



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 06:03 PM EDT

PDB ID : 3E1I
Title : Crystal Structure of BbetaD432A Variant Fibrinogen Fragment D with the Peptide Ligand Gly-His-Arg-Pro-amide
Authors : Bowley, S.R.; Lord, S.T.
Deposited on : 2008-08-04
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

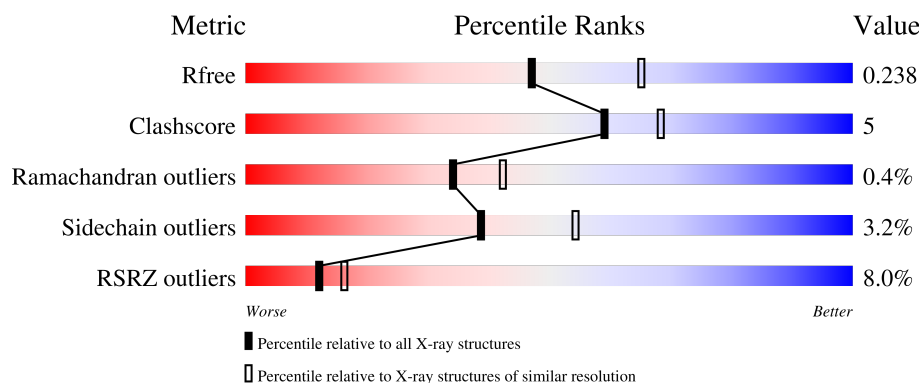
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	87	<div> <div>22%</div> <div>54%</div> <div>9%</div> <div>34%</div> </div>
1	D	87	<div> <div>17%</div> <div>51%</div> <div>11%</div> <div>38%</div> </div>
2	B	328	<div> <div>8%</div> <div>80%</div> <div>9%</div> <div>9%</div> </div>
2	E	328	<div> <div>6%</div> <div>81%</div> <div>9%</div> <div>9%</div> </div>
3	C	319	<div> <div>5%</div> <div>81%</div> <div>8%</div> <div>10%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	319	 2% 81% 8% 10%
4	G	5	 80% 20%
4	H	5	 60% 20% 20%

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	NAG	E	501	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10668 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	57	Total	C	N	O	S	0	0	0
			463	283	88	89	3			
1	D	54	Total	C	N	O	S	0	0	0
			443	269	85	86	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	298	Total	C	N	O	S	0	0	0
			2389	1493	422	452	22			
2	E	298	Total	C	N	O	S	0	0	0
			2389	1493	422	452	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	432	ALA	ASP	engineered mutation	UNP P02675
E	432	ALA	ASP	engineered mutation	UNP P02675

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	288	Total	C	N	O	S	0	0	0
			2311	1467	390	443	11			
3	F	288	Total	C	N	O	S	0	0	0
			2312	1468	390	443	11			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			32	19	9	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	4	Total	C	N	O	0	0	0
			32	19	9	4			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

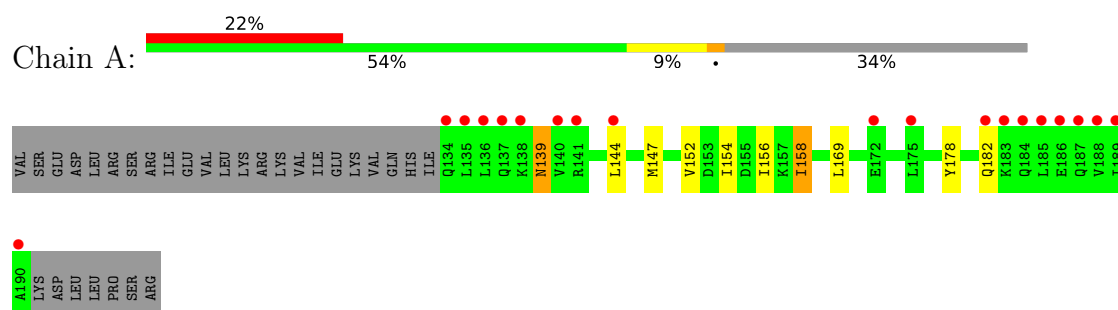
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	O 1	0	0
7	B	49	Total 49	O 49	0	0
7	C	86	Total 86	O 86	0	0
7	D	2	Total 2	O 2	0	0
7	E	44	Total 44	O 44	0	0
7	F	76	Total 76	O 76	0	0
7	G	2	Total 2	O 2	0	0

