Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:52 AM GMT

PDB ID	:	2J3G
Title	:	L-FICOLIN
Authors	:	Garlatti, V.; Gaboriaud, C.
Deposited on	:	2006-08-21
Resolution	:	2.50 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:

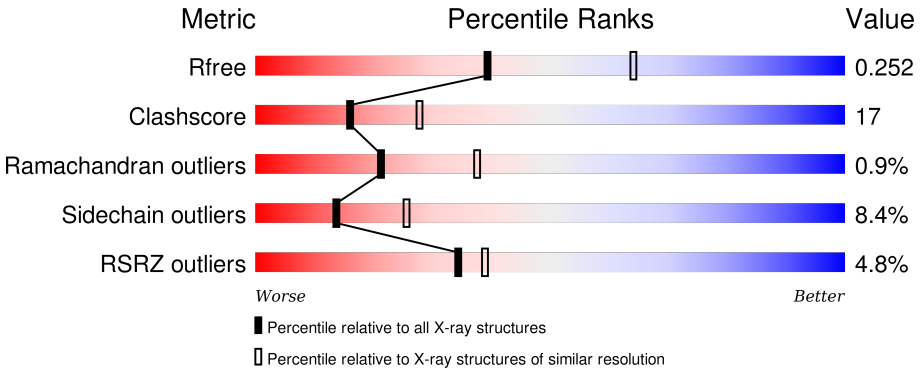
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	218	13% 54% 38% 6% •
1	B	218	2% 74% 22% •
1	C	218	3% 71% 23% • •
1	D	218	6% 71% 26% •
1	E	218	% 70% 26% •

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Mol	Chain	Length	Quality of chain
1	F	218	

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
5	P4C	E	1293	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10729 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	213	Total	C	N	O	S	0	0	0
			1707	1074	301	324	8			
1	B	217	Total	C	N	O	S	0	0	0
			1735	1092	305	329	9			
1	C	213	Total	C	N	O	S	8	1	0
			1719	1083	302	326	8			
1	D	217	Total	C	N	O	S	0	0	0
			1732	1089	305	329	9			
1	E	218	Total	C	N	O	S	0	0	0
			1739	1095	307	328	9			
1	F	214	Total	C	N	O	S	0	0	0
			1714	1078	302	326	8			

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

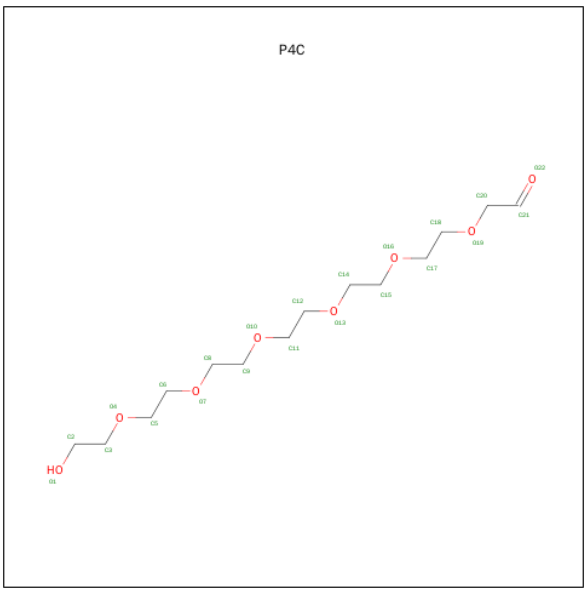
- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	5	Total C N O 60 34 2 24	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	3	Total C N O 39 22 2 15	0	0

- Molecule 5 is O-ACETALDEHYDYL-HEXAETHYLENE GLYCOL (three-letter code: P4C) (formula: $C_{14}H_{28}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	6	0
			22	14	8		

- Molecule 6 is water.

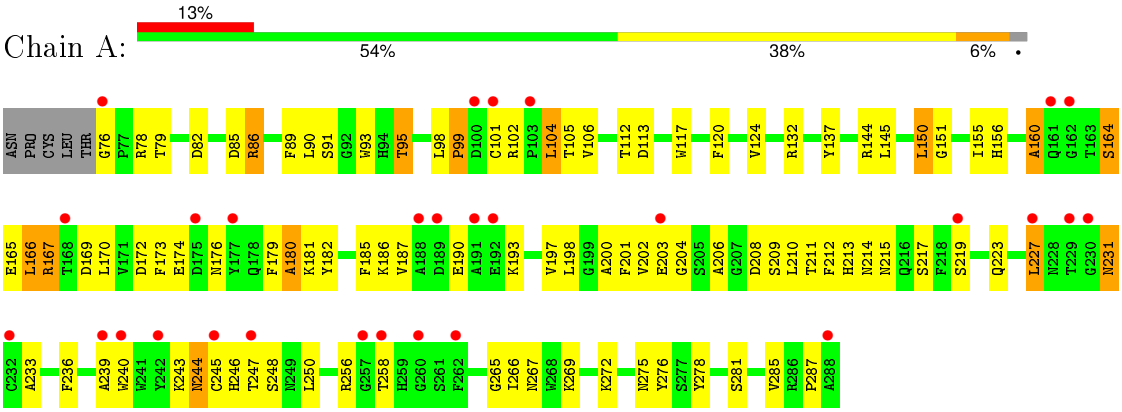
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	23	Total	O	0	0
			23	23		
6	B	60	Total	O	0	0
			60	60		
6	C	52	Total	O	0	0
			52	52		
6	D	29	Total	O	0	0
			29	29		
6	E	55	Total	O	0	0
			55	55		
6	F	37	Total	O	0	0
			37	37		

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.

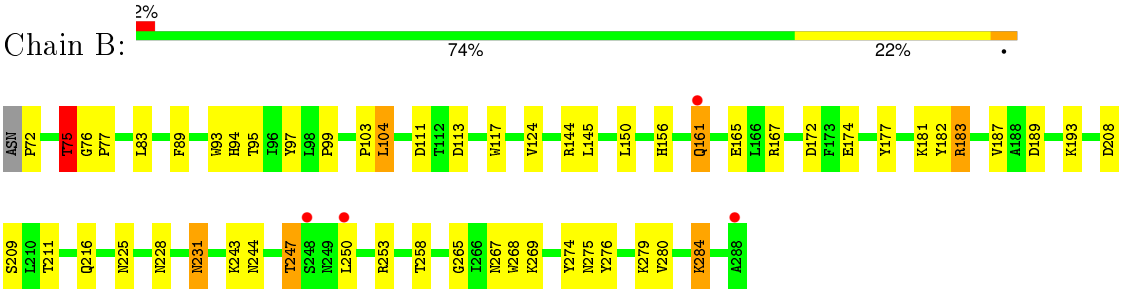
- Molecule 1: FICOLIN-2

Chain A:



