wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:03 PM GMT

PDB ID : 1N86
Title : Crystal structure of human D-dimer from cross-linked fibrin complexed with GPR and GHRPLDK peptide ligands.
Authors : Yang, Z.; Pandi, L.; Doolittle, R.F.
Deposited on : 2002-11-19
Resolution : 3.20 Å(reported)

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

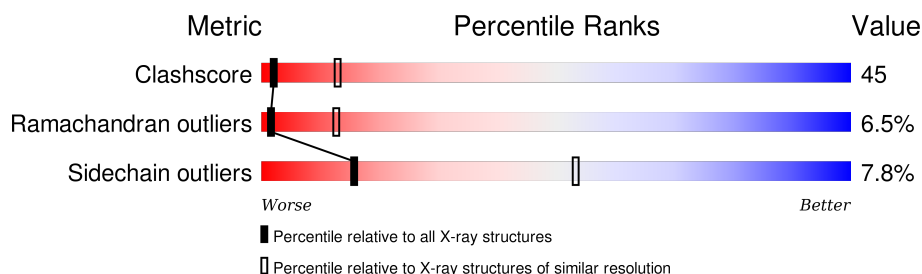|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.20 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	Percentile Ranks	Value
Clashscore		45
Ramachandran outliers		6.5%
Sidechain outliers		7.8%

Worse *Better*

▋ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	87	23% 57% 5% 15%
1	D	87	24% 52% 8% • 15%
2	B	328	34% 50% 8% • 6%
2	E	328	32% 52% 8% • 6%
3	C	324	39% 45% 7% 9%
3	F	324	40% 44% 7% 9%
4	G	3	100%

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Mol	Chain	Length	Quality of chain
4	H	3	67% 33%
5	I	7	57% 43%
5	J	7	57% 43%

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
6	NDG	B	470	-	-	X	-
6	NDG	I	471	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11054 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 Fibrin alpha/alpha-E chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			
1	D	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			

- Molecule 2 is a protein called Fibrin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	307	Total	C	N	O	S	0	0	0
			2462	1535	433	472	22			
2	E	307	Total	C	N	O	S	0	0	0
			2462	1535	433	472	22			

- Molecule 3 is a protein called Fibrin gamma chain.

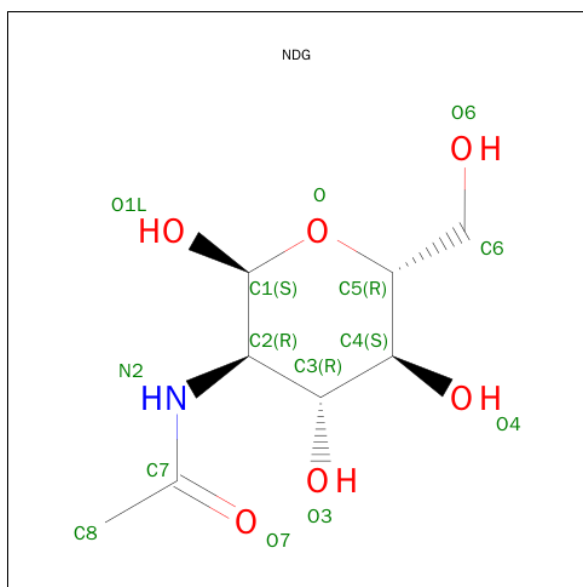| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	295	Total	C	N	O	S	0	0	0
			2364	1498	399	456	11			
3	F	295	Total	C	N	O	S	0	0	0
			2364	1498	399	456	11			

- Molecule 4 is a protein called fibrin alpha chain peptide ligand fragment Gly-Pro-Arg.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			23	13	6	4			
4	H	3	Total	C	N	O	0	0	0
			23	13	6	4			

- Molecule 5 is a protein called fibrin beta chain peptide ligand fragment Gly-His-Arg-Pro-Leu-Asp-Lys.
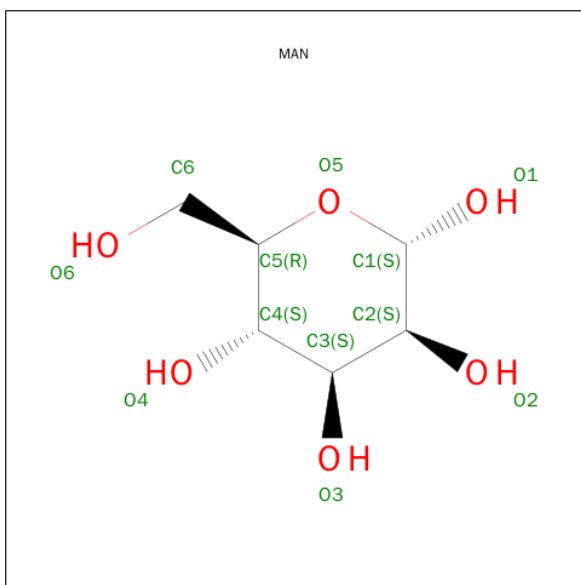
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	4	Total 32	C 19	N 9	O 4	0	0	0
5	J	4	Total 32	C 19	N 9	O 4	0	0	0