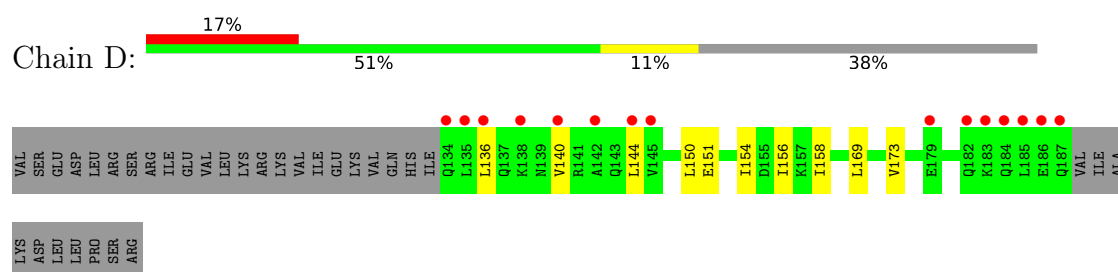
3 Residue-property plots [i](#)

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.

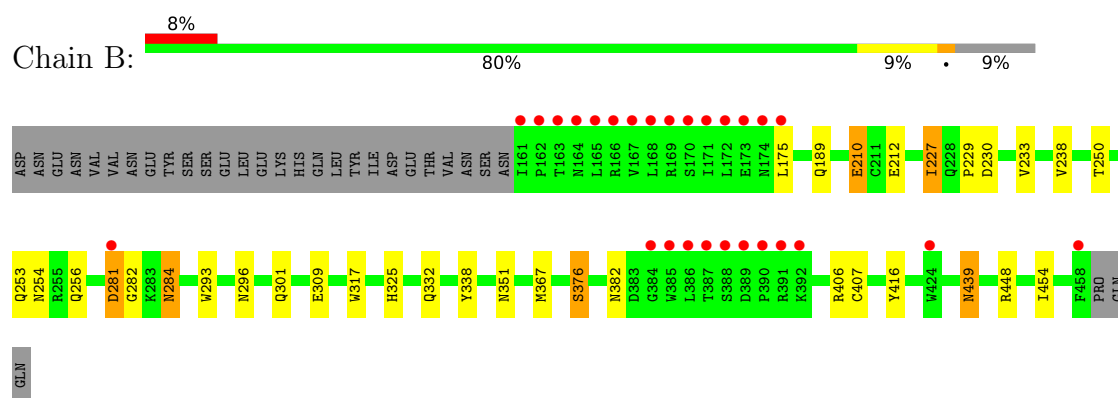
- Molecule 1: Fibrinogen alpha chain



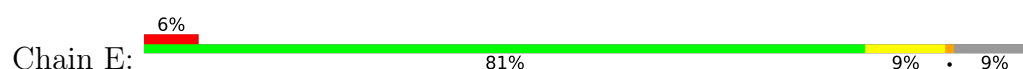
- Molecule 1: Fibrinogen alpha chain

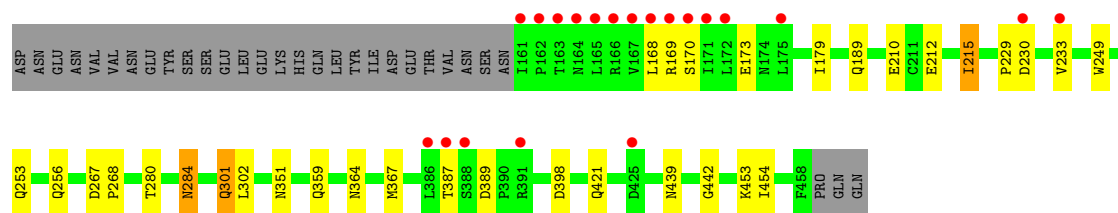


- Molecule 2: Fibrinogen beta chain

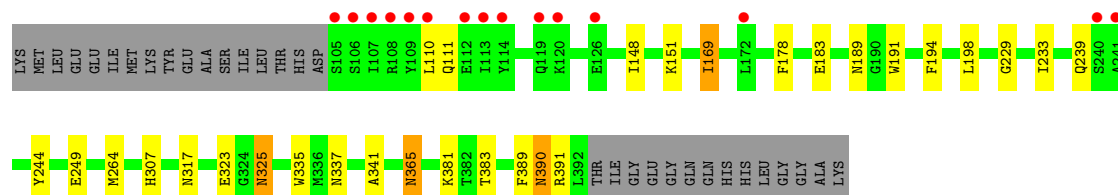
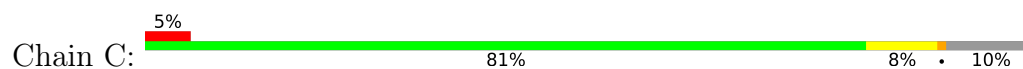


- Molecule 2: Fibrinogen beta chain

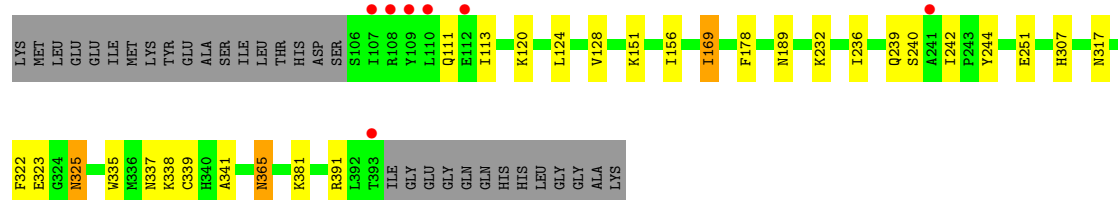
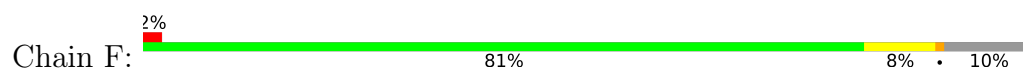




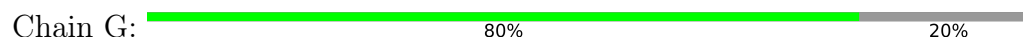
• Molecule 3: Fibrinogen gamma chain



• Molecule 3: Fibrinogen gamma chain



• Molecule 4: Gly-His-Arg-Pro-amide



• Molecule 4: Gly-His-Arg-Pro-amide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.48Å 146.60Å 228.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 2.30 49.19 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.21-2.30) 99.7 (49.19-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.21 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS 1.1	Depositor
R, R_{free}	0.214 , 0.242 0.212 , 0.238	Depositor DCC
R_{free} test set	4129 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10668	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.32	0/463	0.52	0/617
1	D	0.32	0/443	0.54	0/589
2	B	0.42	0/2450	0.54	0/3308
2	E	0.41	0/2450	0.55	0/3308
3	C	0.50	0/2375	0.58	0/3211
3	F	0.48	0/2376	0.56	0/3213
4	G	0.42	0/33	0.62	0/43
4	H	0.70	0/33	0.83	0/43
All	All	0.44	0/10623	0.56	0/14332

There are no bond length outliers.

There are no bond angle outliers.