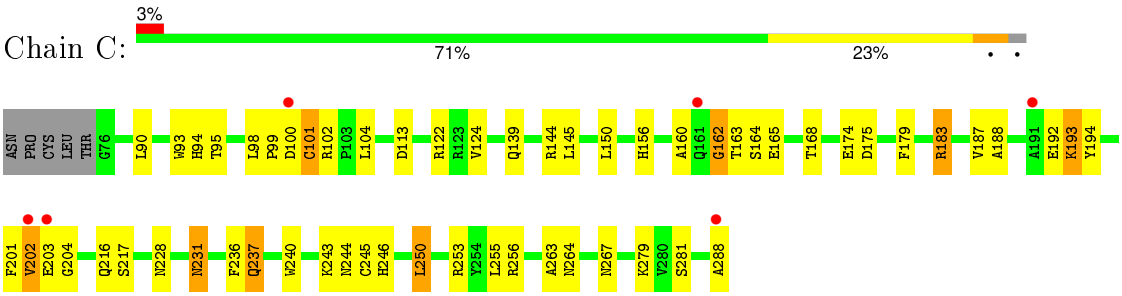
- Molecule 1: FICOLIN-2

Chain B:



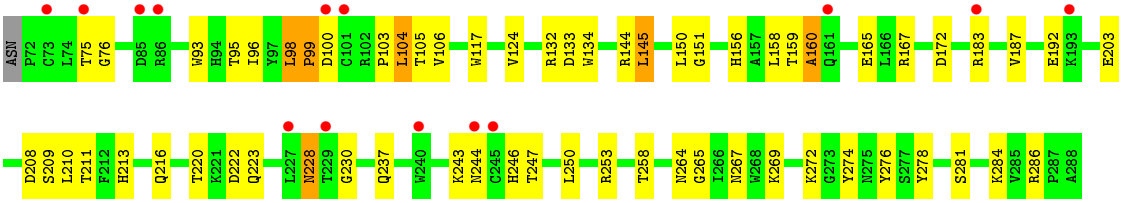
- Molecule 1: FICOLIN-2

Chain C:

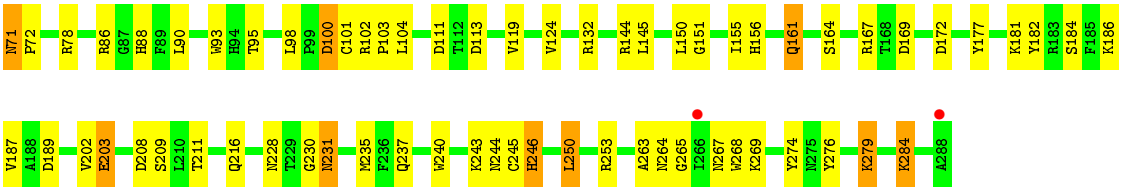


- Molecule 1: FICOLIN-2

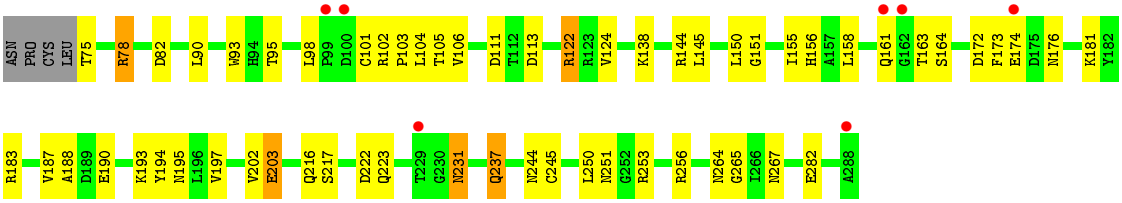
Chain D:



- Molecule 1: FICOLIN-2



- Molecule 1: FICOLIN-2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	98.89Å 98.89Å 141.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.50 19.74 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.50) 97.8 (19.74-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.259 0.199 , 0.252	Depositor DCC
R_{free} test set	2601 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.7	EDS
Estimated twinning fraction	0.033 for -h,-k,l 0.095 for h,-h-k,-l 0.042 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 52154 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10729	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: BMA, NAG, CA, P4C, FUC, MAN

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	0.58	0/1754	0.65	0/2373
1	B	0.64	0/1783	0.70	0/2413
1	C	0.60	0/1767	0.70	1/2391 (0.0%)
1	D	0.57	0/1780	0.62	0/2409
1	E	0.65	0/1787	0.68	0/2419
1	F	0.58	0/1761	0.65	0/2383
All	All	0.60	0/10632	0.67	1/14388 (0.0%)

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
1	C	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	122	ARG	NE-CZ-NH1	-5.50	117.55	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	202	VAL	Peptide
1	C	203	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1707	0	1578	99	0
1	B	1735	0	1606	50	0
1	C	1719	0	1586	40	0
1	D	1732	0	1598	56	0
1	E	1739	0	1609	53	0
1	F	1714	0	1585	48	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	60	0	52	1	0
4	E	39	0	34	0	0
5	E	22	0	27	4	0
6	A	23	0	0	10	0
6	B	60	0	0	4	0
6	C	52	0	0	6	0
6	D	29	0	0	1	0
6	E	55	0	0	5	0
6	F	37	0	0	2	0
All	All	10729	0	9675	339	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 17.

