Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:52 AM GMT

PDB ID	:	2J3O
Title	:	L-FICOLIN COMPLEXED TO N-ACETYL-D-GLUCOSAMINE
Authors	:	Garlatti, V.; Gaboriaud, C.
Deposited on	:	2006-08-22
Resolution	:	2.65 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:

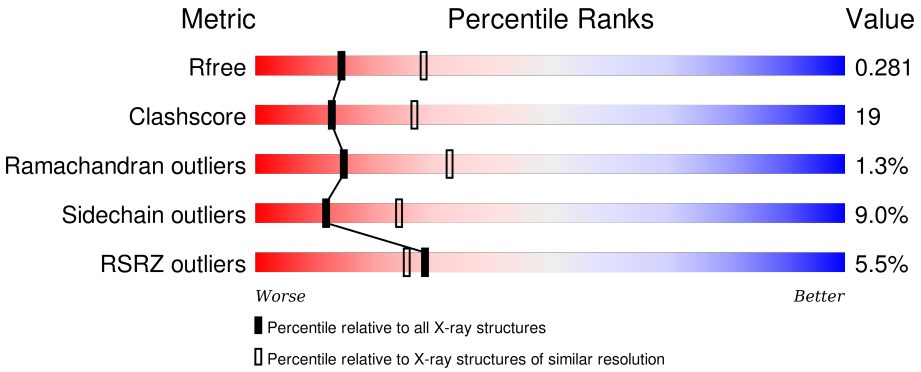
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	219	17% 55% 37% 7%
1	B	219	% 72% 24%
1	C	219	2% 68% 26% 5%
1	D	219	6% 65% 29%
1	E	219	3% 69% 27%

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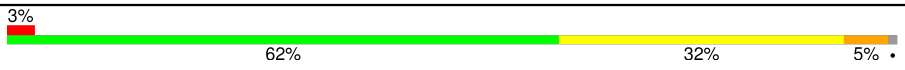
Mol	Chain	Length	Quality of chain
1	F	219	

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
3	ACT	B	1289	-	-	X	X
4	NAG	B	1290[A]	-	-	-	X
4	NAG	B	1290[B]	-	-	-	X
4	NAG	B	1293	X	-	-	-
4	NAG	C	1289	-	-	-	X
4	NAG	C	1290	-	-	-	X
4	NAG	D	1288	-	-	-	X
4	NAG	E	1289	-	-	-	X
4	NAG	E	1292	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10716 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 FICOLIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1735	1092	305	329	9			
1	B	218	Total	C	N	O	S	0	1	0
			1753	1103	310	331	9			
1	C	217	Total	C	N	O	S	0	0	0
			1735	1092	305	329	9			
1	D	216	Total	C	N	O	S	0	0	0
			1730	1089	304	328	9			
1	E	217	Total	C	N	O	S	0	0	0
			1735	1092	305	329	9			
1	F	217	Total	C	N	O	S	0	0	0
			1735	1092	305	329	9			

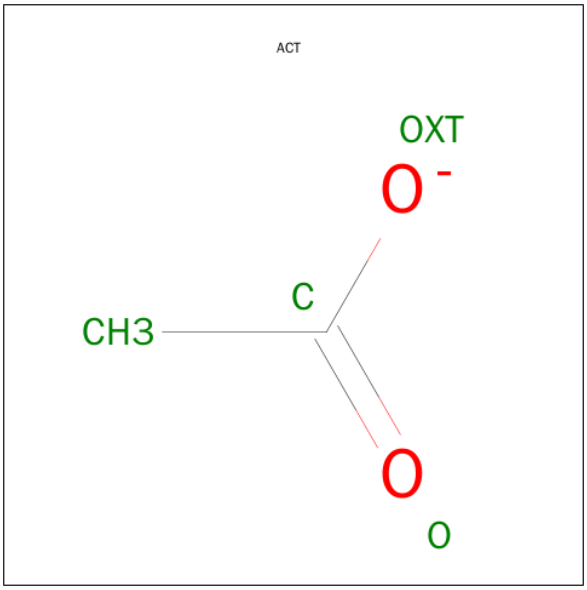
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	THR	VAL	CONFLICT	UNP Q15485
A	247	THR	VAL	CONFLICT	UNP Q15485
B	168	THR	VAL	CONFLICT	UNP Q15485
B	247	THR	VAL	CONFLICT	UNP Q15485
C	168	THR	VAL	CONFLICT	UNP Q15485
C	247	THR	VAL	CONFLICT	UNP Q15485
D	168	THR	VAL	CONFLICT	UNP Q15485
D	247	THR	VAL	CONFLICT	UNP Q15485
E	168	THR	VAL	CONFLICT	UNP Q15485
E	247	THR	VAL	CONFLICT	UNP Q15485
F	168	THR	VAL	CONFLICT	UNP Q15485
F	247	THR	VAL	CONFLICT	UNP Q15485

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

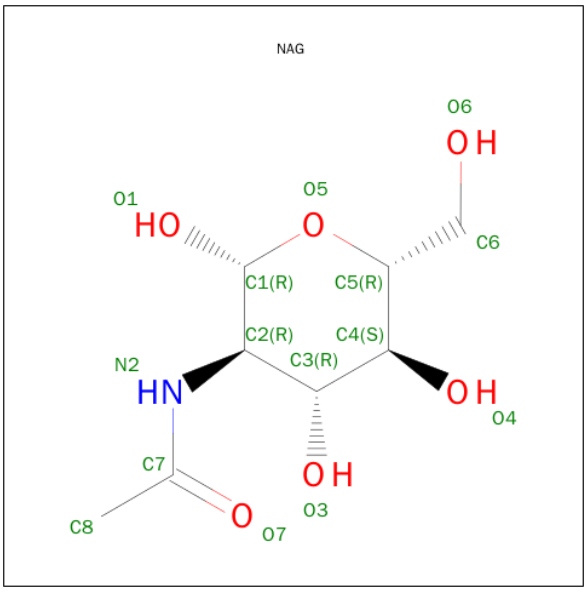
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 30 16 2 12	0	1
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 15 8 1 6	0	0
4	C	1	Total C N O 15 8 1 6	0	0
4	D	1	Total C N O 15 8 1 6	0	0
4	E	1	Total C N O 15 8 1 6	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 15 8 1 6	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	19	Total O 19 19	0	0
5	B	25	Total O 25 25	0	0
5	C	31	Total O 31 31	0	0
5	D	20	Total O 20 20	0	0

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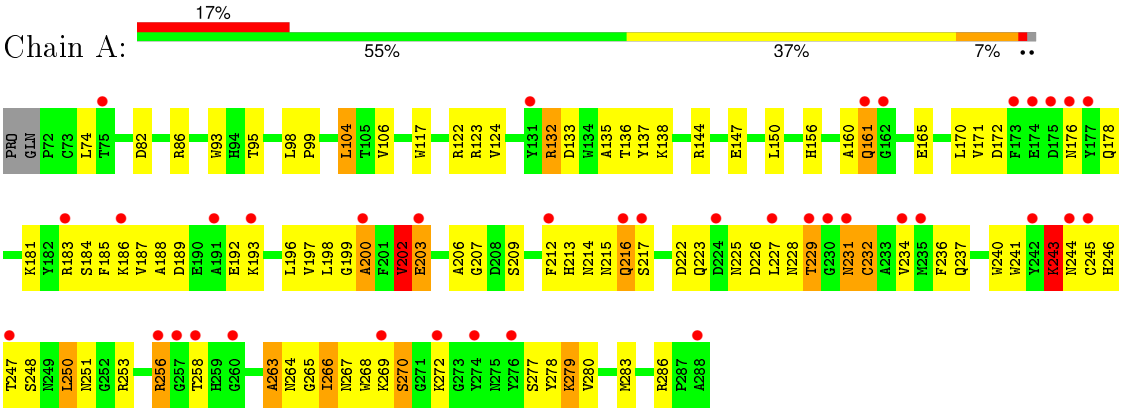
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	22	Total O 22 22	0	0
5	F	29	Total O 29 29	0	0

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.

