



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:41 PM GMT

PDB ID : 4FNU
Title : Crystal structure of GH36 alpha-galactosidase AgaA A355E D478A from Geobacillus stearothermophilus in complex with stachyose
Authors : Merceron, R.; Foucault, M.; Haser, R.; Mattes, R.; Watzlawick, H.; Gouet, P.
Deposited on : 2012-06-20
Resolution : 3.60 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

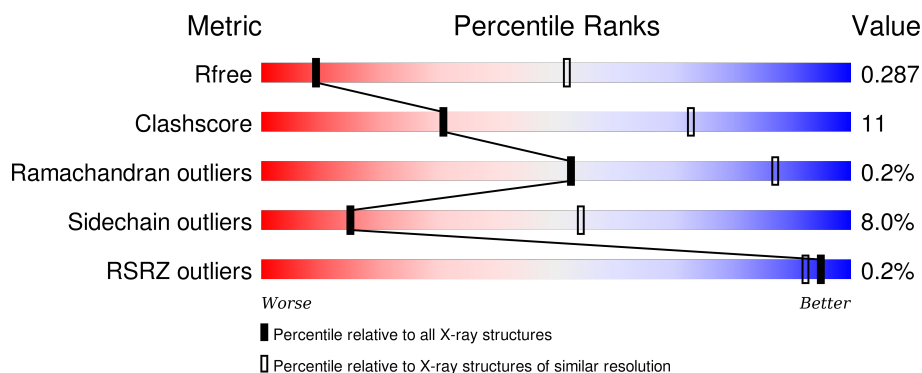
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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	729	 66% 28% . .
1	B	729	 69% 26% . .
1	C	729	 69% 27% . .
1	D	729	 71% 26% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FRU	C	804	-	-	-	X
2	FRU	D	804	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23332 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-galactosidase AgaA.

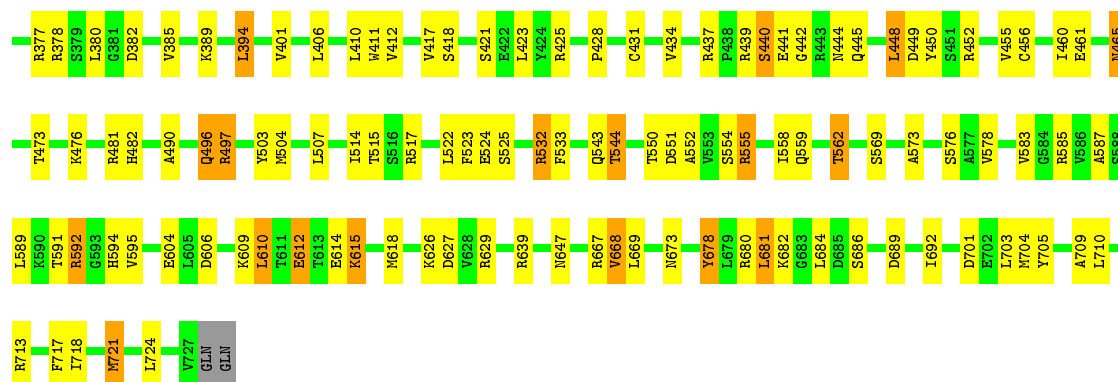
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	718	Total	C	N	O	S	0	0	0
			5788	3675	1020	1070	23			
1	B	718	Total	C	N	O	S	0	0	0
			5788	3675	1020	1070	23			
1	C	718	Total	C	N	O	S	0	0	0
			5788	3675	1020	1070	23			
1	D	718	Total	C	N	O	S	0	0	0
			5788	3675	1020	1070	23			

There are 8 discrepancies between the modelled and reference sequences:

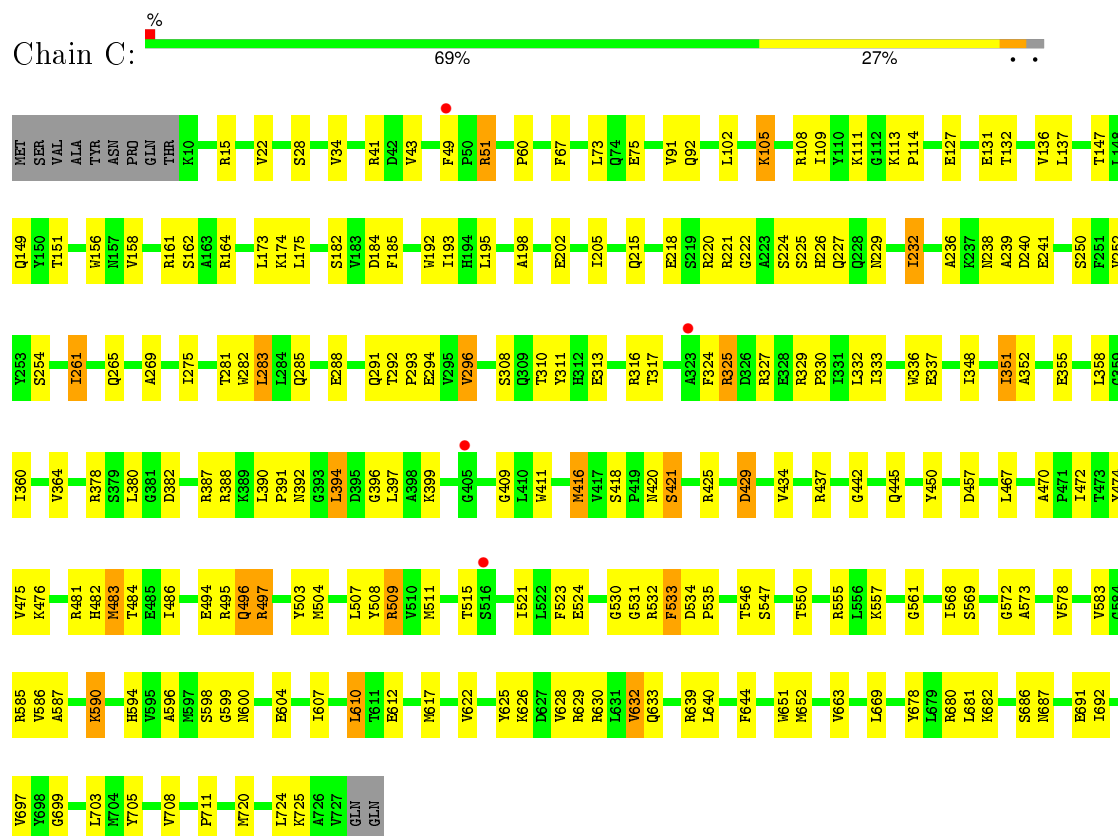
Chain	Residue	Modelled	Actual	Comment	Reference
A	355	GLU	ALA	ENGINEERED MUTATION	UNP Q9ALJ4
A	478	ALA	ASP	ENGINEERED MUTATION	UNP Q9ALJ4
B	355	GLU	ALA	ENGINEERED MUTATION	UNP Q9ALJ4
B	478	ALA	ASP	ENGINEERED MUTATION	UNP Q9ALJ4
C	355	GLU	ALA	ENGINEERED MUTATION	UNP Q9ALJ4
C	478	ALA	ASP	ENGINEERED MUTATION	UNP Q9ALJ4
D	355	GLU	ALA	ENGINEERED MUTATION	UNP Q9ALJ4
D	478	ALA	ASP	ENGINEERED MUTATION	UNP Q9ALJ4

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

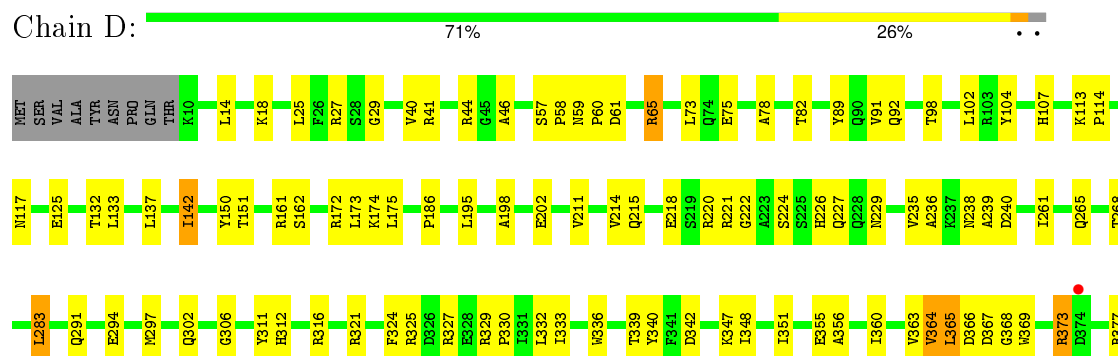
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	4	Total	C	O	0	0
			45	24	21		
2	B	4	Total	C	O	0	0
			45	24	21		
2	C	4	Total	C	O	0	0
			45	24	21		
2	D	4	Total	C	O	0	0
			45	24	21		