All (339) 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:104:LEU:CD2	1:F:106:VAL:HG13	1.74	1.15
1:C:245:CYS:SG	6:C:2043:HOH:O	2.06	1.14
1:F:104:LEU:HD22	1:F:106:VAL:HG13	1.16	1.11
1:F:104:LEU:CD2	1:F:106:VAL:CG1	2.29	1.10
1:A:266:ILE:HA	6:A:2020:HOH:O	1.49	1.10
1:B:183:ARG:HH11	1:B:183:ARG:HG3	0.98	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:LEU:HD22	1:F:106:VAL:CG1	1.84	1.07
1:A:198:LEU:HD22	1:A:210:LEU:CD2	1.89	1.02
1:A:112:THR:CG2	1:A:167:ARG:HH21	1.74	1.01
1:A:164:SER:HB3	1:A:287:PRO:HA	1.46	0.97
1:D:98:LEU:HB3	1:D:99:PRO:HD3	1.44	0.96
1:D:98:LEU:CB	1:D:99:PRO:CD	2.44	0.96
1:A:198:LEU:CD2	1:A:210:LEU:CD2	2.44	0.95
1:A:198:LEU:HD22	1:A:210:LEU:HD23	1.46	0.95
1:C:245:CYS:HB2	6:C:2042:HOH:O	1.66	0.94
1:C:193:LYS:HB3	1:C:217:SER:HB3	1.50	0.93
1:F:104:LEU:HD21	1:F:106:VAL:HG12	1.48	0.93
1:B:183:ARG:CG	1:B:183:ARG:HH11	1.82	0.92
1:A:198:LEU:CD2	1:A:210:LEU:HD23	1.99	0.92
1:A:202:VAL:O	1:A:203:GLU:HG3	1.72	0.90
1:E:237:GLN:HE21	1:E:264:ASN:HD22	1.18	0.88
1:E:237:GLN:NE2	1:E:264:ASN:HD22	1.70	0.88
1:F:104:LEU:HD21	1:F:106:VAL:CG1	2.02	0.85
1:D:98:LEU:HB3	1:D:99:PRO:CD	2.06	0.85
1:D:98:LEU:HB2	1:D:99:PRO:HD2	1.59	0.84
1:D:209:SER:HB3	1:D:247:THR:HG22	1.60	0.84
1:B:183:ARG:NH1	1:B:183:ARG:HG3	1.77	0.84
1:D:98:LEU:CD2	1:D:158:LEU:HD23	2.07	0.84
1:F:237:GLN:HE21	1:F:253:ARG:HE	1.24	0.83
1:D:237:GLN:NE2	1:D:264:ASN:HD22	1.77	0.82
1:E:167:ARG:NH2	1:E:177:TYR:OH	2.11	0.81
1:E:216:GLN:HE21	1:E:243:LYS:NZ	1.80	0.80
1:C:98:LEU:HD12	1:C:102:ARG:HB3	1.64	0.80
1:B:228:ASN:HD22	1:B:244:ASN:ND2	1.81	0.79
1:F:104:LEU:HD23	1:F:104:LEU:C	2.03	0.78
1:D:247:THR:HG23	1:D:269:LYS:HB3	1.66	0.78
1:C:228:ASN:HD22	1:C:244:ASN:ND2	1.81	0.78
1:A:174:GLU:N	1:A:174:GLU:OE1	2.16	0.78
1:A:198:LEU:HD22	1:A:210:LEU:HD21	1.65	0.78
1:D:98:LEU:HB2	1:D:99:PRO:CD	2.12	0.78
1:F:237:GLN:HE22	1:F:264:ASN:HD22	1.30	0.78
1:D:98:LEU:CB	1:D:99:PRO:HD3	2.13	0.77
1:A:272:LYS:HG2	1:A:278:TYR:OH	1.85	0.77
1:D:151:GLY:HA3	6:D:2010:HOH:O	1.83	0.77
1:C:237:GLN:HE22	1:C:264:ASN:HD22	1.33	0.77
1:A:112:THR:HG22	1:A:167:ARG:HH21	1.48	0.75
1:C:237:GLN:HE21	1:C:253:ARG:HE	1.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ASP:O	1:A:170:LEU:HD23	1.87	0.74
1:D:237:GLN:HE22	1:D:264:ASN:HD22	1.36	0.73
1:A:202:VAL:O	1:A:203:GLU:CG	2.36	0.73
1:F:113:ASP:OD2	1:F:181:LYS:CE	2.37	0.72
1:A:250:LEU:HA	6:A:2020:HOH:O	1.87	0.71
1:C:228:ASN:HD22	1:C:244:ASN:HD21	1.39	0.71
1:A:172:ASP:OD1	1:A:176:ASN:HB2	1.90	0.71
1:F:113:ASP:OD2	1:F:181:LYS:NZ	2.25	0.70
1:A:166:LEU:HD13	1:A:167:ARG:N	2.06	0.70
1:C:100:ASP:O	1:C:101:CYS:HB2	1.91	0.70
1:A:198:LEU:HD21	1:A:210:LEU:CD2	2.21	0.69
1:C:183:ARG:HH11	1:C:183:ARG:HB3	1.57	0.68
1:E:71:ASN:N	1:E:72:PRO:CD	2.56	0.68
1:B:167:ARG:NH2	1:B:177:TYR:OH	2.27	0.68
1:F:237:GLN:NE2	1:F:264:ASN:HD22	1.92	0.68
1:A:209:SER:O	1:A:248:SER:HB3	1.94	0.68
1:A:227:LEU:HB2	1:A:243:LYS:HA	1.76	0.67
1:E:228:ASN:HD22	1:E:244:ASN:ND2	1.92	0.67
1:E:113:ASP:OD2	1:E:181:LYS:NZ	2.25	0.67
1:F:78:ARG:NE	1:F:82:ASP:OD2	2.28	0.66
1:E:279:LYS:NZ	5:E:1293:P4C:H52	2.11	0.66
1:E:71:ASN:N	1:E:72:PRO:HD2	2.11	0.66
1:B:72:PRO:O	1:B:75:THR:HG23	1.96	0.66
1:E:265:GLY:H	1:E:267:ASN:HD21	1.42	0.66
1:D:216:GLN:HB2	1:D:243:LYS:HZ2	1.60	0.66
1:A:78:ARG:HG3	1:A:79:THR:HG23	1.75	0.66
1:B:117:TRP:HB3	1:B:284:LYS:HG3	1.79	0.65
1:A:164:SER:HB3	1:A:287:PRO:CA	2.25	0.65
1:E:216:GLN:HE21	1:E:243:LYS:HZ1	1.43	0.65
1:A:202:VAL:C	1:A:203:GLU:HG3	2.18	0.64
1:A:213:HIS:HE1	1:A:246:HIS:HA	1.63	0.63
1:D:228:ASN:HD22	1:D:230:GLY:H	1.46	0.62
1:B:216:GLN:HE21	1:B:243:LYS:HE2	1.64	0.62
1:D:98:LEU:HD21	1:D:158:LEU:CD2	2.28	0.62
1:D:98:LEU:HD22	1:D:158:LEU:HD23	1.80	0.62
1:C:156:HIS:HD2	1:C:187:VAL:O	1.82	0.62
1:D:98:LEU:CD2	1:D:158:LEU:CD2	2.77	0.61
1:D:216:GLN:HB2	1:D:243:LYS:NZ	2.14	0.61
