



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:18 AM GMT

PDB ID : 3HUS
Title : Crystal structure of recombinant gamma N308K fibrinogen fragment D with the peptide ligand Gly-Pro-Arg-Pro-amide
Authors : Lord, S.T.; Bowley, S.R.; Okumura, N.
Deposited on : 2009-06-15
Resolution : 3.04 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

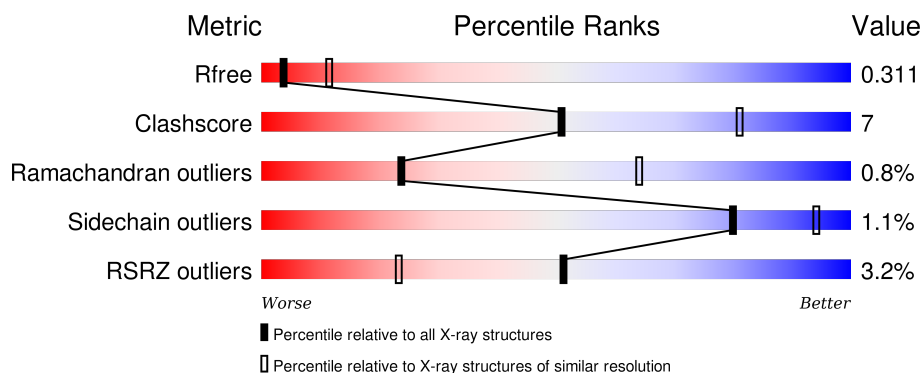
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	1995 (3.08-3.00)
Clashscore	102246	2351 (3.08-3.00)
Ramachandran outliers	100387	2272 (3.08-3.00)
Sidechain outliers	100360	2275 (3.08-3.00)
RSRZ outliers	91569	2013 (3.08-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	66	<div> <div>11%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>8%</div> </div> </div>
1	D	66	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>8%</div> </div> </div>
2	B	313	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>5%</div> </div> </div>
2	E	313	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>3%</div> </div> </div>
3	C	311	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	311	<div><div></div><div>2%</div><div>79%</div><div>14%</div><div>6%</div></div>
4	G	4	<div><div></div><div>100%</div></div>
4	H	4	<div><div></div><div>25%</div><div>50%</div><div>50%</div></div>
4	I	4	<div><div></div><div>75%</div><div>25%</div></div>
4	J	4	<div><div></div><div>50%</div><div>75%</div><div>25%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10837 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 Fibrinogen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	61	Total	C	N	O	S	0	0	0
			497	305	95	94	3			
1	D	61	Total	C	N	O	S	0	0	0
			497	305	95	94	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2428	1514	429	463	22			
2	E	303	Total	C	N	O	S	0	0	0
			2428	1514	429	463	22			

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	291	Total	C	N	O	S	0	0	0
			2335	1483	393	448	11			
3	F	293	Total	C	N	O	S	0	0	0
			2352	1493	397	451	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	308	LYS	ASN	ENGINEERED	UNP P02679
F	308	LYS	ASN	ENGINEERED	UNP P02679

- Molecule 4 is a protein called Peptide Ligand Gly-Pro-Arg-Pro-amide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			30	18	7	5			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	4	Total	C	N	O	0	0	0
			30	18	7	5			
4	I	4	Total	C	N	O	0	0	0
			30	18	7	5			
4	J	4	Total	C	N	O	0	0	0
			30	18	7	5			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		
5	E	1	Total	Ca	0	0
			1	1		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	3	Total	C	N	O	0	0
			38	22	2	14		
6	E	3	Total	C	N	O	0	0
			38	22	2	14		