• Molecule 1: Alpha-galactosidase AgaA



• Molecule 1: Alpha-galactosidase AgaA



R378	S379	L380	V385	G393	L397	A398	V401	I402	I406	G409	L410	I411	E415	I416	V417	S418	I422	P419	I420	L423	L432	H433	V434	R437	Q442	R443	I444	Q445	L446	V447	L448	D449	Y450	S451	D457	V458	I459	L460	E461	I465	V466	L467	P471	I472	T473	Y474
V475	K476	W477	R481	H482	H483	T484	E485	Q496	R497	E498	Y503	R509	V510	E513	I514	T515	I521	I522	F523	C526	S527	R532	F533	M541	P542	Q543	D548	I549	T550	R555	Y560	S563	I568	A573	V578	Q582	V583	R592	A596							
I600	I607	T611	E612	T613	E614	R615	Q616	M617	K626	D627	V628	R629	R630	F637	V638	R639	F653	R658	A661	R667	V668	L669	S677	L681	D685	S686	H687	I692	L703	H704	L710	S714	S715	H721	L724	V727	GLN	GLN								

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.07Å 154.07Å 238.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.92 – 3.60 19.92 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.92-3.60) 99.7 (19.92-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 3.62Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.238 , 0.282 0.250 , 0.287	Depositor DCC
R_{free} test set	1906 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	93.0	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 19.4	EDS
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 38121 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23332	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.22	0/5935	0.42	0/8046
1	B	0.22	0/5935	0.40	0/8046
1	C	0.22	0/5935	0.41	0/8046
1	D	0.22	0/5935	0.42	1/8046 (0.0%)
All	All	0.22	0/23740	0.41	1/32184 (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	D	710	LEU	CA-CB-CG	5.87	128.81	115.30

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	5788	0	5621	147	0
1	B	5788	0	5621	130	0
1	C	5788	0	5621	139	0
1	D	5788	0	5621	124	0
2	A	45	0	39	4	0
2	B	45	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	45	0	39	2	0
2	D	45	0	39	0	0
All	All	23332	0	22640	501	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 11.