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 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	463	0	482	10	0
1	D	443	0	457	7	0
2	B	2389	0	2264	23	0
2	E	2389	0	2264	20	0
3	C	2311	0	2163	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	2312	0	2165	23	0
4	G	32	0	32	0	0
4	H	32	0	32	2	0
5	B	15	0	15	0	0
5	E	15	0	13	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	49	0	0	0	0
7	C	86	0	0	0	0
7	D	2	0	0	0	0
7	E	44	0	0	0	0
7	F	76	0	0	0	0
7	G	2	0	0	0	0
All	All	10668	0	9887	96	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 5.

All (96) 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:307:HIS:HE1	3:F:341:ALA:H	1.28	0.79
3:C:307:HIS:HE1	3:C:341:ALA:H	1.29	0.79
3:C:264:MET:HE1	3:C:389:PHE:CD2	2.20	0.77
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.53	0.74
3:C:249:GLU:HG3	3:C:383:THR:HB	1.72	0.71
1:D:154:ILE:HD11	3:F:128:VAL:HG21	1.75	0.68
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.59	0.67
3:C:189:ASN:HD22	3:C:391:ARG:HE	1.42	0.66
1:A:169:LEU:H	2:B:189:GLN:HE22	1.41	0.66
3:C:307:HIS:CE1	3:C:341:ALA:H	2.14	0.66
2:B:376:SER:HB3	2:B:382:ASN:H	1.62	0.63
3:C:169:ILE:HD11	3:C:178:PHE:CE2	2.32	0.63
3:F:232:LYS:O	3:F:236:ILE:HG12	1.97	0.63
2:B:367:MET:HB2	2:B:406:ARG:HB2	1.81	0.63
2:B:439:ASN:HD22	2:B:439:ASN:H	1.47	0.62
3:F:322:PHE:CZ	4:H:3:ARG:HD3	2.34	0.62
3:F:156:ILE:HD11	3:F:169:ILE:HG22	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:359:GLN:HE22	2:E:442:GLY:HA2	1.66	0.60
3:C:264:MET:CE	3:C:389:PHE:CD2	2.85	0.60
2:B:309:GLU:OE1	2:B:325:HIS:HE1	1.88	0.57
3:C:307:HIS:HD2	3:C:335:TRP:O	1.87	0.57
1:A:147:MET:HG3	2:B:175:LEU:HD22	1.86	0.56
3:F:169:ILE:HD11	3:F:178:PHE:CE2	2.40	0.56
3:C:151:LYS:HB3	3:C:239:GLN:NE2	2.19	0.56
3:F:323:GLU:CD	3:F:323:GLU:H	2.08	0.56
1:A:169:LEU:H	2:B:189:GLN:NE2	2.03	0.55
1:A:144:LEU:HD12	2:B:175:LEU:HD21	1.89	0.55
3:F:307:HIS:CE1	3:F:341:ALA:H	2.17	0.54
2:E:169:ARG:O	2:E:173:GLU:HG3	2.07	0.54
3:C:194:PHE:CG	3:C:233:ILE:HD12	2.43	0.54
2:B:293:TRP:HZ2	2:B:296:ASN:HD21	1.56	0.53
2:B:281:ASP:OD2	2:B:282:GLY:N	2.38	0.53
3:C:229:GLY:O	3:C:233:ILE:HG12	2.09	0.53
3:F:189:ASN:HD22	3:F:391:ARG:HE	1.55	0.52
3:C:189:ASN:ND2	3:C:391:ARG:HE	2.06	0.52
1:A:152:VAL:O	1:A:156:ILE:HG12	2.10	0.52
1:D:150:LEU:HD21	3:F:124:LEU:HD23	1.91	0.52
3:C:194:PHE:HB2	3:C:233:ILE:CD1	2.40	0.51
3:C:249:GLU:CG	3:C:383:THR:HB	2.39	0.51
2:B:439:ASN:HD22	2:B:439:ASN:N	2.09	0.50
3:F:189:ASN:ND2	3:F:391:ARG:HE	2.10	0.50
3:C:390:ASN:C	3:C:390:ASN:HD22	2.15	0.50
1:D:158:ILE:HG23	2:E:189:GLN:HE21	1.77	0.49
3:F:322:PHE:CE2	4:H:3:ARG:HD3	2.46	0.49
3:F:307:HIS:HD2	3:F:335:TRP:O	1.95	0.49
2:E:284:ASN:C	2:E:284:ASN:HD22	2.15	0.49
1:A:178:TYR:O	1:A:182:GLN:HB2	2.13	0.48