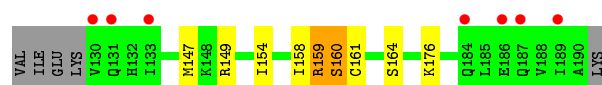
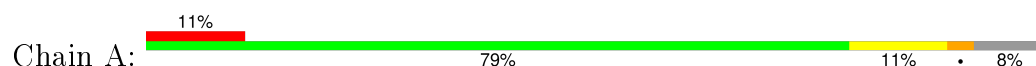
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total	O	0	0
			6	6		
7	B	26	Total	O	0	0
			26	26		
7	C	14	Total	O	0	0
			14	14		
7	D	4	Total	O	0	0
			4	4		
7	E	33	Total	O	0	0
			33	33		
7	F	17	Total	O	0	0
			17	17		

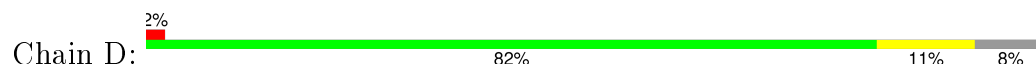
3 Residue-property plots [i](#)

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.

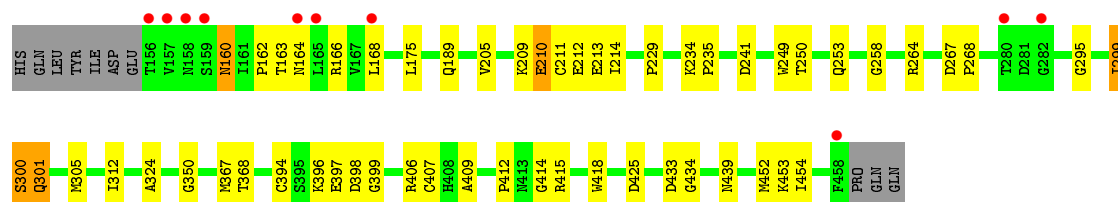
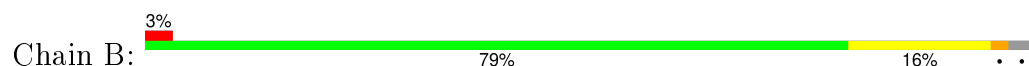
- Molecule 1: Fibrinogen alpha chain



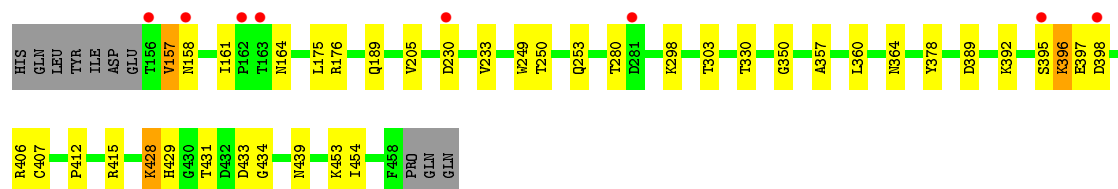
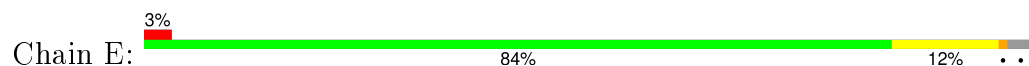
- Molecule 1: Fibrinogen alpha chain



