:587:HIS:HA	2.17	0.45
1:B:135:THR:HG22	1:B:136:VAL:N	2.30	0.45
1:B:2:ARG:HG2	1:B:2:ARG:HH11	1.82	0.45
1:A:196:THR:HB	1:A:197:PRO:CD	2.47	0.45
1:B:259:TRP:HH2	1:B:280:THR:HG23	1.82	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:193:ILE:HG13	1:B:237:ILE:HG21	1.98	0.44
1:B:359:TRP:HA	1:B:377:TYR:HD1	1.82	0.44
1:A:2:ARG:HH12	1:A:4:GLU:HG3	1.81	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:551:ARG:HE	1:B:551:ARG:CA	2.28	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:80:ARG:O	1:A:119:PHE:HA	2.17	0.44
1:A:141:PHE:HD2	1:A:144:ARG:HG2	1.82	0.44
1:A:501:ARG:HD2	1:A:505:ARG:CD	2.43	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:386:PHE:CE1	1:A:394:ALA:HA	2.53	0.43
1:A:551:ARG:NE	1:A:551:ARG:HA	2.31	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:18:TYR:O	1:B:125:LEU:HD11	2.19	0.43
1:B:395:ARG:HD2	1:B:399:ASN:HD21	1.83	0.43
1:B:44:PRO:HB2	1:B:45:TYR:CE1	2.52	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:A:55:GLN:HE21	1:A:55:GLN:HB2	1.63	0.43
1:B:189:GLY:O	1:B:191:THR:HG23	2.18	0.43
1:B:27:LEU:HD22	1:B:86:PHE:CD1	2.54	0.43
1:A:429:LEU:HA	1:A:439:VAL:HG21	2.01	0.43
1:B:436:ILE:O	1:B:440:LYS:HG3	2.18	0.43
1:B:79:TYR:HB3	3:B:1113:HOH:O	2.19	0.43
1:B:320:PHE:O	1:B:321:ASP:CB	2.66	0.43
1:B:137:TRP:NE1	1:B:452:SER:OG	2.51	0.43
1:B:461:ILE:HD11	1:B:475:MET:SD	2.58	0.43
1:B:88:LEU:N	1:B:88:LEU:CD1	2.81	0.43
1:A:149:ASN:HD21	1:A:152:ILE:HG23	1.84	0.43
1:A:4:GLU:CD	1:A:4:GLU:H	2.22	0.43
1:B:186:VAL:HG21	1:B:235:LYS:HD3	2.00	0.43
1:B:326:ARG:HG2	1:B:355:LEU:HD23	2.00	0.43
1:B:435:ASP:OD1	1:B:437:ARG:HB2	2.19	0.43
1:A:318:ARG:HH11	1:A:318:ARG:HG2	1.83	0.43
1:A:397:PHE:HZ	1:A:445:PHE:CE2	2.36	0.43
1:B:389:LYS:O	1:B:390:GLU:HB2	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:242:ASP:OD2	1:B:326:ARG:HD2	2.18	0.43
1:A:208:ASP:OD1	1:A:208:ASP:N	2.52	0.42
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:B:106:VAL:O	1:B:108:THR:HG23	2.19	0.42
1:B:265:SER:C	1:B:267:TYR:H	2.21	0.42
1:B:567:GLU:OE1	1:B:571:LEU:HD21	2.20	0.42
1:B:340:GLU:O	1:B:341:PHE:C	2.56	0.42
1:B:500:TYR:HB3	1:B:529:GLU:OE2	2.19	0.42
1:A:221:ASP:O	1:A:222:LYS:C	2.58	0.42
1:B:31:LYS:HZ1	1:B:395:ARG:NH1	2.18	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:294:GLN:CD	1:A:294:GLN:H	2.23	0.42
1:A:555:LEU:CD2	1:A:555:LEU:N	2.83	0.42
1:B:376:ASN:O	1:B:379:PHE:HB3	2.20	0.42
1:B:40:LEU:O	1:B:84:TYR:HA	2.20	0.42
1:B:420:LEU:CD1	1:B:442:LEU:HB3	2.47	0.42
1:B:83:ARG:NE	1:B:116:CYS:HB2	2.35	0.42
1:A:40:LEU:HD23	1:A:40:LEU:C	2.41	0.42
1:A:515:ASP:HB3	1:A:519:TYR:CE1	2.55	0.42
1:B:79:TYR:O	1:B:80:ARG:HB2	2.18	0.42
1:A:248:CYS:SG	1:A:271:PHE:HE1	2.43	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:131:TRP:CZ3	1:A:238:ARG:HG3	2.55	0.41
1:A:407:SER:HB2	1:B:9:ARG:NH2	2.34	0.41
1:B:199:PHE:CE1	1:B:316:TRP:CZ2	3.08	0.41
1:A:379:PHE:O	1:A:383:VAL:HG23	2.20	0.41
1:B:147:ASN:OD1	1:B:172:GLY:O	2.38	0.41
1:B:255:PHE:HA	1:B:271:PHE:CE2	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:B:286:TYR:CE2	1:B:296:PRO:HB3	2.54	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:A:48:GLN:C	1:A:50:GLY:N	2.74	0.41
1:B:419:LEU:CD2	1:B:419:LEU:H	2.33	0.41
1:B:479:PRO:HA	1:B:482:GLN:CG	2.49	0.41
1:A:258:VAL:HG11	1:A:273:ILE:CD1	2.51	0.41
1:A:243:ALA:HB1	1:A:245:PHE:CE1	2.56	0.41
1:A:331:ASN:ND2	1:A:331:ASN:H	2.17	0.41
1:A:501:ARG:HG3	1:A:501:ARG:HH11	1.85	0.41
1:B:208:ASP:N	1:B:208:ASP:OD1	2.53	0.41
1:B:458:GLY:HA2	1:B:461:ILE:HG12	2.03	0.41
1:A:567:GLU:O	1:A:568:ALA:C	2.59	0.41
1:A:295:MET:HE1	2:A:601:GLC:O5	2.21	0.41
1:B:396:GLN:O	1:B:399:ASN:HB2	2.21	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:B:572:CYS:SG	1:B:572:CYS:O	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LEU:N	1:A:88:LEU:HD12	2.36	0.41
1:A:555:LEU:HD23	1:A:564:PHE:CE1	2.55	0.41
1:A:573:THR:HG22	1:A:575:LEU:HG	2.03	0.41
1:B:23:LEU:HD22	1:B:117:PHE:CD2	2.56	0.41
1:B:278:LEU:N	1:B:278:LEU:CD1	2.84	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:179:ILE:HG12	1:B:228:LEU:HA	2.03	0.41
1:B:221:ASP:O	1:B:224:THR:N	2.54	0.41
1:B:26:ARG:HA	1:B:71:TRP:O	2.21	0.41
1:A:363:MET:HB3	1:A:364:PRO:HD3	2.03	0.40
1:A:545:PRO:HA	1:A:572:CYS:HA	2.03	0.40
1:A:383:VAL:HG12	1:A:442:LEU:CD2	2.50	0.40
1:B:183:ASP:O	1:B:184:TYR:C	2.58	0.40
1:B:265:SER:C	1:B:267:TYR:N	2.75	0.40
1:B:341:PHE:CE2	1:B:354:ILE:HD13	2.56	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:354:ILE:HG22	1:B:354:ILE:O	2.21	0.40
1:B:551:ARG:NE	1:B:551:ARG:CA	2.85	0.40
1:A:2:ARG:HH21	1:B:4:GLU:CG	2.35	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:258:VAL:O	1:B:262:GLY:N	2.50	0.40
1:B:308:TYR:O	1:B:311:ASP:HB2	2.21	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

