



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:15 PM UTC

PDB ID : 2J3O / pdb_00002j3o
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

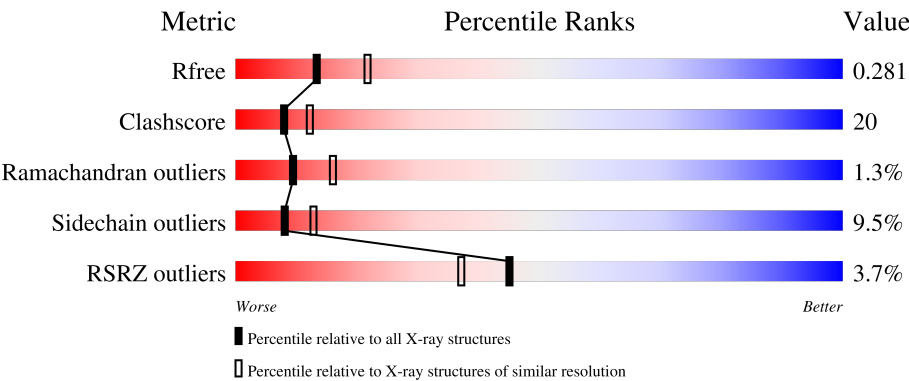
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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

Mol	Chain	Length	Quality of chain
1	A	219	14% 53% 37% 8% ..
1	B	219	% 68% 27% ..
1	C	219	68% 26% 5% .
1	D	219	3% 64% 30% ..
1	E	219	2% 68% 28% ..

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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	-
4	NAG	B	1293	X	-	-	-
4	NAG	E	1292	-	-	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			

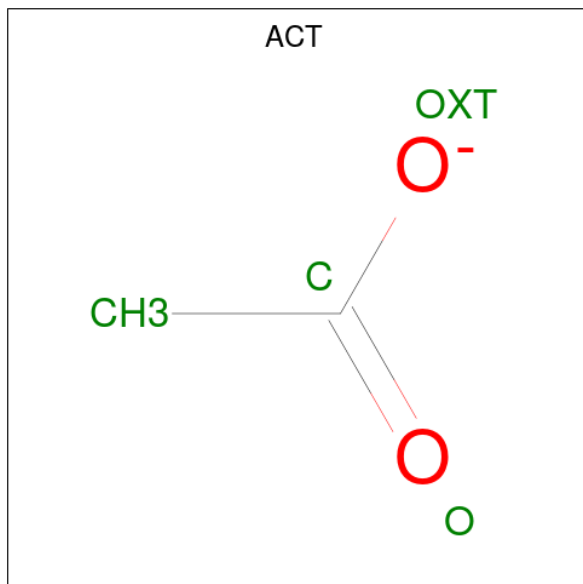
There are 12 discrepancies between the modelled and reference sequences:

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 (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is ACETATE ION (CCD ID: 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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is water.

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

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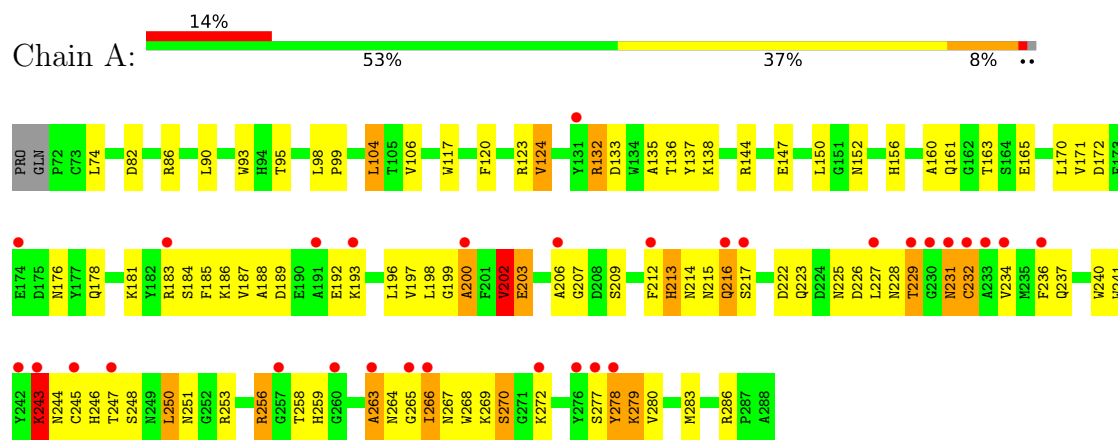
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	22	Total	O	0	0
			22	22		
5	F	29	Total	O	0	0
			29	29		

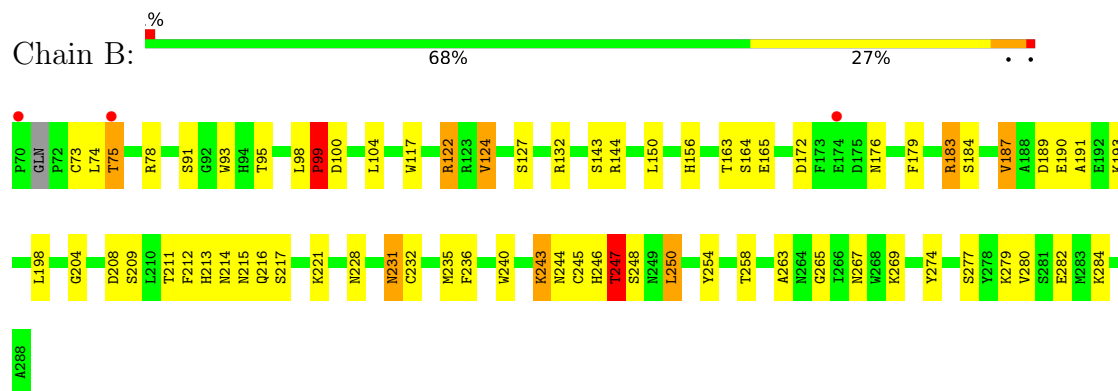
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