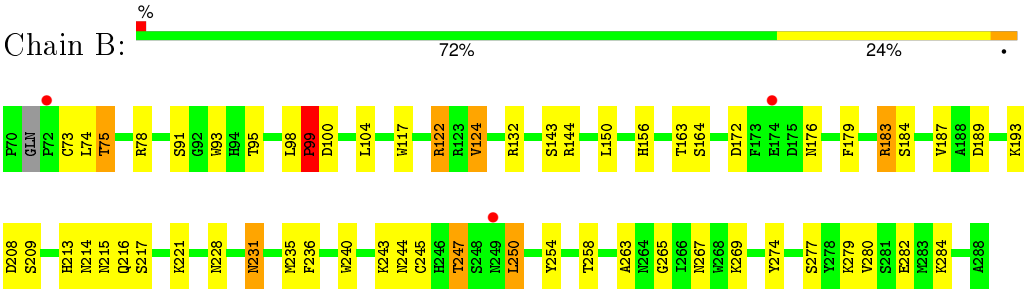
- Molecule 1: FICOLIN-2

Chain A:



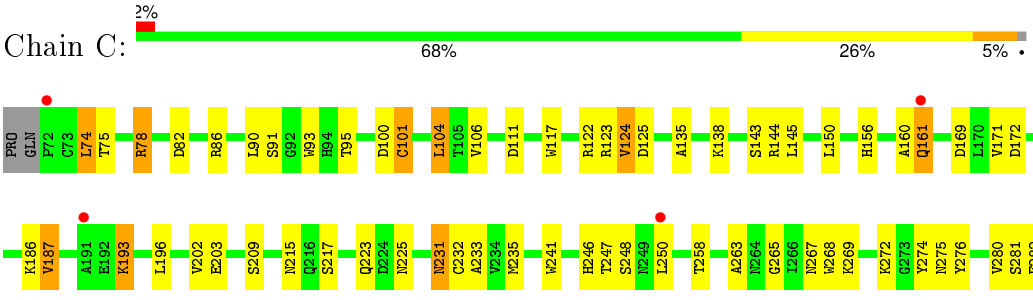
- Molecule 1: FICOLIN-2

Chain B:



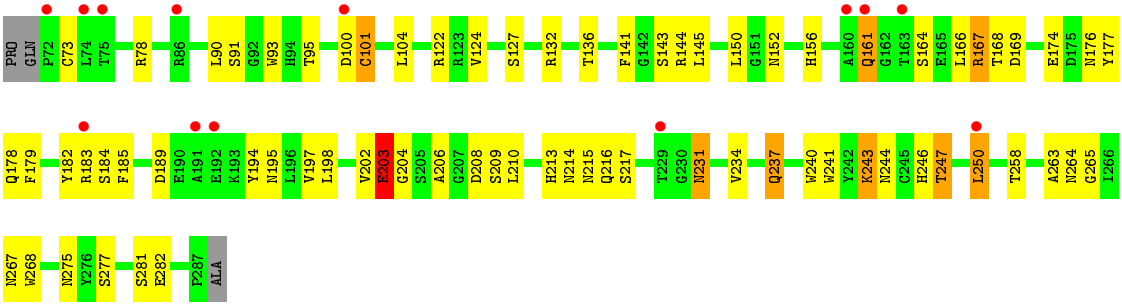
- Molecule 1: FICOLIN-2

Chain C:



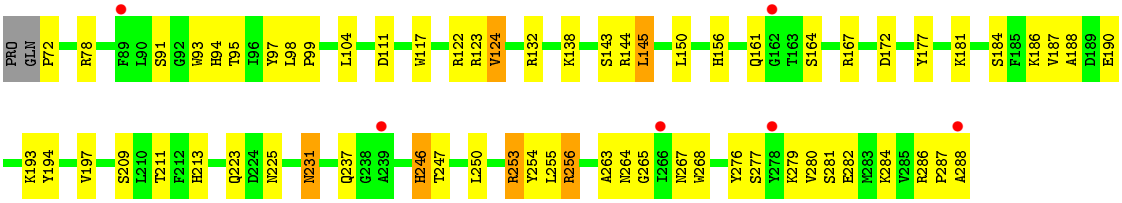
- Molecule 1: FICOLIN-2

Chain D:



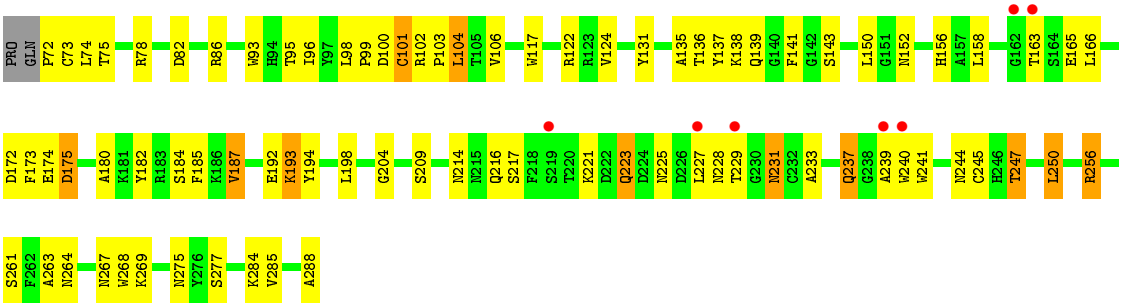
- Molecule 1: FICOLIN-2

Chain E:



- Molecule 1: FICOLIN-2

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	200.52Å 84.51Å 144.09Å 90.00° 123.57° 90.00°	Depositor
Resolution (Å)	19.00 – 2.65 19.75 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.00-2.65) 99.1 (19.75-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 2.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.228 , 0.283 0.230 , 0.281	Depositor DCC
R_{free} test set	5886 reflections (11.33%)	DCC
Wilson B-factor (Å^2)	58.6	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 37.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 57851 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10716	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: CA, NAG, ACT

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	0.92	0/1783	0.74	0/2413
1	B	0.70	0/1801	0.72	0/2436
1	C	0.59	0/1783	0.68	0/2413
1	D	0.63	0/1778	0.66	1/2406 (0.0%)
1	E	0.57	0/1783	0.65	0/2413
1	F	0.58	1/1783 (0.1%)	0.68	0/2413
All	All	0.67	1/10711 (0.0%)	0.69	1/14494 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	101	CYS	CB-SG	-5.02	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	167	ARG	NE-CZ-NH1	-6.38	117.11	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1735	0	1607	107	0
1	B	1753	0	1627	53	0
1	C	1735	0	1607	54	0
1	D	1730	0	1604	63	0
1	E	1735	0	1606	44	0
1	F	1735	0	1607	62	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	B	8	0	6	2	0
4	B	44	0	43	5	0
4	C	30	0	30	8	0
4	D	15	0	15	5	0
4	E	44	0	43	12	0
5	A	19	0	0	2	0
5	B	25	0	0	6	0
5	C	31	0	0	1	0
5	D	20	0	0	7	0
5	E	22	0	0	4	0
5	F	29	0	0	5	0
All	All	10716	0	9795	387	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 19.

