Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:03 AM GMT

PDB ID	:	3NWD
Title	:	Glycoprotein B from Herpes simplex virus type 1, Y179S mutant, low-pH
Authors	:	Stampfer, S.D.; Lou, H.; Cohen, G.H.; Eisenberg, R.J.; Heldwein, E.E.
Deposited on	:	2010-07-09
Resolution	:	2.88 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

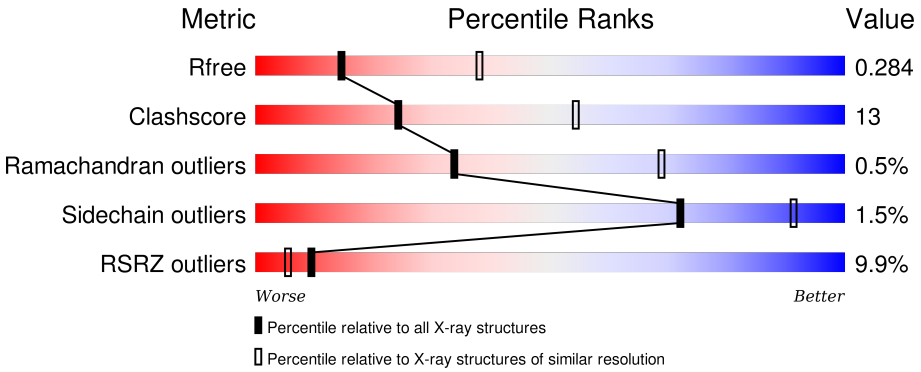
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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 <=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	703	7% 61% 25% • 14%
1	B	703	10% 60% 24% • 15%
1	C	703	10% 55% 30% 15%
1	D	703	8% 65% 21% 14%

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	NAG	B	1141	X	-	-	-
4	CL	D	1	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19481 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 Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	597	Total	C	N	O	S	0	1	0
			4767	3000	835	910	22			
1	A	606	Total	C	N	O	S	0	1	0
			4843	3056	843	922	22			
1	C	601	Total	C	N	O	S	0	0	0
			4766	3003	831	910	22			
1	D	606	Total	C	N	O	S	0	1	0
			4829	3044	846	918	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	28	ASP	-	EXPRESSION TAG	UNP P06437
B	29	PRO	-	EXPRESSION TAG	UNP P06437
B	58	ALA	PRO	SEE REMARK 999	UNP P06437
B	179	SER	TYR	ENGINEERED MUTATION	UNP P06437
B	313	SER	THR	SEE REMARK 999	UNP P06437
B	443	LEU	GLN	SEE REMARK 999	UNP P06437
A	28	ASP	-	EXPRESSION TAG	UNP P06437
A	29	PRO	-	EXPRESSION TAG	UNP P06437
A	58	ALA	PRO	SEE REMARK 999	UNP P06437
A	179	SER	TYR	ENGINEERED MUTATION	UNP P06437
A	313	SER	THR	SEE REMARK 999	UNP P06437
A	443	LEU	GLN	SEE REMARK 999	UNP P06437
C	28	ASP	-	EXPRESSION TAG	UNP P06437
C	29	PRO	-	EXPRESSION TAG	UNP P06437
C	58	ALA	PRO	SEE REMARK 999	UNP P06437
C	179	SER	TYR	ENGINEERED MUTATION	UNP P06437
C	313	SER	THR	SEE REMARK 999	UNP P06437
C	443	LEU	GLN	SEE REMARK 999	UNP P06437
D	28	ASP	-	EXPRESSION TAG	UNP P06437
D	29	PRO	-	EXPRESSION TAG	UNP P06437
D	58	ALA	PRO	SEE REMARK 999	UNP P06437

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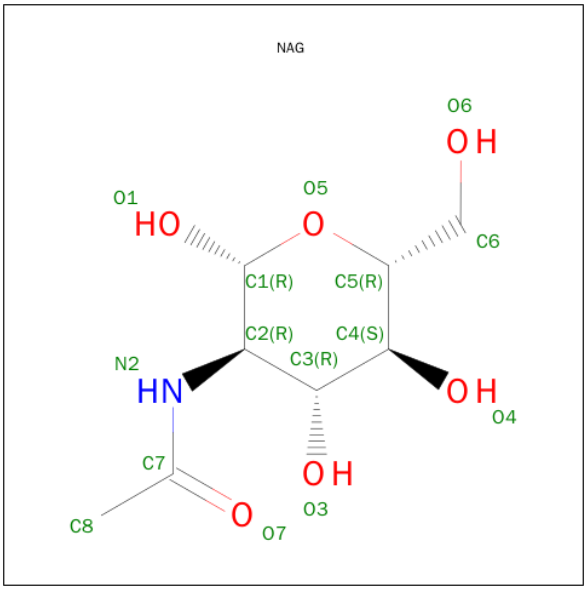
Chain	Residue	Modelled	Actual	Comment	Reference
D	179	SER	TYR	ENGINEERED MUTATION	UNP P06437
D	313	SER	THR	SEE REMARK 999	UNP P06437
D	443	LEU	GLN	SEE REMARK 999	UNP P06437

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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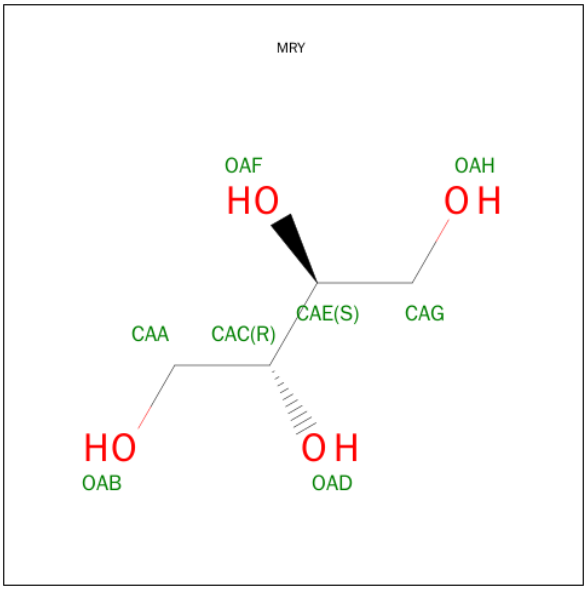
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is MESO-ERYTHRITOL (three-letter code: MRY) (formula: $C_4H_{10}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 8 4 4	0	0

- Molecule 6 is water.

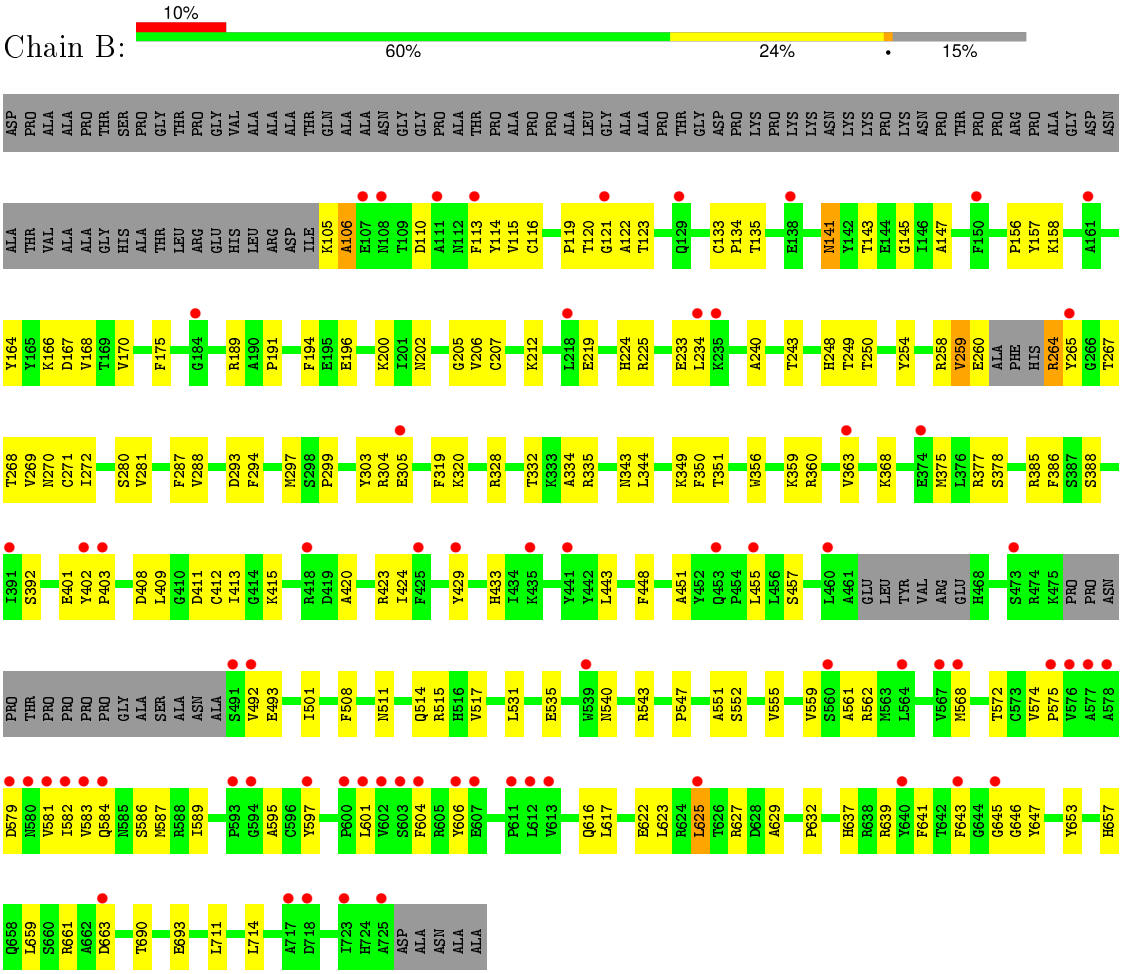
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	16	Total O 16 16	0	0
6	A	25	Total O 25 25	0	0
6	C	18	Total O 18 18	0	0
6	D	25	Total O 25 25	0	0

3 Residue-property plots (i)

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.