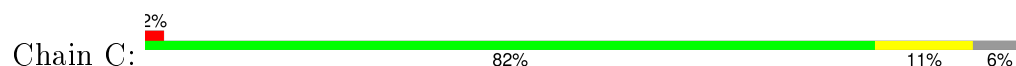
- Molecule 2: Fibrinogen beta chain

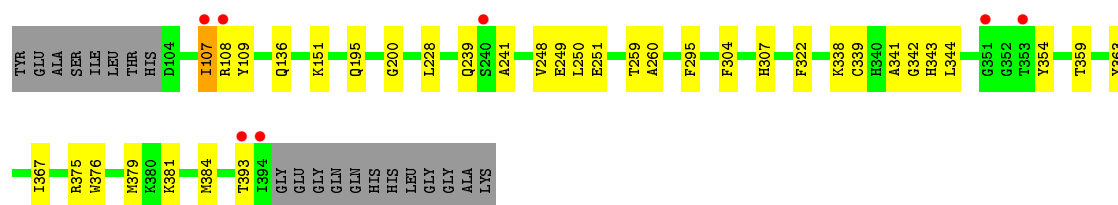


- Molecule 2: Fibrinogen beta chain

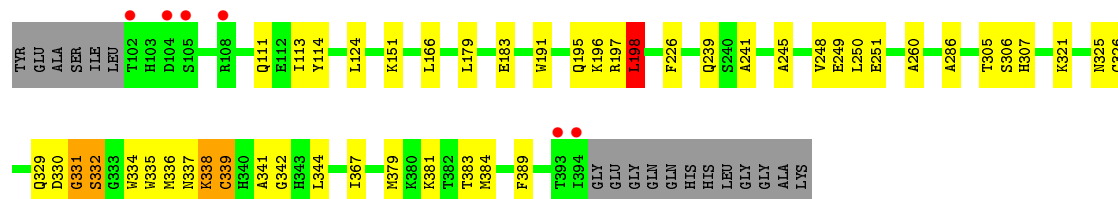
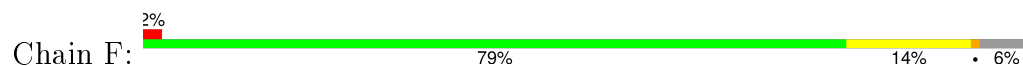


- Molecule 3: Fibrinogen gamma chain





- Molecule 3: Fibrinogen gamma chain



- Molecule 4: Peptide Ligand Gly-Pro-Arg-Pro-amide



There are no outlier residues recorded for this chain.

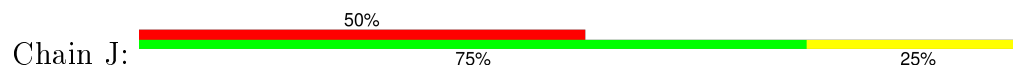
- Molecule 4: Peptide Ligand Gly-Pro-Arg-Pro-amide



- Molecule 4: Peptide Ligand Gly-Pro-Arg-Pro-amide



- Molecule 4: Peptide Ligand Gly-Pro-Arg-Pro-amide



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.01Å 95.01Å 448.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.25 – 3.04 47.24 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.25-3.04) 99.4 (47.24-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.14 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.288 0.287 , 0.311	Depositor DCC
R_{free} test set	2027 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 35.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	3 of 40519 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10837	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.63 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.9848e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, FUC

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	0.38	0/498	0.50	0/665
1	D	0.26	0/498	0.45	0/665
2	B	0.37	0/2489	0.46	0/3362
2	E	0.36	0/2489	0.45	0/3362
3	C	0.32	0/2399	0.42	0/3243
3	F	0.38	0/2417	0.44	1/3268 (0.0%)
4	G	0.49	0/31	0.46	0/40
4	H	0.49	0/31	0.46	0/40
4	I	0.50	0/31	0.52	0/40
4	J	0.50	0/31	0.65	0/40
All	All	0.36	0/10914	0.45	1/14725 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	198	LEU	C-N-CA	-5.29	108.49	121.70

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	497	0	517	12	0
1	D	497	0	517	6	0
2	B	2428	0	2295	42	0
2	E	2428	0	2296	31	0
3	C	2335	0	2192	23	0
3	F	2352	0	2208	44	0
4	G	30	0	32	0	0
4	H	30	0	32	1	0
4	I	30	0	32	1	0
4	J	30	0	32	2	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	B	38	0	34	0	0
6	E	38	0	34	1	0
7	A	6	0	0	0	0
7	B	26	0	0	1	0
7	C	14	0	0	1	0
7	D	4	0	0	0	0
7	E	33	0	0	2	0
7	F	17	0	0	0	0
All	All	10837	0	10221	144	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 7.