All (387) 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:F:158:LEU:HG	5:F:2017:HOH:O	1.43	1.17
1:A:227:LEU:O	1:A:244:ASN:HB2	1.44	1.15
4:C:1289:NAG:H83	4:C:1289:NAG:H3	1.26	1.10
1:D:241:TRP:HE3	5:D:2016:HOH:O	1.40	1.01
1:A:202:VAL:O	1:A:203:GLU:HG2	1.64	0.97
1:A:228:ASN:ND2	1:A:229:THR:H	1.63	0.96
1:B:78:ARG:HD2	5:B:2002:HOH:O	1.68	0.94
1:A:256:ARG:HG3	1:A:256:ARG:HH11	1.31	0.93
4:C:1289:NAG:C8	4:C:1289:NAG:H3	1.95	0.91
1:E:78:ARG:NH1	5:E:2002:HOH:O	1.96	0.90
4:C:1289:NAG:C3	4:C:1289:NAG:H83	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ARG:HH11	1:B:183:ARG:HG3	1.39	0.88
1:C:269:LYS:HD3	1:C:274:TYR:CE2	2.08	0.88
1:F:231:ASN:HD22	1:F:231:ASN:C	1.71	0.88
1:A:98:LEU:HB3	1:A:99:PRO:HD2	1.55	0.87
1:C:161:GLN:HE21	1:C:161:GLN:HA	1.38	0.87
1:B:215:ASN:HD21	4:B:1293:NAG:C1	1.88	0.87
1:A:212:PHE:CE1	1:A:243:LYS:HE3	2.10	0.86
1:F:223:GLN:NE2	1:F:225:ASN:HD21	1.74	0.85
1:F:193:LYS:HB3	1:F:217:SER:HB3	1.57	0.84
1:A:206:ALA:O	1:A:270:SER:HB2	1.77	0.83
1:A:228:ASN:HD22	1:A:229:THR:H	1.26	0.83
1:B:183:ARG:HH11	1:B:183:ARG:CG	1.92	0.83
4:E:1292:NAG:C8	4:E:1292:NAG:O1	2.27	0.81
1:A:231:ASN:HB2	1:A:234:VAL:CG2	2.11	0.81
1:A:178:GLN:HB3	1:A:206:ALA:HB2	1.63	0.81
1:F:223:GLN:HE22	1:F:225:ASN:HD21	1.29	0.80
1:A:231:ASN:HB2	1:A:234:VAL:HG23	1.64	0.80
1:E:231:ASN:HD22	1:E:231:ASN:C	1.86	0.79
1:A:266:ILE:HD11	1:A:278:TYR:O	1.81	0.78
1:E:72:PRO:HB2	1:E:97:TYR:OH	1.84	0.78
1:A:231:ASN:CB	1:A:234:VAL:HG23	2.13	0.78
1:D:143:SER:OG	4:E:1289:NAG:O1	2.00	0.77
1:A:196:LEU:HB2	1:A:241:TRP:CD1	2.19	0.77
1:A:171:VAL:HB	1:A:280:VAL:HB	1.67	0.77
1:D:198:LEU:H	1:D:214:ASN:ND2	1.81	0.77
4:E:1292:NAG:O1	4:E:1292:NAG:H83	1.83	0.77
1:B:213:HIS:HA	5:B:2017:HOH:O	1.85	0.76
1:A:240:TRP:CH2	1:A:250:LEU:HB2	2.21	0.76
1:A:216:GLN:OE1	1:A:243:LYS:HG2	1.85	0.76
1:A:226:ASP:OD2	1:A:232:CYS:HB2	1.85	0.76
1:D:100:ASP:O	1:D:101:CYS:HB2	1.86	0.75
1:A:82:ASP:O	1:A:86:ARG:HG3	1.86	0.75
1:E:237:GLN:NE2	1:E:264:ASN:HD22	1.84	0.74
1:D:203:GLU:HG2	1:D:204:GLY:N	2.02	0.74
1:F:173:PHE:CE1	1:F:256:ARG:O	2.41	0.73
1:F:216:GLN:HE22	1:F:227:LEU:HD23	1.54	0.73
1:C:117:TRP:HB3	1:C:284:LYS:HG3	1.70	0.73
1:A:144:ARG:NH2	3:B:1289:ACT:H2	2.03	0.73
1:A:216:GLN:CD	1:A:243:LYS:HB3	2.09	0.73
1:E:122:ARG:HG3	1:E:282:GLU:HG2	1.69	0.72
1:B:216:GLN:HG2	1:B:243:LYS:NZ	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LYS:HG3	1:A:280:VAL:HG23	1.71	0.71
1:A:212:PHE:HD1	1:A:243:LYS:NZ	1.88	0.71
1:B:216:GLN:HG2	1:B:243:LYS:HZ1	1.54	0.71
1:A:212:PHE:HE1	1:A:243:LYS:HE3	1.56	0.70
1:F:104:LEU:HD13	1:F:106:VAL:CG1	2.21	0.70
1:A:212:PHE:CD1	1:A:243:LYS:HE3	2.26	0.70
1:A:228:ASN:ND2	1:A:229:THR:N	2.38	0.70
1:A:244:ASN:N	1:A:245:CYS:HA	2.05	0.70
1:F:138:LYS:HA	1:F:152:ASN:HB2	1.73	0.70
4:D:1288:NAG:H3	5:D:2020:HOH:O	1.93	0.69
1:B:228:ASN:HD22	1:B:244:ASN:ND2	1.90	0.69
1:D:231:ASN:ND2	1:D:234:VAL:H	1.89	0.69
1:C:100:ASP:O	1:C:101:CYS:HB2	1.93	0.68
1:A:212:PHE:HD1	1:A:243:LYS:HZ2	1.39	0.68
1:B:172:ASP:OD2	1:B:176:ASN:HB2	1.93	0.68
1:F:231:ASN:C	1:F:231:ASN:ND2	2.46	0.67
1:E:209:SER:HB2	1:E:268:TRP:CE2	2.29	0.67
1:A:132:ARG:HG3	1:A:136:THR:HG21	1.78	0.66
1:E:167:ARG:NH2	1:E:177:TYR:OH	2.25	0.66
1:B:269:LYS:HD2	1:B:274:TYR:CE2	2.31	0.66
1:A:172:ASP:HB3	1:A:272:LYS:HE3	1.77	0.66
1:D:198:LEU:H	1:D:214:ASN:HD21	1.42	0.66
1:D:231:ASN:HD22	1:D:234:VAL:H	1.42	0.66
1:A:144:ARG:HH21	3:B:1289:ACT:H2	1.60	0.66
1:F:209:SER:HB2	1:F:268:TRP:CE2	2.32	0.65
1:B:183:ARG:NH1	1:B:183:ARG:CG	2.57	0.65
4:E:1292:NAG:O1	4:E:1292:NAG:H82	1.96	0.65
1:B:156:HIS:HD2	1:B:187:VAL:O	1.79	0.65
1:A:243:LYS:HD2	1:A:243:LYS:O	1.97	0.65
1:E:143:SER:HG	4:E:1292:NAG:HO1	1.45	0.64
1:A:227:LEU:O	1:A:244:ASN:CB	2.35	0.64
1:E:223:GLN:HE21	1:E:225:ASN:HD21	1.45	0.64
1:A:256:ARG:HG3	1:A:256:ARG:NH1	2.09	0.64
1:F:275:ASN:ND2	5:F:2028:HOH:O	2.12	0.64
1:B:98:LEU:HB3	1:B:99:PRO:HD2	1.78	0.63
4:E:1292:NAG:C1	4:E:1292:NAG:C8	2.76	0.63
1:F:98:LEU:HB3	1:F:99:PRO:HD2	1.81	0.62
1:A:256:ARG:CG	1:A:256:ARG:HH11	2.09	0.62
1:D:122:ARG:NH2	4:D:1288:NAG:O3	2.29	0.62
1:B:198:LEU:H	1:B:214:ASN:ND2	1.97	0.62
1:D:237:GLN:HE21	1:D:264:ASN:HD22	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:GLN:HB3	1:D:206:ALA:HB2	1.81	0.62
1:E:287:PRO:O	1:E:288:ALA:O	2.18	0.62
1:B:91:SER:HB3	4:B:1290[B]:NAG:H82	1.82	0.61
1:F:228:ASN:ND2	1:F:229:THR:N	2.48	0.61