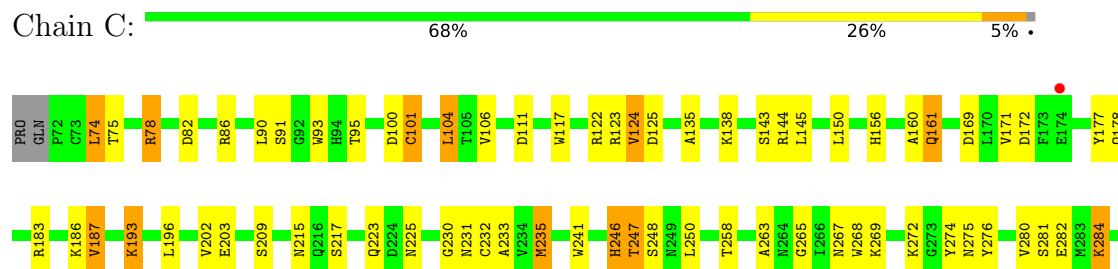
• Molecule 1: FICOLIN-2



• Molecule 1: FICOLIN-2



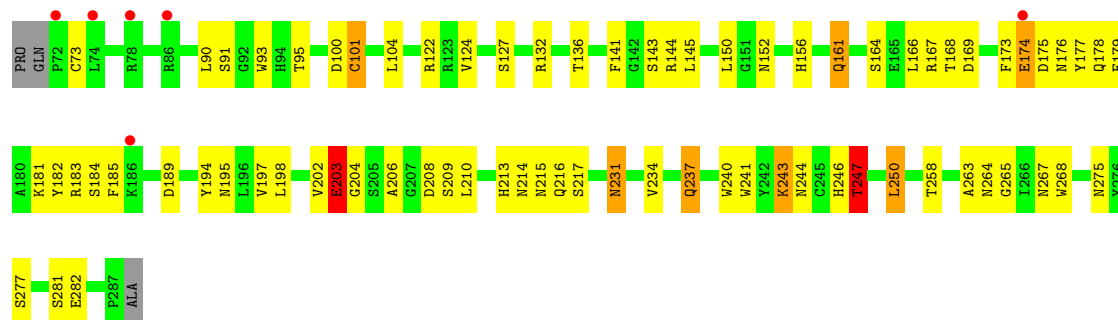
• Molecule 1: FICOLIN-2



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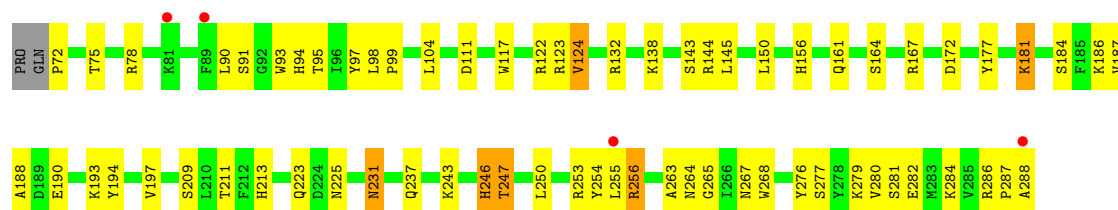
- Molecule 1: FICOLIN-2