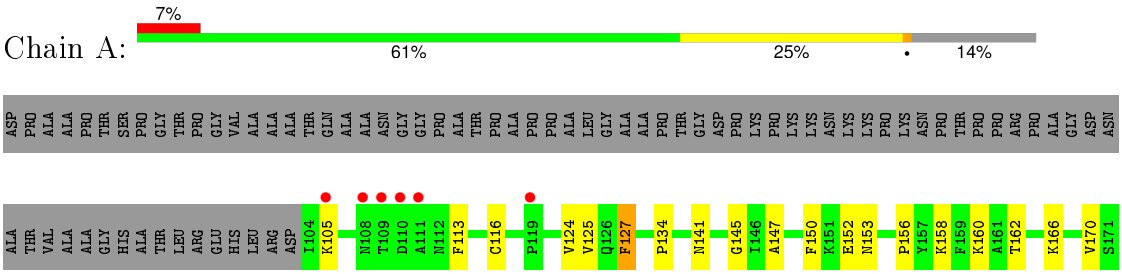
- Molecule 1: Envelope glycoprotein B

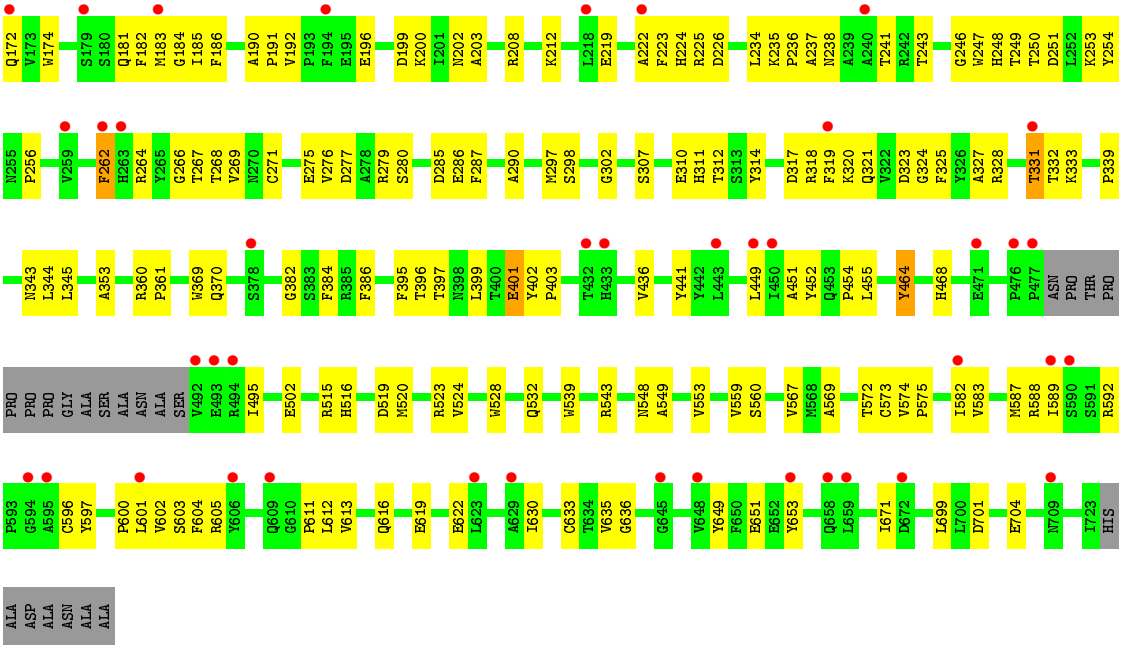
Chain B:



- Molecule 1: Envelope glycoprotein B

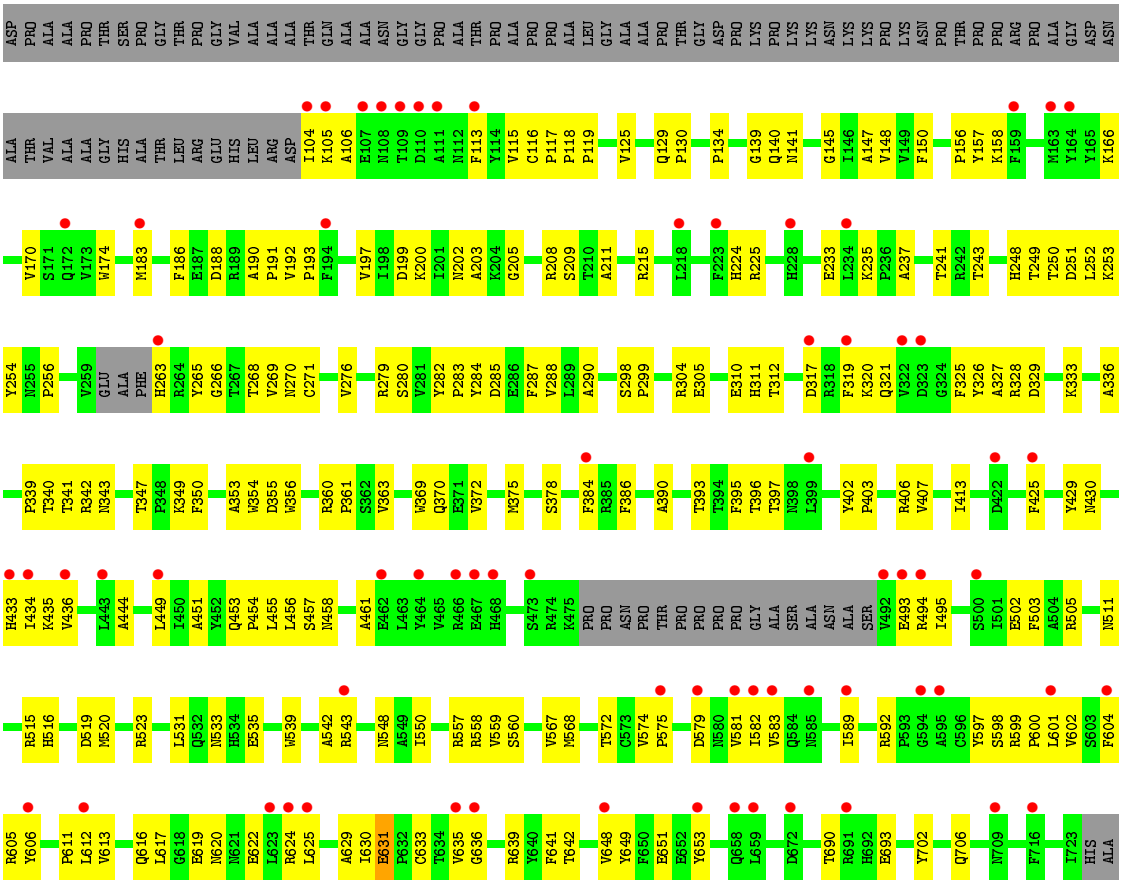
Chain A:





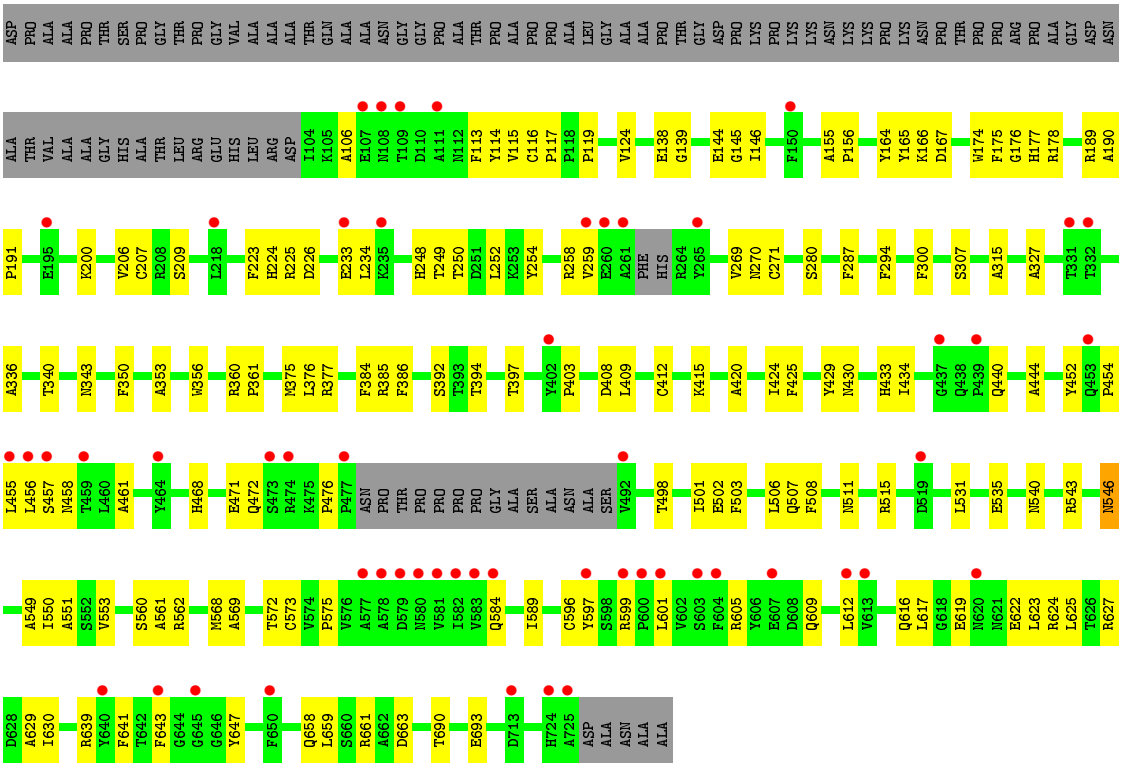
• Molecule 1: Envelope glycoprotein B

Chain C:



- Molecule 1: Envelope glycoprotein B

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	117.76Å 117.76Å 318.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.56 – 2.88 48.56 – 2.88	Depositor EDS
% Data completeness (in resolution range)	88.0 (48.56-2.88) 88.0 (48.56-2.88)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.238 , 0.283 0.235 , 0.284	Depositor DCC
R_{free} test set	4692 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	64.3	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 61.4	EDS
Estimated twinning fraction	0.020 for -h,-k,l 0.468 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 111383 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	19481	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.43 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.8395e-06.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, MRY, NAG

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	0.21	0/4966	0.39	0/6757
1	B	0.22	0/4879	0.38	0/6631
1	C	0.22	0/4880	0.38	0/6639
1	D	0.22	0/4948	0.38	0/6731
All	All	0.22	0/19673	0.38	0/26758

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1141	NAG	C1

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	4843	0	4604	113	0
1	B	4767	0	4540	123	0
1	C	4766	0	4514	144	0
1	D	4829	0	4602	111	0
2	B	28	0	25	2	0
2	D	28	0	25	3	0
3	A	42	0	39	0	0
3	B	28	0	26	0	0
3	C	42	0	39	0	0
3	D	14	0	13	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	C	8	0	10	1	0
6	A	25	0	0	0	0
6	B	16	0	0	0	0
6	C	18	0	0	1	0
6	D	25	0	0	0	0
All	All	19481	0	18437	491	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 13.