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total 15	C 8	N 1	O 6	0	0
6	I	1	Total 15	C 8	N 1	O 6	0	0
6	E	1	Total 15	C 8	N 1	O 6	0	0
6	J	1	Total 15	C 8	N 1	O 6	0	0

- Molecule 7 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).

| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 12	C 6	O 6	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

3 Residue-property plots ⓘ

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.
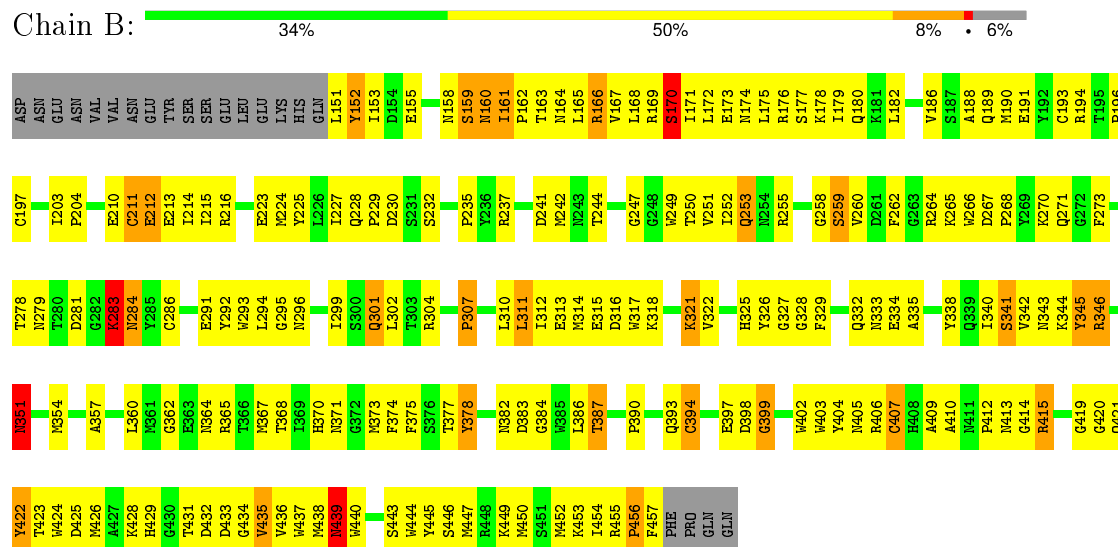
Note EDS was not executed.