Chain D:  3% 64% 30%



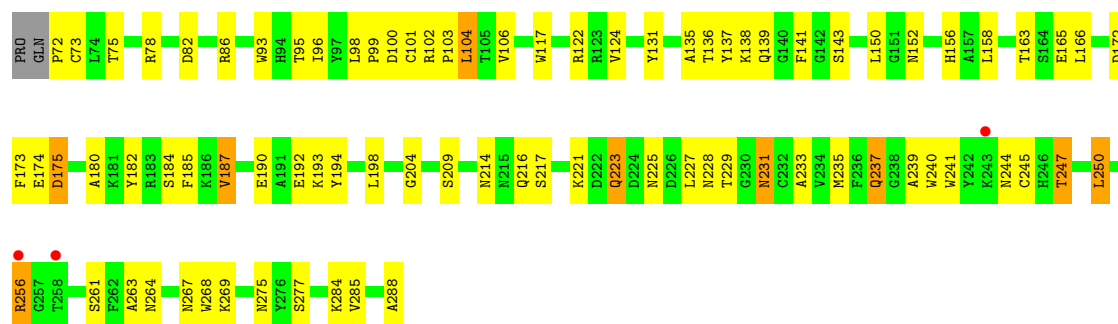
- Molecule 1: FICOLIN-2

Chain E:  2% 68% 28%



- Molecule 1: FICOLIN-2

Chain F:  0% 61% 34%



4 Data and refinement statistics

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 19.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.00-2.65) 98.7 (19.00-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	5889 reflections (10.18%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, CA, 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	1.01	2/1783 (0.1%)	1.05	3/2413 (0.1%)
1	B	0.85	0/1801	0.98	3/2436 (0.1%)
1	C	0.72	0/1783	0.93	1/2413 (0.0%)
1	D	0.75	0/1778	0.89	2/2406 (0.1%)
1	E	0.69	1/1783 (0.1%)	0.90	1/2413 (0.0%)
1	F	0.69	0/1783	0.91	0/2413
All	All	0.79	3/10711 (0.0%)	0.95	10/14494 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	HIS	CE1-NE2	6.43	1.39	1.32
1	A	213	HIS	CG-ND1	6.13	1.45	1.38
1	E	243	LYS	CA-C	5.31	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	ASN	N-CA-C	7.96	119.96	111.28
1	B	127	SER	N-CA-C	6.38	119.05	111.71
1	D	174	GLU	N-CA-C	-6.09	105.83	113.20
1	A	278	TYR	N-CA-C	6.08	118.14	110.24
1	B	246	HIS	N-CA-C	5.90	117.22	108.60
1	D	247	THR	N-CA-C	-5.74	107.27	114.56
1	C	246	HIS	N-CA-C	5.29	116.89	108.79
1	A	259	HIS	N-CA-C	5.28	117.41	109.23
1	B	247	THR	N-CA-C	-5.00	107.03	114.64
1	E	247	THR	N-CA-C	-5.00	107.13	114.39

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	110	0
1	B	1753	0	1627	56	0
1	C	1735	0	1607	56	0
1	D	1730	0	1604	65	0
1	E	1735	0	1606	44	0
1	F	1735	0	1607	63	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	9	0
4	D	15	0	15	5	0
4	E	44	0	43	11	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	397	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 20.