All (501) 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:B:681:LEU:HD11	1:B:703:LEU:HB3	1.61	0.81
1:B:684:LEU:H	1:B:704:MET:HE3	1.45	0.81
1:B:113:LYS:HD2	1:B:151:THR:HG21	1.66	0.78
1:A:113:LYS:HD2	1:A:151:THR:HG21	1.66	0.77
1:C:348:ILE:HD11	1:C:397:LEU:HD11	1.65	0.76
1:D:667:ARG:NH2	1:D:715:SER:O	2.20	0.75
1:A:317:THR:O	1:A:325:ARG:NH1	2.20	0.75
1:D:568:ILE:HD11	1:D:637:PHE:HB2	1.69	0.75
1:C:51:ARG:HH21	1:C:67:PHE:HA	1.51	0.73
1:A:281:THR:HG22	1:A:497:ARG:HB2	1.69	0.73
1:D:548:ASP:O	1:D:582:GLN:NE2	2.21	0.73
1:C:92:GLN:HB3	1:C:174:LYS:HB3	1.70	0.73
1:C:317:THR:O	1:C:325:ARG:NH1	2.22	0.72
1:A:686:SER:O	1:B:41:ARG:NH1	2.23	0.72
1:D:327:ARG:O	1:D:329:ARG:NH1	2.23	0.71
1:A:113:LYS:NZ	1:A:122:THR:O	2.22	0.71
1:B:75:GLU:OE1	1:B:161:ARG:NH1	2.24	0.71
1:C:681:LEU:HD12	1:C:703:LEU:HD13	1.73	0.71
1:C:351:ILE:HD11	1:C:607:ILE:HB	1.72	0.70
1:B:328:GLU:HB3	1:B:629:ARG:HD2	1.72	0.70
1:D:27:ARG:NH2	1:D:61:ASP:OD2	2.25	0.70
1:C:41:ARG:NH2	1:D:686:SER:O	2.24	0.70
1:B:232:ILE:HG12	1:B:259:ALA:HB1	1.73	0.69
1:B:368:GLY:HA2	1:B:373:ARG:HB3	1.73	0.69
1:D:368:GLY:HA2	1:D:373:ARG:HB3	1.74	0.69
1:C:316:ARG:HG3	1:C:317:THR:HG23	1.73	0.69
1:B:86:ALA:O	1:B:270:ARG:NH1	2.26	0.69
1:B:431:CYS:HA	1:B:448:LEU:HA	1.75	0.68
1:A:533:PHE:HE1	1:A:546:THR:HG22	1.58	0.68
1:D:380:LEU:HB2	1:D:418:SER:HB2	1.75	0.68
1:C:691:GLU:HA	1:C:697:VAL:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:ASP:OD1	1:C:509:ARG:NH2	2.27	0.66
1:A:211:VAL:H	1:A:215:GLN:HE21	1.44	0.66
1:A:555:ARG:HH11	1:A:555:ARG:HG3	1.61	0.65
1:D:365:LEU:HD11	1:D:369:TRP:HB3	1.78	0.65
1:D:578:VAL:HG13	1:D:592:ARG:HH11	1.62	0.65
1:C:333:ILE:HG22	1:C:360:ILE:HG21	1.78	0.64
1:B:27:ARG:NH2	1:B:64:ASP:OD2	2.31	0.64
1:B:211:VAL:H	1:B:215:GLN:HE21	1.44	0.64
1:D:401:VAL:HG12	1:D:406:LEU:HB2	1.78	0.64
1:A:70:ASP:O	1:A:85:ARG:NH1	2.30	0.64
1:D:142:ILE:HG13	1:D:173:LEU:HD11	1.79	0.64
1:C:281:THR:HG22	1:C:497:ARG:HB2	1.80	0.64
1:C:625:TYR:OH	1:C:633:GLN:NE2	2.30	0.63
1:D:398:ALA:O	1:D:402:ASN:ND2	2.30	0.63
1:A:497:ARG:NH1	1:D:98:THR:OG1	2.31	0.63
1:A:440:SER:HB3	1:D:60:PRO:HA	1.79	0.63
1:A:41:ARG:NH2	1:B:689:ASP:OD1	2.32	0.62
1:B:440:SER:HB3	1:C:60:PRO:HA	1.80	0.62
1:C:680:ARG:HH21	1:C:705:TYR:HA	1.64	0.62
1:C:652:MET:HE1	1:C:682:LYS:H	1.64	0.62
1:C:442:GLY:H	1:C:481:ARG:HE	1.47	0.62
1:A:364:VAL:HG22	1:A:409:GLY:HA3	1.82	0.61
1:C:283:LEU:HD22	1:C:494:GLU:HG3	1.82	0.61
1:D:218:GLU:OE2	1:D:220:ARG:NH2	2.33	0.61
1:C:250:SER:HB3	1:C:296:VAL:HG13	1.82	0.61
1:C:390:LEU:HD11	1:C:397:LEU:HB2	1.81	0.61
1:A:301:ASP:N	1:A:301:ASP:OD1	2.33	0.61
1:A:546:THR:OG1	1:A:555:ARG:NH2	2.33	0.61
1:A:172:ARG:HH22	1:A:174:LYS:HE2	1.65	0.61
1:A:65:ARG:NH2	1:D:444:ASN:OD1	2.32	0.60
1:C:583:VAL:HG23	1:C:585:ARG:H	1.65	0.60
1:A:431:CYS:HA	1:A:448:LEU:HA	1.83	0.60
1:D:457:ASP:OD1	1:D:509:ARG:NH2	2.32	0.60
1:A:252:VAL:HG12	1:A:535:PRO:HB2	1.83	0.60
1:C:429:ASP:N	1:C:429:ASP:OD1	2.34	0.60
1:C:590:LYS:O	1:C:594:HIS:ND1	2.35	0.59
1:C:474:TYR:OH	1:C:524:GLU:OE2	2.20	0.59
1:D:174:LYS:HB3	1:D:283:LEU:HD12	1.82	0.59
1:C:102:LEU:HD21	1:C:137:LEU:HD13	1.84	0.59
1:B:411:TRP:HD1	1:B:476:LYS:HE2	1.67	0.59
1:B:594:HIS:ND1	1:B:721:MET:SD	2.73	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:ARG:HG2	1:D:420:ASN:HB3	1.84	0.59
1:D:461:GLU:O	1:D:465:ASN:ND2	2.34	0.59
1:D:59:ASN:OD1	1:D:65:ARG:NH1	2.35	0.59
1:C:114:PRO:HD3	1:C:132:THR:HG21	1.85	0.59
1:C:355:GLU:HA	1:C:358:LEU:HD12	1.85	0.59
1:C:193:ILE:HD11	1:C:205:ILE:HB	1.85	0.59
1:B:610:LEU:HD23	1:B:614:GLU:HB3	1.85	0.58
1:B:445:GLN:O	1:B:481:ARG:NH1	2.36	0.58
1:C:699:GLY:H	1:D:44:ARG:HG3	1.68	0.58
1:B:235:VAL:HG12	1:B:246:VAL:HG13	1.85	0.58
1:A:461:GLU:O	1:A:465:ASN:ND2	2.36	0.58
1:C:185:PHE:HB2	1:C:269:ALA:HB3	1.84	0.58
1:D:467:LEU:HD21	1:D:475:VAL:HG21	1.86	0.58
1:C:238:ASN:ND2	1:D:240:ASP:OD2	2.37	0.58
1:A:681:LEU:HD13	1:A:703:LEU:HB3	1.86	0.57
1:D:117:ASN:HB3	1:D:291:GLN:HG3	1.87	0.57
1:C:316:ARG:NH1	1:C:633:GLN:O	2.38	0.57
1:D:434:VAL:HG22	1:D:485:GLU:HB3	1.86	0.57
1:A:452:ARG:HB2	1:A:455:VAL:HG23	1.86	0.57
1:A:595:VAL:O	1:A:598:SER:OG	2.22	0.57
1:A:335:ASN:ND2	1:A:366:ASP:OD2	2.38	0.57
1:A:54:ARG:NH1	1:B:673:ASN:OD1	2.35	0.56
1:D:125:GLU:OE2	1:D:325:ARG:NH2	2.39	0.56
1:C:252:VAL:HG12	1:C:535:PRO:HB2	1.87	0.56
1:B:201:ARG:HA	1:B:558:ILE:HD11	1.86	0.56
1:C:205:ILE:H	1:C:644:PHE:HE2	1.51	0.56
1:C:364:VAL:HG12	1:C:409:GLY:HA3	1.87	0.56
1:A:86:ALA:O	1:A:270:ARG:NH1	2.39	0.56
1:B:377:ARG:NH1	1:B:444:ASN:OD1	2.39	0.56
1:B:175:LEU:HB2	1:B:282:TRP:HB3	1.86	0.56
1:A:497:ARG:HA	1:A:497:ARG:HE	1.71	0.55
1:A:434:VAL:HG23	1:A:437:ARG:HB2	1.89	0.55
1:B:241:GLU:OE2	1:B:639:ARG:NH1	2.39	0.55
1:C:75:GLU:OE1	1:C:161:ARG:NH1	2.39	0.55
1:B:583:VAL:O	1:D:714:SER:OG	2.24	0.55
1:D:339:THR:OG1	1:D:342:ASP:O	2.24	0.55
1:A:27:ARG:NH2	1:A:64:ASP:OD2	2.39	0.55
1:D:447:VAL:HG13	1:D:481:ARG:HD3	1.87	0.55
1:A:85:ARG:HE	1:A:270:ARG:NH2	2.04	0.55
1:C:252:VAL:HG22	1:C:294:GLU:O	2.07	0.55
1:B:504:MET:HE3	1:B:507:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:LEU:HB2	1:C:418:SER:HB2	1.89	0.55
1:A:102:LEU:HD22	1:A:137:LEU:HB3	1.88	0.54
1:B:195:LEU:HB2	1:B:229:ASN:HB3	1.90	0.54
1:C:195:LEU:HB2	1:C:229:ASN:HB3	1.89	0.54
1:A:587:ALA:O	1:A:592:ARG:NH2	2.39	0.54
1:B:203:ARG:NE	1:B:562:THR:OG1	2.34	0.54
1:A:663:VAL:HG21	1:A:681:LEU:HD21	1.90	0.54
1:D:411:TRP:HD1	1:D:476:LYS:HE2	1.73	0.54
1:A:10:LYS:HB3	1:A:25:LEU:HB2	1.90	0.54
1:A:612:GLU:HA	1:A:615:LYS:HE3	1.90	0.54
1:A:680:ARG:NH2	1:B:245:GLU:OE2	2.39	0.54
1:C:158:VAL:HG13	1:C:296:VAL:HG23	1.91	0.53
1:A:250:SER:HB3	1:A:296:VAL:HG13	1.89	0.53