1:B:72:PRO:O	1:B:75:THR:CG2	2.49	0.61
1:D:265:GLY:H	1:D:267:ASN:HD21	1.47	0.61
1:F:156:HIS:HD2	1:F:187:VAL:O	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:CYS:O	1:E:103:PRO:HD3	2.01	0.61
1:A:213:HIS:CE1	1:A:246:HIS:HA	2.35	0.61
1:A:198:LEU:CD2	1:A:210:LEU:HD21	2.26	0.60
1:A:213:HIS:HE1	1:A:246:HIS:CB	2.14	0.60
1:A:213:HIS:HE1	1:A:246:HIS:CA	2.14	0.60
1:A:213:HIS:HE1	1:A:246:HIS:HB2	1.66	0.60
1:C:162:GLY:O	1:C:163:THR:HG23	2.01	0.60
1:F:244:ASN:O	1:F:244:ASN:ND2	2.34	0.60
1:B:265:GLY:H	1:B:267:ASN:HD21	1.50	0.60
1:B:253:ARG:HD3	6:B:2010:HOH:O	2.02	0.60
1:A:151:GLY:O	1:A:155:ILE:HG13	2.02	0.60
1:A:258:THR:HA	1:A:275:ASN:O	2.02	0.59
1:B:174:GLU:O	1:B:174:GLU:HG3	2.02	0.59
1:A:156:HIS:HD2	1:A:187:VAL:O	1.85	0.59
1:D:237:GLN:HE21	1:D:253:ARG:HE	1.51	0.59
1:A:214:ASN:OD1	1:A:215:ASN:N	2.36	0.59
1:D:216:GLN:HE21	1:D:243:LYS:NZ	2.01	0.58
1:F:265:GLY:H	1:F:267:ASN:HD21	1.51	0.58
1:A:193:LYS:HB2	1:A:217:SER:OG	2.03	0.58
1:E:244:ASN:N	1:E:245:CYS:HA	2.16	0.57
1:B:89:PHE:HB2	6:B:2003:HOH:O	2.04	0.57
1:F:173:PHE:CZ	1:F:256:ARG:HA	2.39	0.57
1:A:86:ARG:O	1:A:86:ARG:HG3	2.05	0.57
1:B:113:ASP:OD2	1:B:181:LYS:NZ	2.37	0.57
1:A:112:THR:HG22	1:A:167:ARG:NH2	2.18	0.57
1:B:209:SER:HB3	1:B:247:THR:HG23	1.86	0.57
1:A:98:LEU:HD13	1:A:102:ARG:NH2	2.20	0.57
1:B:167:ARG:HH21	1:B:177:TYR:HH	1.49	0.56
1:E:279:LYS:HZ1	5:E:1293:P4C:H52	1.70	0.56
1:B:72:PRO:HA	1:B:75:THR:CG2	2.35	0.56
1:E:156:HIS:HD2	1:E:187:VAL:O	1.88	0.56
1:F:102:ARG:HG2	1:F:103:PRO:HD2	1.86	0.56
1:A:179:PHE:O	1:A:206:ALA:HB3	2.05	0.56
1:F:75:THR:HG21	6:F:2001:HOH:O	2.06	0.56
1:D:237:GLN:NE2	1:D:253:ARG:HE	2.03	0.56
1:A:266:ILE:HG23	6:A:2020:HOH:O	2.05	0.55
1:D:156:HIS:HD2	1:D:187:VAL:O	1.89	0.55
1:E:88:HIS:HD2	6:E:2003:HOH:O	1.88	0.55
1:F:104:LEU:CD2	1:F:104:LEU:C	2.74	0.55
1:A:210:LEU:C	1:A:210:LEU:HD23	2.27	0.55
1:E:237:GLN:HE22	1:E:253:ARG:HH21	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:HIS:CE1	1:A:246:HIS:HB2	2.42	0.55
1:B:208:ASP:OD1	1:B:211:THR:HB	2.07	0.55
1:A:98:LEU:O	1:A:101:CYS:N	2.30	0.54
1:C:279:LYS:HE3	6:C:2051:HOH:O	2.06	0.54
1:D:265:GLY:H	1:D:267:ASN:ND2	2.05	0.54
1:A:117:TRP:CZ3	1:A:167:ARG:HB2	2.43	0.54
1:F:98:LEU:HD12	1:F:102:ARG:HB3	1.89	0.54
1:F:78:ARG:HD3	1:F:78:ARG:N	2.23	0.54
1:A:236:PHE:HE2	1:A:245:CYS:SG	2.30	0.54
1:B:93:TRP:CE3	1:B:144:ARG:HD3	2.42	0.54
1:C:113:ASP:HA	6:C:2009:HOH:O	2.08	0.54
1:C:216:GLN:HE21	1:C:243:LYS:NZ	2.06	0.54
1:F:104:LEU:HD23	1:F:105:THR:N	2.23	0.54
1:B:231:ASN:HD22	1:B:231:ASN:C	2.11	0.53
1:A:76:GLY:N	6:A:2001:HOH:O	2.41	0.53
1:F:172:ASP:OD1	1:F:174:GLU:HG2	2.07	0.53
1:F:188:ALA:O	1:F:194:TYR:HA	2.08	0.53
1:C:237:GLN:NE2	1:C:264:ASN:HD22	2.04	0.53
1:B:93:TRP:CD2	1:B:144:ARG:HD3	2.44	0.53
1:B:228:ASN:HD22	1:B:244:ASN:HD21	1.56	0.53
1:C:201:PHE:CD1	1:C:202:VAL:O	2.61	0.53
1:A:166:LEU:CD1	1:A:167:ARG:N	2.71	0.53
1:B:156:HIS:HD2	1:B:187:VAL:O	1.91	0.53
1:A:231:ASN:HD21	1:A:233:ALA:HB3	1.73	0.53
1:A:272:LYS:HG2	1:A:278:TYR:CZ	2.44	0.52
1:E:144:ARG:NH1	6:E:2015:HOH:O	2.41	0.52
1:A:93:TRP:HE3	1:A:105:THR:HG22	1.74	0.52
1:D:272:LYS:HG3	1:D:278:TYR:OH	2.09	0.52
1:E:265:GLY:H	1:E:267:ASN:ND2	2.08	0.52
1:E:88:HIS:CD2	6:E:2003:HOH:O	2.61	0.52
1:A:244:ASN:N	1:A:245:CYS:HA	2.24	0.52
1:A:95:THR:HA	1:A:104:LEU:O	2.09	0.52
1:B:258:THR:HG22	1:B:276:TYR:HD2	1.72	0.52
1:C:193:LYS:CB	1:C:217:SER:HB3	2.30	0.52
1:E:216:GLN:HE21	1:E:243:LYS:HZ2	1.53	0.52
1:A:227:LEU:HB2	1:A:243:LYS:CA	2.39	0.52
1:F:193:LYS:CB	1:F:217:SER:HB3	2.40	0.52
1:A:201:PHE:HB2	1:A:208:ASP:OD2	2.10	0.52
1:E:228:ASN:HD22	1:E:244:ASN:HD22	1.55	0.52
1:A:113:ASP:HB2	1:A:167:ARG:NH2	2.25	0.52
1:E:100:ASP:O	1:E:101:CYS:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LYS:CB	1:A:217:SER:OG	2.58	0.51
1:A:190:GLU:O	1:A:193:LYS:HD3	2.10	0.51