All (397) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:231:ASN:C	1:F:231:ASN:HD22	1.71	0.96
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:H3	4:C:1289:NAG:C8	1.95	0.91
1:E:78:ARG:NH1	5:E:2002:HOH:O	1.96	0.90
4:C:1289:NAG:H83	4:C:1289:NAG:C3	2.02	0.89
1:B:183:ARG:HG3	1:B:183:ARG:HH11	1.39	0.88
1:C:269:LYS:HD3	1:C:274:TYR:CE2	2.08	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:E:231:ASN:C	1:E:231:ASN:HD22	1.86	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
1:A:231:ASN:HB2	1:A:234:VAL:CG2	2.11	0.81
4:E:1292:NAG:C8	4:E:1292:NAG:O1	2.27	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: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:A:216:GLN:CD	1:A:243:LYS:HB3	2.09	0.78
1:D:143:SER:OG	4:E:1289:NAG:O1	2.00	0.77
1:A:171:VAL:HB	1:A:280:VAL:HB	1.67	0.77
1:A:196:LEU:HB2	1:A:241:TRP:CD1	2.19	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:A:240:TRP:CH2	1:A:250:LEU:HB2	2.21	0.76
1:B:213:HIS:HA	5:B:2017:HOH:O	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:HZ2	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
1:F:231:ASN:C	1:F:231:ASN:ND2	2.46	0.69
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:B:172:ASP:OD2	1:B:176:ASN:HB2	1.93	0.68
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:CG	1:B:183:ARG:NH1	2.57	0.65
1:B:156:HIS:HD2	1:B:187:VAL:O	1.79	0.65
4:E:1292:NAG:O1	4:E:1292:NAG:H82	1.96	0.65
1:A:243:LYS:HD2	1:A:243:LYS:O	1.97	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:231:ASN:HD22	1:C:231:ASN:C	2.05	0.63
1:D:231:ASN:HD22	1:D:231:ASN:C	2.06	0.63
4:E:1292:NAG:C8	4:E:1292:NAG:C1	2.76	0.63
1:C:74:LEU:O	1:C:75:THR:OG1	2.13	0.63
1:A:256:ARG:HH11	1:A:256:ARG:CG	2.09	0.62
1:D:122:ARG:NH2	4:D:1288:NAG:O3	2.29	0.62
1:F:98:LEU:HB3	1:F:99:PRO:HD2	1.81	0.62
1:B:198:LEU:H	1:B:214:ASN:ND2	1.97	0.62
1:D:178:GLN:HB3	1:D:206:ALA:HB2	1.81	0.62
1:D:237:GLN:HE21	1:D:264:ASN:HD22	1.47	0.62
1:E:287:PRO:O	1:E:288:ALA:O	2.18	0.62
1:F:72:PRO:O	1:F:73:CYS:C	2.42	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:F:228:ASN:OD1	1:F:235:MET:HE1	2.01	0.60
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:A:209:SER:HG	1:A:268:TRP:CD1	2.19	0.59
1:A:120:PHE:CZ	1:A:283:MET:HE2	2.37	0.59
1:A:165:GLU:OE1	1:A:181:LYS:HE2	2.02	0.59
1:D:167:ARG:NH2	1:D:177:TYR:OH	2.35	0.59
1:C:209:SER:HB3	1:C:247:THR:HG22	1.84	0.59
1:D:174:GLU:HA	5:D:2010:HOH:O	2.03	0.59
1:F:223:GLN:NE2	1:F:225:ASN:ND2	2.48	0.59
1:A:243:LYS:O	1:A:244:ASN:C	2.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1292:NAG:H83	4:E:1292:NAG:C1	2.33	0.58
1:B:231:ASN:N	1:B:235:MET:HE2	2.19	0.58
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: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:B:117:TRP:HB3	1:B:284:LYS:HB2	1.86	0.57
1:E:143:SER:OG	4:E:1292:NAG:O1	2.22	0.57
1:F:209:SER:HB3	1:F:247:THR:HG23	1.87	0.57
1:A:209:SER:HB2	1:A:268:TRP:CE2	2.40	0.56
1:A:237:GLN:HE21	1:A:264:ASN:HD22	1.53	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: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:E:287:PRO:O	1:E:288:ALA:C	2.48	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:A:183:ARG:HD2	1:A:200:ALA:HB3	1.87	0.55
1:D:213:HIS:CE1	1:D:246:HIS:HA	2.42	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:B:231:ASN:C	1:B:231:ASN:HD22	2.14	0.54
1:C:145:LEU:HD12	4:C:1289:NAG:H1	1.89	0.54
1:A:196:LEU:HD13	1:A:196:LEU:C	2.33	0.54
1:B:93:TRP:CZ2	1:B:144:ARG:HA	2.43	0.54
1:D:195:ASN:HD21	1:D:215:ASN:C	2.15	0.54
1:D:258:THR:HA	1:D:275:ASN:O	2.07	0.54
1:A:98:LEU:HB3	1:A:99:PRO:CD	2.35	0.54
1:A:217:SER:HB2	1:A:225:ASN:HB3	1.89	0.54
1:A:243:LYS:O	1:A:243:LYS:CD	2.55	0.54
1:D:213:HIS:HE1	1:D:246:HIS:HA	1.73	0.54
1:F:231:ASN:HD21	1:F:233:ALA:HB3	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:LEU:HB3	1:E:99:PRO:HD2	1.90	0.54
1:C:169:ASP:OD2	1:C:284:LYS:NZ	2.35	0.53
1:B:215:ASN:ND2	4:B:1293:NAG:C1	2.66	0.53
1:B:156:HIS:CE1	1:B:189:ASP:HB3	2.42	0.53
1:C:209:SER:O	1:C:248:SER:HB3	2.09	0.53
1:A:202:VAL:O	1:A:202:VAL:HG13	2.08	0.53
1:B:184:SER:OG	5:B:2015:HOH:O	2.19	0.53
1:C:160:ALA:HA	1:C:186:LYS:NZ	2.23	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: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:D:152:ASN:HB3	1:D:194:TYR:CE1	2.45	0.51
1:F:158:LEU:N	5:F:2017:HOH:O	2.43	0.51
1:D:156:HIS:CE1	1:D:189:ASP:HB3	2.45	0.51
1:B:164:SER:O	1:B:184:SER:HA	2.10	0.51
1:B:228:ASN:ND2	1:B:244:ASN:ND2	2.58	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:282:GLU:CD	4:D:1288:NAG:H2	2.35	0.51
1:A:231:ASN:HB3	1:A:234:VAL:HG23	1.90	0.51
1:B:198:LEU:H	1:B:214:ASN:HD21	1.59	0.51
1:D:217:SER:O	1:D:241:TRP:HA	2.10	0.51
1:D:231:ASN:ND2	1:D:231:ASN:C	2.67	0.51
1:F:82:ASP:O	1:F:86:ARG:HG3	2.10	0.51
1:A:185:PHE:C	1:A:185:PHE:CD1	2.88	0.51
1:B:91:SER:HB3	4:B:1290[B]:NAG:C8	2.41	0.51
1:F:256:ARG:O	1:F:277:SER:O	2.29	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:D:169:ASP:OD1	1:D:177:TYR:OH	2.25	0.50
1:E:122:ARG:HH12	4:E:1289:NAG:H5	1.76	0.50
1:B:132:ARG:NH2	1:C:111:ASP:OD2	2.44	0.50
1:E:186:LYS:HG2	1:E:197:VAL:HB	1.93	0.50
1:F:98:LEU:HB3	1:F:99:PRO:CD	2.40	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:D:208:ASP:OD1	1:D:208:ASP:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:GLY:H	1:B:267:ASN:ND2	2.10	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: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:O	1:A:202:VAL:CG1	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:156:HIS:HD2	1:A:187:VAL:O	1.96	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:212:PHE:HD1	1:A:243:LYS:CE	2.26	0.49
1:C:246:HIS:CD2	1:C:246:HIS:C	2.91	0.48
1:B:240:TRP:CH2	1:B:250:LEU:HB2	2.48	0.48
1:C:247:THR:HG23	1:C:269:LYS:HB3	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:D:143:SER:HB2	1:E:91:SER:HB2	1.96	0.48
1:D:237:GLN:HG3	1:D:264:ASN:HB2	1.95	0.48