All (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:NH1	2:B:418:TRP:CE3	2.08	1.22
3:F:198:LEU:N	3:F:198:LEU:HD12	1.50	1.17
3:F:326:CYS:HB3	3:F:339:CYS:SG	1.85	1.16
3:F:326:CYS:CB	3:F:339:CYS:SG	2.41	1.08
1:A:159:ARG:O	2:B:258:GLY:O	1.70	1.07
3:F:338:LYS:NZ	4:I:3:ARG:O	1.97	0.96
2:E:397:GLU:HG2	2:E:431:THR:HG21	1.52	0.90
3:F:198:LEU:H	3:F:198:LEU:HD12	1.15	0.90
3:F:338:LYS:H	3:F:339:CYS:HA	1.37	0.88
3:F:338:LYS:O	3:F:338:LYS:HG3	1.75	0.86
3:F:338:LYS:N	3:F:339:CYS:HA	1.89	0.86
3:F:331:GLY:O	3:F:332:SER:HB3	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:378:TYR:HB2	2:E:396:LYS:HG3	1.62	0.82
3:C:200:GLY:HA2	7:C:83:HOH:O	1.81	0.80
3:F:198:LEU:N	3:F:198:LEU:CD1	2.30	0.78
3:F:338:LYS:H	3:F:339:CYS:CA	1.96	0.77
2:E:395:SER:O	2:E:396:LYS:HB2	1.84	0.76
2:B:160:ASN:O	2:B:162:PRO:HD3	1.85	0.76
4:J:3:ARG:HH11	4:J:3:ARG:HG3	1.53	0.73
3:F:338:LYS:O	3:F:338:LYS:CG	2.36	0.72
2:B:295:GLY:O	2:B:299:ILE:HG13	1.89	0.71
2:B:399:GLY:HA3	2:B:414:GLY:HA2	1.73	0.69
2:B:264:ARG:HH21	3:C:136:GLN:HA	1.59	0.67
3:F:337:ASN:O	3:F:338:LYS:CB	2.42	0.67
1:A:154:ILE:O	1:A:158:ILE:HG13	1.95	0.66
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.79	0.65
3:F:307:HIS:HE1	3:F:342:GLY:H	1.43	0.65
2:B:253:GLN:HE22	2:B:412:PRO:HB2	1.62	0.65
2:B:301:GLN:NE2	2:B:305:MET:SD	2.69	0.64
3:F:326:CYS:CB	3:F:339:CYS:HG	2.00	0.63
2:E:397:GLU:HG2	2:E:431:THR:CG2	2.26	0.63
2:E:453:LYS:NZ	7:E:50:HOH:O	2.31	0.62
1:A:158:ILE:HG23	2:B:189:GLN:HE21	1.64	0.62
3:F:334:TRP:O	3:F:336:MET:N	2.30	0.62
2:B:396:LYS:O	2:B:397:GLU:HG2	2.00	0.61
3:C:307:HIS:HE1	3:C:342:GLY:H	1.48	0.61
3:F:338:LYS:N	3:F:339:CYS:CA	2.60	0.60
3:F:196:LYS:O	3:F:197:ARG:HG2	2.01	0.60
3:F:251:GLU:HB3	3:F:381:LYS:HB2	1.84	0.60
2:B:209:LYS:HG3	2:B:213:GLU:OE2	2.02	0.59
2:B:367:MET:HB2	2:B:406:ARG:HB2	1.82	0.59
3:F:344:LEU:HA	3:F:367:ILE:HG23	1.85	0.59
2:B:209:LYS:C	2:B:210:GLU:HG3	2.23	0.59
2:B:398:ASP:HA	2:B:433:ASP:HB3	1.85	0.59
2:B:300:SER:O	2:B:301:GLN:C	2.37	0.58
2:E:428:LYS:O	2:E:428:LYS:CG	2.52	0.58
3:F:196:LYS:O	3:F:197:ARG:CG	2.52	0.58
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.68	0.57
3:F:305:THR:HB	3:F:341:ALA:HB2	1.86	0.57
2:E:364:ASN:HD21	6:E:3:NAG:H2	1.70	0.57
2:E:253:GLN:HE22	2:E:412:PRO:HB2	1.70	0.55
3:C:304:PHE:HB3	3:C:338:LYS:HB3	1.88	0.55