3:C:323:GLU:H	3:C:323:GLU:CD	2.17	0.48
1:A:156:ILE:HD12	2:B:416:TYR:O	2.14	0.48
2:E:168:LEU:C	2:E:170:SER:H	2.16	0.47
1:D:151:GLU:HG2	1:D:173:VAL:HG13	1.97	0.46
2:B:238:VAL:HG21	2:B:250:THR:CG2	2.45	0.46
1:D:140:VAL:O	1:D:144:LEU:HB2	2.15	0.46
2:B:317:TRP:CE3	2:B:448:ARG:HD2	2.51	0.46
2:B:210:GLU:OE1	2:B:212:GLU:HB3	2.16	0.46
2:E:229:PRO:CB	2:E:301:GLN:HE22	2.29	0.46
1:A:139:ASN:H	1:A:139:ASN:HD22	1.65	0.45
1:A:139:ASN:HD22	1:A:139:ASN:N	2.13	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:359:GLN:NE2	2:E:442:GLY:HA2	2.31	0.45
3:C:148:ILE:HD12	3:C:148:ILE:H	1.82	0.45
3:C:390:ASN:HD22	3:C:391:ARG:N	2.15	0.44
3:F:325:ASN:HD22	3:F:325:ASN:C	2.20	0.44
2:B:284:ASN:HD22	2:B:284:ASN:C	2.20	0.44
3:C:365:ASN:HD22	3:C:365:ASN:H	1.64	0.44
3:C:189:ASN:ND2	3:C:391:ARG:HH21	2.15	0.44
3:F:251:GLU:HB3	3:F:381:LYS:HB2	1.99	0.44
1:D:169:LEU:H	2:E:189:GLN:HE22	1.64	0.44
2:E:364:ASN:HA	2:E:367:MET:CE	2.48	0.43
2:B:230:ASP:HB3	2:B:233:VAL:HG23	2.00	0.43
3:F:240:SER:O	3:F:242:ILE:HG13	2.19	0.43
2:B:227:ILE:HG12	2:B:229:PRO:HD3	1.99	0.43
2:B:254:ASN:HD21	2:B:256:GLN:NE2	2.17	0.43
2:E:364:ASN:HA	2:E:367:MET:HE3	2.01	0.42
3:C:198:LEU:CD2	3:C:381:LYS:HD3	2.50	0.42
2:E:387:THR:C	2:E:389:ASP:H	2.22	0.42
2:E:230:ASP:OD2	2:E:233:VAL:HG23	2.19	0.42
3:F:124:LEU:O	3:F:128:VAL:HG23	2.19	0.42
2:E:169:ARG:HB2	3:F:111:GLN:NE2	2.35	0.42
2:E:212:GLU:O	2:E:215:ILE:HG22	2.20	0.42
1:D:169:LEU:H	2:E:189:GLN:NE2	2.18	0.42
2:E:267:ASP:HB3	2:E:268:PRO:HD3	2.02	0.42
2:E:179:ILE:HG21	3:F:120:LYS:HB3	2.00	0.41
3:F:365:ASN:HD22	3:F:365:ASN:H	1.66	0.41
1:A:154:ILE:HG23	1:A:158:ILE:HD12	2.03	0.41
2:E:249:TRP:HB3	2:E:453:LYS:HB3	2.03	0.41
3:C:183:GLU:HB3	3:C:191:TRP:HB2	2.03	0.41
2:E:302:LEU:HD13	2:E:454:ILE:HD11	2.02	0.41
2:B:238:VAL:HG21	2:B:250:THR:HG23	2.03	0.41
2:B:332:GLN:O	2:B:338:TYR:HA	2.20	0.41
2:B:406:ARG:N	2:B:407:CYS:HA	2.36	0.41
2:B:439:ASN:N	2:B:439:ASN:ND2	2.69	0.41
3:C:325:ASN:HD22	3:C:325:ASN:C	2.24	0.41
3:C:323:GLU:CD	3:C:323:GLU:N	2.74	0.40
2:E:439:ASN:HD22	2:E:439:ASN:H	1.70	0.40
3:F:338:LYS:N	3:F:339:CYS:HA	2.35	0.40
3:F:365:ASN:HD22	3:F:365:ASN:N	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	55/87 (63%)	49 (89%)	6 (11%)	0	100	100
1	D	52/87 (60%)	46 (88%)	5 (10%)	1 (2%)	8	7
2	B	296/328 (90%)	281 (95%)	14 (5%)	1 (0%)	41	50
2	E	296/328 (90%)	284 (96%)	11 (4%)	1 (0%)	41	50
3	C	286/319 (90%)	272 (95%)	12 (4%)	2 (1%)	22	26
3	F	286/319 (90%)	273 (96%)	13 (4%)	0	100	100
4	G	2/5 (40%)	2 (100%)	0	0	100	100
4	H	2/5 (40%)	2 (100%)	0	0	100	100
All	All	1275/1478 (86%)	1209 (95%)	61 (5%)	5 (0%)	34	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	110	LEU
3	C	111	GLN
2	B	281	ASP
1	D	136	LEU
2	E	256	GLN