All (491) 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:183:MET:H	1:A:184:GLY:HA3	1.20	1.05
1:A:183:MET:N	1:A:184:GLY:HA3	1.88	0.88
1:B:259:VAL:HG22	1:B:260:GLU:H	1.45	0.82
1:C:256:PRO:HD3	1:C:266:GLY:HA2	1.64	0.79
1:D:403:PRO:HG3	1:D:476:PRO:HB3	1.65	0.79
1:C:393:THR:HG22	1:C:505:ARG:HG2	1.66	0.77
1:A:150:PHE:HB2	1:A:449:LEU:HB3	1.68	0.75
1:C:599:ARG:HH12	1:C:617:LEU:HG	1.53	0.73
1:A:436:VAL:HB	1:A:454:PRO:HB2	1.70	0.71
1:B:166:LYS:HG2	1:B:271:CYS:HA	1.72	0.71
1:C:174:TRP:HB2	1:C:183:MET:SD	2.30	0.70
1:C:397:THR:HG22	1:C:444:ALA:HA	1.73	0.69
1:C:116:CYS:HB3	1:C:560:SER:HB2	1.74	0.69
1:D:375:MET:SD	1:D:386:PHE:HB3	2.33	0.68
1:A:298:SER:HB3	1:A:310:GLU:HB3	1.76	0.67
1:B:385:ARG:HH22	1:B:515:ARG:NH2	1.93	0.67
1:C:156:PRO:HG2	1:C:279:ARG:NH2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:LEU:HD21	1:D:461:ALA:HA	1.75	0.67
1:D:224:HIS:HB2	1:D:269:VAL:HB	1.77	0.66
1:A:156:PRO:HG2	1:A:279:ARG:NH2	2.11	0.66
1:A:174:TRP:HB2	1:A:183:MET:SD	2.36	0.66
1:D:546:ASN:HB3	1:D:549:ALA:HB3	1.78	0.66
1:C:202:ASN:O	1:C:328:ARG:HB3	1.95	0.65
1:D:584:GLN:HG3	1:D:601:LEU:HB2	1.79	0.65
1:C:158:LYS:HD3	1:C:279:ARG:NH1	2.12	0.65
1:D:166:LYS:HG2	1:D:271:CYS:HA	1.77	0.65
1:C:606:TYR:CD2	1:C:613:VAL:HG21	2.31	0.64
1:C:436:VAL:HB	1:C:454:PRO:HB2	1.79	0.64
1:D:166:LYS:HE3	1:D:207:CYS:SG	2.37	0.64
1:C:156:PRO:HG2	1:C:279:ARG:HH21	1.62	0.64
1:D:119:PRO:HG2	1:D:562:ARG:HG2	1.80	0.64
1:D:206:VAL:HG12	1:D:233:GLU:HG2	1.79	0.64
1:D:280:SER:HB2	1:D:287:PHE:HB3	1.80	0.63
1:A:105:LYS:HG2	1:A:582:ILE:HG22	1.81	0.63
1:C:166:LYS:HG2	1:C:271:CYS:HA	1.80	0.63
1:A:202:ASN:O	1:A:328:ARG:HB3	1.98	0.63
1:B:156:PRO:HB3	1:B:281:VAL:HG12	1.81	0.62
1:D:550:ILE:O	1:D:553:VAL:HG12	1.99	0.62
1:C:145:GLY:HA2	1:C:455:LEU:HG	1.81	0.62
1:C:583:VAL:HA	1:C:602:VAL:HG12	1.80	0.62
1:A:116:CYS:HB3	1:A:560:SER:HB2	1.82	0.61
1:B:224:HIS:HB2	1:B:269:VAL:HB	1.81	0.61
1:A:235:LYS:HG2	1:A:248:HIS:O	2.00	0.61
1:A:464:TYR:O	1:A:468:HIS:HB2	2.00	0.61
1:D:223:PHE:HB2	1:D:226:ASP:HA	1.83	0.60
1:D:119:PRO:HG3	1:D:561:ALA:HA	1.82	0.60
1:A:325:PHE:HE2	1:A:327:ALA:HB2	1.66	0.60
1:B:189:ARG:HB2	1:B:349:LYS:HE2	1.83	0.60
1:C:386:PHE:HB2	1:C:395:PHE:HB2	1.83	0.60
1:C:601:LEU:HD23	1:C:616:GLN:HB3	1.83	0.60
1:B:105:LYS:N	1:B:582:ILE:HG13	2.16	0.60
1:A:237:ALA:HA	1:A:248:HIS:CD2	2.37	0.60
1:D:377:ARG:HD3	1:D:386:PHE:CZ	2.38	0.59
1:D:616:GLN:HG3	1:D:624:ARG:HB2	1.83	0.59
1:A:235:LYS:HE3	1:A:248:HIS:CE1	2.37	0.59
1:C:649:TYR:CE2	1:C:651:GLU:HB2	2.37	0.59
1:D:360:ARG:HG2	1:D:409:LEU:HD23	1.84	0.58
1:B:343:ASN:HD21	1:B:356:TRP:HD1	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:LYS:HE3	1:C:248:HIS:CE1	2.38	0.58
1:D:252:LEU:H	1:D:252:LEU:HD23	1.68	0.58
1:D:115:VAL:O	1:D:117:PRO:HD3	2.02	0.58
1:B:280:SER:HB2	1:B:287:PHE:HB3	1.84	0.58
1:A:324:GLY:HA2	1:A:339:PRO:HB2	1.85	0.58
1:B:175:PHE:CD2	1:B:259:VAL:HG12	2.38	0.58
1:C:166:LYS:HD2	1:C:211:ALA:HB2	1.86	0.58
1:A:589:ILE:HG22	1:A:592:ARG:H	1.69	0.58
1:B:531:LEU:O	1:B:535:GLU:HG2	2.04	0.58
1:D:377:ARG:HB2	1:D:386:PHE:CE2	2.39	0.58
1:A:253:LYS:HA	1:A:268:THR:HG21	1.86	0.58
1:C:511:ASN:O	1:C:515:ARG:HG2	2.04	0.57
1:A:314:TYR:HB3	1:A:318:ARG:HD2	1.84	0.57
1:B:690:THR:OG1	1:B:693:GLU:HG3	2.04	0.57
1:A:600:PRO:O	1:A:616:GLN:HG3	2.04	0.57
1:B:170:VAL:HG22	1:B:267:THR:HG22	1.86	0.57
1:B:119:PRO:HG2	1:B:562:ARG:HG2	1.87	0.57
1:A:603:SER:HB3	1:A:612:LEU:HG	1.87	0.57
1:D:429:TYR:CE2	1:D:455:LEU:HD13	2.39	0.57
1:B:240:ALA:HB1	1:B:243:THR:OG1	2.05	0.57
1:B:375:MET:HE1	1:B:388:SER:HB2	1.86	0.56
1:D:248:HIS:HA	1:D:271:CYS:O	2.05	0.56
1:A:401:GLU:HG2	1:A:441:TYR:O	2.06	0.56
1:A:582:ILE:HD11	1:A:603:SER:HB2	1.87	0.56
1:A:588:ARG:HG2	1:A:596:CYS:SG	2.46	0.56
1:C:118:PRO:HD3	1:C:625:LEU:CD2	2.35	0.56
1:A:331:THR:HG22	1:A:332:THR:HG23	1.87	0.56
1:B:141:ASN:HD22	1:B:141:ASN:N	2.02	0.56
1:D:343:ASN:HD21	1:D:356:TRP:HD1	1.54	0.56
1:C:113:PHE:O	1:C:575:PRO:HA	2.04	0.56
1:A:325:PHE:CE2	1:A:327:ALA:HB2	2.41	0.56
1:A:147:ALA:HA	1:A:451:ALA:O	2.06	0.56
1:C:250:THR:HG22	1:C:252:LEU:H	1.72	0.55
1:A:539:TRP:O	1:A:543:ARG:HG3	2.06	0.55
1:B:540:ASN:O	1:B:543:ARG:HG2	2.07	0.55
1:B:625:LEU:H	1:B:625:LEU:HD22	1.72	0.55
1:B:205:GLY:O	1:B:233:GLU:HG3	2.06	0.55
1:C:241:THR:O	1:C:243:THR:HG23	2.07	0.55
1:B:595:ALA:HA	1:B:632:PRO:HA	1.89	0.55
1:A:649:TYR:CE2	1:A:651:GLU:HB2	2.41	0.55
1:A:597:TYR:HA	1:A:630:ILE:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:HIS:O	1:C:520:MET:HG2	2.07	0.54
1:B:167:ASP:OD2	1:B:189:ARG:HG2	2.07	0.54
1:B:234:LEU:HD23	1:B:249:THR:HG23	1.89	0.54
1:D:498:THR:HG21	1:D:503:PHE:HE2	1.73	0.54
1:A:223:PHE:HB2	1:A:226:ASP:HA	1.89	0.54
1:C:200:LYS:HE3	1:C:208:ARG:CZ	2.37	0.54
1:A:360:ARG:HB2	1:A:361:PRO:HD3	1.89	0.54
1:C:633:CYS:HA	1:C:653:TYR:OH	2.08	0.54
1:C:150:PHE:HB2	1:C:449:LEU:HB3	1.90	0.54
1:B:191:PRO:HA	1:B:350:PHE:HA	1.88	0.54
1:B:196:GLU:O	1:B:200:LYS:HB2	2.07	0.54
1:C:372:VAL:HG11	1:C:375:MET:HE2	1.90	0.54
1:C:597:TYR:CE1	1:C:601:LEU:HD11	2.43	0.53
1:B:711:LEU:HD12	1:B:714:LEU:HD12	1.89	0.53
1:A:285:ASP:HA	1:A:298:SER:HB2	1.89	0.53
1:C:105:LYS:HE2	1:C:579:ASP:O	2.08	0.53
1:B:551:ALA:O	1:B:555:VAL:HG23	2.09	0.53
1:D:225:ARG:HD2	1:D:254:TYR:CD1	2.43	0.53
1:B:559:VAL:HG12	1:B:572:THR:HA	1.91	0.53
1:B:647:TYR:HE2	1:B:661:ARG:HE	1.55	0.53
1:D:502:GLU:O	1:D:506:LEU:HB2	2.08	0.53
1:D:531:LEU:O	1:D:535:GLU:HG2	2.08	0.53
1:D:209:SER:HB2	1:D:224:HIS:HB3	1.91	0.53
1:B:551:ALA:HB2	1:B:568:MET:SD	2.49	0.53
1:B:250:THR:HB	1:B:270:ASN:HB2	1.90	0.52
1:D:124:VAL:HG12	1:D:569:ALA:HA	1.90	0.52
1:B:639:ARG:HB3	1:B:641:PHE:CE1	2.44	0.52
1:D:206:VAL:HA	1:D:233:GLU:HA	1.90	0.52
1:A:515:ARG:HD2	1:A:515:ARG:N	2.23	0.52
1:B:375:MET:SD	1:B:386:PHE:HB3	2.49	0.52
1:C:317:ASP:O	1:C:320:LYS:HE2	2.09	0.52
1:A:145:GLY:HA2	1:A:455:LEU:HG	1.92	0.52
1:A:280:SER:HB2	1:A:287:PHE:HB3	1.91	0.52
1:A:212:LYS:HE2	1:A:219:GLU:OE2	2.10	0.52
1:A:516:HIS:O	1:A:520:MET:HG2	2.10	0.52
1:A:225:ARG:HD2	1:A:254:TYR:CD1	2.44	0.52
1:B:206:VAL:HA	1:B:233:GLU:HA	1.91	0.52
1:C:225:ARG:HD2	1:C:254:TYR:CD1	2.45	0.52
1:D:601:LEU:HB3	1:D:627:ARG:CZ	2.40	0.52
1:A:343:ASN:O	1:A:353:ALA:HA	2.09	0.52
1:C:360:ARG:HB2	1:C:361:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:620:ASN:HA	1:C:642:THR:HG21	1.92	0.52
1:D:601:LEU:HD13	1:D:627:ARG:NH1	2.25	0.52
1:D:639:ARG:HB3	1:D:641:PHE:CE1	2.44	0.52
1:B:429:TYR:CD2	1:B:455:LEU:HD13	2.45	0.51
1:D:178:ARG:HG2	1:D:178:ARG:O	2.11	0.51
1:D:605:ARG:HB3	1:D:612:LEU:HD23	1.92	0.51
1:B:429:TYR:CE2	1:B:455:LEU:HD13	2.45	0.51
1:C:433:HIS:HD2	1:C:457:SER:HA	1.75	0.51
1:B:616:GLN:CD	1:B:627:ARG:HA	2.31	0.51
1:D:165:TYR:CE1	1:D:189:ARG:HD2	2.45	0.51
1:A:158:LYS:HD3	1:A:279:ARG:NH1	2.26	0.51
1:B:343:ASN:CG	1:B:356:TRP:HB2	2.31	0.51
1:D:138:GLU:CB	2:D:1141:NAG:H83	2.41	0.51
1:A:328:ARG:HH21	1:A:333:LYS:HG2	1.76	0.50
1:A:597:TYR:CE1	1:A:601:LEU:HD11	2.46	0.50
1:D:139:GLY:C	2:D:1141:NAG:H82	2.31	0.50
1:B:420:ALA:O	1:B:423:ARG:HB3	2.10	0.50
1:D:540:ASN:O	1:D:543:ARG:HG2	2.12	0.50
1:A:319:PHE:CZ	1:A:321:GLN:HB2	2.47	0.50
1:C:325:PHE:CD2	1:C:342:ARG:HB2	2.47	0.50
2:B:1141:NAG:O7	2:B:1141:NAG:H3	2.12	0.50
1:B:584:GLN:HG2	1:B:586:SER:H	1.76	0.50
1:A:605:ARG:HB3	1:A:611:PRO:O	2.12	0.50
1:C:117:PRO:HA	1:C:625:LEU:HD21	1.92	0.50