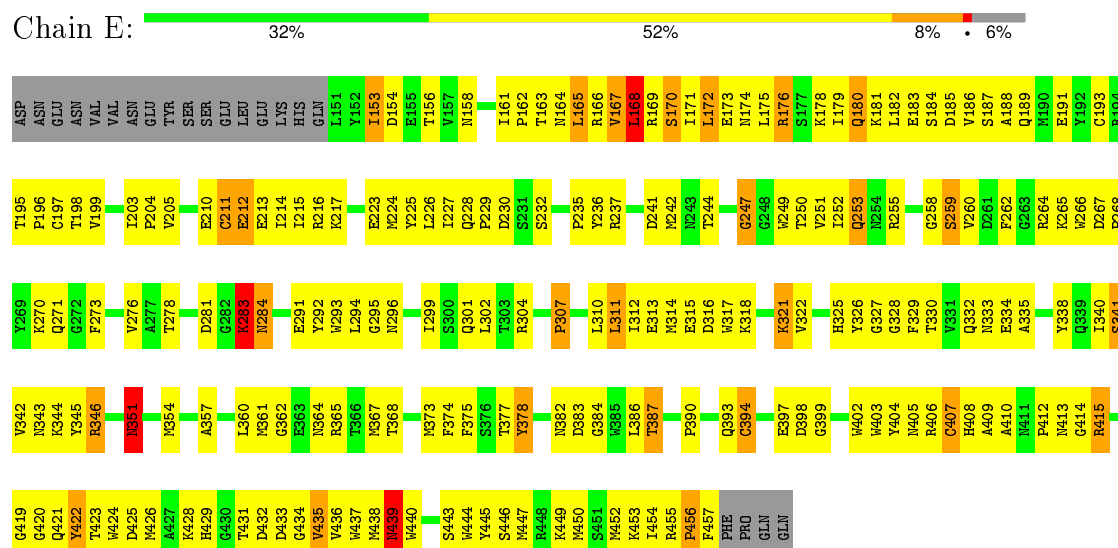- Molecule 1: Fibrin alpha/alpha-E chain
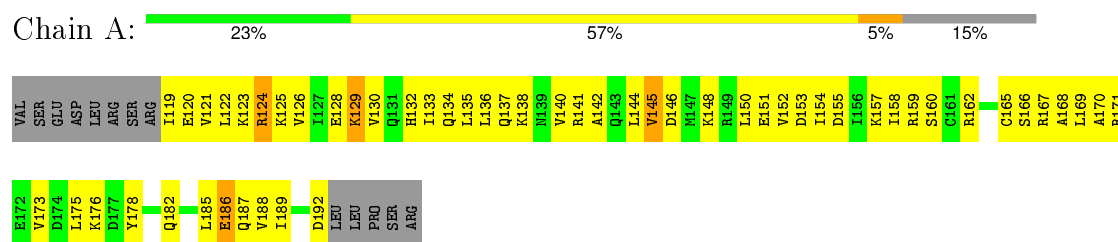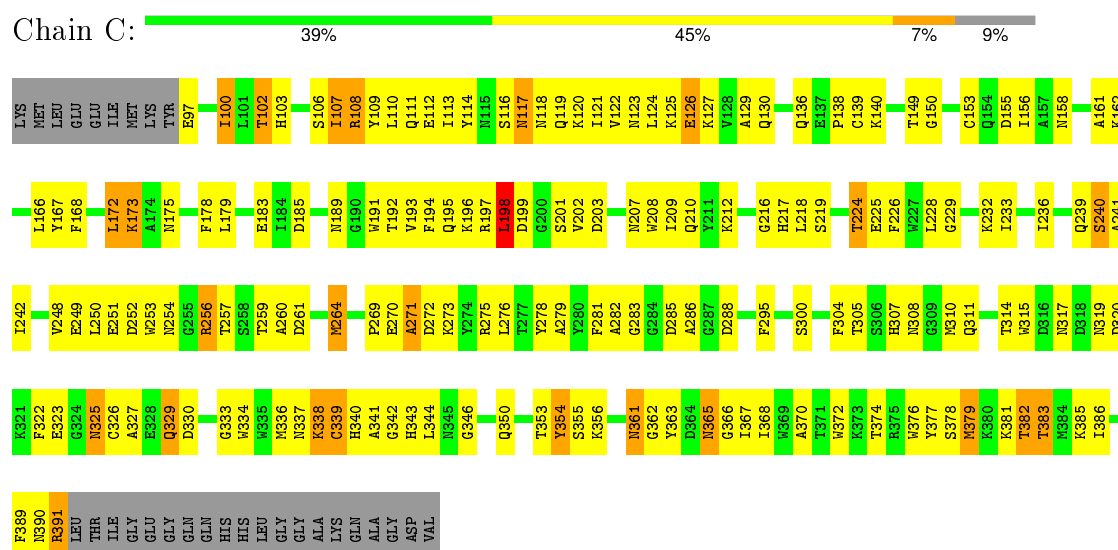

- Molecule 1: Fibrin alpha/alpha-E chain
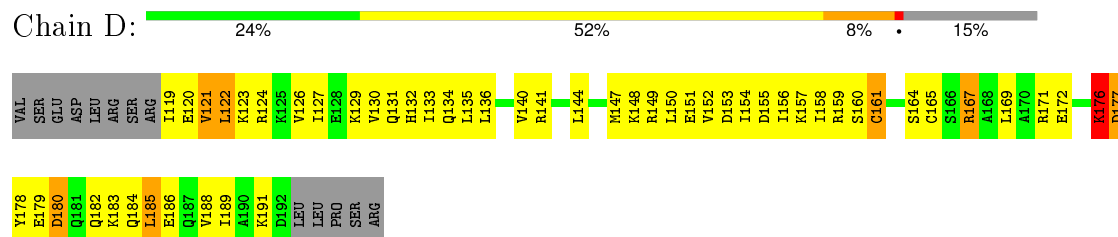
- Molecule 2: Fibrin beta chain

● Molecule 2: Fibrin beta chain

Chain E:

● Molecule 3: Fibrin gamma chain

Chain C:

● Molecule 3: Fibrin gamma chain

Chain F:

N319 D320 K321 F322 E323 G324 N325 C326 A327 E328 Q329 D330 G333 W334 W335 M336 N337 K338 C339 H340 A341 G342 H343 L344 V347 Y348 Y349 Q350 T353 Y354 S355 K356 N361 G362 Y363 D364 N365 G366 I367 I368 M369 A370 T371 W372 K373 T374 R375 W376 Y377 S378 M379 K380 K381 T382 T383 M384

K385 I386 F389 N390 R391 LEU THR ILE GLY GLU GLY GLN GLN HIS HIS LEU GLY GLY ALA LYS GLN ALA GLY ASP VAL

• Molecule 4: fibrin alpha chain peptide ligand fragment Gly-Pro-Arg

Chain G: 100%

G1 P2 R3

• Molecule 4: fibrin alpha chain peptide ligand fragment Gly-Pro-Arg

Chain H: 67%   33%

G1 P2 R3

• Molecule 5: fibrin beta chain peptide ligand fragment Gly-His-Arg-Pro-Leu-Asp-Lys

Chain I: 57%   43%
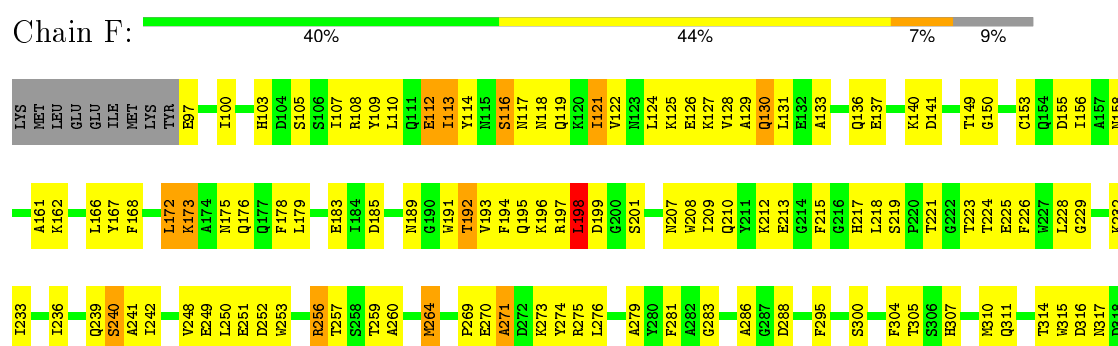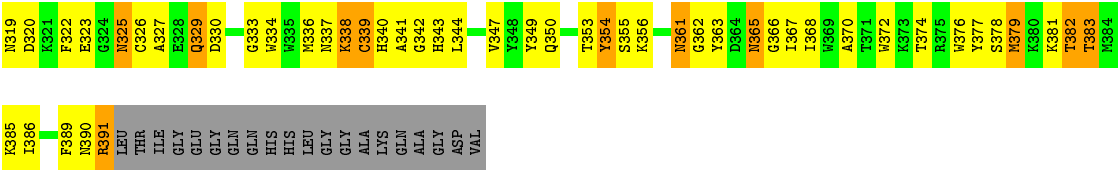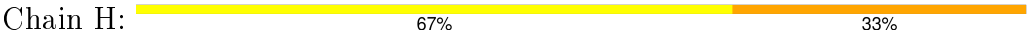
G1 H2 R3 P4 LEU ASP LYS

• Molecule 5: fibrin beta chain peptide ligand fragment Gly-His-Arg-Pro-Leu-Asp-Lys

Chain J: 57%   43%
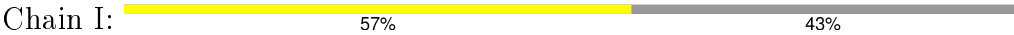
G1 H2 R3 P4 LEU ASP LYS
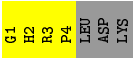
4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.33Å 130.09Å 298.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20	Depositor
% Data completeness (in resolution range)	84.0 (20.00-3.20)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.226 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11054	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NDG, 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	0.41	0/609	0.69	0/811
1	D	0.38	0/609	0.64	0/811
2	B	0.38	0/2523	0.70	1/3409 (0.0%)
2	E	0.40	0/2523	0.69	1/3409 (0.0%)
3	C	0.43	0/2429	0.69	2/3285 (0.1%)
3	F	0.44	0/2429	0.69	1/3285 (0.0%)
4	G	0.71	0/23	0.74	0/28
4	H	0.61	0/23	0.76	0/28
5	I	0.55	0/33	0.56	0/43
5	J	0.47	0/33	0.54	0/43
All	All	0.41	0/11234	0.69	5/15152 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	338	LYS	N-CA-C	-5.44	96.30	111.00
3	F	338	LYS	N-CA-C	-5.27	96.78	111.00
2	E	346	ARG	N-CA-C	-5.26	96.79	111.00
2	B	346	ARG	N-CA-C	-5.14	97.13	111.00
3	C	102	THR	N-CA-C	-5.01	97.46	111.00

There are no chirality outliers.