1:D:373:ARG:NH1	1:D:378:ARG:O	2.42	0.53
1:A:158:VAL:HG13	1:A:296:VAL:HG23	1.90	0.53
1:C:434:VAL:HG23	1:C:437:ARG:HB2	1.91	0.53
1:C:149:GLN:HE22	1:C:164:ARG:HB2	1.74	0.53
1:A:198:ALA:HB2	1:D:265:GLN:HB2	1.91	0.53
1:C:175:LEU:HB2	1:C:282:TRP:HB3	1.90	0.53
1:B:450:TYR:HE2	1:B:507:LEU:HD13	1.73	0.53
1:A:705:TYR:CD1	1:B:38:LYS:HE3	2.43	0.53
1:C:313:GLU:HA	1:C:316:ARG:HG2	1.91	0.52
1:A:714:SER:OG	1:C:583:VAL:O	2.27	0.52
1:C:687:ASN:HA	1:D:41:ARG:HH22	1.74	0.52
1:B:452:ARG:HE	1:B:490:ALA:HB2	1.74	0.52
1:C:507:LEU:HD21	1:C:532:ARG:HH12	1.74	0.52
1:C:467:LEU:HG	1:C:472:ILE:HG21	1.91	0.52
1:B:198:ALA:HB2	1:C:265:GLN:HB2	1.91	0.52
1:A:555:ARG:HD2	1:A:559:GLN:HG3	1.90	0.52
1:A:227:GLN:HG3	1:D:265:GLN:HB3	1.92	0.52
1:C:475:VAL:HG23	1:C:521:ILE:HD11	1.90	0.52
1:C:22:VAL:HG21	1:C:43:VAL:HG21	1.92	0.52
1:B:265:GLN:HB2	1:C:198:ALA:HB2	1.91	0.52
1:A:203:ARG:HE	1:A:562:THR:HB	1.74	0.52
1:A:232:ILE:HG12	1:A:259:ALA:HB1	1.91	0.52
1:B:373:ARG:NH1	1:B:378:ARG:O	2.43	0.52
1:B:578:VAL:HG11	1:B:587:ALA:H	1.75	0.52
1:A:591:THR:HG21	1:A:717:PHE:O	2.10	0.52
1:D:329:ARG:O	1:D:629:ARG:NH2	2.43	0.51
1:D:481:ARG:NH1	1:D:482:HIS:O	2.43	0.51
1:D:385:VAL:HG21	1:D:393:GLY:HA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:VAL:HG13	1:D:215:GLN:NE2	2.25	0.51
1:D:133:LEU:HB3	1:D:150:TYR:HB2	1.92	0.51
1:C:392:ASN:HB3	1:C:396:GLY:HA3	1.92	0.51
1:A:162:SER:HB3	1:A:294:GLU:HA	1.92	0.51
1:C:337:GLU:HB2	1:C:604:GLU:HG2	1.92	0.51
1:C:218:GLU:OE2	1:C:220:ARG:NH2	2.44	0.51
1:B:555:ARG:HD2	1:B:559:GLN:HG3	1.93	0.51
1:D:543:GLN:OE1	1:D:600:ASN:ND2	2.44	0.51
1:D:333:ILE:HG22	1:D:360:ILE:HG21	1.93	0.51
1:C:275:ILE:HD11	1:C:293:PRO:HD2	1.92	0.51
1:A:530:GLY:N	1:A:546:THR:O	2.44	0.51
1:A:211:VAL:HG22	1:A:215:GLN:HG3	1.92	0.51
1:A:725:LYS:NZ	1:A:726:ALA:O	2.31	0.51
1:C:546:THR:OG1	1:C:555:ARG:NH1	2.40	0.51
1:C:324:PHE:HA	1:C:327:ARG:HG3	1.92	0.51
1:B:434:VAL:HG23	1:B:437:ARG:HB2	1.93	0.51
1:B:626:LYS:HB3	1:B:629:ARG:HH21	1.75	0.51
1:A:215:GLN:OE1	1:A:215:GLN:N	2.42	0.50
1:C:573:ALA:HB1	1:C:596:ALA:HA	1.93	0.50
1:B:441:GLU:HA	1:B:481:ARG:HH12	1.77	0.50
1:B:116:LEU:HD12	1:B:121:ALA:HB2	1.93	0.50
1:C:411:TRP:HD1	1:C:476:LYS:HE3	1.74	0.50
1:D:75:GLU:OE1	1:D:161:ARG:NH1	2.44	0.50
1:C:202:GLU:HG3	1:C:226:HIS:HB3	1.94	0.50
1:A:447:VAL:HG23	1:A:481:ARG:HD3	1.94	0.50
1:C:483:MET:HB2	1:C:486:ILE:HD11	1.93	0.50
1:B:552:ALA:HB2	1:B:592:ARG:HA	1.93	0.50
1:A:252:VAL:HG22	1:A:294:GLU:O	2.12	0.49
1:A:22:VAL:HG21	1:A:43:VAL:HG21	1.94	0.49
1:D:363:VAL:HG23	1:D:406:LEU:HD22	1.94	0.49
1:A:41:ARG:NH1	1:B:686:SER:O	2.43	0.49
1:D:661:ALA:HB3	1:D:724:LEU:HB2	1.93	0.49
1:B:496:GLN:NE2	1:B:497:ARG:HG2	2.27	0.49
1:B:70:ASP:OD2	1:C:221:ARG:NH2	2.40	0.49
1:C:240:ASP:OD1	1:D:238:ASN:ND2	2.38	0.49
1:D:195:LEU:HB2	1:D:229:ASN:HB3	1.95	0.49
1:A:161:ARG:HE	1:A:181:MET:HB2	1.77	0.49
1:A:442:GLY:O	1:A:445:GLN:HG2	2.11	0.49
1:B:92:GLN:HB2	1:B:176:LEU:HD11	1.94	0.49
1:D:202:GLU:HG3	1:D:226:HIS:HB3	1.94	0.49
1:C:192:TRP:HZ3	1:C:232:ILE:HD11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:691:GLU:HG3	1:C:725:LYS:HG3	1.95	0.49
1:D:113:LYS:HD3	1:D:151:THR:HG21	1.95	0.49
1:C:578:VAL:HG21	1:C:587:ALA:H	1.77	0.49
1:B:576:SER:O	1:B:592:ARG:NH1	2.45	0.49
1:B:380:LEU:HB2	1:B:418:SER:HB2	1.95	0.49
1:C:622:VAL:HG12	1:C:626:LYS:HE3	1.95	0.48
1:B:460:ILE:HA	1:B:514:ILE:HD11	1.94	0.48
1:D:611:THR:O	1:D:615:LYS:HG2	2.13	0.48
1:D:92:GLN:HB3	1:D:174:LYS:HG3	1.95	0.48
1:B:411:TRP:CD1	1:B:476:LYS:HE2	2.48	0.48
1:B:51:ARG:HA	1:B:51:ARG:HD2	1.56	0.48
1:D:555:ARG:HH22	1:D:573:ALA:HA	1.78	0.48
1:C:496:GLN:NE2	1:C:497:ARG:HG2	2.28	0.48
1:D:582:GLN:OE1	1:D:582:GLN:N	2.46	0.48
1:D:509:ARG:NH1	1:D:513:GLU:OE2	2.46	0.48
1:B:428:PRO:O	1:B:439:ARG:NH1	2.46	0.48
1:B:551:ASP:OD2	1:B:585:ARG:NH1	2.44	0.48
1:A:161:ARG:HH21	1:A:182:SER:H	1.61	0.48
1:C:697:VAL:HG22	1:D:44:ARG:HH21	1.78	0.48
1:A:184:ASP:OD1	1:A:270:ARG:NE	2.30	0.48
1:A:440:SER:OG	1:A:485:GLU:OE2	2.31	0.48
1:B:606:ASP:OD2	1:B:609:LYS:NZ	2.30	0.48
1:A:709:ALA:HB3	1:B:48:ALA:HB3	1.96	0.48
1:A:38:LYS:HB3	1:B:705:TYR:CG	2.49	0.48
1:A:669:LEU:HD21	1:C:669:LEU:HD21	1.96	0.48
1:D:460:ILE:HD11	1:D:510:VAL:HA	1.95	0.48
1:D:560:TYR:CZ	1:D:639:ARG:HD2	2.49	0.48
1:C:568:ILE:HD11	1:C:599:GLY:HA2	1.96	0.47
1:C:113:LYS:HD2	1:C:151:THR:HG21	1.96	0.47
1:C:51:ARG:HD2	1:C:51:ARG:HA	1.56	0.47
1:A:459:ILE:O	1:A:463:ILE:HG12	2.14	0.47
1:C:111:LYS:NZ	1:C:131:GLU:HB3	2.29	0.47
1:C:442:GLY:N	1:C:481:ARG:HE	2.12	0.47
1:A:99:VAL:HG21	1:D:485:GLU:HA	1.95	0.47
1:B:496:GLN:HE22	1:B:497:ARG:HG2	1.78	0.47
1:A:147:THR:HB	1:A:164:ARG:HB3	1.97	0.47
1:B:22:VAL:HG21	1:B:43:VAL:HG21	1.96	0.47
1:A:382:ASP:OD1	1:A:382:ASP:N	2.46	0.47
1:B:85:ARG:HE	1:B:270:ARG:NH2	2.12	0.47
1:A:705:TYR:HB3	1:B:38:LYS:HB3	1.96	0.47
1:B:680:ARG:HH21	1:B:705:TYR:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:HB2	1:A:282:TRP:HB3	1.96	0.47
1:B:525:SER:OG	1:B:544:THR:HG23	2.15	0.47
1:D:235:VAL:HG13	1:D:239:ALA:HB3	1.96	0.47
1:C:394:LEU:HB3	1:C:470:ALA:HB2	1.96	0.47
1:D:356:ALA:HB2	1:D:406:LEU:HD11	1.96	0.47
1:A:53:ASP:OD1	1:A:65:ARG:HD2	2.15	0.47
1:B:377:ARG:HH11	1:B:377:ARG:HG2	1.80	0.47
1:C:388:ARG:HD3	1:C:388:ARG:HA	1.70	0.47
1:A:265:GLN:HB2	1:D:198:ALA:HB2	1.96	0.47
1:C:73:LEU:HD22	1:C:184:ASP:HB3	1.96	0.47
1:C:215:GLN:HG2	1:C:261:ILE:HG23	1.97	0.46
1:C:533:PHE:HE1	1:C:546:THR:HG22	1.80	0.46
1:D:366:ASP:OD1	1:D:367:ASP:N	2.43	0.46
1:D:677:SER:HB2	1:D:710:LEU:HD11	1.97	0.46
1:D:161:ARG:HD3	1:D:297:MET:HE1	1.97	0.46
1:B:329:ARG:HA	1:B:330:PRO:HD3	1.82	0.46
1:D:397:LEU:O	1:D:401:VAL:HG23	2.16	0.46