1:A:158:ILE:HG23	2:B:189:GLN:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:245:ALA:HB2	3:F:389:PHE:HD1	1.71	0.54
2:E:428:LYS:O	2:E:428:LYS:HG3	2.08	0.54
1:A:158:ILE:CG2	2:B:189:GLN:HE21	2.21	0.54
2:B:164:ASN:O	2:B:168:LEU:HB2	2.09	0.53
2:E:249:TRP:HB3	2:E:453:LYS:HB3	1.91	0.52
4:J:3:ARG:HG3	4:J:3:ARG:NH1	2.19	0.52
1:A:149:ARG:HH21	2:B:425:ASP:HA	1.75	0.52
2:E:157:VAL:HG22	2:E:158:ASN:H	1.74	0.51
3:F:306:SER:O	3:F:337:ASN:ND2	2.27	0.51
1:D:137:GLN:HE21	1:D:188:VAL:HG12	1.75	0.50
2:B:209:LYS:CG	2:B:213:GLU:OE2	2.59	0.50
3:C:195:GLN:HB3	3:C:384:MET:HB2	1.94	0.50
3:C:338:LYS:N	3:C:339:CYS:HA	2.25	0.49
1:A:159:ARG:NH1	2:B:418:TRP:CZ3	2.69	0.49
1:A:159:ARG:O	1:A:160:SER:OG	2.30	0.49
3:F:325:ASN:O	3:F:329:GLN:HG2	2.13	0.49
2:B:312:ILE:HB	2:B:324:ALA:HB3	1.95	0.49
2:E:389:ASP:HB3	2:E:392:LYS:HB2	1.95	0.49
2:B:211:CYS:HA	2:B:214:ILE:HD12	1.95	0.48
2:B:209:LYS:CD	2:B:213:GLU:OE2	2.61	0.48
3:F:183:GLU:HB3	3:F:191:TRP:HB2	1.94	0.48
2:B:350:GLY:HA3	2:B:439:ASN:HB3	1.95	0.48
3:F:111:GLN:HA	3:F:114:TYR:HB3	1.95	0.48
1:A:159:ARG:C	1:A:160:SER:OG	2.50	0.48
2:E:176:ARG:HE	3:F:113:ILE:HD11	1.78	0.48
3:F:337:ASN:O	3:F:338:LYS:HB3	2.12	0.48
2:B:295:GLY:O	2:B:299:ILE:CG1	2.61	0.48
2:E:398:ASP:HA	2:E:433:ASP:HB3	1.95	0.48
2:E:250:THR:HB	2:E:454:ILE:HG13	1.96	0.48
2:E:397:GLU:O	2:E:431:THR:OG1	2.32	0.47
2:B:415:ARG:O	2:B:434:GLY:HA2	2.14	0.47
3:F:321:LYS:HB2	3:F:337:ASN:O	2.14	0.47
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.97	0.47
2:B:368:THR:HB	2:B:409:ALA:HB2	1.96	0.47
2:E:298:LYS:HA	7:E:60:HOH:O	2.14	0.46
3:C:249:GLU:HG2	3:C:259:THR:HG22	1.97	0.46
2:E:428:LYS:HG2	2:E:429:HIS:CD2	2.51	0.46
2:E:161:ILE:O	2:E:164:ASN:HB3	2.14	0.46
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.97	0.46
3:F:250:LEU:HD22	3:F:379:MET:HG3	1.97	0.46
3:F:337:ASN:O	3:F:338:LYS:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:TRP:HB3	2:B:453:LYS:HB2	1.98	0.45
2:B:210:GLU:OE2	2:B:212:GLU:HB3	2.17	0.45
1:D:150:LEU:HD21	3:F:124:LEU:HD23	1.99	0.45
2:E:406:ARG:CG	2:E:406:ARG:O	2.63	0.45
2:E:406:ARG:N	2:E:407:CYS:HA	2.31	0.45
3:C:307:HIS:CE1	3:C:341:ALA:H	2.35	0.44
1:D:139:ASN:HB3	3:F:114:TYR:CZ	2.52	0.44
3:F:331:GLY:O	3:F:332:SER:CB	2.54	0.44
2:E:415:ARG:O	2:E:434:GLY:HA2	2.17	0.44
3:C:307:HIS:HE1	3:C:341:ALA:H	1.65	0.44