There are no planarity outliers.

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

wwPDB X-ray Structure Validation Summary Report

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	608	0	649	62	0
1	D	608	0	649	69	0
2	B	2462	0	2328	250	0
2	E	2462	0	2328	261	0
3	C	2364	0	2208	194	0
3	F	2364	0	2208	194	0
4	G	23	0	25	5	0
4	H	23	0	25	7	0
5	I	32	0	32	5	0
5	J	32	0	32	5	0
6	B	15	0	15	12	0
6	E	15	0	15	4	0
6	I	15	0	15	7	0
6	J	15	0	15	0	0
7	B	12	0	12	2	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
All	All	11054	0	10556	979	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 45.

The worst 5 of 979 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)
3:F:365:ASN:HD22	3:F:365:ASN:H	1.03	1.02
3:C:326:CYS:HB3	3:C:336:MET:HE2	1.42	0.97
1:D:188:VAL:HG21	2:E:167:VAL:HG21	1.46	0.96
2:B:166:ARG:HH11	2:B:166:ARG:HB2	1.31	0.95
2:E:398:ASP:HA	2:E:433:ASP:HB3	1.48	0.95

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	72/87 (83%)	51 (71%)	18 (25%)	3 (4%)	3	26
1	D	72/87 (83%)	44 (61%)	23 (32%)	5 (7%)	1	10
2	B	305/328 (93%)	232 (76%)	50 (16%)	23 (8%)	1	9
2	E	305/328 (93%)	228 (75%)	54 (18%)	23 (8%)	1	9
3	C	293/324 (90%)	230 (78%)	46 (16%)	17 (6%)	2	17
3	F	293/324 (90%)	235 (80%)	42 (14%)	16 (6%)	2	18
4	G	1/3 (33%)	0	1 (100%)	0	100	100
4	H	1/3 (33%)	0	1 (100%)	0	100	100
5	I	2/7 (29%)	2 (100%)	0	0	100	100
5	J	2/7 (29%)	2 (100%)	0	0	100	100
All	All	1346/1498 (90%)	1024 (76%)	235 (18%)	87 (6%)	1	13

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
1	A	145	VAL
2	B	152	TYR
2	B	159	SER
2	B	160	ASN

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	69/82 (84%)	62 (90%)	7 (10%)	9	36
1	D	69/82 (84%)	60 (87%)	9 (13%)	5	24
2	B	265/286 (93%)	247 (93%)	18 (7%)	20	59
2	E	265/286 (93%)	247 (93%)	18 (7%)	20	59
3	C	248/270 (92%)	229 (92%)	19 (8%)	16	54
3	F	248/270 (92%)	229 (92%)	19 (8%)	16	54
4	G	2/2 (100%)	2 (100%)	0	100	100
4	H	2/2 (100%)	1 (50%)	1 (50%)	0	0
5	I	3/6 (50%)	3 (100%)	0	100	100
5	J	3/6 (50%)	3 (100%)	0	100	100
All	All	1174/1292 (91%)	1083 (92%)	91 (8%)	16	53

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	382	THR
1	D	180	ASP
3	F	365	ASN
3	C	383	THR
1	D	167	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	365	ASN
2	E	243	ASN
3	F	307	HIS
2	E	158	ASN
2	E	256	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	#$\|Z\| > 2$
6	NDG	B	470	-	15,15,15	0.64	0	17,21,21	0.78	0
7	MAN	B	472	-	12,12,12	0.48	0	17,17,17	0.40	0
6	NDG	E	570	-	15,15,15	0.42	0	17,21,21	0.53	0
6	NDG	I	471	-	15,15,15	0.47	0	17,21,21	0.51	0
6	NDG	J	571	-	15,15,15	0.58	0	17,21,21	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NDG	B	470	-	-	0/6/26/26	0/1/1/1
7	MAN	B	472	-	-	0/2/22/22	0/1/1/1
6	NDG	E	570	-	-	0/6/26/26	0/1/1/1
6	NDG	I	471	-	-	0/6/26/26	0/1/1/1
6	NDG	J	571	-	-	0/6/26/26	0/1/1/1

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.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	470	NDG	12	0
7	B	472	MAN	2	0
6	E	570	NDG	4	0
6	I	471	NDG	7	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.