1:E:231:ASN:HD22	1:E:231:ASN:C	2.13	0.51
1:F:183:ARG:HG3	1:F:202:VAL:CG2	2.41	0.51
1:F:202:VAL:HG12	1:F:203:GLU:HG2	1.93	0.51
1:E:269:LYS:HD3	1:E:274:TYR:CZ	2.46	0.51
1:F:122:ARG:HD2	1:F:282:GLU:OE2	2.11	0.51
1:A:198:LEU:HD23	1:A:211:THR:HA	1.93	0.51
1:E:172:ASP:HB2	1:E:276:TYR:OH	2.10	0.51
1:A:250:LEU:C	6:A:2020:HOH:O	2.50	0.51
1:D:75:THR:HG22	1:D:76:GLY:N	2.26	0.50
1:E:151:GLY:O	1:E:155:ILE:HG13	2.11	0.50
1:D:213:HIS:HE1	1:D:246:HIS:HA	1.76	0.50
1:F:173:PHE:CE1	1:F:256:ARG:HA	2.47	0.50
1:E:209:SER:HB2	1:E:268:TRP:CE2	2.46	0.50
1:E:279:LYS:HE3	5:E:1293:P4C:O10	2.12	0.50
1:E:240:TRP:CH2	1:E:250:LEU:HB2	2.47	0.50
1:E:132:ARG:HH22	1:F:111:ASP:CG	2.14	0.50
1:C:201:PHE:CE1	1:C:202:VAL:O	2.65	0.49
1:B:72:PRO:HA	1:B:75:THR:HG21	1.93	0.49
1:C:188:ALA:O	1:C:194:TYR:HA	2.11	0.49
1:A:198:LEU:HD21	1:A:210:LEU:HD23	1.87	0.49
1:F:244:ASN:N	1:F:245:CYS:HA	2.26	0.49
1:A:165:GLU:O	1:A:285:VAL:HA	2.12	0.49
1:D:208:ASP:OD2	1:D:211:THR:OG1	2.30	0.49
1:D:96:ILE:O	1:D:103:PRO:HA	2.13	0.49
1:B:75:THR:HG23	1:B:76:GLY:N	2.28	0.49
1:F:195:ASN:ND2	1:F:216:GLN:C	2.66	0.49
1:F:93:TRP:CD2	1:F:144:ARG:HD3	2.47	0.49
1:E:216:GLN:NE2	1:E:243:LYS:NZ	2.58	0.48
1:C:93:TRP:CD2	1:C:144:ARG:HD3	2.47	0.48
1:A:98:LEU:HD13	1:A:102:ARG:CZ	2.43	0.48
1:C:113:ASP:CA	6:C:2009:HOH:O	2.61	0.48
1:A:240:TRP:CH2	1:A:250:LEU:HB2	2.48	0.48
1:E:119:VAL:O	6:E:2008:HOH:O	2.20	0.48
1:C:236:PHE:HE2	1:C:245:CYS:SG	2.37	0.48
1:F:237:GLN:HE22	1:F:264:ASN:ND2	2.06	0.48
1:B:156:HIS:CE1	1:B:189:ASP:HB3	2.49	0.48
1:D:132:ARG:NH2	1:E:111:ASP:OD1	2.40	0.48
1:D:272:LYS:HG3	1:D:278:TYR:CZ	2.48	0.48
1:F:183:ARG:HG3	1:F:202:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:GLU:C	1:E:203:GLU:OE2	2.53	0.47
1:E:208:ASP:OD1	1:E:211:THR:HB	2.13	0.47
1:A:156:HIS:O	1:A:160:ALA:HB2	2.13	0.47
1:D:98:LEU:HD21	1:D:158:LEU:HD21	1.96	0.47
1:B:208:ASP:OD1	1:B:211:THR:CB	2.62	0.47
1:D:132:ARG:HH22	1:E:111:ASP:CG	2.17	0.47
1:A:89:PHE:CE1	1:C:139:GLN:HB2	2.50	0.47
1:A:250:LEU:CA	6:A:2020:HOH:O	2.54	0.47
1:B:183:ARG:CG	1:B:183:ARG:NH1	2.52	0.47
1:A:180:ALA:HB1	1:A:201:PHE:HE1	1.80	0.47
1:D:228:ASN:ND2	1:D:230:GLY:H	2.12	0.47
1:E:100:ASP:OD2	1:E:100:ASP:O	2.33	0.47
1:D:213:HIS:CE1	1:D:246:HIS:HA	2.49	0.47
1:B:209:SER:HB2	1:B:268:TRP:CE2	2.50	0.47
1:B:182:TYR:CE2	1:B:208:ASP:OD2	2.68	0.47
1:E:98:LEU:HD12	1:E:102:ARG:HB3	1.96	0.47
1:D:98:LEU:HD21	1:D:158:LEU:HD23	1.85	0.47
1:B:117:TRP:CB	1:B:284:LYS:HG3	2.44	0.47
1:A:173:PHE:CZ	1:A:256:ARG:HA	2.49	0.46
1:D:145:LEU:HD21	1:E:93:TRP:HE1	1.80	0.46
3:B:1292:FUC:H3	6:B:2056:HOH:O	2.15	0.46
1:C:240:TRP:CH2	1:C:250:LEU:HB2	2.51	0.46
1:A:144:ARG:NH2	1:B:94:HIS:NE2	2.64	0.46
1:C:174:GLU:O	1:C:175:ASP:HB2	2.16	0.46
1:F:265:GLY:H	1:F:267:ASN:ND2	2.14	0.46
1:F:222:ASP:OD1	1:F:222:ASP:N	2.40	0.46
1:A:166:LEU:HD23	1:A:185:PHE:CG	2.50	0.45
1:E:156:HIS:CE1	1:E:189:ASP:HB3	2.52	0.45
1:A:86:ARG:CG	1:A:86:ARG:O	2.64	0.45
1:C:165:GLU:HG3	1:C:288:ALA:HA	1.99	0.45
1:B:144:ARG:NH2	1:C:94:HIS:NE2	2.65	0.45
1:E:208:ASP:OD1	1:E:211:THR:CB	2.65	0.45
1:D:172:ASP:HB2	1:D:276:TYR:OH	2.16	0.45
1:D:133:ASP:HB2	1:D:222:ASP:OD2	2.16	0.45
1:D:117:TRP:HB3	1:D:284:LYS:HB2	1.98	0.45
1:D:237:GLN:HE22	1:D:264:ASN:ND2	2.08	0.45
1:B:193:LYS:HE3	1:B:225:ASN:OD1	2.16	0.45
1:F:151:GLY:O	1:F:155:ILE:HG13	2.16	0.45
1:F:195:ASN:HD22	1:F:216:GLN:C	2.20	0.45
1:C:231:ASN:C	1:C:231:ASN:HD22	2.19	0.45
1:D:209:SER:CB	1:D:247:THR:HG22	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ASP:CG	1:A:174:GLU:OE1	2.55	0.45
1:F:193:LYS:HB2	1:F:217:SER:HB3	1.99	0.45
1:D:93:TRP:CZ2	1:D:144:ARG:HA	2.52	0.45
1:A:180:ALA:HA	1:A:204:GLY:HA3	1.97	0.44
1:A:172:ASP:HB2	1:A:276:TYR:OH	2.18	0.44
1:A:236:PHE:HE2	1:A:245:CYS:CB	2.30	0.44
1:E:208:ASP:CG	1:E:211:THR:HG1	2.21	0.44
1:D:167:ARG:O	1:D:284:LYS:HG2	2.16	0.44