1:E:237:GLN:NE2	1:E:253:ARG:HE	2.11	0.48
1:F:172:ASP:OD1	1:F:172:ASP:C	2.57	0.48
1:F:268:TRP:O	1:F:269:LYS:C	2.56	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:E:246:HIS:HE1	1:E:263:ALA:O	1.96	0.48
1:F:228:ASN:ND2	1:F:229:THR:H	2.11	0.48
1:C:161:GLN:HA	1:C:161:GLN:NE2	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:A:186:LYS:HG2	1:A:197:VAL:HB	1.96	0.47
1:B:124:VAL:O	1:B:254:TYR:OH	2.32	0.47
1:E:181:LYS:HG2	5:E:2015:HOH:O	2.14	0.47
1:F:131:TYR:O	1:F:221:LYS:HE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:228:ASN:HD22	1:F:229:THR:N	2.12	0.47
1:A:213:HIS:HE1	1:A:246:HIS:HA	1.79	0.47
1:B:208:ASP:C	1:B:208:ASP:OD1	2.57	0.47
1:C:169:ASP:OD1	1:C:177:TYR:OH	2.18	0.47
1:A:231:ASN:CB	1:A:234:VAL:CG2	2.82	0.47
1:F:135:ALA:O	1:F:139:GLN:HB2	2.14	0.47
1:E:246:HIS:C	1:E:246:HIS:CD2	2.92	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:A:120:PHE:HZ	1:A:283:MET:HE2	1.78	0.46
1:D:265:GLY:H	1:D:267:ASN:ND2	2.13	0.46
1:A:196:LEU:HD12	1:A:214:ASN:HA	1.96	0.46
1:A:263:ALA:HA	1:A:267:ASN:ND2	2.31	0.46
1:C:82:ASP:O	1:C:86:ARG:HG3	2.14	0.46
1:C:223:GLN:HE21	1:C:225:ASN:HD21	1.63	0.46
1:E:231:ASN:C	1:E:231:ASN:ND2	2.59	0.46
1:A:256:ARG:NH1	1:A:256:ARG:CG	2.71	0.46
1:D:209:SER:HB3	1:D:247:THR:CG2	2.46	0.46
1:A:189:ASP:O	1:A:193:LYS:O	2.33	0.46
1:C:74:LEU:C	1:C:75:THR:HG23	2.40	0.46
1:F:192:GLU:O	1:F:192:GLU:HG2	2.16	0.46
1:A:172:ASP:OD1	1:A:172:ASP:C	2.60	0.45
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:C:230:GLY:HA3	1:C:235:MET:HE1	1.98	0.45
1:D:73:CYS:CB	1:D:101:CYS:SG	3.04	0.45
1:F:98:LEU:HD22	5:F:2017:HOH:O	2.17	0.45
1:C:178:GLN:HE22	1:C:272:LYS:HD3	1.80	0.45
1:D:136:THR:HG22	1:D:141:PHE:CD2	2.52	0.45
1:E:99:PRO:HG3	1:E:161:GLN:NE2	2.31	0.45
1:A:123:ARG:HA	1:A:147:GLU:HG2	1.98	0.45
1:F:152:ASN:HB3	1:F:194:TYR:CE1	2.50	0.45
1:A:236:PHE:O	1:A:237:GLN:C	2.60	0.45
1:A:247:THR:HG23	1:A:269:LYS:HD3	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:HIS:HD2	1:E:187:VAL:O	2.00	0.45
1:E:255:LEU:O	1:E:277:SER:HB3	2.17	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:B:190:GLU:O	1:B:191:ALA:C	2.60	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:C:282:GLU:CD	4:C:1290:NAG:H2	2.41	0.45
1:B:216:GLN:HG3	1:B:243:LYS:HG3	1.99	0.44
1:A:133:ASP:OD1	1:A:133:ASP:C	2.59	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: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:C:231:ASN:HD22	1:C:232:CYS:N	2.15	0.44
1:E:123:ARG:O	1:E:280:VAL:HA	2.18	0.44
1:C:135:ALA:O	1:C:138:LYS:HB3	2.18	0.44
1:D:173:PHE:C	1:D:175:ASP:H	2.25	0.44
1:E:213:HIS:CE1	1:E:246:HIS:HA	2.53	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
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:A:161:GLN:HE21	1:A:161:GLN:HB3	1.60	0.43
1:B:228:ASN:ND2	1:B:244:ASN:HD21	2.16	0.43
1:E:211:THR:C	1:E:213:HIS:N	2.73	0.43
1:E:190:GLU:O	1:E:193:LYS:N	2.36	0.43
1:A:120:PHE:CD1	1:A:120:PHE:C	2.97	0.43
1:A:156:HIS:NE2	1:A:189:ASP:HB3	2.33	0.43
1:A:207:GLY:HA3	1:A:270:SER:CB	2.49	0.43
1:C:231:ASN:C	1:C:231:ASN:ND2	2.72	0.43
1:D:250:LEU:HD12	1:D:250:LEU:HA	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ARG:HD2	1:B:282:GLU:OE2	2.19	0.43
1:B:236:PHE:HE2	1:B:245:CYS:SG	2.42	0.43
1:E:138:LYS:HG3	1:E:194:TYR:OH	2.19	0.43
1:E:265:GLY:H	1:E:267:ASN:HD21	1.67	0.43
1:B:193:LYS:HB3	1:B:217:SER:HB3	2.00	0.42
1:B:263:ALA:HA	1:B:267:ASN:ND2	2.35	0.42
1:D:91:SER:HB2	1:F:143:SER:HB2	2.01	0.42
1:F:174:GLU:O	1:F:175:ASP:HB2	2.19	0.42
1:C:93:TRP:CZ2	1:C:144:ARG:HA	2.53	0.42
1:D:197:VAL:HG12	1:D:197:VAL:O	2.17	0.42
1:C:123:ARG:HB2	1:C:281:SER:HB3	2.02	0.42
1:C:231:ASN:ND2	1:C:233:ALA:H	2.16	0.42
1:F:216:GLN:HA	1:F:216:GLN:OE1	2.18	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:A:247:THR:HG23	1:A:269:LYS:CD	2.49	0.42
1:B:244:ASN:N	1:B:245:CYS:HA	2.35	0.42
1:A:132:ARG:HB2	1:A:137:TYR:HE1	1.84	0.42
1:C:217:SER:O	1:C:241:TRP:HA	2.20	0.42
1:C:282:GLU:OE1	4:C:1290:NAG:H2	2.19	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
1:B:232:CYS:N	1:B:235:MET:HE3	2.35	0.42
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:A:202:VAL:C	1:A:203:GLU:HG2	2.42	0.41
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: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:B:211:THR:O	1:B:212:PHE:C	2.62	0.41
1:C:104:LEU:HD13	1:C:106:VAL:CG1	2.50	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLN:OE1	1:A:253:ARG:NH2	2.53	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:B:179:PHE:O	1:B:204:GLY:HA3	2.20	0.41
1:D:216:GLN:HG2	1:D:243:LYS:HD3	2.02	0.41
1:F:96:ILE:HD11	1:F:158:LEU:HD21	2.02	0.41
1:A:209:SER:HB2	1:A:268:TRP:CD2	2.55	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:D:210:LEU:HD12	1:D:210:LEU:HA	1.81	0.41
1:D:241:TRP:HB2	5:D:2016:HOH:O	2.21	0.41
1:A:266:ILE:HG12	1:A:277:SER:HB2	2.03	0.41
1:F:190:GLU:C	1:F:192:GLU:N	2.78	0.41
1:E:256:ARG:HG3	1:E:256:ARG:HH11	1.85	0.40
1:F:117:TRP:HB3	1:F:284:LYS:HB2	2.03	0.40
1:F:180:ALA:HA	1:F:204:GLY:HA3	2.03	0.40
1:F:182:TYR:CD2	1:F:198:LEU:HD21	2.57	0.40
1:A:117:TRP:CZ2	1:A:286:ARG:NH2	2.74	0.40
1:D:132:ARG:HH22	1:E:111:ASP:CG	2.29	0.40
1:F:93:TRP:HA	1:F:106:VAL:O	2.21	0.40
1:C:172:ASP:HB2	1:C:276:TYR:OH	2.22	0.40
1:A:265:GLY:H	1:A:267:ASN:HD21	1.68	0.40
1:C:215:ASN:ND2	5:C:2023:HOH:O	2.54	0.40
1:E:172:ASP:HB2	1:E:276:TYR:OH	2.21	0.40
1:C:143:SER:OG	4:C:1289:NAG:O1	2.09	0.40
1:D:161:GLN:HE21	1:D:161:GLN:HA	1.86	0.40
1:D:282:GLU:OE1	4:D:1288:NAG:H2	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	215/219 (98%)	177 (82%)	30 (14%)	8 (4%)	2	4
1	B	216/219 (99%)	196 (91%)	19 (9%)	1 (0%)	24	39
1	C	215/219 (98%)	199 (93%)	14 (6%)	2 (1%)	14	24
1	D	214/219 (98%)	188 (88%)	23 (11%)	3 (1%)	9	14
1	E	215/219 (98%)	195 (91%)	17 (8%)	3 (1%)	9	14
1	F	215/219 (98%)	189 (88%)	26 (12%)	0	100	100
All	All	1290/1314 (98%)	1144 (89%)	129 (10%)	17 (1%)	9	16