1:D:177:HIS:O	1:D:178:ARG:HB3	2.12	0.50
1:A:319:PHE:O	1:A:320:LYS:HD3	2.11	0.50
1:A:633:CYS:HA	1:A:653:TYR:OH	2.12	0.50
1:C:125:VAL:O	1:C:567:VAL:HG13	2.11	0.50
1:C:567:VAL:HG12	1:C:568:MET:N	2.27	0.50
1:D:597:TYR:CZ	1:D:601:LEU:HD11	2.47	0.50
1:B:420:ALA:O	1:B:424:ILE:HG13	2.12	0.50
1:D:468:HIS:O	1:D:472:GLN:HG3	2.12	0.50
1:A:241:THR:O	1:A:243:THR:HG23	2.12	0.50
1:D:343:ASN:ND2	1:D:356:TRP:HB2	2.28	0.49
1:B:552:SER:HA	1:B:559:VAL:HG22	1.93	0.49
1:B:412:CYS:HA	1:B:415:LYS:HD2	1.94	0.49
1:B:377:ARG:HA	1:B:385:ARG:O	2.12	0.49
1:A:262:PHE:CD1	1:A:262:PHE:N	2.78	0.49
1:B:287:PHE:CD2	1:B:299:PRO:HG3	2.46	0.49
1:B:616:GLN:HB3	1:B:627:ARG:HG2	1.93	0.49
1:C:639:ARG:HB3	1:C:641:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:702:TYR:O	1:C:706:GLN:HG2	2.13	0.49
1:A:183:MET:N	1:A:184:GLY:CA	2.71	0.49
1:C:604:PHE:CZ	1:C:613:VAL:HB	2.47	0.49
1:D:425:PHE:CE2	1:D:430:ASN:HA	2.47	0.49
1:B:501:ILE:O	1:B:501:ILE:HG13	2.12	0.49
1:C:166:LYS:HZ1	1:C:192:VAL:HG22	1.77	0.49
1:D:501:ILE:HG13	1:D:501:ILE:O	2.13	0.49
1:B:114:TYR:HA	1:B:574:VAL:O	2.13	0.49
1:B:617:LEU:HD12	1:B:622:GLU:O	2.11	0.49
1:B:212:LYS:HE2	1:B:219:GLU:OE2	2.13	0.49
1:A:285:ASP:HB2	1:A:311:HIS:HB3	1.93	0.48
1:B:511:ASN:O	1:B:515:ARG:HG2	2.13	0.48
1:C:287:PHE:CD2	1:C:299:PRO:HG3	2.48	0.48
1:A:311:HIS:CG	1:A:312:THR:N	2.81	0.48
1:C:494:ARG:HG2	1:C:495:ILE:N	2.27	0.48
1:C:304:ARG:HB3	1:C:305:GLU:OE1	2.12	0.48
1:C:597:TYR:CE2	1:C:601:LEU:HD21	2.49	0.48
1:B:543:ARG:O	1:B:547:PRO:HG3	2.13	0.48
1:D:119:PRO:HG3	1:D:561:ALA:CA	2.43	0.48
1:B:106:ALA:HA	1:B:643:PHE:CE2	2.49	0.48
1:A:386:PHE:HB2	1:A:395:PHE:HB2	1.95	0.48
1:C:531:LEU:O	1:C:535:GLU:HG2	2.13	0.48
1:C:253:LYS:HA	1:C:268:THR:HG21	1.95	0.48
1:D:412:CYS:HA	1:D:415:LYS:NZ	2.29	0.48
1:D:551:ALA:HB2	1:D:568:MET:SD	2.53	0.48
1:D:377:ARG:HH21	1:D:454:PRO:HG3	1.78	0.48
1:A:286:GLU:HA	1:A:297:MET:O	2.13	0.48
1:D:507:GLN:HG3	1:D:511:ASN:OD1	2.14	0.48
1:B:305:GLU:HG2	1:B:305:GLU:O	2.14	0.48
1:D:647:TYR:CE2	1:D:661:ARG:HG2	2.49	0.48
1:B:166:LYS:HE3	1:B:207:CYS:SG	2.54	0.48
1:D:377:ARG:HA	1:D:385:ARG:O	2.13	0.48
1:D:300:PHE:O	1:D:307:SER:HB2	2.14	0.48
1:A:172:GLN:HB3	1:A:184:GLY:HA2	1.95	0.48
1:C:105:LYS:HG3	1:C:582:ILE:HG22	1.95	0.48
1:D:599:ARG:NH2	1:D:619:GLU:HG2	2.29	0.48
1:A:234:LEU:HD23	1:A:249:THR:HG23	1.96	0.48
1:B:304:ARG:HG2	1:A:320:LYS:NZ	2.29	0.47
1:A:199:ASP:O	1:A:203:ALA:HB3	2.14	0.47
1:C:205:GLY:HA3	1:C:328:ARG:NH1	2.29	0.47
1:C:559:VAL:HG12	1:C:572:THR:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:GLU:O	1:A:622:GLU:HB2	2.15	0.47
1:C:311:HIS:CG	1:C:312:THR:N	2.83	0.47
1:D:596:CYS:O	1:D:630:ILE:HG23	2.13	0.47
1:A:559:VAL:HA	1:A:573:CYS:H	1.80	0.47
1:D:434:ILE:HG23	1:D:458:ASN:HD21	1.80	0.47
1:C:158:LYS:HD3	1:C:279:ARG:HH12	1.77	0.47
1:C:616:GLN:HG3	1:C:624:ARG:HD2	1.96	0.47
1:D:360:ARG:N	1:D:361:PRO:HD2	2.30	0.47
1:B:433:HIS:HA	1:B:457:SER:HA	1.97	0.47
1:B:360:ARG:HE	1:B:409:LEU:HD23	1.79	0.47
1:D:106:ALA:HA	1:D:658:GLN:OE1	2.13	0.47
1:A:172:GLN:HG2	1:A:183:MET:CE	2.45	0.47
1:A:519:ASP:O	1:A:523:ARG:HG3	2.14	0.47
1:B:115:VAL:HB	1:B:623:LEU:HB2	1.96	0.47
1:B:259:VAL:HG13	1:B:260:GLU:N	2.30	0.47
1:B:264:ARG:HG3	1:B:265[A]:TYR:H	1.79	0.47
1:B:105:LYS:HE3	1:B:579:ASP:O	2.15	0.47
1:B:119:PRO:HG3	1:B:561:ALA:CA	2.44	0.47
1:A:583:VAL:HA	1:A:602:VAL:HG12	1.97	0.47
1:C:116:CYS:HB3	1:C:560:SER:CB	2.43	0.47
1:B:115:VAL:HG23	1:B:623:LEU:O	2.15	0.47
1:C:598:SER:HB3	1:C:631:GLU:HG2	1.97	0.47
1:A:113:PHE:O	1:A:575:PRO:HA	2.15	0.46
1:C:599:ARG:NH1	1:C:617:LEU:HG	2.25	0.46
1:B:114:TYR:O	1:B:622:GLU:HA	2.15	0.46
1:B:194:PHE:HE1	1:B:344:LEU:HD13	1.79	0.46
1:D:138:GLU:HB2	2:D:1141:NAG:H83	1.98	0.46
1:D:690:THR:OG1	1:D:693:GLU:HG3	2.14	0.46
1:A:222:ALA:HB1	1:A:267:THR:HG21	1.96	0.46
1:C:543:ARG:HB3	1:C:550:ILE:HG21	1.97	0.46
1:D:174:TRP:CZ3	1:D:176:GLY:HA3	2.51	0.46
1:D:572:THR:HG22	1:D:573:CYS:H	1.80	0.46
1:C:166:LYS:NZ	1:C:192:VAL:HG22	2.31	0.46
1:D:167:ASP:OD2	1:D:189:ARG:HG2	2.14	0.46
1:C:548:ASN:HB3	1:C:622:GLU:OE2	2.15	0.46
1:B:589:ILE:HG12	1:B:597:TYR:CE1	2.51	0.46
1:C:199:ASP:O	1:C:203:ALA:HB3	2.14	0.46
1:D:113:PHE:O	1:D:575:PRO:HA	2.15	0.46
1:A:548:ASN:OD1	1:A:560:SER:HA	2.15	0.46
1:B:601:LEU:HD13	1:B:627:ARG:NH1	2.30	0.46
1:A:559:VAL:HG12	1:A:572:THR:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:601:LEU:HA	1:D:616:GLN:HA	1.97	0.46
1:B:250:THR:HB	1:B:270:ASN:CB	2.45	0.46
1:A:124:VAL:HG12	1:A:569:ALA:HA	1.98	0.46
1:C:190:ALA:HA	1:C:191:PRO:HD3	1.77	0.46
1:B:581:VAL:HG22	1:B:604:PHE:HB3	1.97	0.46
1:B:248:HIS:HA	1:B:271:CYS:O	2.16	0.46
1:B:270:ASN:O	1:B:272:ILE:HG13	2.16	0.46
1:D:457:SER:O	1:D:458:ASN:HB2	2.16	0.46
1:C:329:ASP:O	1:C:333:LYS:HA	2.16	0.46
1:C:157:TYR:CD1	1:C:363:VAL:HG12	2.51	0.46
1:B:202:ASN:O	1:B:328:ARG:HB3	2.16	0.46
1:D:252:LEU:N	1:D:252:LEU:HD23	2.31	0.45
1:A:520:MET:O	1:A:524:VAL:HG23	2.16	0.45
1:C:285:ASP:HA	1:C:298:SER:HB2	1.97	0.45
1:C:140:GLN:HE21	1:C:378:SER:HB2	1.80	0.45
1:B:646:GLY:HA3	1:B:659:LEU:O	2.17	0.45
1:D:440:GLN:NE2	1:D:471:GLU:HB3	2.32	0.45
1:D:616:GLN:CD	1:D:627:ARG:HA	2.36	0.45
1:D:498:THR:HG21	1:D:503:PHE:CE2	2.50	0.45
1:C:319:PHE:CZ	1:C:321:GLN:HB2	2.51	0.45
1:C:224:HIS:HB2	1:C:269:VAL:HB	1.97	0.45
1:C:147:ALA:HA	1:C:451:ALA:O	2.16	0.45
1:D:584:GLN:CG	1:D:601:LEU:HB2	2.45	0.45
1:B:657:HIS:HD2	1:B:659:LEU:HG	1.81	0.45
1:C:502:GLU:HG3	1:C:503:PHE:N	2.31	0.45
1:B:164:TYR:HD1	1:B:351:THR:O	2.00	0.45
1:C:425:PHE:CZ	1:C:430:ASN:HA	2.51	0.45
1:A:701:ASP:OD1	1:A:704:GLU:HG3	2.16	0.45
1:A:202:ASN:OD1	1:A:327:ALA:HA	2.16	0.45
1:D:408:ASP:OD1	1:D:409:LEU:HG	2.16	0.45
1:D:164:TYR:HE1	1:D:353:ALA:HB3	1.81	0.45
1:A:343:ASN:C	1:A:344:LEU:HD12	2.37	0.45
1:D:394:THR:N	1:D:508:PHE:HB2	2.32	0.45
1:A:236:PRO:HA	1:A:246:GLY:O	2.17	0.45
1:C:567:VAL:CG1	1:C:568:MET:N	2.80	0.45
1:C:369:TRP:CD2	1:C:370:GLN:HG2	2.51	0.45
1:A:162:THR:HA	1:A:275:GLU:HA	1.99	0.45
1:B:378:SER:O	1:B:385:ARG:N	2.50	0.45
1:A:314:TYR:CE1	1:A:345:LEU:HD21	2.52	0.45
1:B:194:PHE:CD1	1:B:320:LYS:HD2	2.51	0.45
1:C:407:VAL:HA	1:C:493:GLU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:ALA:H	1:C:336:ALA:HB3	1.81	0.45
1:D:207:CYS:HB3	1:D:249:THR:HG21	1.98	0.45
1:A:328:ARG:HE	1:A:333:LYS:HA	1.82	0.45
1:C:340:THR:HG21	1:C:355:ASP:OD2	2.17	0.45
1:C:325:PHE:O	1:C:339:PRO:HA	2.16	0.45
1:B:259:VAL:HG22	1:B:260:GLU:N	2.23	0.44
1:C:342:ARG:HD2	1:C:354:TRP:O	2.17	0.44
1:B:443:LEU:HD12	1:B:448:PHE:O	2.17	0.44
1:C:115:VAL:O	1:C:117:PRO:HD3	2.17	0.44
1:B:202:ASN:O	1:B:328:ARG:HD3	2.18	0.44
1:A:160:LYS:HE3	1:A:277:ASP:OD1	2.17	0.44
1:C:605:ARG:HG2	1:C:611:PRO:O	2.16	0.44
1:A:200:LYS:HE3	1:A:208:ARG:CZ	2.48	0.44
1:B:328:ARG:HG3	1:B:335:ARG:HB3	1.99	0.44
1:B:297:MET:HE1	1:B:319:PHE:HB2	1.99	0.44
1:B:212:LYS:HE2	1:B:219:GLU:CD	2.38	0.44
1:D:191:PRO:HG3	1:D:350:PHE:N	2.32	0.44
1:B:587:MET:HB2	1:B:653:TYR:HB3	1.99	0.44
1:B:175:PHE:CE1	1:B:258:ARG:HA	2.53	0.44
1:A:635:VAL:HG12	1:A:636:GLY:N	2.32	0.44
1:B:147:ALA:HA	1:B:451:ALA:O	2.17	0.44
1:A:125:VAL:O	1:A:567:VAL:HG13	2.18	0.44
1:D:659:LEU:HB2	1:D:663:ASP:OD1	2.17	0.44
1:C:406:ARG:HG2	1:C:406:ARG:O	2.17	0.44
1:C:186:PHE:CZ	1:C:188:ASP:HB2	2.52	0.44
1:C:116:CYS:CB	1:C:560:SER:HB2	2.45	0.44
1:A:166:LYS:NZ	1:A:192:VAL:HG22	2.33	0.44
1:B:343:ASN:OD1	1:B:356:TRP:HB2	2.18	0.44