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	52/82 (63%)	50 (96%)	2 (4%)	33	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	50/82 (61%)	49 (98%)	1 (2%)	55	72
2	B	255/285 (90%)	246 (96%)	9 (4%)	36	50
2	E	255/285 (90%)	246 (96%)	9 (4%)	36	50
3	C	242/267 (91%)	235 (97%)	7 (3%)	42	58
3	F	242/267 (91%)	235 (97%)	7 (3%)	42	58
4	G	3/3 (100%)	3 (100%)	0	100	100
4	H	3/3 (100%)	3 (100%)	0	100	100
All	All	1102/1274 (86%)	1067 (97%)	35 (3%)	39	54

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	158	ILE
2	B	210	GLU
2	B	227	ILE
2	B	253	GLN
2	B	284	ASN
2	B	301	GLN
2	B	351	ASN
2	B	376	SER
2	B	439	ASN
2	B	454	ILE
3	C	169	ILE
3	C	244	TYR
3	C	317	ASN
3	C	325	ASN
3	C	337	ASN
3	C	365	ASN
3	C	390	ASN
1	D	156	ILE
2	E	210	GLU
2	E	215	ILE
2	E	253	GLN
2	E	280	THR
2	E	284	ASN
2	E	301	GLN
2	E	351	ASN
2	E	398	ASP
2	E	421	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	113	ILE
3	F	169	ILE
3	F	244	TYR
3	F	317	ASN
3	F	325	ASN
3	F	337	ASN
3	F	365	ASN

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

Mol	Chain	Res	Type
2	B	164	ASN
2	B	180	GLN
2	B	189	GLN
2	B	253	GLN
2	B	256	GLN
2	B	284	ASN
2	B	296	ASN
2	B	301	GLN
2	B	325	HIS
2	B	339	GLN
2	B	351	ASN
2	B	421	GLN
2	B	439	ASN
3	C	117	ASN
3	C	118	ASN
3	C	119	GLN
3	C	136	GLN
3	C	189	ASN
3	C	239	GLN
3	C	254	ASN
3	C	307	HIS
3	C	317	ASN
3	C	319	ASN
3	C	325	ASN
3	C	337	ASN
3	C	365	ASN
3	C	390	ASN
2	E	189	GLN
2	E	253	GLN
2	E	256	GLN
2	E	284	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	296	ASN
2	E	301	GLN
2	E	339	GLN
2	E	351	ASN
2	E	421	GLN
2	E	439	ASN
3	F	111	GLN
3	F	115	ASN
3	F	117	ASN
3	F	136	GLN
3	F	177	GLN
3	F	189	ASN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	337	ASN
3	F	365	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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	NAG	B	501	-	15,15,15	0.47	0	21,21,21	0.82	0
5	NAG	E	501	-	15,15,15	1.68	2 (13%)	21,21,21	5.04	5 (23%)