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
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 ⓘ

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%)	159 (87%)	23 (13%)	4	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	184/184 (100%)	164 (89%)	20 (11%)	6	9
1	C	182/184 (99%)	166 (91%)	16 (9%)	9	15
1	D	182/184 (99%)	165 (91%)	17 (9%)	8	13
1	E	182/184 (99%)	169 (93%)	13 (7%)	13	23
1	F	182/184 (99%)	167 (92%)	15 (8%)	10	18
All	All	1094/1104 (99%)	990 (90%)	104 (10%)	8	13

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LEU
1	A	90	LEU
1	A	95	THR
1	A	104	LEU
1	A	124	VAL
1	A	132	ARG
1	A	150	LEU
1	A	163	THR
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

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Mol	Chain	Res	Type
1	B	124	VAL
1	B	150	LEU
1	B	163	THR
1	B	165	GLU
1	B	183	ARG
1	B	187	VAL
1	B	231	ASN
1	B	243	LYS
1	B	247	THR
1	B	248	SER
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
1	C	187	VAL
1	C	193	LYS
1	C	235	MET
1	C	247	THR
1	C	250	LEU
1	C	284	LYS
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	181	LYS
1	D	184	SER
1	D	203	GLU
1	D	231	ASN
1	D	237	GLN
1	D	243	LYS

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Mol	Chain	Res	Type
1	D	247	THR
1	D	250	LEU
1	D	277	SER
1	D	281	SER
1	E	75	THR
1	E	90	LEU
1	E	95	THR
1	E	104	LEU
1	E	124	VAL
1	E	145	LEU
1	E	150	LEU
1	E	181	LYS
1	E	231	ASN
1	E	246	HIS
1	E	247	THR
1	E	250	LEU
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
1	F	187	VAL
1	F	223	GLN
1	F	231	ASN
1	F	237	GLN
1	F	247	THR
1	F	250	LEU
1	F	256	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	139	GLN
1	A	156	HIS
1	A	161	GLN
1	A	178	GLN
1	A	214	ASN