2:E:230:ASP:HB2	2:E:233:VAL:HG22	1.99	0.44
3:C:248:VAL:HB	3:C:260:ALA:HB3	1.99	0.44
3:C:344:LEU:HA	3:C:367:ILE:HG23	1.99	0.43
3:C:107:ILE:C	3:C:109:TYR:H	2.22	0.43
3:C:107:ILE:HG22	3:C:108:ARG:H	1.82	0.43
2:B:205:VAL:HG11	3:C:228:LEU:HA	1.99	0.43
2:E:205:VAL:HG21	3:F:226:PHE:HB2	2.00	0.43
2:B:253:GLN:HB3	2:B:452:MET:HB2	2.01	0.43
2:E:357:ALA:HB3	2:E:360:LEU:HD12	1.99	0.43
3:C:359:THR:HG21	3:C:363:TYR:O	2.18	0.43
3:F:326:CYS:O	3:F:330:ASP:HB2	2.19	0.42
2:E:406:ARG:HG2	2:E:406:ARG:O	2.19	0.42
2:E:350:GLY:HA3	2:E:439:ASN:HB3	2.01	0.42
2:B:250:THR:HB	2:B:454:ILE:HG13	2.00	0.42
1:A:147:MET:HG3	2:B:175:LEU:HD22	2.01	0.42
3:F:260:ALA:HB2	3:F:286:ALA:HB3	2.02	0.42
3:F:248:VAL:HB	3:F:260:ALA:HB3	2.01	0.42
2:B:406:ARG:N	2:B:407:CYS:HA	2.35	0.42
2:B:394:CYS:O	2:B:398:ASP:HB2	2.19	0.42
4:H:1:GLY:H3	4:H:3:ARG:HH12	1.68	0.42
3:C:343:HIS:O	3:C:367:ILE:HA	2.18	0.42
3:F:195:GLN:HB3	3:F:384:MET:HB2	2.02	0.42
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.84	0.42
2:E:395:SER:O	2:E:396:LYS:CB	2.63	0.41
2:B:163:THR:HG22	2:B:166:ARG:NH2	2.35	0.41
2:B:163:THR:HG22	2:B:166:ARG:HH21	1.85	0.41
3:C:307:HIS:CE1	3:C:342:GLY:H	2.34	0.41
3:C:295:PHE:HB3	3:C:375:ARG:HH21	1.84	0.41
3:C:322:PHE:HD1	3:C:338:LYS:HE2	1.85	0.41
3:C:354:TYR:O	3:C:376:TRP:HB3	2.20	0.41
1:A:161:CYS:HA	1:A:164:SER:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:250:LEU:HD22	3:C:379:MET:HG3	2.02	0.41
1:D:169:LEU:H	2:E:189:GLN:HE22	1.69	0.41
1:D:147:MET:HG3	2:E:175:LEU:HD22	2.01	0.41
3:F:249:GLU:HB3	3:F:383:THR:HB	2.03	0.41
3:F:166:LEU:HD13	3:F:179:LEU:HD21	2.02	0.41
2:B:229:PRO:HG2	7:B:81:HOH:O	2.21	0.40
2:B:234:LYS:HA	2:B:235:PRO:HD3	1.99	0.40
1:D:136:LEU:HD21	3:F:111:GLN:HB3	2.02	0.40
2:E:303:THR:HB	2:E:330:THR:HA	2.02	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	59/66 (89%)	55 (93%)	3 (5%)	1 (2%)	11	43
1	D	59/66 (89%)	58 (98%)	1 (2%)	0	100	100
2	B	301/313 (96%)	271 (90%)	29 (10%)	1 (0%)	46	82
2	E	301/313 (96%)	275 (91%)	24 (8%)	2 (1%)	26	67
3	C	289/311 (93%)	267 (92%)	21 (7%)	1 (0%)	46	82
3	F	291/311 (94%)	265 (91%)	21 (7%)	5 (2%)	11	43
4	G	2/4 (50%)	2 (100%)	0	0	100	100
4	H	2/4 (50%)	2 (100%)	0	0	100	100
4	I	2/4 (50%)	2 (100%)	0	0	100	100
4	J	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1308/1396 (94%)	1199 (92%)	99 (8%)	10 (1%)	24	64