1:B:265:GLN:HB3	1:C:227:GLN:HG3	1.96	0.46
2:C:802:GLA:O2	2:C:804:FRU:H4	2.15	0.46
1:C:628:VAL:O	1:C:632:VAL:HG13	2.15	0.46
1:B:23:MET:HE3	1:B:75:GLU:HG3	1.97	0.46
1:D:221:ARG:HD3	1:D:482:HIS:CE1	2.50	0.46
1:D:14:LEU:HD11	1:D:150:TYR:HB3	1.97	0.46
1:D:58:PRO:HB2	1:D:82:THR:HG22	1.97	0.46
1:A:149:GLN:HE21	1:A:149:GLN:HB2	1.53	0.46
1:A:236:ALA:HB3	1:A:239:ALA:HB2	1.98	0.46
1:A:555:ARG:NH1	1:A:555:ARG:HG3	2.27	0.46
1:A:535:PRO:HD3	1:A:566:TYR:HE1	1.81	0.46
1:A:415:GLU:HA	1:A:450:TYR:HE2	1.80	0.46
1:A:227:GLN:OE1	1:A:227:GLN:N	2.48	0.46
1:B:227:GLN:N	1:B:227:GLN:OE1	2.47	0.46
1:A:375:ASP:N	1:A:375:ASP:OD1	2.47	0.46
1:C:222:GLY:HA3	1:C:483:MET:SD	2.56	0.46
1:B:93:LEU:HD13	1:B:142:ILE:HD11	1.96	0.46
1:D:432:LEU:HB2	1:D:447:VAL:HG23	1.97	0.46
1:D:227:GLN:N	1:D:227:GLN:OE1	2.47	0.46
1:D:283:LEU:N	1:D:498:GLU:OE2	2.43	0.46
1:D:236:ALA:HB3	1:D:239:ALA:HB2	1.98	0.46
1:D:442:GLY:O	1:D:445:GLN:HG2	2.15	0.46
1:D:415:GLU:OE2	1:D:477:TRP:NE1	2.48	0.46
1:A:394:LEU:HD12	1:A:395:ASP:N	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:VAL:HG12	1:B:394:LEU:HD13	1.98	0.46
1:A:417:VAL:HG23	1:A:448:LEU:HD22	1.97	0.45
1:C:147:THR:HB	1:C:164:ARG:HB3	1.98	0.45
1:C:472:ILE:HG23	1:C:521:ILE:HD12	1.97	0.45
1:D:102:LEU:HD22	1:D:137:LEU:HB3	1.99	0.45
1:C:91:VAL:HG11	1:C:173:LEU:HD23	1.97	0.45
1:C:640:LEU:HA	1:C:640:LEU:HD12	1.81	0.45
1:B:460:ILE:HG13	1:B:461:GLU:N	2.31	0.45
1:B:337:GLU:HB2	1:B:604:GLU:HG2	1.98	0.45
1:A:640:LEU:HD13	1:A:679:LEU:HD11	1.97	0.45
1:B:38:LYS:HB2	1:B:38:LYS:HE2	1.84	0.45
1:A:324:PHE:CD2	1:A:522:LEU:HD12	2.51	0.45
1:C:416:MET:HE2	1:C:445:GLN:HE21	1.82	0.45
1:A:336:TRP:CE3	2:A:801:GLA:H62	2.52	0.45
1:D:687:ASN:O	1:D:687:ASN:ND2	2.43	0.45
1:B:532:ARG:HB3	1:B:532:ARG:HE	1.54	0.45
1:A:526:CYS:SG	2:A:801:GLA:H2	2.56	0.45
1:C:351:ILE:HG12	1:C:607:ILE:HD13	1.99	0.45
1:A:262:GLU:HB3	1:A:270:ARG:HB3	1.98	0.45
1:C:227:GLN:N	1:C:227:GLN:OE1	2.49	0.45
1:C:598:SER:OG	1:C:651:TRP:NE1	2.50	0.45
1:C:105:LYS:HD2	1:C:105:LYS:HA	1.76	0.45
1:B:373:ARG:HD2	1:B:373:ARG:HA	1.54	0.45
1:B:167:ASN:ND2	1:B:173:LEU:HD13	2.31	0.45
1:A:559:GLN:HA	1:A:562:THR:HG22	1.98	0.45
1:B:221:ARG:HD3	1:B:482:HIS:ND1	2.32	0.45
1:A:663:VAL:HB	1:A:722:TRP:HB2	1.99	0.45
1:C:467:LEU:HD21	1:C:475:VAL:HG21	1.99	0.45
1:C:421:SER:O	1:C:425:ARG:HG3	2.17	0.45
1:B:180:SER:H	1:B:274:GLY:HA3	1.82	0.45
1:D:162:SER:HB3	1:D:294:GLU:HA	1.98	0.45
1:B:583:VAL:HG23	1:B:585:ARG:H	1.81	0.44
1:B:355:GLU:HB3	1:B:360:ILE:HD12	1.98	0.44
1:A:502:ARG:HA	1:A:505:LEU:HB2	1.99	0.44
1:B:58:PRO:HB2	1:B:82:THR:HG22	1.99	0.44
1:B:442:GLY:H	1:B:481:ARG:NH1	2.15	0.44
1:D:475:VAL:HG23	1:D:521:ILE:HD11	1.97	0.44
1:B:450:TYR:HB2	1:B:503:TYR:CD1	2.52	0.44
1:D:541:MET:HA	1:D:542:PRO:HD3	1.82	0.44
1:D:91:VAL:HG13	1:D:175:LEU:HD23	2.00	0.44
1:C:261:ILE:HD11	1:C:269:ALA:HB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:SER:OG	1:A:715:SER:N	2.51	0.44
1:B:554:SER:O	1:B:558:ILE:HG12	2.17	0.44
1:D:351:ILE:O	1:D:355:GLU:HG3	2.16	0.44
1:C:205:ILE:HG23	1:C:561:GLY:HA2	1.99	0.44
1:A:572:GLY:HA2	1:A:600:ASN:OD1	2.18	0.44
1:D:398:ALA:HB3	1:D:471:PRO:HD2	1.99	0.44
1:C:652:MET:HG2	1:C:663:VAL:HA	1.98	0.44
1:A:172:ARG:HG3	1:A:172:ARG:HH11	1.82	0.44
1:A:541:MET:HA	1:A:542:PRO:HD3	1.85	0.44
1:A:677:SER:HB2	1:A:710:LEU:HD22	2.00	0.44
1:D:73:LEU:H	1:D:73:LEU:HD12	1.82	0.44
1:B:194:HIS:CD2	1:B:196:PRO:HD3	2.53	0.44
1:D:568:ILE:HD13	1:D:653:PHE:HE1	1.83	0.44
1:A:551:ASP:O	1:A:555:ARG:HB2	2.18	0.44
1:C:225:SER:N	1:C:531:GLY:O	2.50	0.44
1:A:354:THR:O	1:A:358:LEU:HD13	2.17	0.44
1:A:92:GLN:HB2	1:A:176:LEU:HD11	1.99	0.44
1:D:450:TYR:HB2	1:D:503:TYR:CD1	2.53	0.44
1:C:352:ALA:HA	1:C:355:GLU:HG2	1.99	0.44
1:D:434:VAL:HG23	1:D:437:ARG:HB2	1.99	0.44
1:C:387:ARG:NH2	1:C:391:PRO:O	2.51	0.44
1:A:551:ASP:OD1	1:A:585:ARG:HB3	2.18	0.44
1:B:158:VAL:HG13	1:B:296:VAL:HG13	2.00	0.43
1:C:156:TRP:NE1	1:C:313:GLU:OE2	2.50	0.43
1:B:51:ARG:HH21	1:B:67:PHE:HA	1.82	0.43
1:A:223:ALA:HA	1:A:254:SER:O	2.18	0.43
1:B:465:ASN:OD1	1:B:465:ASN:N	2.50	0.43
1:B:692:ILE:HG13	1:B:724:LEU:HG	2.00	0.43
1:A:168:LYS:HB3	1:A:168:LYS:HE3	1.79	0.43
1:D:104:TYR:OH	1:D:107:HIS:ND1	2.28	0.43
1:C:316:ARG:HH12	1:C:569:SER:HB3	1.83	0.43
1:C:275:ILE:H	1:C:275:ILE:HD12	1.84	0.43
1:D:523:PHE:HB3	1:D:541:MET:HG2	2.01	0.43
1:C:236:ALA:HB3	1:C:239:ALA:HB2	1.99	0.43
1:A:385:VAL:HG11	1:A:393:GLY:HA2	1.99	0.43
1:A:430:TRP:CE3	1:A:455:VAL:HG13	2.54	0.43
1:A:254:SER:HA	1:A:534:ASP:OD2	2.18	0.43
1:C:450:TYR:HB2	1:C:503:TYR:CD1	2.54	0.43
1:C:224:SER:HB2	1:C:532:ARG:HA	2.00	0.43
1:C:202:GLU:N	1:C:202:GLU:OE1	2.46	0.43
1:B:18:LYS:HG2	1:B:157:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:MET:HG3	1:C:508:TYR:CE2	2.54	0.43
1:A:667:ARG:HH11	1:A:667:ARG:HG2	1.83	0.43
1:D:312:HIS:NE2	1:D:563:SER:O	2.41	0.43
1:D:222:GLY:HA3	1:D:483:MET:SD	2.58	0.43
1:B:686:SER:HB2	1:B:701:ASP:HB3	2.01	0.43
1:C:162:SER:HB3	1:C:294:GLU:HA	2.00	0.43
1:C:308:SER:OG	1:C:639:ARG:NH2	2.37	0.43
1:C:607:ILE:HA	1:C:610:LEU:HD21	1.99	0.43
1:D:373:ARG:NH1	1:D:378:ARG:H	2.16	0.43
1:A:18:LYS:HE3	1:A:38:LYS:HD2	2.01	0.43
1:B:421:SER:O	1:B:425:ARG:HG3	2.19	0.43
1:C:285:GLN:N	1:C:288:GLU:OE2	2.46	0.43
1:A:454:ASP:N	1:A:454:ASP:OD2	2.52	0.43
1:C:333:ILE:HD11	1:C:607:ILE:HD11	2.01	0.43
1:A:652:MET:SD	1:A:681:LEU:HD23	2.59	0.43
1:C:578:VAL:HG11	1:C:586:VAL:HG13	2.01	0.43
1:A:218:GLU:OE2	1:A:220:ARG:NH2	2.52	0.43
1:B:332:LEU:HB3	1:B:362:LEU:HD23	2.01	0.43
1:D:613:THR:O	1:D:616:GLN:HG2	2.18	0.42
1:B:401:VAL:HG13	1:B:406:LEU:HB2	2.01	0.42
1:C:49:PHE:CZ	1:C:51:ARG:HD3	2.54	0.42