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Mol	Chain	Res	Type
1	A	225	ASN
1	A	228	ASN
1	A	244	ASN
1	A	264	ASN
1	A	267	ASN
1	B	94	HIS
1	B	139	GLN
1	B	156	HIS
1	B	161	GLN
1	B	178	GLN
1	B	214	ASN
1	B	215	ASN
1	B	223	GLN
1	B	231	ASN
1	B	244	ASN
1	B	246	HIS
1	B	267	ASN
1	B	275	ASN
1	C	88	HIS
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	C	275	ASN
1	D	88	HIS
1	D	94	HIS
1	D	139	GLN
1	D	156	HIS
1	D	161	GLN
1	D	176	ASN
1	D	178	GLN
1	D	195	ASN
1	D	214	ASN
1	D	231	ASN
1	D	237	GLN
1	D	246	HIS
1	D	267	ASN
1	D	275	ASN

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Mol	Chain	Res	Type
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	88	HIS
1	F	156	HIS
1	F	195	ASN
1	F	214	ASN
1	F	216	GLN
1	F	223	GLN
1	F	228	ASN
1	F	231	ASN
1	F	237	GLN
1	F	246	HIS
1	F	264	ASN
1	F	267	ASN
1	F	275	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 oligosaccharides 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
4	NAG	C	1289	-	15,15,15	0.55	0	21,21,21	1.55	1 (4%)
4	NAG	D	1288	-	15,15,15	1.10	1 (6%)	21,21,21	1.96	4 (19%)
4	NAG	E	1291	1	14,14,15	0.58	0	17,19,21	1.44	3 (17%)
4	NAG	B	1293	-	14,14,15	0.56	0	17,19,21	1.50	2 (11%)
4	NAG	B	1290[A]	-	15,15,15	0.60	0	21,21,21	1.87	5 (23%)
3	ACT	B	1292	-	3,3,3	0.87	0	3,3,3	1.37	0
4	NAG	E	1292	-	15,15,15	0.66	0	21,21,21	1.52	6 (28%)
3	ACT	B	1289	-	3,3,3	1.02	0	3,3,3	1.23	0
4	NAG	B	1290[B]	-	15,15,15	0.50	0	21,21,21	1.96	4 (19%)
4	NAG	E	1289	-	15,15,15	0.74	0	21,21,21	1.86	4 (19%)
4	NAG	C	1290	-	15,15,15	0.54	0	21,21,21	1.07	2 (9%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1288	NAG	C1-C2	3.03	1.56	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1288	NAG	O5-C1-C2	6.55	116.09	109.52
4	E	1289	NAG	C4-C3-C2	5.39	118.25	110.40
4	C	1289	NAG	C1-C2-N2	-5.36	104.52	110.73
4	B	1290[B]	NAG	C4-C3-C2	4.91	117.56	110.40
4	B	1290[A]	NAG	C3-C4-C5	4.78	118.90	110.23
4	B	1290[A]	NAG	C4-C3-C2	4.30	116.66	110.40
4	B	1290[B]	NAG	C1-C2-C3	4.22	116.30	110.54
4	B	1293	NAG	C4-C3-C2	-4.06	105.07	111.02
4	B	1290[B]	NAG	O5-C1-C2	3.88	113.41	109.52
4	E	1289	NAG	C1-O5-C5	-3.67	106.56	113.65
4	D	1288	NAG	C1-C2-C3	3.14	114.82	110.54
4	E	1291	NAG	O5-C1-C2	-3.08	106.53	111.29
4	B	1290[A]	NAG	O5-C5-C6	2.79	113.36	106.44
4	B	1290[A]	NAG	C6-C5-C4	-2.77	106.22	113.02
4	E	1289	NAG	C1-C2-N2	-2.75	107.55	110.73
4	E	1292	NAG	O7-C7-N2	2.70	126.75	121.98
4	E	1292	NAG	O5-C5-C6	2.64	112.99	106.44
4	B	1290[B]	NAG	C1-C2-N2	-2.59	107.72	110.73
4	D	1288	NAG	C1-O5-C5	2.55	118.59	113.65
4	E	1292	NAG	C4-C3-C2	2.52	114.07	110.40
4	E	1291	NAG	O5-C5-C6	2.51	112.55	107.66
4	E	1291	NAG	C2-N2-C7	-2.50	119.55	122.90
4	E	1292	NAG	C8-C7-N2	-2.44	112.07	116.12
4	E	1289	NAG	C3-C2-N2	2.39	115.02	110.62
4	C	1290	NAG	C1-C2-N2	2.13	113.19	110.73
4	B	1293	NAG	C1-C2-N2	2.11	113.76	110.43
4	E	1292	NAG	C1-O5-C5	-2.07	109.65	113.65
4	C	1290	NAG	O5-C1-C2	2.05	111.58	109.52
4	B	1290[A]	NAG	C1-O5-C5	-2.05	109.68	113.65
4	D	1288	NAG	C1-C2-N2	2.05	113.10	110.73
4	E	1292	NAG	C3-C4-C5	2.01	113.88	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1293	NAG	C5