1:B:77:PRO:HG3	1:B:83:LEU:HD21	1.98	0.44
1:A:266:ILE:CB	6:A:2020:HOH:O	2.61	0.44
1:A:179:PHE:O	1:A:180:ALA:HB2	2.17	0.44
1:B:228:ASN:ND2	1:B:244:ASN:ND2	2.57	0.44
1:E:182:TYR:CE2	1:E:208:ASP:OD2	2.71	0.44
1:D:216:GLN:HE21	1:D:243:LYS:HZ1	1.61	0.44
1:B:269:LYS:NZ	6:B:2044:HOH:O	2.45	0.44
1:B:228:ASN:HB2	1:B:244:ASN:HD22	1.81	0.44
1:D:222:ASP:O	1:D:223:GLN:HG2	2.18	0.44
1:B:97:TYR:CE2	1:B:103:PRO:HB3	2.52	0.44
1:F:138:LYS:HE2	1:F:190:GLU:OE1	2.17	0.44
1:A:91:SER:O	1:C:144:ARG:HG3	2.17	0.44
1:D:269:LYS:HD2	1:D:274:TYR:CE2	2.52	0.43
1:B:161:GLN:HE21	1:B:161:GLN:HB3	1.64	0.43
1:C:162:GLY:O	1:C:163:THR:CG2	2.65	0.43
1:F:193:LYS:HB3	1:F:217:SER:HB3	2.00	0.43
1:E:78:ARG:HD3	1:E:78:ARG:HA	1.52	0.43
1:F:93:TRP:CE3	1:F:144:ARG:HD3	2.53	0.43
1:C:168:THR:O	1:C:179:PHE:HA	2.19	0.43
1:A:132:ARG:HH22	1:B:111:ASP:CG	2.21	0.43
1:A:219:SER:HB2	6:A:2016:HOH:O	2.17	0.43
1:F:104:LEU:HD23	1:F:105:THR:C	2.39	0.43
1:C:100:ASP:O	1:C:101:CYS:CB	2.62	0.43
1:A:137:TYR:CZ	1:A:239:ALA:HB3	2.53	0.43
1:C:192:GLU:O	1:C:193:LYS:HB2	2.19	0.43
1:E:164:SER:O	1:E:184:SER:HA	2.19	0.43
1:D:134:TRP:HA	1:D:220:THR:HG21	2.01	0.43
1:E:230:GLY:HA3	1:E:235:MET:CE	2.48	0.43
1:A:182:TYR:HA	1:A:200:ALA:O	2.19	0.43
1:A:150:LEU:HD23	1:A:150:LEU:HA	1.85	0.43
1:D:158:LEU:HA	1:D:158:LEU:HD23	1.82	0.42
1:A:247:THR:HB	1:A:269:LYS:HB3	2.01	0.42
1:A:120:PHE:CD1	1:A:155:ILE:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ASP:OD1	1:D:208:ASP:C	2.58	0.42
1:C:98:LEU:HB3	1:C:99:PRO:HD2	2.00	0.42
5:E:1293:P4C:H62	5:E:1293:P4C:H32	1.70	0.42
1:B:269:LYS:HD2	1:B:274:TYR:CZ	2.54	0.42
1:D:99:PRO:HG2	1:D:100:ASP:H	1.84	0.42
1:A:215:ASN:HA	6:A:2012:HOH:O	2.18	0.42
1:B:182:TYR:HE2	1:B:208:ASP:OD2	2.01	0.42
1:A:112:THR:HG23	1:A:167:ARG:HH21	1.72	0.42
1:B:172:ASP:HB2	1:B:276:TYR:OH	2.20	0.42
1:B:279:LYS:HG2	1:B:280:VAL:HG23	2.00	0.42
1:C:246:HIS:C	1:C:246:HIS:CD2	2.93	0.42
1:E:202:VAL:HG12	1:E:203:GLU:HG3	2.02	0.42
1:C:279:LYS:CE	6:C:2051:HOH:O	2.64	0.42
1:A:167:ARG:HG2	1:A:181:LYS:HB3	2.02	0.41
1:D:165:GLU:HG2	1:D:286:ARG:O	2.20	0.41
1:D:104:LEU:HD13	1:D:106:VAL:CG1	2.50	0.41
1:E:169:ASP:OD1	1:E:284:LYS:NZ	2.43	0.41
1:A:212:PHE:O	1:A:243:LYS:NZ	2.36	0.41
1:A:231:ASN:ND2	1:A:233:ALA:HB3	2.33	0.41
1:D:228:ASN:HD22	1:D:230:GLY:N	2.14	0.41
1:A:164:SER:CB	1:A:287:PRO:HA	2.34	0.41
1:E:216:GLN:NE2	1:E:243:LYS:HZ1	2.13	0.41
1:A:98:LEU:O	1:A:99:PRO:C	2.59	0.41
1:A:265:GLY:H	1:A:267:ASN:ND2	2.18	0.41
1:A:236:PHE:CE2	1:A:245:CYS:SG	3.11	0.41
1:E:161:GLN:NE2	6:E:2022:HOH:O	2.53	0.41
1:A:167:ARG:NH1	1:A:179:PHE:CD1	2.89	0.41
1:C:93:TRP:CE3	1:C:144:ARG:HD3	2.55	0.41
1:E:246:HIS:HE1	1:E:263:ALA:O	2.03	0.41
1:B:104:LEU:HA	1:B:104:LEU:HD23	1.93	0.41
1:C:255:LEU:O	1:C:256:ARG:HB2	2.21	0.41
1:D:159:THR:O	1:D:160:ALA:C	2.59	0.41
1:D:210:LEU:HD12	1:D:210:LEU:HA	1.82	0.41
1:A:197:VAL:HA	6:A:2012:HOH:O	2.20	0.40
1:A:166:LEU:C	1:A:166:LEU:CD1	2.89	0.40
1:B:258:THR:HA	1:B:275:ASN:O	2.21	0.40
1:F:231:ASN:C	1:F:231:ASN:HD22	2.24	0.40
1:A:82:ASP:O	1:A:85:ASP:HB2	2.20	0.40
1:F:172:ASP:OD2	1:F:176:ASN:HB2	2.22	0.40
1:A:93:TRP:HA	1:A:106:VAL:O	2.21	0.40
1:E:182:TYR:HE2	1:E:208:ASP:OD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:ALA:HA	1:C:267:ASN:ND2	2.36	0.40
1:B:165:GLU:H	1:B:165:GLU:HG2	1.68	0.40
1:F:251:ASN:HB2	6:F:2032:HOH:O	2.21	0.40
1:B:75:THR:HG23	1:B:76:GLY:H	1.85	0.40
1:A:93:TRP:CD2	1:A:144:ARG:HD3	2.57	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	211/218 (97%)	185 (88%)	23 (11%)	3 (1%)	14	24
1	B	215/218 (99%)	197 (92%)	17 (8%)	1 (0%)	34	55
1	C	212/218 (97%)	193 (91%)	16 (8%)	3 (1%)	14	24
1	D	215/218 (99%)	193 (90%)	19 (9%)	3 (1%)	14	24
1	E	216/218 (99%)	200 (93%)	16 (7%)	0	100	100
1	F	212/218 (97%)	198 (93%)	13 (6%)	1 (0%)	34	55
All	All	1281/1308 (98%)	1166 (91%)	104 (8%)	11 (1%)	21	37