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	157	VAL
3	F	335	TRP
3	F	338	LYS
1	A	160	SER
2	E	396	LYS
3	F	331	GLY
3	F	332	SER
3	C	241	ALA
3	F	241	ALA
2	B	160	ASN

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	56/61 (92%)	54 (96%)	2 (4%)	42	78
1	D	56/61 (92%)	56 (100%)	0	100	100
2	B	261/271 (96%)	257 (98%)	4 (2%)	72	91
2	E	261/271 (96%)	259 (99%)	2 (1%)	86	95
3	C	245/259 (95%)	243 (99%)	2 (1%)	86	95
3	F	247/259 (95%)	245 (99%)	2 (1%)	86	95
4	G	3/3 (100%)	3 (100%)	0	100	100
4	H	3/3 (100%)	3 (100%)	0	100	100
4	I	3/3 (100%)	3 (100%)	0	100	100
4	J	3/3 (100%)	3 (100%)	0	100	100
All	All	1138/1194 (95%)	1126 (99%)	12 (1%)	80	94

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	ARG
1	A	176	LYS
2	B	210	GLU
2	B	299	ILE

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Mol	Chain	Res	Type
2	B	300	SER
2	B	301	GLN
3	C	107	ILE
3	C	393	THR
2	E	280	THR
2	E	428	LYS
3	F	198	LEU
3	F	339	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
2	B	189	GLN
2	B	202	ASN
2	B	253	GLN
2	B	339	GLN
2	B	408	HIS
3	C	111	GLN
3	C	136	GLN
3	C	189	ASN
3	C	230	ASN
3	C	239	GLN
3	C	307	HIS
3	C	319	ASN
2	E	189	GLN
2	E	253	GLN
2	E	301	GLN
2	E	339	GLN
2	E	364	ASN
2	E	408	HIS
2	E	429	HIS
3	F	103	HIS
3	F	115	ASN
3	F	117	ASN
3	F	136	GLN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS

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 ⓘ

6 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$
6	NAG	B	3	2,6	14,14,15	0.49	0	15,19,21	0.74	0
6	NAG	B	4	6	14,14,15	0.74	0	15,19,21	2.57	5 (33%)
6	FUC	B	5	6	10,10,11	0.60	0	14,14,16	0.92	1 (7%)
6	NAG	E	3	6	14,14,15	0.53	0	15,19,21	0.86	1 (6%)
6	NAG	E	4	6	14,14,15	0.61	0	15,19,21	1.57	2 (13%)
6	FUC	E	5	6	10,10,11	0.59	0	14,14,16	1.00	2 (14%)

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
6	NAG	B	3	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	4	6	-	0/6/23/26	0/1/1/1
6	FUC	B	5	6	-	0/0/17/20	0/1/1/1
6	NAG	E	3	6	-	0/6/23/26	0/1/1/1
6	NAG	E	4	6	-	0/6/23/26	0/1/1/1
6	FUC	E	5	6	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	4	NAG	O7-C7-C8	-2.42	117.62	122.06
6	E	3	NAG	C3-C4-C5	2.03	113.74	110.20
6	E	5	FUC	C1-C2-C3	2.17	112.11	109.54
6	E	5	FUC	O5-C5-C6	2.43	110.14	106.13
6	B	5	FUC	O5-C5-C6	2.51	110.27	106.13
6	B	4	NAG	C3-C4-C5	2.52	114.59	110.20
6	E	4	NAG	C4-C3-C2	2.94	115.80	111.23
6	B	4	NAG	C8-C7-N2	3.19	122.21	116.11
6	B	4	NAG	C4-C3-C2	3.90	117.29	111.23
6	E	4	NAG	C2-N2-C7	3.94	128.10	123.04
6	B	4	NAG	C2-N2-C7	7.48	132.66	123.04