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	41
1	B	586/588 (100%)	521 (89%)	56 (10%)	9 (2%)	12	51
All	All	1172/1176 (100%)	1043 (89%)	107 (9%)	22 (2%)	9	46

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%)	45	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	521/521 (100%)	501 (96%)	20 (4%)	38	74
All	All	1042/1042 (100%)	1006 (96%)	36 (4%)	41	76

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	0.62	0	13,15,17	0.47	0
2	GLC	A	602	2	11,11,12	0.35	0	13,15,17	1.11	2 (15%)
2	GLC	A	603	2	12,12,12	0.51	0	17,17,17	0.64	0
2	GLC	B	604	2	11,11,12	0.48	0	13,15,17	0.84	1 (7%)
2	GLC	B	605	2	11,11,12	0.43	0	13,15,17	0.82	1 (7%)
2	GLC	B	606	2	12,12,12	0.50	0	17,17,17	0.72	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	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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	GLC	C1-C2-C3	-2.05	107.06	109.65
2	B	604	GLC	C1-O5-C5	2.27	115.30	112.17
2	B	605	GLC	C1-O5-C5	2.40	115.48	112.17
2	A	602	GLC	C1-O5-C5	2.43	115.52	112.17

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%)	-0.60	7 (1%) 79 67	1, 14, 34, 73	0
1	B	588/588 (100%)	-0.61	5 (0%) 84 75	1, 14, 39, 69	0
All	All	1176/1176 (100%)	-0.60	12 (1%) 82 72	1, 14, 36, 73	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	568	ALA	5.7
1	A	568	ALA	4.9
1	B	569	GLU	4.2
1	B	570	THR	3.8
1	A	569	GLU	3.6
1	A	514	ASP	3.5
1	B	567	GLU	3.3
1	B	514	ASP	3.0
1	A	49	ASN	2.7
1	A	570	THR	2.6
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.