1:D:375:MET:O	1:D:452:TYR:HE1	2.01	0.44
1:C:600:PRO:O	1:C:616:GLN:HB2	2.18	0.44
1:B:583:VAL:HG22	1:B:584:GLN:N	2.33	0.44
1:D:250:THR:HB	1:D:270:ASN:HB2	2.00	0.44
1:C:279:ARG:O	1:C:288:VAL:HG22	2.18	0.43
1:D:433:HIS:HA	1:D:456:LEU:O	2.17	0.43
1:B:116:CYS:HB2	1:B:622:GLU:CD	2.39	0.43
1:D:280:SER:HB2	1:D:287:PHE:CB	2.47	0.43
1:A:332:THR:O	1:A:333:LYS:HB2	2.18	0.43
1:C:235:LYS:HG2	1:C:248:HIS:O	2.18	0.43
1:B:145:GLY:HA2	1:B:455:LEU:HD12	2.00	0.43
1:B:175:PHE:HD1	1:B:258:ARG:HH11	1.66	0.43
1:C:209:SER:HB2	1:C:224:HIS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLN:HG2	1:A:182:PHE:O	2.17	0.43
1:A:250:THR:HG22	1:A:251:ASP:N	2.34	0.43
1:B:168:VAL:HA	1:B:268:THR:O	2.18	0.43
1:C:434:ILE:HD12	1:C:434:ILE:O	2.18	0.43
1:C:170:VAL:HA	1:C:266:GLY:O	2.18	0.43
1:C:559:VAL:HG12	1:C:572:THR:HG23	2.00	0.43
1:B:265[B]:TYR:C	1:B:265[B]:TYR:CD1	2.91	0.43
1:A:384:PHE:CE2	1:A:399:LEU:HA	2.54	0.43
1:A:382:GLY:HA2	1:A:399:LEU:HD11	2.00	0.43
1:C:635:VAL:HG22	1:C:636:GLY:H	1.83	0.43
1:B:156:PRO:O	1:B:158:LYS:HG3	2.18	0.43
1:A:402:TYR:HA	1:A:403:PRO:HD3	1.72	0.43
1:C:384:PHE:O	1:C:396:THR:HA	2.19	0.43
1:A:172:GLN:HG2	1:A:183:MET:HE2	2.00	0.43
1:C:193:PRO:O	1:C:197:VAL:HG23	2.18	0.43
1:B:106:ALA:HA	1:B:643:PHE:HE2	1.83	0.43
1:A:574:VAL:HA	1:A:575:PRO:HD3	1.86	0.43
1:C:327:ALA:H	1:C:336:ALA:CB	2.32	0.43
1:D:327:ALA:HB3	1:D:336:ALA:HB2	2.00	0.43
1:B:175:PHE:CD1	1:B:258:ARG:HD2	2.54	0.43
1:C:113:PHE:CD1	1:C:581:VAL:HG21	2.54	0.43
1:B:616:GLN:NE2	1:B:629:ALA:HB3	2.33	0.43
1:B:110:ASP:OD1	1:B:645:GLY:HA3	2.18	0.43
1:D:616:GLN:HE22	1:D:629:ALA:H	1.65	0.42
1:C:104:ILE:O	1:C:582:ILE:HB	2.19	0.42
1:C:105:LYS:HB3	1:C:106:ALA:H	1.51	0.42
1:D:106:ALA:HB2	1:D:643:PHE:CZ	2.54	0.42
1:D:392:SER:HA	1:D:508:PHE:CZ	2.54	0.42
1:C:406:ARG:HG2	1:C:493:GLU:HB3	2.00	0.42
1:C:435:LYS:HD2	1:C:453:GLN:CD	2.40	0.42
1:A:276:VAL:HB	1:A:290:ALA:HB3	2.01	0.42
1:C:319:PHE:O	1:C:320:LYS:HD3	2.20	0.42
1:A:236:PRO:HA	1:A:247:TRP:CD1	2.54	0.42
1:A:256:PRO:HG3	1:A:266:GLY:N	2.35	0.42
1:C:458:ASN:HA	1:C:461:ALA:HB2	2.02	0.42
1:D:234:LEU:HD23	1:D:249:THR:HG23	2.00	0.42
1:B:225:ARG:HD2	1:B:254:TYR:CD1	2.53	0.42
1:B:574:VAL:HA	1:B:575:PRO:HD3	1.88	0.42
1:B:408:ASP:OD1	1:B:409:LEU:HG	2.20	0.42
1:C:619:GLU:O	1:C:622:GLU:HB3	2.19	0.42
1:A:402:TYR:OH	1:A:495:ILE:HD11	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:629:ALA:C	1:C:630:ILE:HD12	2.39	0.42
1:D:343:ASN:O	1:D:353:ALA:HA	2.20	0.42
1:C:304:ARG:NH1	5:C:2001:MRY:HAA2	2.35	0.42
1:D:113:PHE:CD2	1:D:623:LEU:HD21	2.55	0.42
1:A:369:TRP:CD2	1:A:370:GLN:HG2	2.55	0.42
1:D:144:GLU:HA	1:D:376:LEU:HD23	2.01	0.42
1:A:298:SER:CB	1:A:310:GLU:HB3	2.48	0.42
1:A:166:LYS:HG2	1:A:271:CYS:HA	2.00	0.42
1:A:147:ALA:HB2	1:A:452:TYR:HD1	1.85	0.42
1:C:148:VAL:HB	1:C:451:ALA:HB3	2.01	0.42
1:D:155:ALA:HA	1:D:156:PRO:HD3	1.82	0.42
1:D:616:GLN:NE2	1:D:629:ALA:HB3	2.35	0.42
1:C:574:VAL:HA	1:C:575:PRO:HD3	1.90	0.42
1:C:276:VAL:HB	1:C:290:ALA:HB3	2.00	0.42
1:D:617:LEU:HD12	1:D:622:GLU:O	2.20	0.42
1:C:589:ILE:HG22	1:C:592:ARG:H	1.84	0.42
1:A:587:MET:O	1:A:596:CYS:HB3	2.19	0.42
1:A:196:GLU:O	1:A:200:LYS:HB2	2.19	0.42
1:A:127:PHE:HA	1:A:127:PHE:HD2	1.75	0.42
1:C:237:ALA:HA	1:C:248:HIS:CD2	2.53	0.42
1:D:175:PHE:CD1	1:D:258:ARG:HD2	2.54	0.42
1:C:604:PHE:O	1:C:612:LEU:HA	2.19	0.42
1:D:511:ASN:O	1:D:515:ARG:HG2	2.19	0.42
1:C:157:TYR:HB2	1:C:284:TYR:CE2	2.55	0.42
1:D:397:THR:HG22	1:D:444:ALA:HA	2.01	0.42
1:A:190:ALA:HA	1:A:191:PRO:HD3	1.74	0.42
1:D:589:ILE:HG12	1:D:597:TYR:CE1	2.54	0.42
1:C:130:PRO:HB3	1:C:533:ASN:HB3	2.02	0.42
1:B:392:SER:HA	1:B:508:PHE:CE2	2.55	0.42
1:C:119:PRO:HG3	1:C:560:SER:O	2.20	0.41
1:C:606:TYR:HD2	1:C:613:VAL:HG21	1.81	0.41
1:C:280:SER:HB2	1:C:287:PHE:HB3	2.02	0.41
1:B:492:VAL:HG12	1:B:493:GLU:N	2.35	0.41
1:B:402:TYR:HA	1:B:403:PRO:HD3	1.89	0.41
1:B:637:HIS:CE1	1:B:639:ARG:HD2	2.54	0.41
1:C:433:HIS:HA	1:C:456:LEU:O	2.20	0.41
1:C:557:ARG:HG3	1:C:559:VAL:HG13	2.02	0.41
1:C:425:PHE:O	1:C:430:ASN:HB3	2.20	0.41
1:C:233:GLU:O	1:C:249:THR:HG22	2.18	0.41
1:A:671:ILE:N	1:A:671:ILE:HD12	2.35	0.41
1:C:248:HIS:HE1	6:C:733:HOH:O	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:ARG:NH2	1:C:622:GLU:HB2	2.36	0.41
1:A:528:TRP:O	1:A:532:GLN:HG2	2.20	0.41
1:C:402:TYR:HA	1:C:403:PRO:HD3	1.79	0.41
1:B:359:LYS:O	1:B:363:VAL:HG22	2.19	0.41
1:B:288:VAL:HG12	1:B:294:PHE:HA	2.02	0.41
1:B:120:THR:O	1:B:121:GLY:C	2.59	0.41
1:A:248:HIS:HA	1:A:271:CYS:O	2.21	0.41
1:D:572:THR:HG22	1:D:573:CYS:N	2.35	0.41
1:C:191:PRO:HA	1:C:350:PHE:HA	2.02	0.41
1:C:298:SER:HB3	1:C:310:GLU:HB3	2.02	0.41
1:C:129:GLN:HB3	1:C:130:PRO:HD2	2.02	0.41
1:D:146:ILE:HD11	1:D:429:TYR:CD1	2.55	0.41
1:B:659:LEU:HB3	1:B:663:ASP:OD1	2.20	0.41
1:B:514:GLN:O	1:B:517:VAL:HG22	2.21	0.41
1:D:145:GLY:HA3	1:D:452:TYR:CZ	2.55	0.41
1:A:604:PHE:O	1:A:613:VAL:N	2.49	0.41
1:D:605:ARG:HH11	1:D:609:GLN:HA	1.85	0.41
2:B:1141:NAG:O7	2:B:1141:NAG:C3	2.69	0.41
1:B:411:ASP:HB3	1:B:415:LYS:HE3	2.02	0.41
1:D:190:ALA:HA	1:D:191:PRO:HD3	1.87	0.41
1:A:384:PHE:O	1:A:396:THR:HA	2.20	0.41
1:D:420:ALA:O	1:D:424:ILE:HG13	2.21	0.41
1:D:647:TYR:HE2	1:D:661:ARG:HG2	1.86	0.41
1:C:282:TYR:CG	1:C:283:PRO:HA	2.56	0.41
1:C:519:ASP:O	1:C:523:ARG:HG3	2.21	0.41
1:B:133:CYS:HA	1:B:134:PRO:HD3	1.91	0.41
1:D:639:ARG:HB3	1:D:641:PHE:CZ	2.55	0.41
1:B:264:ARG:HG3	1:B:265[B]:TYR:H	1.84	0.41
1:C:326:TYR:HD1	1:C:336:ALA:O	2.04	0.41
1:B:401:GLU:HB3	1:B:402:TYR:H	1.75	0.41
1:C:539:TRP:HA	1:C:542:ALA:HB3	2.03	0.41
1:B:368:LYS:NZ	1:B:368:LYS:HB3	2.35	0.41
1:A:152:GLU:HG2	1:A:153:ASN:N	2.36	0.41
1:C:690:THR:OG1	1:C:693:GLU:HG3	2.21	0.41
1:B:122:ALA:HA	1:B:123:THR:HA	1.66	0.41
1:A:441:TYR:HB3	1:A:449:LEU:HD11	2.02	0.41
1:B:555:VAL:HG12	1:B:555:VAL:O	2.21	0.41
1:A:302:GLY:O	1:A:307:SER:HB2	2.21	0.41
1:C:321:GLN:NE2	1:C:341:THR:HG22	2.36	0.40
1:C:641:PHE:HB2	1:C:648:VAL:HG13	2.03	0.40
1:D:175:PHE:CE1	1:D:258:ARG:HA	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:CYS:HB3	1:D:560:SER:HB3	2.03	0.40
1:B:332:THR:C	1:B:334:ALA:H	2.24	0.40
1:C:568:MET:HE3	1:C:568:MET:HB2	1.85	0.40
1:D:174:TRP:CH2	1:D:176:GLY:HA3	2.56	0.40
1:D:114:TYR:HB3	1:D:573:CYS:HB3	2.04	0.40
1:C:347:THR:N	1:C:350:PHE:O	2.54	0.40
1:D:659:LEU:N	1:D:659:LEU:HD23	2.36	0.40
1:B:392:SER:HA	1:B:508:PHE:CZ	2.56	0.40
1:D:200:LYS:HB3	1:D:206:VAL:HG23	2.04	0.40
1:C:340:THR:HG22	1:C:341:THR:N	2.36	0.40
1:A:200:LYS:HE3	1:A:208:ARG:NH1	2.36	0.40
1:A:549:ALA:O	1:A:553:VAL:HG12	2.22	0.40
1:B:224:HIS:CD2	1:B:225:ARG:HG2	2.56	0.40
1:C:601:LEU:HA	1:C:616:GLN:HA	2.03	0.40
1:C:250:THR:HG22	1:C:251:ASP:N	2.36	0.40
1:B:157:TYR:CD1	1:B:363:VAL:HG12	2.57	0.40
1:C:343:ASN:O	1:C:353:ALA:HA	2.21	0.40
1:C:215:ARG:NH2	1:C:349:LYS:HG2	2.37	0.40
1:A:224:HIS:HB2	1:A:269:VAL:HB	2.02	0.40
1:B:303:TYR:O	1:A:317:ASP:HB3	2.21	0.40
1:C:597:TYR:HA	1:C:630:ILE:HA	2.04	0.40
1:C:304:ARG:HD3	1:C:356:TRP:CZ3	2.57	0.40
1:D:175:PHE:HB2	1:D:259:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	603/703 (86%)	543 (90%)	56 (9%)	4 (1%)	26	61
1	B	590/703 (84%)	523 (89%)	64 (11%)	3 (0%)	34	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	595/703 (85%)	532 (89%)	58 (10%)	5 (1%)	24 58
1	D	601/703 (86%)	548 (91%)	52 (9%)	1 (0%)	52 83
All	All	2389/2812 (85%)	2146 (90%)	230 (10%)	13 (0%)	34 69