1:D:211:VAL:HG13	1:D:215:GLN:HE21	1.84	0.42
1:A:473:THR:O	1:A:473:THR:OG1	2.36	0.42
1:D:626:LYS:HA	1:D:629:ARG:HD2	2.00	0.42
1:A:449:ASP:OD2	1:A:451:SER:OG	2.25	0.42
1:D:25:LEU:HD11	1:D:29:GLY:HA2	2.01	0.42
1:B:555:ARG:HH12	1:B:573:ALA:HA	1.83	0.42
1:C:530:GLY:N	1:C:546:THR:O	2.53	0.42
1:A:163:ALA:H	1:A:292:THR:HG22	1.83	0.42
1:D:459:ILE:HD13	1:D:459:ILE:HA	1.86	0.42
1:A:78:ALA:HB2	1:A:89:TYR:CE2	2.55	0.42
1:A:525:SER:HB2	1:A:544:THR:HG23	2.01	0.42
1:A:194:HIS:CD2	1:A:196:PRO:HD3	2.54	0.42
1:C:511:MET:HB2	1:C:511:MET:HE3	1.87	0.42
1:A:179:LEU:HD13	1:A:272:SER:HB2	2.01	0.42
1:D:364:VAL:HG13	1:D:409:GLY:HA3	2.01	0.42
1:A:573:ALA:HB1	1:A:596:ALA:HA	2.01	0.42
1:C:557:LYS:HB3	1:C:644:PHE:HE1	1.85	0.42
1:B:236:ALA:HB3	1:B:239:ALA:HB2	2.02	0.42
1:A:527:SER:OG	1:A:532:ARG:HD2	2.20	0.42
1:D:302:GLN:HB3	1:D:306:GLY:HA3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:THR:HG22	1:C:523:PHE:CD2	2.55	0.42
1:A:251:PHE:CE1	1:A:293:PRO:HB2	2.55	0.42
1:B:461:GLU:OE2	1:B:517:ARG:NH2	2.52	0.42
1:B:417:VAL:HG13	1:B:423:LEU:HD21	2.01	0.42
1:C:692:ILE:HG12	1:C:724:LEU:HG	2.01	0.42
1:D:347:LYS:HA	1:D:347:LYS:HD3	1.76	0.42
1:A:319:LEU:HD23	1:A:538:LEU:HD23	2.01	0.42
1:A:96:GLY:O	1:D:497:ARG:HD2	2.19	0.42
1:C:252:VAL:HG23	1:C:252:VAL:O	2.20	0.42
1:B:49:PHE:CZ	1:B:51:ARG:HD3	2.54	0.42
1:A:524:GLU:OE1	1:A:543:GLN:NE2	2.49	0.42
1:A:480:ASN:ND2	2:A:802:GLA:O4	2.53	0.42
1:B:251:PHE:CE1	1:B:293:PRO:HB2	2.55	0.42
1:B:151:THR:O	1:B:159:ILE:HA	2.20	0.42
1:D:329:ARG:HA	1:D:330:PRO:HD3	1.86	0.42
1:B:481:ARG:HG2	1:B:482:HIS:N	2.35	0.42
1:C:161:ARG:NH2	1:C:182:SER:H	2.18	0.42
1:A:180:SER:HA	1:A:292:THR:HG21	2.02	0.42
1:A:196:PRO:HB3	1:A:228:GLN:HE22	1.83	0.42
1:A:264:ASP:OD1	1:A:268:THR:HG23	2.19	0.42
1:B:524:GLU:OE1	1:B:543:GLN:NE2	2.52	0.42
1:D:78:ALA:HB2	1:D:89:TYR:CE2	2.54	0.42
1:C:711:PRO:HG2	1:C:720:MET:HE1	2.02	0.42
1:C:625:TYR:CE2	1:C:629:ARG:HB2	2.55	0.41
1:B:229:ASN:O	1:B:231:PHE:N	2.52	0.41
1:B:76:TYR:HB2	1:B:148:LEU:HD21	2.01	0.41
1:A:284:LEU:HD23	1:A:288:GLU:HG3	2.01	0.41
1:C:254:SER:OG	1:C:534:ASP:OD2	2.25	0.41
1:A:222:GLY:HA3	1:A:483:MET:SD	2.60	0.41
1:D:373:ARG:HD2	1:D:373:ARG:HA	1.61	0.41
1:B:449:ASP:O	1:B:455:VAL:HG21	2.19	0.41
1:A:109:ILE:HG12	1:A:133:LEU:HD13	2.01	0.41
1:B:113:LYS:HA	1:B:114:PRO:HD3	1.94	0.41
1:D:316:ARG:O	1:D:325:ARG:HG3	2.20	0.41
1:A:18:LYS:HG2	1:A:157:ASN:HD21	1.84	0.41
1:A:625:TYR:OH	1:A:633:GLN:NE2	2.41	0.41
1:B:196:PRO:HD2	1:B:204:TRP:O	2.20	0.41
1:D:692:ILE:HG13	1:D:724:LEU:HG	2.02	0.41
1:D:336:TRP:O	1:D:340:TYR:HD1	2.04	0.41
1:D:18:LYS:HA	1:D:18:LYS:HD2	1.82	0.41
1:A:504:MET:HE3	1:A:507:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:701:ASP:OD1	1:B:701:ASP:N	2.53	0.41
1:B:456:CYS:O	1:B:460:ILE:HG12	2.21	0.41
1:B:681:LEU:HD13	1:B:684:LEU:HD12	2.02	0.41
1:A:495:ARG:O	1:A:497:ARG:N	2.54	0.41
1:A:484:THR:HG23	1:D:82:THR:H	1.86	0.41
1:A:395:ASP:OD1	1:A:396:GLY:N	2.53	0.41
1:A:275:ILE:HD11	1:A:293:PRO:HD2	2.02	0.41
1:B:515:THR:HG22	1:B:523:PHE:CD2	2.56	0.41
1:A:197:GLY:O	1:A:227:GLN:HA	2.20	0.41
1:D:113:LYS:HA	1:D:114:PRO:HD3	1.89	0.41
1:A:480:ASN:HB3	2:A:802:GLA:O4	2.21	0.41
1:C:678:TYR:CE2	1:D:186:PRO:HB2	2.55	0.41
1:B:551:ASP:O	1:B:555:ARG:HB2	2.20	0.41
1:C:467:LEU:HD11	1:C:475:VAL:HG21	2.03	0.41
1:B:669:LEU:HD21	1:D:669:LEU:HD21	2.01	0.41
1:C:329:ARG:HA	1:C:330:PRO:HD3	1.80	0.41
1:D:324:PHE:HA	1:D:327:ARG:HB2	2.03	0.41
1:C:495:ARG:O	1:C:497:ARG:N	2.54	0.41
1:C:336:TRP:HB3	1:C:604:GLU:OE2	2.21	0.41
1:D:573:ALA:HB1	1:D:596:ALA:HA	2.03	0.41
1:B:82:THR:H	1:C:484:THR:HG23	1.86	0.41
1:B:196:PRO:HB3	1:B:228:GLN:HE22	1.86	0.41
1:C:285:GLN:O	1:C:288:GLU:HG2	2.21	0.41
1:A:94:GLU:OE2	1:A:171:GLU:HG2	2.21	0.41
1:C:572:GLY:HA2	1:C:600:ASN:HB3	2.03	0.41
1:A:258:LEU:O	1:A:273:MET:HA	2.21	0.41
1:D:526:CYS:SG	1:D:527:SER:N	2.94	0.41
1:B:678:TYR:HA	1:B:709:ALA:HA	2.03	0.41
1:C:708:VAL:HA	1:D:46:ALA:O	2.21	0.41
1:B:78:ALA:HB2	1:B:89:TYR:CE2	2.56	0.41
1:C:607:ILE:O	1:C:610:LEU:HG	2.21	0.41
1:B:227:GLN:HG3	1:C:265:GLN:HB3	2.02	0.41
1:D:630:ARG:HD3	1:D:630:ARG:HA	1.63	0.41
1:A:328:GLU:OE1	1:A:630:ARG:HG2	2.21	0.41
1:A:70:ASP:HB2	1:A:82:THR:O	2.20	0.40
1:C:221:ARG:HD3	1:C:482:HIS:ND1	2.36	0.40
1:D:449:ASP:OD1	1:D:451:SER:OG	2.23	0.40
1:A:202:GLU:OE2	1:A:226:HIS:HD2	2.03	0.40
1:B:27:ARG:HB3	1:B:28:SER:H	1.59	0.40
1:A:443:ARG:H	1:D:65:ARG:NH1	2.20	0.40
1:B:53:ASP:OD2	2:C:804:FRU:O4	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:THR:HG21	1:B:717:PHE:O	2.21	0.40
1:B:647:ASN:OD1	1:B:668:VAL:HG13	2.20	0.40
1:B:161:ARG:NH2	1:B:182:SER:H	2.19	0.40
1:B:626:LYS:HB3	1:B:629:ARG:NH2	2.36	0.40
1:A:460:ILE:HG13	1:A:461:GLU:N	2.35	0.40
1:D:57:SER:HA	1:D:58:PRO:HD3	1.94	0.40
1:D:515:THR:HG22	1:D:523:PHE:CD2	2.57	0.40
1:D:681:LEU:CD1	1:D:703:LEU:HB2	2.50	0.40
1:B:612:GLU:OE2	1:B:615:LYS:NZ	2.54	0.40
1:D:172:ARG:HH11	1:D:172:ARG:HG2	1.86	0.40
1:C:547:SER:O	1:C:555:ARG:NH2	2.54	0.40
1:A:38:LYS:HG2	1:B:705:TYR:CE2	2.57	0.40
1:A:600:ASN:HA	1:A:625:TYR:OH	2.21	0.40
1:B:713:ARG:HB2	1:B:718:ILE:HD13	2.03	0.40
1:A:418:SER:O	1:A:421:SER:OG	2.33	0.40
1:B:351:ILE:O	1:B:355:GLU:HG3	2.21	0.40
1:A:47:ARG:HH21	1:B:678:TYR:HE1	1.69	0.40
1:D:658:ARG:HB3	1:D:685:ASP:HB2	2.04	0.40
1:B:344:ASN:HA	1:B:389:LYS:HB2	2.03	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	716/729 (98%)	683 (95%)	32 (4%)	1 (0%)	56	90
1	B	716/729 (98%)	685 (96%)	30 (4%)	1 (0%)	56	90
1	C	716/729 (98%)	683 (95%)	32 (4%)	1 (0%)	56	90
1	D	716/729 (98%)	682 (95%)	32 (4%)	2 (0%)	46	83
All	All	2864/2916 (98%)	2733 (95%)	126 (4%)	5 (0%)	52	87