1:D:265:GLY:H	1:D:267:ASN:HD21	1.48	0.61
1:D:152:ASN:HB3	1:D:194:TYR:CD1	2.35	0.61
1:B:265:GLY:H	1:B:267:ASN:HD21	1.45	0.61
1:D:73:CYS:HB3	1:D:101:CYS:SG	2.41	0.61
1:F:100:ASP:O	1:F:101:CYS:HB2	2.01	0.61
1:D:167:ARG:NH1	1:D:179:PHE:CD2	2.70	0.60
1:D:183:ARG:HG3	1:D:202:VAL:CG2	2.31	0.60
1:A:202:VAL:O	1:A:203:GLU:CG	2.46	0.60
1:D:167:ARG:NH2	1:D:177:TYR:OH	2.35	0.59
1:A:165:GLU:OE1	1:A:181:LYS:HE2	2.02	0.59
1:C:231:ASN:C	1:C:231:ASN:HD22	2.05	0.59
1:C:209:SER:HB3	1:C:247:THR:HG22	1.84	0.59
1:F:223:GLN:NE2	1:F:225:ASN:ND2	2.48	0.59
1:D:174:GLU:HA	5:D:2010:HOH:O	2.03	0.59
1:B:243:LYS:HD2	5:B:2017:HOH:O	2.01	0.59
1:E:223:GLN:NE2	1:E:225:ASN:HD21	2.01	0.59
4:E:1292:NAG:H1	1:F:122:ARG:NH2	2.17	0.58
1:D:231:ASN:HD22	1:D:231:ASN:C	2.06	0.58
1:B:156:HIS:CD2	1:B:187:VAL:O	2.56	0.58
1:D:246:HIS:HE1	1:D:263:ALA:O	1.86	0.58
1:A:216:GLN:OE1	1:A:243:LYS:HB3	2.04	0.58
1:F:217:SER:O	1:F:241:TRP:HA	2.03	0.58
1:F:198:LEU:H	1:F:214:ASN:ND2	2.02	0.58
4:E:1292:NAG:C1	4:E:1292:NAG:H83	2.33	0.58
1:B:231:ASN:N	1:B:235:MET:HE2	2.19	0.57
1:A:198:LEU:H	1:A:214:ASN:HD22	1.52	0.57
1:F:198:LEU:H	1:F:214:ASN:HD21	1.51	0.57
1:C:209:SER:HB2	1:C:268:TRP:CE2	2.40	0.57
1:F:72:PRO:O	1:F:73:CYS:C	2.42	0.57
1:A:272:LYS:HG2	1:A:278:TYR:OH	2.04	0.57
1:D:209:SER:HB3	1:D:247:THR:HG22	1.85	0.57
1:F:209:SER:HB3	1:F:247:THR:HG23	1.87	0.57
1:B:117:TRP:HB3	1:B:284:LYS:HB2	1.86	0.57
1:A:209:SER:HB2	1:A:268:TRP:CE2	2.40	0.56
1:D:93:TRP:CZ2	1:D:144:ARG:HA	2.41	0.56
1:D:166:LEU:HD22	1:D:185:PHE:CD1	2.39	0.56
1:A:237:GLN:HE21	1:A:264:ASN:HD22	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ARG:CD	1:A:200:ALA:HB3	2.34	0.56
1:C:282:GLU:OE2	4:C:1290:NAG:H2	2.06	0.56
1:C:171:VAL:HB	1:C:280:VAL:HB	1.87	0.56
1:A:212:PHE:CD1	1:A:243:LYS:CE	2.89	0.55
1:A:198:LEU:HG	1:A:199:GLY:H	1.70	0.55
1:D:213:HIS:CE1	1:D:246:HIS:HA	2.42	0.55
1:A:183:ARG:HD2	1:A:200:ALA:HB3	1.87	0.55
1:F:137:TYR:CZ	1:F:239:ALA:HB3	2.42	0.55
1:A:272:LYS:HG2	1:A:278:TYR:CZ	2.42	0.55
1:B:243:LYS:HB2	5:B:2017:HOH:O	2.06	0.55
1:F:165:GLU:HG3	1:F:288:ALA:HB2	1.88	0.55
1:D:174:GLU:CA	5:D:2010:HOH:O	2.54	0.54
1:F:165:GLU:O	1:F:285:VAL:HA	2.07	0.54
1:C:145:LEU:HD12	4:C:1289:NAG:H1	1.89	0.54
1:D:258:THR:HA	1:D:275:ASN:O	2.07	0.54
1:B:93:TRP:CZ2	1:B:144:ARG:HA	2.43	0.54
1:A:243:LYS:O	1:A:244:ASN:C	2.46	0.54
1:A:98:LEU:HB3	1:A:99:PRO:CD	2.35	0.54
1:A:243:LYS:O	1:A:243:LYS:CD	2.55	0.54
1:A:217:SER:HB2	1:A:225:ASN:HB3	1.89	0.54
1:F:231:ASN:HD21	1:F:233:ALA:HB3	1.72	0.54
1:D:213:HIS:HE1	1:D:246:HIS:HA	1.73	0.54
1:F:228:ASN:HD22	1:F:229:THR:H	1.55	0.54
1:D:282:GLU:OE2	4:D:1288:NAG:H2	2.08	0.54
1:E:98:LEU:HB3	1:E:99:PRO:HD2	1.90	0.54
1:B:215:ASN:ND2	4:B:1293:NAG:C1	2.66	0.53
1:C:209:SER:O	1:C:248:SER:HB3	2.09	0.53
1:B:156:HIS:CE1	1:B:189:ASP:HB3	2.42	0.53
1:A:202:VAL:O	1:A:202:VAL:HG13	2.08	0.53
1:C:160:ALA:HA	1:C:186:LYS:NZ	2.23	0.53
1:B:184:SER:OG	5:B:2015:HOH:O	2.19	0.53
1:D:132:ARG:NH2	1:E:111:ASP:OD2	2.41	0.52
1:A:188:ALA:HB1	1:A:192:GLU:HB2	1.91	0.52
1:C:258:THR:HA	1:C:275:ASN:O	2.09	0.52
1:C:169:ASP:OD2	1:C:284:LYS:NZ	2.35	0.52
1:C:117:TRP:CB	1:C:284:LYS:HG3	2.39	0.52
1:A:93:TRP:CZ2	1:A:144:ARG:HA	2.44	0.52
1:A:228:ASN:HD22	1:A:229:THR:N	1.99	0.52
1:F:158:LEU:N	5:F:2017:HOH:O	2.43	0.51
1:D:152:ASN:HB3	1:D:194:TYR:CE1	2.45	0.51
1:D:156:HIS:CE1	1:D:189:ASP:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ASN:ND2	1:B:244:ASN:ND2	2.58	0.51
1:B:164:SER:O	1:B:184:SER:HA	2.10	0.51
1:C:193:LYS:HB3	1:C:217:SER:HB3	1.92	0.51
1:B:209:SER:HB3	1:B:247:THR:HG23	1.91	0.51
1:D:217:SER:O	1:D:241:TRP:HA	2.10	0.51
1:B:198:LEU:H	1:B:214:ASN:HD21	1.59	0.51
1:A:231:ASN:HB3	1:A:234:VAL:HG23	1.90	0.51
1:E:287:PRO:O	1:E:288:ALA:C	2.48	0.51
1:F:82:ASP:O	1:F:86:ARG:HG3	2.10	0.51
1:C:74:LEU:O	1:C:75:THR:OG1	2.13	0.51
1:F:256:ARG:O	1:F:277:SER:O	2.29	0.51
1:B:91:SER:HB3	4:B:1290[B]:NAG:C8	2.41	0.51
1:D:168:THR:O	1:D:179:PHE:HA	2.11	0.51
1:E:286:ARG:HG3	1:E:287:PRO:HD2	1.93	0.51
1:E:122:ARG:HH12	4:E:1289:NAG:H5	1.76	0.50
1:D:169:ASP:OD1	1:D:177:TYR:OH	2.25	0.50
1:F:98:LEU:HB3	1:F:99:PRO:CD	2.40	0.50
1:E:186:LYS:HG2	1:E:197:VAL:HB	1.93	0.50
1:B:132:ARG:NH2	1:C:111:ASP:OD2	2.44	0.50
1:A:132:ARG:HB2	1:A:137:TYR:CE1	2.46	0.50
1:C:75:THR:O	1:C:86:ARG:NH2	2.36	0.50
1:D:246:HIS:CE1	1:D:263:ALA:O	2.65	0.50