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	VAL
1	B	413	ILE
1	A	238	ASN
1	C	429	TYR
1	B	106	ALA
1	D	315	ALA
1	A	134	PRO
1	A	264	ARG
1	A	699	LEU
1	C	390	ALA
1	C	413	ILE
1	C	134	PRO
1	C	139	GLY

5.3.2 Protein sidechains (i)

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	517/593 (87%)	505 (98%)	12 (2%)	58 86
1	B	509/593 (86%)	501 (98%)	8 (2%)	70 90
1	C	506/593 (85%)	501 (99%)	5 (1%)	82 95
1	D	514/593 (87%)	509 (99%)	5 (1%)	82 95
All	All	2046/2372 (86%)	2016 (98%)	30 (2%)	72 91

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	113	PHE
1	B	135	THR
1	B	141	ASN
1	B	143	THR
1	B	264	ARG
1	B	293	ASP
1	B	606	TYR
1	B	625	LEU
1	A	127	PHE
1	A	141	ASN
1	A	170	VAL
1	A	185	ILE
1	A	186	PHE
1	A	262	PHE
1	A	323	ASP
1	A	331	THR
1	A	397	THR
1	A	401	GLU
1	A	464	TYR
1	A	502	GLU
1	C	141	ASN
1	C	263	HIS
1	C	265	TYR
1	C	270	ASN
1	C	631	GLU
1	D	294	PHE
1	D	340	THR
1	D	384	PHE
1	D	546	ASN
1	D	625	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	453	GLN
1	B	709	ASN
1	A	440	GLN
1	A	620	ASN
1	C	140	GLN
1	C	270	ASN
1	C	433	HIS
1	C	468	HIS
1	D	472	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

4 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	NAG	B	1141	1,2	14,14,15	0.59	0	15,19,21	1.10	1 (6%)
2	NAG	B	1142	2	14,14,15	0.45	0	15,19,21	0.74	0
2	NAG	D	1141	1,2	14,14,15	0.52	0	15,19,21	1.60	4 (26%)
2	NAG	D	1142	2	14,14,15	0.49	0	15,19,21	0.82	1 (6%)

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	NAG	B	1141	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	1142	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1141	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	1142	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1141	NAG	C2-N2-C7	-3.92	118.00	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1141	NAG	O7-C7-C8	-2.48	117.51	122.06
2	D	1142	NAG	C2-N2-C7	-2.32	120.06	123.04
2	D	1141	NAG	O7-C7-N2	2.10	126.15	121.86
2	B	1141	NAG	C2-N2-C7	2.57	126.34	123.04
2	D	1141	NAG	C1-O5-C5	2.66	115.63	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1141	NAG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1141	NAG	2	0
2	D	1141	NAG	3	0

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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	$\#\|Z\| > 2$
3	NAG	A	1141	1	14,14,15	0.49	0	15,19,21	0.64	0
3	NAG	A	1430	1	14,14,15	0.54	0	15,19,21	0.88	1 (6%)
3	NAG	A	1674	1	14,14,15	0.49	0	15,19,21	0.67	0
3	NAG	B	1398	1	14,14,15	0.53	0	15,19,21	0.66	0
3	NAG	B	1430	1	14,14,15	0.57	0	15,19,21	1.00	1 (6%)
3	NAG	C	1141	1	14,14,15	0.51	0	15,19,21	0.61	0
3	NAG	C	1430	1	14,14,15	0.46	0	15,19,21	1.16	2 (13%)
3	NAG	C	1674	1	14,14,15	0.51	0	15,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MRY	C	2001	-	7,7,7	0.36	0	6,8,8	0.20	0
3	NAG	D	1398	1	14,14,15	0.53	0	15,19,21	0.54	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
3	NAG	A	1141	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1430	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1674	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1398	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1430	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1141	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1430	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1674	1	-	0/6/23/26	0/1/1/1
5	MRY	C	2001	-	-	0/8/8/8	0/0/0/0
3	NAG	D	1398	1	-	1/6/23/26	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(^{o})	Ideal(^{o})
3	C	1430	NAG	C2-N2-C7	-2.11	120.33	123.04
3	A	1430	NAG	C1-O5-C5	2.47	115.39	112.25
3	B	1430	NAG	C1-O5-C5	2.97	116.02	112.25
3	C	1430	NAG	C1-O5-C5	3.45	116.63	112.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1398	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2001	MRY	1	0