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	496	GLN
1	B	496	GLN
1	C	496	GLN
1	D	496	GLN
1	D	526	CYS

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	608/618 (98%)	545 (90%)	63 (10%)	9	42
1	B	608/618 (98%)	555 (91%)	53 (9%)	13	51
1	C	608/618 (98%)	567 (93%)	41 (7%)	20	62
1	D	608/618 (98%)	570 (94%)	38 (6%)	22	64
All	All	2432/2472 (98%)	2237 (92%)	195 (8%)	15	54

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	15	ARG
1	A	38	LYS
1	A	43	VAL
1	A	51	ARG
1	A	72	LEU
1	A	90	GLN
1	A	94	GLU
1	A	108	ARG
1	A	115	ARG
1	A	124	VAL
1	A	136	VAL
1	A	149	GLN
1	A	154	GLU
1	A	155	LYS

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Mol	Chain	Res	Type
1	A	215	GLN
1	A	224	SER
1	A	232	ILE
1	A	268	THR
1	A	296	VAL
1	A	301	ASP
1	A	302	GLN
1	A	311	TYR
1	A	325	ARG
1	A	349	VAL
1	A	357	GLU
1	A	365	LEU
1	A	375	ASP
1	A	377	ARG
1	A	382	ASP
1	A	389	LYS
1	A	394	LEU
1	A	404	LEU
1	A	410	LEU
1	A	412	VAL
1	A	420	ASN
1	A	423	LEU
1	A	440	SER
1	A	448	LEU
1	A	455	VAL
1	A	463	ILE
1	A	473	THR
1	A	497	ARG
1	A	514	ILE
1	A	522	LEU
1	A	527	SER
1	A	533	PHE
1	A	550	THR
1	A	555	ARG
1	A	575	VAL
1	A	589	LEU
1	A	590	LYS
1	A	598	SER
1	A	607	ILE
1	A	618	MET
1	A	652	MET
1	A	676	LEU

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Mol	Chain	Res	Type
1	A	681	LEU
1	A	682	LYS
1	A	692	ILE
1	A	703	LEU
1	A	710	LEU
1	A	725	LYS
1	B	10	LYS
1	B	40	VAL
1	B	90	GLN
1	B	91	VAL
1	B	126	HIS
1	B	129	GLU
1	B	132	THR
1	B	142	ILE
1	B	155	LYS
1	B	215	GLN
1	B	232	ILE
1	B	263	VAL
1	B	310	THR
1	B	311	TYR
1	B	321	ARG
1	B	325	ARG
1	B	348	ILE
1	B	351	ILE
1	B	354	THR
1	B	364	VAL
1	B	373	ARG
1	B	382	ASP
1	B	394	LEU
1	B	410	LEU
1	B	412	VAL
1	B	440	SER
1	B	448	LEU
1	B	465	ASN
1	B	473	THR
1	B	497	ARG
1	B	522	LEU
1	B	532	ARG
1	B	533	PHE
1	B	544	THR
1	B	550	THR
1	B	555	ARG

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Mol	Chain	Res	Type
1	B	562	THR
1	B	569	SER
1	B	589	LEU
1	B	592	ARG
1	B	595	VAL
1	B	610	LEU
1	B	612	GLU
1	B	615	LYS
1	B	618	MET
1	B	627	ASP
1	B	667	ARG
1	B	668	VAL
1	B	678	TYR
1	B	681	LEU
1	B	682	LYS
1	B	710	LEU
1	B	721	MET
1	C	15	ARG
1	C	28	SER
1	C	34	VAL
1	C	51	ARG
1	C	105	LYS
1	C	108	ARG
1	C	109	ILE
1	C	127	GLU
1	C	136	VAL
1	C	232	ILE
1	C	241	GLU
1	C	261	ILE
1	C	283	LEU
1	C	291	GLN
1	C	292	THR
1	C	296	VAL
1	C	310	THR
1	C	311	TYR
1	C	325	ARG
1	C	332	LEU
1	C	351	ILE
1	C	378	ARG
1	C	382	ASP
1	C	394	LEU
1	C	399	LYS

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Mol	Chain	Res	Type
1	C	416	MET
1	C	420	ASN
1	C	421	SER
1	C	429	ASP
1	C	483	MET
1	C	497	ARG
1	C	509	ARG
1	C	533	PHE
1	C	550	THR
1	C	590	LYS
1	C	610	LEU
1	C	612	GLU
1	C	617	MET
1	C	630	ARG
1	C	632	VAL
1	C	686	SER
1	D	40	VAL
1	D	65	ARG
1	D	132	THR
1	D	142	ILE
1	D	214	VAL
1	D	224	SER
1	D	261	ILE
1	D	268	THR
1	D	283	LEU
1	D	311	TYR
1	D	321	ARG
1	D	332	LEU
1	D	348	ILE
1	D	364	VAL
1	D	365	LEU
1	D	373	ARG
1	D	377	ARG
1	D	416	MET
1	D	423	LEU
1	D	459	ILE
1	D	473	THR
1	D	483	MET
1	D	497	ARG
1	D	532	ARG
1	D	533	PHE
1	D	550	THR

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Mol	Chain	Res	Type
1	D	583	VAL
1	D	607	ILE
1	D	615	LYS
1	D	617	MET
1	D	627	ASP
1	D	630	ARG
1	D	668	VAL
1	D	681	LEU
1	D	687	ASN
1	D	704	MET
1	D	710	LEU
1	D	721	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	291	GLN
1	A	302	GLN
1	C	291	GLN
1	C	445	GLN
1	C	621	GLN
1	D	580	ASN

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](#)

16 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	GLA	A	801	2	11,11,12	2.68	2 (18%)	14,15,17	0.95	0
2	GLA	A	802	2	11,11,12	2.62	2 (18%)	14,15,17	1.62	2 (14%)
2	GLC	A	803	2	11,11,12	2.46	2 (18%)	14,15,17	1.38	1 (7%)
2	FRU	A	804	2	11,12,12	1.62	4 (36%)	10,18,18	1.76	2 (20%)
2	GLA	B	801	2	11,11,12	2.74	2 (18%)	14,15,17	1.21	1 (7%)
2	GLA	B	802	2	11,11,12	2.57	3 (27%)	14,15,17	2.40	7 (50%)
2	GLC	B	803	2	11,11,12	2.66	4 (36%)	14,15,17	1.60	3 (21%)
2	FRU	B	804	2	11,12,12	1.62	4 (36%)	10,18,18	2.07	4 (40%)
2	GLA	C	801	2	11,11,12	2.73	2 (18%)	14,15,17	1.31	1 (7%)
2	GLA	C	802	2	11,11,12	2.58	2 (18%)	14,15,17	2.17	5 (35%)
2	GLC	C	803	2	11,11,12	2.39	2 (18%)	14,15,17	2.20	6 (42%)
2	FRU	C	804	2	11,12,12	1.59	2 (18%)	10,18,18	2.00	4 (40%)
2	GLA	D	801	2	11,11,12	2.66	2 (18%)	14,15,17	1.36	1 (7%)
2	GLA	D	802	2	11,11,12	2.47	3 (27%)	14,15,17	2.24	6 (42%)
2	GLC	D	803	2	11,11,12	2.50	2 (18%)	14,15,17	1.72	4 (28%)
2	FRU	D	804	2	11,12,12	1.62	2 (18%)	10,18,18	2.14	4 (40%)