1:B:265:GLY:H	1:B:267:ASN:ND2	2.10	0.50
1:B:231:ASN:HD22	1:B:231:ASN:C	2.14	0.50
1:B:73:CYS:SG	1:B:75:THR:HB	2.52	0.50
1:A:135:ALA:O	1:A:138:LYS:HB3	2.12	0.49
1:A:196:LEU:HD13	1:A:196:LEU:C	2.33	0.49
1:D:195:ASN:HD21	1:D:215:ASN:C	2.15	0.49
1:E:231:ASN:C	1:E:231:ASN:ND2	2.59	0.49
1:C:156:HIS:HD2	1:C:187:VAL:O	1.95	0.49
1:F:263:ALA:HA	1:F:267:ASN:ND2	2.28	0.49
1:A:104:LEU:HD13	1:A:106:VAL:CG1	2.43	0.49
1:A:202:VAL:CG1	1:A:202:VAL:O	2.61	0.49
1:D:100:ASP:O	1:D:101:CYS:CB	2.58	0.49
1:E:93:TRP:CE2	1:E:144:ARG:HG2	2.48	0.49
1:A:165:GLU:OE1	1:A:181:LYS:CE	2.61	0.49
1:E:263:ALA:HA	1:E:267:ASN:ND2	2.27	0.49
1:A:156:HIS:HD2	1:A:187:VAL:O	1.96	0.49
1:A:212:PHE:HD1	1:A:243:LYS:CE	2.26	0.49
1:C:247:THR:HG23	1:C:269:LYS:HB3	1.95	0.48
1:B:240:TRP:CH2	1:B:250:LEU:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:SER:HB2	1:E:91:SER:HB2	1.96	0.48
1:E:237:GLN:NE2	1:E:253:ARG:HE	2.11	0.48
1:D:237:GLN:HG3	1:D:264:ASN:HB2	1.95	0.48
1:C:78:ARG:HD3	1:C:82:ASP:OD2	2.13	0.48
1:C:246:HIS:CE1	1:C:263:ALA:HB1	2.49	0.48
1:A:123:ARG:NH1	1:A:251:ASN:HA	2.29	0.48
1:F:261:SER:HB3	1:F:264:ASN:HD21	1.77	0.48
1:A:117:TRP:HZ2	1:A:286:ARG:HH21	1.50	0.48
1:F:228:ASN:ND2	1:F:229:THR:H	2.11	0.48
1:E:246:HIS:HE1	1:E:263:ALA:O	1.96	0.48
1:C:161:GLN:NE2	1:C:161:GLN:HA	2.20	0.48
1:E:132:ARG:HD2	5:E:2012:HOH:O	2.13	0.48
1:F:131:TYR:CE1	1:F:237:GLN:HA	2.49	0.48
1:F:152:ASN:HB3	1:F:194:TYR:CD1	2.49	0.47
1:F:244:ASN:N	1:F:245:CYS:HA	2.28	0.47
1:A:216:GLN:OE1	1:A:243:LYS:CG	2.58	0.47
1:C:202:VAL:HG12	1:C:203:GLU:HG2	1.96	0.47
1:F:104:LEU:HD13	1:F:106:VAL:HG13	1.97	0.47
1:D:241:TRP:CE3	5:D:2016:HOH:O	2.31	0.47
1:F:131:TYR:O	1:F:221:LYS:HE2	2.15	0.47
1:A:186:LYS:HG2	1:A:197:VAL:HB	1.96	0.47
1:E:181:LYS:HG2	5:E:2015:HOH:O	2.14	0.47
1:F:228:ASN:HD22	1:F:229:THR:N	2.12	0.47
1:D:209:SER:HB2	1:D:268:TRP:CE2	2.50	0.47
1:E:164:SER:O	1:E:184:SER:HA	2.14	0.47
1:C:169:ASP:OD1	1:C:177:TYR:OH	2.18	0.47
1:A:213:HIS:HE1	1:A:246:HIS:HA	1.79	0.47
1:A:231:ASN:CB	1:A:234:VAL:CG2	2.82	0.47
1:D:231:ASN:C	1:D:231:ASN:ND2	2.67	0.47
1:F:135:ALA:O	1:F:139:GLN:HB2	2.14	0.47
1:B:215:ASN:HD21	4:B:1293:NAG:C2	2.28	0.46
1:A:170:LEU:HD23	1:A:278:TYR:CE1	2.50	0.46
1:E:246:HIS:CE1	1:E:263:ALA:HB1	2.50	0.46
1:F:78:ARG:HB3	5:F:2006:HOH:O	2.16	0.46
1:D:265:GLY:H	1:D:267:ASN:ND2	2.13	0.46
1:A:185:PHE:C	1:A:185:PHE:CD1	2.88	0.46
1:A:196:LEU:HD12	1:A:214:ASN:HA	1.96	0.46
1:C:223:GLN:HE21	1:C:225:ASN:HD21	1.63	0.46
1:C:82:ASP:O	1:C:86:ARG:HG3	2.14	0.46
1:A:263:ALA:HA	1:A:267:ASN:ND2	2.31	0.46
1:A:256:ARG:NH1	1:A:256:ARG:CG	2.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:SER:HB3	1:D:247:THR:CG2	2.46	0.46
1:E:145:LEU:HB2	4:E:1292:NAG:HO1	1.81	0.46
1:A:189:ASP:O	1:A:193:LYS:O	2.33	0.46
1:D:282:GLU:CD	4:D:1288:NAG:H2	2.35	0.46
1:D:208:ASP:OD1	1:D:208:ASP:C	2.54	0.46
1:F:192:GLU:O	1:F:192:GLU:HG2	2.16	0.46
1:D:145:LEU:HB2	4:E:1289:NAG:O1	2.16	0.45
1:B:214:ASN:O	1:B:215:ASN:CB	2.65	0.45
1:B:221:LYS:HG2	5:B:2009:HOH:O	2.16	0.45
1:F:98:LEU:HD22	5:F:2017:HOH:O	2.17	0.45
1:D:73:CYS:CB	1:D:101:CYS:SG	3.04	0.45
1:D:136:THR:HG22	1:D:141:PHE:CD2	2.52	0.45
1:C:178:GLN:HE22	1:C:272:LYS:HD3	1.80	0.45
1:E:99:PRO:HG3	1:E:161:GLN:NE2	2.31	0.45
1:F:152:ASN:HB3	1:F:194:TYR:CE1	2.50	0.45
1:A:123:ARG:HA	1:A:147:GLU:HG2	1.98	0.45
1:C:145:LEU:HB2	4:C:1289:NAG:O1	2.16	0.45
1:D:127:SER:HB2	4:E:1289:NAG:H4	1.97	0.45
1:E:255:LEU:O	1:E:277:SER:HB3	2.17	0.45
1:E:156:HIS:HD2	1:E:187:VAL:O	2.00	0.45
1:A:247:THR:HG23	1:A:269:LYS:HD3	1.99	0.45
1:A:170:LEU:HD23	1:A:278:TYR:CZ	2.51	0.45
1:E:237:GLN:HE21	1:E:264:ASN:HD22	1.61	0.45
1:F:240:TRP:CH2	1:F:250:LEU:HB2	2.51	0.45
1:A:196:LEU:HB2	1:A:241:TRP:CG	2.52	0.45
1:E:254:TYR:OH	1:E:279:LYS:O	2.35	0.45
1:A:266:ILE:CD1	1:A:278:TYR:O	2.58	0.45
1:B:124:VAL:O	1:B:254:TYR:OH	2.32	0.45
1:B:216:GLN:HG3	1:B:243:LYS:HG3	1.99	0.44
1:A:240:TRP:NE1	1:A:248:SER:O	2.50	0.44
1:D:240:TRP:CH2	1:D:250:LEU:HB2	2.52	0.44
1:A:198:LEU:H	1:A:214:ASN:ND2	2.13	0.44
1:C:231:ASN:HD22	1:C:232:CYS:N	2.15	0.44
1:A:213:HIS:CE1	1:A:246:HIS:HA	2.52	0.44
1:B:279:LYS:HG2	1:B:280:VAL:HG23	1.99	0.44
1:E:123:ARG:O	1:E:280:VAL:HA	2.18	0.44
1:E:213:HIS:CE1	1:E:246:HIS:HA	2.53	0.44
1:C:246:HIS:C	1:C:246:HIS:CD2	2.91	0.44
1:C:135:ALA:O	1:C:138:LYS:HB3	2.18	0.44
1:A:93:TRP:CE2	1:A:144:ARG:HG2	2.52	0.44