5.7 Other polymers

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

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, 95^{th} 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	606/703 (86%)	0.57	47 (7%) 16 11	20, 66, 145, 550	0
1	B	597/703 (84%)	0.77	68 (11%) 7 4	23, 71, 174, 550	0
1	C	601/703 (85%)	0.73	69 (11%) 6 4	20, 76, 176, 550	0
1	D	606/703 (86%)	0.62	54 (8%) 12 7	22, 65, 151, 550	0
All	All	2410/2812 (85%)	0.67	238 (9%) 9 5	20, 69, 164, 550	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	612	LEU	9.9
1	B	600	PRO	9.4
1	B	577	ALA	8.6
1	C	111	ALA	7.9
1	B	579	ASP	7.8
1	D	600	PRO	7.3
1	C	594	GLY	7.2
1	A	109	THR	7.1
1	B	491	SER	7.0
1	B	580	ASN	6.9
1	B	640	TYR	6.5
1	C	109	THR	6.3
1	D	577	ALA	6.3
1	D	597	TYR	6.2
1	B	150	PHE	6.2
1	D	604	PHE	6.2
1	D	402	TYR	6.1
1	B	643	PHE	6.0
1	B	402	TYR	6.0
1	D	579	ASP	5.8
1	C	623	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	612	LEU	5.7
1	B	594	GLY	5.7
1	A	623	LEU	5.5
1	B	717	ALA	5.5
1	D	725	ALA	5.4
1	C	595	ALA	5.4
1	A	582	ILE	5.3
1	B	578	ALA	5.2
1	D	613	VAL	5.2
1	C	107	GLU	5.1
1	D	439	PRO	5.0
1	B	597	TYR	5.0
1	A	443	LEU	4.9
1	D	581	VAL	4.9
1	A	111	ALA	4.9
1	C	672	ASP	4.9
1	B	581	VAL	4.9
1	D	582	ILE	4.8
1	C	582	ILE	4.8
1	D	233	GLU	4.8
1	C	110	ASP	4.8
1	A	672	ASP	4.8
1	D	455	LEU	4.7
1	B	613	VAL	4.7
1	C	648	VAL	4.6
1	B	645	GLY	4.6
1	B	455	LEU	4.5
1	D	437	GLY	4.4
1	B	725	ALA	4.3
1	A	262	PHE	4.3
1	B	583	VAL	4.2
1	A	331	THR	4.2
1	B	564	LEU	4.1
1	C	653	TYR	4.0
1	A	319	PHE	4.0
1	C	606	TYR	4.0
1	B	567	VAL	4.0
1	C	468	HIS	4.0
1	C	601	LEU	3.9
1	A	433	HIS	3.9
1	B	492	VAL	3.9
1	A	105	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	603	SER	3.9
1	B	606	TYR	3.9
1	A	110	ASP	3.9
1	D	645	GLY	3.8
1	B	604	PHE	3.8
1	A	629	ALA	3.7
1	A	492	VAL	3.7
1	A	108	ASN	3.7
1	A	601	LEU	3.7
1	D	599	ARG	3.7
1	C	464	TYR	3.7
1	D	453	GLN	3.7
1	A	653	TYR	3.7
1	C	104	ILE	3.7
1	C	583	VAL	3.6
1	B	453	GLN	3.6
1	C	500	SER	3.6
1	B	602	VAL	3.6
1	A	259	VAL	3.6
1	A	595	ALA	3.5
1	C	319	PHE	3.5
1	C	612	LEU	3.5
1	B	603	SER	3.5
1	D	108	ASN	3.5
1	D	492	VAL	3.4
1	D	261	ALA	3.4
1	B	218	LEU	3.4
1	D	109	THR	3.4
1	A	172	GLN	3.3
1	A	589	ILE	3.3
1	A	432	THR	3.3
1	A	648	VAL	3.2
1	B	305	GLU	3.2
1	C	159	PHE	3.2
1	B	601	LEU	3.2
1	C	492	VAL	3.2
1	A	494	ARG	3.2
1	D	650	PHE	3.1
1	C	624	ARG	3.1
1	C	493	GLU	3.1
1	D	620	ASN	3.1
1	C	636	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	108	ASN	3.1
1	A	709	ASN	3.0
1	B	473	SER	3.0
1	C	575	PRO	3.0
1	D	218	LEU	3.0
1	D	331	THR	3.0
1	D	265[A]	TYR	2.9
1	C	105	LYS	2.9
1	C	462	GLU	2.9
1	D	260	GLU	2.9
1	A	222	ALA	2.9
1	C	322	VAL	2.9
1	D	724	HIS	2.9
1	C	473	SER	2.9
1	B	429	TYR	2.8
1	D	477	PRO	2.8
1	C	399	LEU	2.8
1	B	575	PRO	2.8
1	B	403	PRO	2.8
1	B	425	PHE	2.7
1	B	568	MET	2.7
1	C	164	TYR	2.7
1	C	543	ARG	2.7
1	B	723	ILE	2.7
1	C	228	HIS	2.7
1	A	477	PRO	2.7
1	B	718	ASP	2.7
1	C	172	GLN	2.7
1	D	584	GLN	2.6
1	C	433	HIS	2.6
1	C	581	VAL	2.6
1	D	583	VAL	2.6
1	D	456	LEU	2.6
1	C	658	GLN	2.6
1	D	578	ALA	2.6
1	D	643	PHE	2.6
1	C	691	ARG	2.6
1	D	195	GLU	2.6
1	B	441	TYR	2.6
1	A	471	GLU	2.6
1	C	625	LEU	2.5
1	C	716	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	460	LEU	2.5
1	B	560	SER	2.5
1	B	129	GLN	2.5
1	C	422	ASP	2.5
1	C	384	PHE	2.5
1	B	161	ALA	2.4
1	C	323	ASP	2.4
1	D	332	THR	2.4
1	C	467	GLU	2.4
1	D	235	LYS	2.4
1	C	443	LEU	2.4
1	B	184	GLY	2.4
1	C	635	VAL	2.4
1	A	594	GLY	2.4
1	A	449	LEU	2.4
1	C	234	LEU	2.4
1	B	265[A]	TYR	2.4
1	B	625	LEU	2.4
1	A	183	MET	2.4
1	A	240	ALA	2.4
1	C	317	ASP	2.4
1	A	590	SER	2.3
1	C	585	ASN	2.3
1	D	464	TYR	2.3
1	C	163	MET	2.3
1	D	640	TYR	2.3
1	D	111	ALA	2.3
1	B	582	ILE	2.3
1	D	150	PHE	2.3
1	A	493	GLU	2.3
1	D	519	ASP	2.3
1	A	263	HIS	2.3
1	B	611	PRO	2.3
1	C	194	PHE	2.3
1	C	659	LEU	2.3
1	B	107	GLU	2.3
1	B	374	GLU	2.3
1	C	223	PHE	2.2
1	B	234	LEU	2.2
1	B	113	PHE	2.2
1	A	194	PHE	2.2
1	C	589	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	473	SER	2.2
1	B	138	GLU	2.2
1	B	111	ALA	2.2
1	B	593	PRO	2.2
1	A	450	ILE	2.2
1	A	658	GLN	2.2
1	B	363	VAL	2.2
1	A	606	TYR	2.2
1	B	584	GLN	2.2
1	A	179	SER	2.2
1	D	607	GLU	2.2
1	D	601	LEU	2.2
1	D	580	ASN	2.2
1	A	119	PRO	2.1
1	C	466	ARG	2.1
1	A	659	LEU	2.1
1	C	604	PHE	2.1
1	A	609	GLN	2.1
1	C	425	PHE	2.1
1	A	645	GLY	2.1
1	B	235	LYS	2.1
1	B	576	VAL	2.1
1	C	449	LEU	2.1
1	D	459	THR	2.1
1	B	607	GLU	2.1
1	D	107	GLU	2.1
1	C	579	ASP	2.1
1	C	709	ASN	2.1
1	B	121	GLY	2.1
1	B	435	LYS	2.1
1	C	434	ILE	2.1
1	B	418	ARG	2.1
1	B	108	ASN	2.1
1	C	263	HIS	2.1
1	B	539	TRP	2.1
1	C	113	PHE	2.1
1	C	218	LEU	2.1
1	C	436	VAL	2.1
1	C	183	MET	2.1
1	D	713	ASP	2.0
1	B	391	ILE	2.0
1	A	218	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	476	PRO	2.0
1	D	457	SER	2.0
1	C	494	ARG	2.0
1	D	474	ARG	2.0
1	B	663	ASP	2.0
1	D	259	VAL	2.0
1	A	378	SER	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, 95^{th} 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(Å^2)	Q<0.9
2	NAG	B	1141	14/15	0.69	0.21	-	104,104,104,104	0
2	NAG	D	1142	14/15	0.80	0.25	-	91,91,91,91	0
2	NAG	D	1141	14/15	0.83	0.23	-	77,77,77,77	0
2	NAG	B	1142	14/15	0.83	0.22	-	89,89,89,89	0

6.4 Ligands (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, 95^{th} 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(Å^2)	Q<0.9
4	CL	D	1	1/1	0.73	0.38	5.54	59,59,59,59	0
5	MRY	C	2001	8/8	0.83	0.36	1.22	69,69,69,69	0
4	CL	A	2	1/1	0.81	0.17	-1.33	78,78,78,78	0
3	NAG	C	1674	14/15	0.81	0.20	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	1674	14/15	0.83	0.23	-	89,89,89,89	0
3	NAG	A	1141	14/15	0.81	0.27	-	120,120,120,120	0
3	NAG	B	1398	14/15	0.86	0.25	-	92,92,92,92	0
3	NAG	C	1141	14/15	0.71	0.25	-	113,113,113,113	0
3	NAG	D	1398	14/15	0.81	0.17	-	87,87,87,87	0
3	NAG	C	1430	14/15	0.77	0.31	-	117,117,117,117	0
3	NAG	B	1430	14/15	0.82	0.27	-	117,117,117,117	0
3	NAG	A	1430	14/15	0.44	0.43	-	118,118,118,118	0

6.5 Other polymers

There are no such residues in this entry.