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	98	LEU
1	B	75	THR
1	C	162	GLY
1	C	204	GLY
1	A	180	ALA
1	D	99	PRO
1	A	160	ALA

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Mol	Chain	Res	Type
1	C	160	ALA
1	D	160	ALA
1	F	161	GLN
1	A	99	PRO

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	178/183 (97%)	162 (91%)	16 (9%)	12	22
1	B	182/183 (100%)	169 (93%)	13 (7%)	18	34
1	C	179/183 (98%)	165 (92%)	14 (8%)	16	29
1	D	181/183 (99%)	167 (92%)	14 (8%)	16	30
1	E	182/183 (100%)	165 (91%)	17 (9%)	11	21
1	F	179/183 (98%)	162 (90%)	17 (10%)	11	20
All	All	1081/1098 (98%)	990 (92%)	91 (8%)	14	25

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	A	90	LEU
1	A	95	THR
1	A	104	LEU
1	A	124	VAL
1	A	145	LEU
1	A	150	LEU
1	A	164	SER
1	A	166	LEU
1	A	167	ARG
1	A	186	LYS
1	A	223	GLN
1	A	227	LEU
1	A	231	ASN

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Mol	Chain	Res	Type
1	A	244	ASN
1	A	281	SER
1	B	75	THR
1	B	95	THR
1	B	99	PRO
1	B	104	LEU
1	B	124	VAL
1	B	145	LEU
1	B	150	LEU
1	B	161	GLN
1	B	183	ARG
1	B	231	ASN
1	B	247	THR
1	B	250	LEU
1	B	284	LYS
1	C	90	LEU
1	C	95	THR
1	C	101	CYS
1	C	104	LEU
1	C	124	VAL
1	C	145	LEU
1	C	150	LEU
1	C	164	SER
1	C	183	ARG
1	C	193	LYS
1	C	231	ASN
1	C	237	GLN
1	C	250	LEU
1	C	281	SER
1	D	95	THR
1	D	104	LEU
1	D	105	THR
1	D	124	VAL
1	D	145	LEU
1	D	150	LEU
1	D	183	ARG
1	D	192	GLU
1	D	203	GLU
1	D	228	ASN
1	D	244	ASN
1	D	250	LEU
1	D	258	THR

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Mol	Chain	Res	Type
1	D	281	SER
1	E	71	ASN
1	E	86	ARG
1	E	90	LEU
1	E	95	THR
1	E	100	ASP
1	E	104	LEU
1	E	124	VAL
1	E	145	LEU
1	E	150	LEU
1	E	161	GLN
1	E	186	LYS
1	E	203	GLU
1	E	231	ASN
1	E	246	HIS
1	E	250	LEU
1	E	279	LYS
1	E	284	LYS
1	F	78	ARG
1	F	90	LEU
1	F	95	THR
1	F	101	CYS
1	F	122	ARG
1	F	124	VAL
1	F	145	LEU
1	F	150	LEU
1	F	158	LEU
1	F	163	THR
1	F	164	SER
1	F	197	VAL
1	F	203	GLU
1	F	223	GLN
1	F	231	ASN
1	F	237	GLN
1	F	250	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	156	HIS
1	A	176	ASN

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Mol	Chain	Res	Type
1	A	228	ASN
1	A	231	ASN
1	A	244	ASN
1	A	246	HIS
1	A	267	ASN
1	A	275	ASN
1	B	139	GLN
1	B	156	HIS
1	B	176	ASN
1	B	216	GLN
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	195	ASN
1	C	216	GLN
1	C	231	ASN
1	C	237	GLN
1	C	244	ASN
1	C	246	HIS
1	C	267	ASN
1	D	139	GLN
1	D	156	HIS
1	D	216	GLN
1	D	228	ASN
1	D	237	GLN
1	D	244	ASN
1	D	246	HIS
1	D	267	ASN
1	E	139	GLN
1	E	156	HIS
1	E	161	GLN
1	E	216	GLN
1	E	231	ASN
1	E	237	GLN
1	E	244	ASN
1	E	246	HIS
1	E	267	ASN
1	F	139	GLN
1	F	156	HIS

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Mol	Chain	Res	Type
1	F	195	ASN
1	F	216	GLN
1	F	231	ASN
1	F	237	GLN
1	F	246	HIS
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

8 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	$\#\|Z\| > 2$
3	NAG	B	1290	1,3	14,14,15	0.67	0	15,19,21	1.48	2 (13%)
3	NAG	B	1291	3	14,14,15	0.78	1 (7%)	15,19,21	1.47	2 (13%)
3	FUC	B	1292	3	10,10,11	0.70	0	14,14,16	1.56	3 (21%)
3	BMA	B	1293	3	11,11,12	0.60	0	14,15,17	1.12	0
3	MAN	B	1294	3	11,11,12	0.73	0	14,15,17	1.38	2 (14%)
4	NAG	E	1290	1,4	14,14,15	0.52	0	15,19,21	1.48	2 (13%)
4	NAG	E	1291	4	14,14,15	0.36	0	15,19,21	1.32	1 (6%)
4	BMA	E	1292	4	11,11,12	0.63	0	14,15,17	2.06	4 (28%)