1:C:122:ARG:HD2	1:C:282:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:LYS:NZ	1:C:223:GLN:NE2	2.65	0.44
1:A:199:GLY:HA2	5:A:2013:HOH:O	2.17	0.44
1:F:261:SER:CB	1:F:264:ASN:HD21	2.31	0.44
1:F:172:ASP:C	1:F:172:ASP:OD1	2.57	0.44
1:B:228:ASN:ND2	1:B:244:ASN:HD21	2.16	0.43
1:F:268:TRP:O	1:F:269:LYS:C	2.56	0.43
1:A:161:GLN:HE21	1:A:161:GLN:HB3	1.60	0.43
1:E:190:GLU:O	1:E:193:LYS:N	2.36	0.43
1:A:207:GLY:HA3	1:A:270:SER:CB	2.49	0.43
1:A:156:HIS:NE2	1:A:189:ASP:HB3	2.33	0.43
1:D:250:LEU:HD12	1:D:250:LEU:HA	1.90	0.43
1:A:283:MET:HB3	1:A:283:MET:HE2	1.65	0.43
1:C:196:LEU:HB2	1:C:241:TRP:CD1	2.53	0.43
1:A:240:TRP:CZ3	1:A:250:LEU:HB2	2.54	0.43
1:A:251:ASN:N	5:A:2018:HOH:O	2.45	0.43
1:C:265:GLY:H	1:C:267:ASN:HD21	1.67	0.43
1:B:243:LYS:HB3	1:B:244:ASN:H	1.68	0.43
1:B:236:PHE:HE2	1:B:245:CYS:SG	2.42	0.43
1:E:265:GLY:H	1:E:267:ASN:HD21	1.67	0.43
1:E:138:LYS:HG3	1:E:194:TYR:OH	2.19	0.43
1:B:122:ARG:HD2	1:B:282:GLU:OE2	2.19	0.43
1:B:263:ALA:HA	1:B:267:ASN:ND2	2.35	0.42
1:B:193:LYS:HB3	1:B:217:SER:HB3	2.00	0.42
1:D:91:SER:HB2	1:F:143:SER:HB2	2.01	0.42
1:B:208:ASP:OD1	1:B:208:ASP:C	2.57	0.42
1:F:174:GLU:O	1:F:175:ASP:HB2	2.19	0.42
1:D:197:VAL:O	1:D:197:VAL:HG12	2.17	0.42
1:C:93:TRP:CZ2	1:C:144:ARG:HA	2.53	0.42
1:F:216:GLN:OE1	1:F:216:GLN:HA	2.18	0.42
1:C:231:ASN:ND2	1:C:233:ALA:H	2.16	0.42
1:C:123:ARG:HB2	1:C:281:SER:HB3	2.02	0.42
1:C:193:LYS:HZ1	1:C:223:GLN:NE2	2.18	0.42
1:F:136:THR:HG22	1:F:141:PHE:CD1	2.55	0.42
1:B:244:ASN:N	1:B:245:CYS:HA	2.35	0.42
1:A:247:THR:HG23	1:A:269:LYS:CD	2.49	0.42
1:A:132:ARG:HB2	1:A:137:TYR:HE1	1.84	0.42
1:C:282:GLU:OE1	4:C:1290:NAG:H2	2.19	0.42
1:C:217:SER:O	1:C:241:TRP:HA	2.20	0.42
1:E:246:HIS:C	1:E:246:HIS:CD2	2.92	0.42
1:D:243:LYS:HB3	1:D:244:ASN:H	1.64	0.42
1:A:172:ASP:OD2	1:A:176:ASN:ND2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:LEU:O	1:C:75:THR:CB	2.68	0.42
1:F:102:ARG:HA	1:F:103:PRO:HD3	1.93	0.42
1:A:266:ILE:HG13	1:A:278:TYR:N	2.34	0.42
1:F:156:HIS:HD2	1:F:187:VAL:O	2.03	0.42
1:B:244:ASN:HA	1:B:245:CYS:HA	1.95	0.41
1:C:74:LEU:HD12	1:C:74:LEU:HA	1.88	0.41
1:C:74:LEU:C	1:C:75:THR:HG23	2.40	0.41
1:E:211:THR:C	1:E:213:HIS:N	2.73	0.41
1:C:246:HIS:HE1	1:C:263:ALA:O	2.02	0.41
1:D:182:TYR:N	1:D:182:TYR:CD1	2.88	0.41
1:B:143:SER:HB2	1:C:91:SER:HB2	2.01	0.41
1:A:93:TRP:CD2	1:A:144:ARG:HG2	2.55	0.41
1:F:166:LEU:HD22	1:F:185:PHE:CD1	2.54	0.41
1:C:231:ASN:C	1:C:231:ASN:ND2	2.72	0.41
1:D:174:GLU:N	5:D:2010:HOH:O	2.53	0.41
1:E:94:HIS:HD2	5:E:2007:HOH:O	2.02	0.41
1:C:104:LEU:HD13	1:C:106:VAL:CG1	2.50	0.41
1:E:117:TRP:HB3	1:E:284:LYS:HB2	2.01	0.41
1:A:216:GLN:OE1	1:A:243:LYS:CB	2.68	0.41
1:B:228:ASN:HD22	1:B:244:ASN:HD21	1.64	0.41
1:C:100:ASP:O	1:C:101:CYS:CB	2.65	0.41
1:A:237:GLN:OE1	1:A:253:ARG:NH2	2.53	0.41
1:F:96:ILE:HD11	1:F:158:LEU:HD21	2.02	0.41
1:D:216:GLN:HG2	1:D:243:LYS:HD3	2.02	0.41
1:B:179:PHE:O	1:B:204:GLY:HA3	2.20	0.41
1:D:241:TRP:HB2	5:D:2016:HOH:O	2.21	0.41
1:A:172:ASP:OD1	1:A:172:ASP:C	2.60	0.41
1:A:250:LEU:HA	1:A:250:LEU:HD12	1.78	0.41
1:D:73:CYS:O	1:D:73:CYS:SG	2.79	0.41
1:A:209:SER:HB2	1:A:268:TRP:CD2	2.55	0.41
1:D:210:LEU:HD12	1:D:210:LEU:HA	1.81	0.41
1:A:266:ILE:HG12	1:A:277:SER:HB2	2.03	0.41
1:F:182:TYR:CD2	1:F:198:LEU:HD21	2.57	0.40
1:F:72:PRO:O	1:F:74:LEU:N	2.54	0.40
1:F:117:TRP:HB3	1:F:284:LYS:HB2	2.03	0.40
1:E:256:ARG:HG3	1:E:256:ARG:HH11	1.85	0.40
1:F:180:ALA:HA	1:F:204:GLY:HA3	2.03	0.40
1:F:93:TRP:HA	1:F:106:VAL:O	2.21	0.40
1:A:117:TRP:CZ2	1:A:286:ARG:NH2	2.74	0.40
1:C:172:ASP:HB2	1:C:276:TYR:OH	2.22	0.40
1:A:236:PHE:O	1:A:237:GLN:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:GLY:H	1:A:267:ASN:HD21	1.68	0.40
1:A:133:ASP:OD1	1:A:133:ASP:C	2.59	0.40
1:E:172:ASP:HB2	1:E:276:TYR:OH	2.21	0.40
1:C:215:ASN:ND2	5:C:2023:HOH:O	2.54	0.40
1:C:143:SER:OG	4:C:1289:NAG:O1	2.09	0.40
1:D:282:GLU:OE1	4:D:1288:NAG:H2	2.21	0.40
1:D:161:GLN:HA	1:D:161:GLN:HE21	1.86	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	215/219 (98%)	177 (82%)	30 (14%)	8 (4%)	4 8
1	B	216/219 (99%)	196 (91%)	19 (9%)	1 (0%)	34 59
1	C	215/219 (98%)	199 (93%)	14 (6%)	2 (1%)	21 44
1	D	214/219 (98%)	188 (88%)	23 (11%)	3 (1%)	14 31
1	E	215/219 (98%)	195 (91%)	17 (8%)	3 (1%)	14 31
1	F	215/219 (98%)	189 (88%)	26 (12%)	0	100 100
All	All	1290/1314 (98%)	1144 (89%)	129 (10%)	17 (1%)	15 33