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
6	E	3	NAG	1	0

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	61/66 (92%)	0.88	7 (11%) 6 2	72, 87, 102, 102	0
1	D	61/66 (92%)	0.16	1 (1%) 74 47	60, 67, 78, 78	0
2	B	303/313 (96%)	0.20	10 (3%) 50 22	49, 58, 75, 88	0
2	E	303/313 (96%)	0.07	8 (2%) 59 29	46, 55, 68, 81	0
3	C	291/311 (93%)	0.10	7 (2%) 62 32	50, 59, 72, 83	0
3	F	293/311 (94%)	0.17	6 (2%) 68 39	50, 61, 73, 87	0
4	G	4/4 (100%)	0.46	0 100 100	85, 85, 86, 86	0
4	H	4/4 (100%)	1.14	1 (25%) 1 0	88, 88, 88, 89	0
4	I	4/4 (100%)	0.54	0 100 100	95, 95, 96, 96	0
4	J	4/4 (100%)	1.79	2 (50%) 0 0	78, 78, 78, 80	0
All	All	1328/1396 (95%)	0.18	42 (3%) 51 23	46, 59, 82, 102	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	156	THR	8.7
2	B	157	VAL	5.9
2	E	163	THR	5.3
1	A	131	GLN	5.0
1	A	130	VAL	4.6
3	C	394	ILE	4.3
2	B	158	ASN	3.9
2	B	458	PHE	3.7
1	A	186	GLU	3.7
3	C	240	SER	3.5
1	A	187	GLN	3.5
2	B	159	SER	3.4
2	B	164	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
3	F	104	ASP	3.1
3	F	394	ILE	3.0
3	F	393	THR	2.8
2	E	395	SER	2.8
4	J	4	PRO	2.7
2	B	168	LEU	2.7
2	B	280	THR	2.7
3	C	353	THR	2.7
1	A	133	ILE	2.7
4	J	1	GLY	2.6
2	E	281	ASP	2.6
2	E	158	ASN	2.6
3	C	108	ARG	2.5
2	B	282	GLY	2.5
2	E	230	ASP	2.5
3	C	107	ILE	2.5
1	A	189	ILE	2.5
2	E	156	THR	2.4
1	A	184	GLN	2.4
2	E	162	PRO	2.2
3	F	108	ARG	2.2
3	F	102	THR	2.2
4	H	1	GLY	2.2
3	C	351	GLY	2.1
1	D	187	GLN	2.1
3	C	393	THR	2.1
2	B	165	LEU	2.1
2	E	398	ASP	2.0
3	F	105	SER	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	E	4	14/15	0.74	0.43	-	134,135,135,135	0
6	NAG	E	3	14/15	0.59	0.29	-	132,134,135,135	0
6	FUC	E	5	10/11	0.78	0.30	-	135,135,135,135	0
6	NAG	B	3	14/15	0.75	0.27	-	89,92,97,97	0
6	NAG	B	4	14/15	0.62	0.48	-	100,101,102,102	0
6	FUC	B	5	10/11	0.72	0.52	-	99,99,100,100	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	CA	B	2	1/1	0.40	0.26	0.98	69,69,69,69	0
5	CA	E	2	1/1	0.91	0.15	-	64,64,64,64	0
5	CA	F	1	1/1	0.68	0.37	-	90,90,90,90	0
5	CA	C	1	1/1	-0.03	0.29	-	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.