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	B	1290	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1291	3	-	0/6/23/26	0/1/1/1
3	FUC	B	1292	3	-	0/0/17/20	0/1/1/1
3	BMA	B	1293	3	-	0/2/19/22	0/1/1/1
3	MAN	B	1294	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1290	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	1291	4	-	0/6/23/26	0/1/1/1
4	BMA	E	1292	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1291	NAG	O5-C1	-2.07	1.40	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1290	NAG	C3-C4-C5	-3.40	104.27	110.20
3	B	1291	NAG	C2-N2-C7	-3.34	118.75	123.04
3	B	1294	MAN	O2-C2-C3	-3.07	103.95	110.12
4	E	1290	NAG	C3-C4-C5	-2.53	105.78	110.20
4	E	1292	BMA	O5-C1-C2	-2.48	106.84	110.86
3	B	1291	NAG	C6-C5-C4	-2.29	107.37	113.02
3	B	1294	MAN	C2-C3-C4	-2.27	107.19	111.04
3	B	1292	FUC	O5-C1-C2	-2.16	107.35	110.86
3	B	1292	FUC	C1-C2-C3	-2.16	106.98	109.54
3	B	1290	NAG	O4-C4-C3	-2.04	105.74	110.34
4	E	1291	NAG	C1-O5-C5	3.46	116.64	112.25
3	B	1292	FUC	C1-O5-C5	3.62	117.97	112.38
4	E	1292	BMA	C1-C2-C3	3.68	113.89	109.54
4	E	1292	BMA	C3-C4-C5	3.73	116.71	110.20
4	E	1290	NAG	C1-O5-C5	3.78	117.05	112.25
4	E	1292	BMA	C2-C3-C4	3.82	117.53	111.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1292	FUC	1	0

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
5	P4C	E	1293	-	21,21,21	2.40	4 (19%)	19,20,20	2.70	2 (10%)

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
5	P4C	E	1293	-	-	0/18/19/19	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1293	P4C	O1-C2	-3.25	1.24	1.42
5	E	1293	P4C	O22-C21	3.60	1.43	1.19
5	E	1293	P4C	O19-C20	4.02	1.56	1.42
5	E	1293	P4C	O16-C17	8.66	1.78	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1293	P4C	O16-C17-C18	-4.50	90.34	110.36
5	E	1293	P4C	C17-O16-C15	10.63	158.99	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1293	P4C	4	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	213/218 (97%)	0.70	29 (13%) 4 4	20, 42, 71, 74	0
1	B	217/218 (99%)	-0.12	4 (1%) 71 75	14, 30, 45, 52	0
1	C	213/218 (97%)	-0.01	6 (2%) 56 61	18, 33, 49, 56	1 (0%)
1	D	217/218 (99%)	0.11	14 (6%) 22 25	20, 38, 59, 71	0
1	E	218/218 (100%)	-0.20	2 (0%) 85 88	18, 31, 46, 59	1 (0%)
1	F	214/218 (98%)	0.05	7 (3%) 50 55	20, 34, 54, 66	0
All	All	1292/1308 (98%)	0.09	62 (4%) 34 39	14, 34, 60, 74	2 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	ALA	5.0
1	A	227	LEU	5.0
1	A	288	ALA	4.9
1	A	245	CYS	4.7
1	A	230	GLY	4.4
1	A	191	ALA	4.4
1	D	73	CYS	4.0
1	A	240	TRP	4.0
1	F	100	ASP	3.9
1	D	101	CYS	3.8
1	A	239	ALA	3.7
1	F	288	ALA	3.6
1	A	100	ASP	3.5
1	A	203	GLU	3.5
1	A	101	CYS	3.4
1	A	161	GLN	3.4
1	F	161	GLN	3.4
1	A	162	GLY	3.3
1	C	203	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	100	ASP	3.0
1	A	219	SER	3.0
1	C	100	ASP	2.9
1	B	161	GLN	2.8
1	D	183	ARG	2.8
1	D	227	LEU	2.8
1	F	162	GLY	2.8
1	D	244	ASN	2.7
1	E	288	ALA	2.7
1	B	250	LEU	2.7
1	A	177	TYR	2.6
1	C	288	ALA	2.6
1	A	262	PHE	2.6
1	A	260	GLY	2.6
1	D	75	THR	2.6
1	A	232	CYS	2.5
1	C	161	GLN	2.5
1	D	85	ASP	2.5
1	A	258	THR	2.5
1	A	175	ASP	2.4
1	A	192	GLU	2.4
1	C	191	ALA	2.4
1	A	188	ALA	2.4
1	D	245	CYS	2.3
1	F	229	THR	2.3
1	A	247	THR	2.3
1	A	229	THR	2.3
1	E	266	ILE	2.3
1	D	240	TRP	2.3
1	D	161	GLN	2.3
1	D	193	LYS	2.2
1	A	257	GLY	2.2
1	F	174	GLU	2.2
1	A	103	PRO	2.2
1	A	242	TYR	2.1
1	A	168	THR	2.1
1	F	99	PRO	2.1
1	A	76	GLY	2.1
1	A	189	ASP	2.1
1	D	86	ARG	2.0
1	D	229	THR	2.0
1	C	202	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	248	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
3	FUC	B	1292	10/11	0.93	0.15	0.64	37,40,41,42	0
3	MAN	B	1294	11/12	0.96	0.11	-1.08	50,50,51,52	0
3	BMA	B	1293	11/12	0.93	0.16	-	47,49,50,51	0
3	NAG	B	1291	14/15	0.95	0.17	-	34,37,42,44	0
4	NAG	E	1290	14/15	0.94	0.17	-	45,48,50,52	0
4	NAG	E	1291	14/15	0.91	0.25	-	55,57,59,61	0
3	NAG	B	1290	14/15	0.96	0.11	-	26,29,35,37	0
4	BMA	E	1292	11/12	0.79	0.35	-	63,65,66,66	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
5	P4C	E	1293	22/22	0.85	0.21	3.13	20,51,69,71	6
2	CA	B	1289	1/1	0.88	0.14	1.11	36,36,36,36	0
2	CA	F	1289	1/1	0.96	0.03	-1.66	44,44,44,44	0
2	CA	E	1289	1/1	0.99	0.11	-1.89	28,28,28,28	0
2	CA	A	1289	1/1	0.86	0.06	-2.47	76,76,76,76	0
2	CA	D	1289	1/1	0.88	0.05	-2.52	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	1289	1/1	0.98	0.04	-4.53	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.