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	GLU
1	A	160	ALA
1	A	215	ASN
1	A	243	LYS
1	D	101	CYS

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Mol	Chain	Res	Type
1	D	203	GLU
1	E	188	ALA
1	E	256	ARG
1	A	200	ALA
1	A	202	VAL
1	A	263	ALA
1	B	99	PRO
1	C	125	ASP
1	A	124	VAL
1	D	124	VAL
1	C	124	VAL
1	E	124	VAL

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	182/184 (99%)	160 (88%)	22 (12%)	6 12
1	B	184/184 (100%)	168 (91%)	16 (9%)	13 26
1	C	182/184 (99%)	166 (91%)	16 (9%)	12 25
1	D	182/184 (99%)	165 (91%)	17 (9%)	11 23
1	E	182/184 (99%)	171 (94%)	11 (6%)	24 47
1	F	182/184 (99%)	166 (91%)	16 (9%)	12 25
All	All	1094/1104 (99%)	996 (91%)	98 (9%)	12 24

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LEU
1	A	95	THR
1	A	104	LEU
1	A	122	ARG
1	A	132	ARG
1	A	150	LEU

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Mol	Chain	Res	Type
1	A	161	GLN
1	A	184	SER
1	A	202	VAL
1	A	216	GLN
1	A	222	ASP
1	A	223	GLN
1	A	229	THR
1	A	231	ASN
1	A	232	CYS
1	A	243	LYS
1	A	250	LEU
1	A	256	ARG
1	A	258	THR
1	A	266	ILE
1	A	270	SER
1	A	279	LYS
1	B	74	LEU
1	B	75	THR
1	B	95	THR
1	B	99	PRO
1	B	100	ASP
1	B	104	LEU
1	B	122	ARG
1	B	124	VAL
1	B	150	LEU
1	B	163	THR
1	B	183	ARG
1	B	231	ASN
1	B	247	THR
1	B	250	LEU
1	B	258	THR
1	B	277	SER
1	C	74	LEU
1	C	78	ARG
1	C	90	LEU
1	C	95	THR
1	C	101	CYS
1	C	104	LEU
1	C	124	VAL
1	C	150	LEU
1	C	161	GLN
1	C	183	ARG

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Mol	Chain	Res	Type
1	C	187	VAL
1	C	193	LYS
1	C	231	ASN
1	C	235	MET
1	C	250	LEU
1	C	284	LYS
1	D	78	ARG
1	D	90	LEU
1	D	95	THR
1	D	104	LEU
1	D	150	LEU
1	D	161	GLN
1	D	164	SER
1	D	176	ASN
1	D	184	SER
1	D	203	GLU
1	D	231	ASN
1	D	237	GLN
1	D	243	LYS
1	D	247	THR
1	D	250	LEU
1	D	277	SER
1	D	281	SER
1	E	95	THR
1	E	104	LEU
1	E	124	VAL
1	E	145	LEU
1	E	150	LEU
1	E	231	ASN
1	E	246	HIS
1	E	247	THR
1	E	250	LEU
1	E	253	ARG
1	E	281	SER
1	F	75	THR
1	F	95	THR
1	F	104	LEU
1	F	124	VAL
1	F	150	LEU
1	F	163	THR
1	F	175	ASP
1	F	184	SER

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Mol	Chain	Res	Type
1	F	187	VAL
1	F	193	LYS
1	F	223	GLN
1	F	231	ASN
1	F	237	GLN
1	F	247	THR
1	F	250	LEU
1	F	256	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	156	HIS
1	A	161	GLN
1	A	214	ASN
1	A	228	ASN
1	A	264	ASN
1	A	267	ASN
1	A	275	ASN
1	B	139	GLN
1	B	156	HIS
1	B	214	ASN
1	B	215	ASN
1	B	231	ASN
1	B	244	ASN
1	B	246	HIS
1	B	267	ASN
1	C	139	GLN
1	C	156	HIS
1	C	161	GLN
1	C	178	GLN
1	C	223	GLN
1	C	231	ASN
1	C	246	HIS
1	C	267	ASN
1	D	139	GLN
1	D	156	HIS
1	D	161	GLN
1	D	195	ASN
1	D	214	ASN
1	D	231	ASN

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Mol	Chain	Res	Type
1	D	237	GLN
1	D	246	HIS
1	D	267	ASN
1	E	88	HIS
1	E	139	GLN
1	E	156	HIS
1	E	161	GLN
1	E	223	GLN
1	E	231	ASN
1	E	237	GLN
1	E	246	HIS
1	E	267	ASN
1	F	156	HIS
1	F	176	ASN
1	F	195	ASN
1	F	214	ASN
1	F	223	GLN
1	F	231	ASN
1	F	237	GLN
1	F	246	HIS
1	F	264	ASN
1	F	267	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	ACT	B	1289	-	1,3,3	2.45	1 (100%)	0,3,3	0.00	-
4	NAG	B	1290[A]	-	15,15,15	0.59	0	17,21,21	2.10	5 (29%)
4	NAG	B	1290[B]	-	15,15,15	0.50	0	17,21,21	1.57	1 (5%)
3	ACT	B	1292	-	1,3,3	1.85	0	0,3,3	0.00	-
4	NAG	B	1293	-	14,14,15	0.54	0	15,19,21	1.48	1 (6%)
4	NAG	C	1289	-	15,15,15	0.54	0	17,21,21	1.03	1 (5%)
4	NAG	C	1290	-	15,15,15	0.52	0	17,21,21	0.92	0
4	NAG	D	1288	-	15,15,15	1.07	1 (6%)	17,21,21	1.19	2 (11%)
4	NAG	E	1289	-	15,15,15	0.73	0	17,21,21	1.96	4 (23%)
4	NAG	E	1291	1	14,14,15	0.57	0	15,19,21	1.26	3 (20%)
4	NAG	E	1292	-	15,15,15	0.64	0	17,21,21	1.57	6 (35%)