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1290[A]	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	B	1290[A]	NAG	C3-C2-N2-C7
4	B	1290[A]	NAG	C8-C7-N2-C2
4	B	1290[A]	NAG	O7-C7-N2-C2
4	B	1290[B]	NAG	C8-C7-N2-C2
4	B	1290[B]	NAG	O7-C7-N2-C2
4	C	1289	NAG	C1-C2-N2-C7
4	C	1289	NAG	C3-C2-N2-C7
4	C	1289	NAG	C8-C7-N2-C2
4	C	1289	NAG	O7-C7-N2-C2
4	C	1290	NAG	C8-C7-N2-C2
4	C	1290	NAG	O7-C7-N2-C2
4	D	1288	NAG	C1-C2-N2-C7
4	D	1288	NAG	C8-C7-N2-C2
4	D	1288	NAG	O7-C7-N2-C2
4	E	1292	NAG	C8-C7-N2-C2
4	E	1292	NAG	O7-C7-N2-C2
4	C	1290	NAG	O5-C5-C6-O6
4	E	1291	NAG	C4-C5-C6-O6
4	B	1290[A]	NAG	O5-C5-C6-O6
4	E	1289	NAG	C8-C7-N2-C2
4	E	1289	NAG	O7-C7-N2-C2
4	E	1291	NAG	C8-C7-N2-C2
4	E	1291	NAG	O5-C5-C6-O6
4	C	1290	NAG	C4-C5-C6-O6
4	E	1291	NAG	O7-C7-N2-C2
4	E	1292	NAG	O5-C5-C6-O6
4	B	1293	NAG	C8-C7-N2-C2
4	D	1288	NAG	O5-C5-C6-O6
4	C	1289	NAG	O5-C5-C6-O6
4	B	1290[A]	NAG	C4-C5-C6-O6
4	B	1293	NAG	O7-C7-N2-C2
4	D	1288	NAG	C3-C2-N2-C7
4	E	1289	NAG	C1-C2-N2-C7
4	E	1289	NAG	C3-C2-N2-C7

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
4	C	1289	NAG	6	0
4	D	1288	NAG	5	0
4	B	1293	NAG	3	0
4	E	1292	NAG	7	0
3	B	1289	ACT	2	0
4	B	1290[B]	NAG	2	0
4	E	1289	NAG	4	0
4	C	1290	NAG	3	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	217/219 (99%)	0.92	31 (14%) 6 5	44, 57, 62, 70	4 (1%)
1	B	218/219 (99%)	-0.10	3 (1%) 73 69	26, 47, 56, 73	1 (0%)
1	C	217/219 (99%)	-0.19	1 (0%) 87 85	26, 51, 60, 68	1 (0%)
1	D	216/219 (98%)	0.47	6 (2%) 55 48	23, 61, 67, 83	4 (1%)
1	E	217/219 (99%)	0.15	4 (1%) 67 63	28, 59, 66, 71	1 (0%)
1	F	217/219 (99%)	0.10	3 (1%) 73 69	26, 58, 64, 69	1 (0%)
All	All	1302/1314 (99%)	0.23	48 (3%) 45 37	23, 57, 65, 83	12 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	86	ARG	13.2
1	D	78	ARG	12.3
1	D	186	LYS	8.8
1	C	174	GLU	7.9
1	E	81	LYS	7.8
1	A	231	ASN	6.5
1	F	243	LYS	6.2
1	A	263	ALA	6.1
1	D	174	GLU	5.9
1	B	174	GLU	5.4
1	A	212	PHE	4.4
1	A	242	TYR	3.8
1	A	229	THR	3.7
1	A	247	THR	3.4
1	A	276	TYR	3.2
1	D	74	LEU	3.1
1	A	217	SER	3.1
1	A	277	SER	3.0
1	D	72	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	183	ARG	2.9
1	A	232	CYS	2.8
1	A	216	GLN	2.7
1	A	245	CYS	2.7
1	A	257	GLY	2.7
1	E	288	ALA	2.7
1	A	266	ILE	2.6
1	A	230	GLY	2.6
1	A	234	VAL	2.5
1	A	243	LYS	2.4
1	A	206	ALA	2.4
1	A	227	LEU	2.4
1	B	70	PRO	2.4
1	A	200	ALA	2.3
1	A	272	LYS	2.2
1	A	174	GLU	2.2
1	A	265	GLY	2.2
1	A	193	LYS	2.2
1	F	256	ARG	2.1
1	E	255	LEU	2.1
1	A	131	TYR	2.1
1	A	260	GLY	2.1
1	A	236	PHE	2.1
1	E	89	PHE	2.1
1	A	278	TYR	2.1
1	A	233	ALA	2.0
1	A	191	ALA	2.0
1	B	75	THR	2.0
1	F	258	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	D	1288	15/15	0.67	0.17	67,71,72,73	4
4	NAG	B	1293	14/15	0.71	0.13	62,65,67,68	14
4	NAG	C	1290	15/15	0.73	0.17	62,66,67,67	11
4	NAG	E	1291	14/15	0.76	0.16	65,66,67,68	14
4	NAG	C	1289	15/15	0.78	0.18	59,62,64,64	11
3	ACT	B	1289	4/4	0.78	0.22	54,55,56,56	0
4	NAG	E	1292	15/15	0.81	0.19	56,58,60,61	9
4	NAG	B	1290[A]	15/15	0.82	0.23	45,52,53,54	15
4	NAG	B	1290[B]	15/15	0.82	0.23	47,50,51,51	15
4	NAG	E	1289	15/15	0.83	0.18	57,62,64,65	9
2	CA	B	1291	1/1	0.89	0.09	60,60,60,60	0
3	ACT	B	1292	4/4	0.93	0.09	58,59,60,60	0
2	CA	E	1290	1/1	0.93	0.06	60,60,60,60	0
2	CA	F	1289	1/1	0.95	0.07	72,72,72,72	0
2	CA	D	1289	1/1	0.95	0.05	75,75,75,75	0
2	CA	A	1289	1/1	0.96	0.16	78,78,78,78	0
2	CA	C	1291	1/1	0.96	0.06	61,61,61,61	0

6.5 Other polymers ⓘ

There are no such residues in this entry.