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	GLA	A	801	2	-	0/2/19/22	0/1/1/1
2	GLA	A	802	2	-	0/2/19/22	0/1/1/1
2	GLC	A	803	2	-	0/2/19/22	0/1/1/1
2	FRU	A	804	2	-	0/5/24/24	0/1/1/1
2	GLA	B	801	2	-	0/2/19/22	0/1/1/1
2	GLA	B	802	2	-	0/2/19/22	0/1/1/1
2	GLC	B	803	2	-	0/2/19/22	0/1/1/1
2	FRU	B	804	2	-	0/5/24/24	0/1/1/1
2	GLA	C	801	2	-	0/2/19/22	0/1/1/1
2	GLA	C	802	2	-	0/2/19/22	0/1/1/1
2	GLC	C	803	2	-	0/2/19/22	0/1/1/1
2	FRU	C	804	2	-	0/5/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLA	D	801	2	-	0/2/19/22	0/1/1/1
2	GLA	D	802	2	-	0/2/19/22	0/1/1/1
2	GLC	D	803	2	-	0/2/19/22	0/1/1/1
2	FRU	D	804	2	-	0/5/24/24	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	GLA	C2-C3	-7.94	1.41	1.52
2	B	801	GLA	C2-C3	-7.90	1.41	1.52
2	A	801	GLA	C2-C3	-7.81	1.41	1.52
2	A	802	GLA	C2-C3	-7.67	1.42	1.52
2	D	801	GLA	C2-C3	-7.57	1.42	1.52
2	B	802	GLA	C2-C3	-7.46	1.42	1.52
2	C	802	GLA	C2-C3	-7.40	1.42	1.52
2	B	803	GLC	C2-C3	-7.01	1.42	1.52
2	D	802	GLA	C2-C3	-6.95	1.43	1.52
2	D	803	GLC	C2-C3	-6.87	1.43	1.52
2	A	803	GLC	C2-C3	-6.79	1.43	1.52
2	C	803	GLC	C2-C3	-6.25	1.43	1.52
2	C	804	FRU	C4-C5	-2.81	1.45	1.53
2	D	804	FRU	C4-C5	-2.70	1.45	1.53
2	B	804	FRU	C4-C5	-2.66	1.45	1.53
2	A	804	FRU	C4-C5	-2.55	1.46	1.53
2	A	804	FRU	O5-C2	-2.49	1.39	1.43
2	D	804	FRU	O3-C3	-2.47	1.37	1.42
2	C	804	FRU	O3-C3	-2.32	1.37	1.42
2	B	804	FRU	O3-C3	-2.32	1.37	1.42
2	A	804	FRU	O3-C3	-2.29	1.38	1.42
2	D	802	GLA	C4-C3	-2.13	1.46	1.52
2	B	803	GLC	C4-C3	-2.12	1.46	1.52
2	B	802	GLA	C4-C3	-2.10	1.46	1.52
2	B	803	GLC	O2-C2	-2.07	1.38	1.43
2	B	804	FRU	O5-C2	-2.04	1.40	1.43
2	A	804	FRU	O2-C2	2.05	1.44	1.41
2	B	804	FRU	O2-C2	2.08	1.44	1.41
2	A	802	GLA	O5-C1	2.13	1.47	1.43
2	B	802	GLA	O5-C1	2.28	1.47	1.43
2	C	802	GLA	O5-C1	2.32	1.47	1.43
2	D	802	GLA	O5-C1	2.45	1.47	1.43
2	A	803	GLC	O5-C1	3.11	1.48	1.43
2	A	801	GLA	O5-C1	3.14	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	GLA	O5-C1	3.15	1.49	1.43
2	D	803	GLC	O5-C1	3.25	1.49	1.43
2	C	801	GLA	O5-C1	3.33	1.49	1.43
2	D	801	GLA	O5-C1	3.36	1.49	1.43
2	C	803	GLC	O5-C1	3.61	1.49	1.43
2	B	803	GLC	O5-C1	3.93	1.50	1.43

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	803	GLC	O5-C1-C2	-2.79	106.34	110.86
2	D	804	FRU	C6-C5-C4	-2.75	108.58	115.08
2	D	802	GLA	O3-C3-C4	-2.74	104.17	110.34
2	B	802	GLA	O2-C2-C3	-2.56	104.97	110.12
2	D	803	GLC	O4-C4-C3	-2.54	104.61	110.34
2	C	804	FRU	C6-C5-C4	-2.44	109.31	115.08
2	B	803	GLC	O2-C2-C3	-2.33	105.44	110.12
2	B	802	GLA	O3-C3-C4	-2.27	105.22	110.34
2	B	804	FRU	C6-C5-C4	-2.27	109.71	115.08
2	B	803	GLC	O4-C4-C3	-2.23	105.31	110.34
2	C	803	GLC	O2-C2-C3	-2.19	105.71	110.12
2	C	803	GLC	O4-C4-C3	-2.12	105.56	110.34
2	D	803	GLC	C2-C3-C4	2.02	114.48	111.04
2	D	802	GLA	C2-C3-C4	2.08	114.57	111.04
2	D	802	GLA	O6-C6-C5	2.08	118.21	111.33
2	B	802	GLA	C1-O5-C5	2.17	115.00	112.25
2	C	802	GLA	O6-C6-C5	2.17	118.50	111.33
2	B	801	GLA	C1-C2-C3	2.19	112.14	109.54
2	B	804	FRU	O6-C6-C5	2.19	118.58	111.33
2	C	803	GLC	O6-C6-C5	2.22	118.67	111.33
2	D	804	FRU	O6-C6-C5	2.27	118.83	111.33
2	A	804	FRU	O5-C5-C6	2.27	115.45	108.57
2	B	804	FRU	O5-C5-C6	2.33	115.63	108.57
2	D	804	FRU	O5-C5-C6	2.38	115.77	108.57
2	C	804	FRU	O6-C6-C5	2.49	119.56	111.33
2	C	803	GLC	C3-C4-C5	2.60	114.72	110.20
2	C	804	FRU	O5-C5-C6	2.60	116.43	108.57
2	C	802	GLA	C2-C3-C4	2.64	115.52	111.04
2	C	802	GLA	C3-C4-C5	2.68	114.87	110.20
2	A	802	GLA	O5-C5-C6	2.73	113.26	107.35
2	C	801	GLA	C1-C2-C3	3.02	113.11	109.54
2	B	802	GLA	C3-C4-C5	3.10	115.60	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	803	GLC	C1-C2-C3	3.11	113.22	109.54
2	B	802	GLA	O5-C5-C6	3.12	114.11	107.35
2	C	803	GLC	C2-C3-C4	3.20	116.47	111.04
2	D	801	GLA	C1-C2-C3	3.20	113.33	109.54
2	D	802	GLA	O5-C5-C6	3.22	114.33	107.35
2	B	802	GLA	C2-C3-C4	3.28	116.62	111.04
2	D	803	GLC	C3-C4-C5	3.36	116.06	110.20
2	C	802	GLA	O5-C5-C6	3.53	114.99	107.35
2	B	803	GLC	C1-C2-C3	3.80	114.04	109.54
2	A	802	GLA	C3-C4-C5	3.82	116.85	110.20
2	D	802	GLA	C1-C2-C3	3.97	114.24	109.54
2	A	804	FRU	O1-C1-C2	4.02	119.20	111.39
2	D	802	GLA	C1-O5-C5	4.14	117.50	112.25
2	C	804	FRU	O1-C1-C2	4.20	119.56	111.39
2	B	804	FRU	O1-C1-C2	4.57	120.28	111.39
2	C	802	GLA	C1-C2-C3	4.59	114.97	109.54
2	D	804	FRU	O1-C1-C2	4.65	120.43	111.39
2	B	802	GLA	C1-C2-C3	5.16	115.65	109.54
2	C	803	GLC	C1-C2-C3	5.48	116.02	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	GLA	2	0
2	A	802	GLA	2	0
2	C	802	GLA	1	0
2	C	804	FRU	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	718/729 (98%)	-0.32	2 (0%) 94 90	61, 101, 145, 173	0
1	B	718/729 (98%)	-0.47	0 100 100	56, 90, 127, 144	0
1	C	718/729 (98%)	-0.27	4 (0%) 90 83	71, 113, 139, 163	0
1	D	718/729 (98%)	-0.42	1 (0%) 95 94	62, 93, 126, 151	0
All	All	2872/2916 (98%)	-0.37	7 (0%) 95 92	56, 100, 136, 173	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	516	SER	2.9
1	C	323	ALA	2.7
1	A	376	ASP	2.7
1	A	374	ASP	2.2
1	C	405	GLY	2.2
1	D	374	ASP	2.1
1	C	49	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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	FRU	D	804	12/12	0.87	0.31	5.85	102,121,135,143	0
2	FRU	C	804	12/12	0.68	0.52	5.04	99,131,142,146	0
2	GLA	C	802	11/12	0.88	0.27	1.84	99,110,115,119	0
2	GLA	B	802	11/12	0.86	0.28	1.58	104,109,124,127	0
2	GLA	B	801	11/12	0.89	0.23	0.70	95,103,109,110	0
2	GLA	C	801	11/12	0.84	0.25	0.52	114,119,123,125	0
2	GLA	D	802	11/12	0.91	0.18	0.46	94,102,110,110	0
2	GLA	A	801	11/12	0.86	0.26	0.42	105,123,130,131	0
2	GLA	A	802	11/12	0.80	0.29	0.27	106,116,119,121	0
2	GLA	D	801	11/12	0.93	0.19	-0.01	87,98,102,103	0
2	FRU	B	804	12/12	0.81	0.39	-	104,131,137,140	0
2	GLC	B	803	11/12	0.86	0.38	-	122,129,136,138	0
2	FRU	A	804	12/12	0.69	0.51	-	117,138,149,157	0
2	GLC	A	803	11/12	0.80	0.47	-	125,141,146,151	0
2	GLC	C	803	11/12	0.72	0.63	-	124,139,148,150	0
2	GLC	D	803	11/12	0.73	0.33	-	109,129,137,138	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.