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	ACT	B	1289	-	-	0/0/0/0	0/0/0/0
4	NAG	B	1290[A]	-	-	0/6/26/26	0/1/1/1
4	NAG	B	1290[B]	-	-	0/6/26/26	0/1/1/1
3	ACT	B	1292	-	-	0/0/0/0	0/0/0/0
4	NAG	B	1293	-	1/1/5/7	0/6/23/26	1/1/1/1
4	NAG	C	1289	-	-	2/6/26/26	0/1/1/1
4	NAG	C	1290	-	-	0/6/26/26	0/1/1/1
4	NAG	D	1288	-	-	0/6/26/26	0/1/1/1
4	NAG	E	1289	-	-	0/6/26/26	0/1/1/1
4	NAG	E	1291	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1292	-	-	0/6/26/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1289	ACT	CH3-C	2.45	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1288	NAG	C1-C2	2.97	1.56	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1293	NAG	C4-C3-C2	-3.96	105.07	111.23
4	E	1289	NAG	C1-O5-C5	-3.74	106.56	113.47
4	B	1290[A]	NAG	C6-C5-C4	-2.75	106.22	113.02
4	E	1291	NAG	C2-N2-C7	-2.72	119.55	123.04
4	E	1292	NAG	C8-C7-N2	-2.11	112.07	116.11
4	E	1292	NAG	C1-O5-C5	-2.07	109.65	113.47
4	B	1290[A]	NAG	C1-O5-C5	-2.05	109.68	113.47
4	E	1291	NAG	C1-O5-C5	-2.04	109.67	112.25
4	E	1289	NAG	C3-C4-C5	2.01	113.71	110.20
4	D	1288	NAG	C4-C3-C2	2.03	113.24	110.43
4	E	1289	NAG	C3-C2-N2	2.11	115.02	110.66
4	E	1292	NAG	C3-C4-C5	2.11	113.88	110.20
4	C	1289	NAG	C1-O5-C5	2.14	117.42	113.47
4	E	1292	NAG	O7-C7-N2	2.40	126.75	121.86
4	E	1291	NAG	O5-C5-C6	2.40	112.55	107.35
4	E	1292	NAG	O5-C5-C6	2.63	112.99	106.36
4	E	1292	NAG	C4-C3-C2	2.63	114.07	110.43
4	D	1288	NAG	C1-O5-C5	2.77	118.59	113.47
4	B	1290[A]	NAG	O5-C5-C6	2.77	113.36	106.36
4	B	1290[A]	NAG	C4-C3-C2	4.50	116.66	110.43
4	B	1290[A]	NAG	C3-C4-C5	4.99	118.90	110.20
4	B	1290[B]	NAG	C4-C3-C2	5.14	117.56	110.43
4	E	1289	NAG	C4-C3-C2	5.64	118.25	110.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1293	NAG	C5

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1289	NAG	O7-C7-N2-C2
4	C	1289	NAG	C8-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1293	NAG	C1-C2-C3-C4-C5-O5

8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1289	ACT	2	0
4	B	1290[B]	NAG	2	0
4	B	1293	NAG	3	0
4	C	1289	NAG	6	0
4	C	1290	NAG	2	0
4	D	1288	NAG	5	0
4	E	1289	NAG	4	0
4	E	1292	NAG	8	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	217/219 (99%)	0.70	38 (17%) 2 1	44, 57, 62, 70	4 (1%)
1	B	218/219 (99%)	-0.09	3 (1%) 78 76	40, 47, 56, 73	0
1	C	217/219 (99%)	-0.06	5 (2%) 64 62	43, 51, 60, 68	1 (0%)
1	D	216/219 (98%)	0.21	13 (6%) 25 23	55, 61, 67, 83	4 (1%)
1	E	217/219 (99%)	0.09	6 (2%) 56 55	51, 59, 66, 71	1 (0%)
1	F	217/219 (99%)	0.06	7 (3%) 51 50	51, 58, 64, 69	1 (0%)
All	All	1302/1314 (99%)	0.15	72 (5%) 29 26	40, 57, 65, 83	11 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	PHE	6.8
1	A	231	ASN	5.5
1	A	288	ALA	5.5
1	A	245	CYS	4.8
1	A	183	ARG	4.4
1	A	229	THR	4.3
1	D	161	GLN	4.3
1	F	239	ALA	4.0
1	D	72	PRO	4.0
1	E	288	ALA	4.0
1	D	74	LEU	3.9
1	C	161	GLN	3.8
1	A	177	TYR	3.7
1	A	227	LEU	3.7
1	A	230	GLY	3.7
1	A	247	THR	3.5
1	C	72	PRO	3.4
1	D	163	THR	3.4
1	A	191	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	244	ASN	3.3
1	F	162	GLY	3.3
1	B	174	GLU	3.2
1	C	191	ALA	3.1
1	A	131	TYR	3.1
1	A	242	TYR	3.0
1	F	229	THR	3.0
1	A	272	LYS	3.0
1	C	250	LEU	2.8
1	A	256	ARG	2.8
1	A	276	TYR	2.7
1	D	75	THR	2.7
1	A	235	MET	2.7
1	D	192	GLU	2.7
1	A	274	TYR	2.7
1	A	269	LYS	2.7
1	A	193	LYS	2.6
1	E	162	GLY	2.5
1	A	175	ASP	2.5
1	A	174	GLU	2.4
1	F	219	SER	2.4
1	A	260	GLY	2.4
1	E	266	ILE	2.4
1	D	229	THR	2.4
1	A	257	GLY	2.4
1	D	86	ARG	2.4
1	A	200	ALA	2.3
1	A	216	GLN	2.3
1	A	234	VAL	2.3
1	C	288	ALA	2.3
1	A	217	SER	2.3
1	E	239	ALA	2.3
1	F	163	THR	2.3
1	F	240	TRP	2.3
1	F	227	LEU	2.2
1	D	100	ASP	2.2
1	A	186	LYS	2.2
1	D	191	ALA	2.2
1	A	162	GLY	2.2
1	A	258	THR	2.2
1	B	72	PRO	2.1
1	E	89	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	224	ASP	2.1
1	B	249	ASN	2.1
1	A	173	PHE	2.1
1	E	278	TYR	2.1
1	A	203	GLU	2.1
1	A	176	ASN	2.1
1	A	161	GLN	2.1
1	D	160	ALA	2.1
1	D	183	ARG	2.0
1	D	250	LEU	2.0
1	A	75	THR	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)

There are no carbohydrates in this entry.

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	NAG	D	1288	15/15	0.69	0.43	8.61	67,71,72,73	4
4	NAG	E	1292	15/15	0.74	0.41	7.28	56,58,60,61	9
4	NAG	B	1290[B]	15/15	0.83	0.42	5.19	47,50,51,51	15
4	NAG	E	1289	15/15	0.80	0.33	5.12	57,62,64,65	9
4	NAG	C	1290	15/15	0.71	0.36	4.78	62,66,67,67	11
4	NAG	B	1290[A]	15/15	0.83	0.42	4.68	45,52,53,54	15
4	NAG	C	1289	15/15	0.77	0.33	4.07	59,62,64,64	11
3	ACT	B	1289	4/4	0.91	0.27	3.88	54,55,56,56	0
3	ACT	B	1292	4/4	0.94	0.19	0.31	58,59,60,60	0
2	CA	B	1291	1/1	0.90	0.08	-1.41	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CA	C	1291	1/1	0.96	0.07	-1.62	61,61,61,61	0
2	CA	D	1289	1/1	0.98	0.04	-2.00	75,75,75,75	0
2	CA	F	1289	1/1	0.96	0.06	-2.08	72,72,72,72	0
2	CA	A	1289	1/1	0.95	0.03	-2.62	78,78,78,78	0
2	CA	E	1290	1/1	0.94	0.04	-3.66	60,60,60,60	0
4	NAG	E	1291	14/15	0.76	0.33	-	65,66,67,68	14
4	NAG	B	1293	14/15	0.80	0.26	-	62,65,67,68	14

6.5 Other polymers (i)

There are no such residues in this entry.