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	NAG	B	501	-	-	4/6/26/26	0/1/1/1
5	NAG	E	501	-	1/1/6/7	2/6/26/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	501	NAG	C1-C2	-4.95	1.47	1.52
5	E	501	NAG	O5-C1	-3.59	1.34	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	501	NAG	O5-C1-C2	12.34	121.92	109.52
5	E	501	NAG	O1-C1-C2	11.52	133.15	109.22
5	E	501	NAG	O1-C1-O5	-9.95	80.53	110.38
5	E	501	NAG	C1-O5-C5	8.55	129.79	113.66
5	E	501	NAG	C1-C2-N2	8.12	120.13	110.73

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	501	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	NAG	O7-C7-N2-C2
5	E	501	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	E	501	NAG	O7-C7-N2-C2
5	B	501	NAG	C8-C7-N2-C2
5	B	501	NAG	C4-C5-C6-O6
5	B	501	NAG	O5-C5-C6-O6

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 [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	57/87 (65%)	1.77	19 (33%) 0 0	34, 65, 96, 97	0
1	D	54/87 (62%)	1.54	15 (27%) 0 0	32, 51, 79, 82	0
2	B	298/328 (90%)	0.37	27 (9%) 9 12	17, 32, 76, 102	0
2	E	298/328 (90%)	0.18	20 (6%) 17 23	21, 31, 58, 96	0
3	C	288/319 (90%)	-0.04	15 (5%) 27 34	13, 20, 64, 100	0
3	F	288/319 (90%)	0.03	7 (2%) 59 66	14, 23, 45, 90	0
4	G	4/5 (80%)	-0.17	0 100 100	30, 31, 33, 39	0
4	H	4/5 (80%)	-0.20	0 100 100	25, 26, 29, 35	0
All	All	1291/1478 (87%)	0.27	103 (7%) 12 16	13, 28, 77, 102	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	167	VAL	10.3
3	C	109	TYR	9.6
1	A	190	ALA	9.5
3	C	105	SER	8.7
2	B	161	ILE	8.3
3	C	106	SER	8.0
2	B	166	ARG	7.7
2	B	163	THR	7.6
1	D	185	LEU	7.3
3	F	107	ILE	7.3
2	B	392	LYS	7.2
1	A	185	LEU	7.1
1	D	136	LEU	6.5
1	A	189	ILE	6.4
2	B	390	PRO	6.2
1	A	137	GLN	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	165	LEU	5.8
3	F	109	TYR	5.8
2	E	168	LEU	5.6
1	D	187	GLN	5.5
1	A	188	VAL	5.4
2	E	167	VAL	5.4
3	C	107	ILE	5.2
3	F	110	LEU	5.2
1	A	187	GLN	5.1
1	D	140	VAL	5.0
2	B	388	SER	4.9
2	B	458	PHE	4.9
1	D	186	GLU	4.9
2	B	387	THR	4.8
2	B	168	LEU	4.7
2	E	386	LEU	4.7
2	B	169	ARG	4.7
2	E	162	PRO	4.4
2	E	171	ILE	4.4
2	B	424	TRP	4.3
1	D	182	GLN	4.2
2	E	165	LEU	4.1
1	A	172	GLU	4.1
1	D	134	GLN	4.1
1	D	142	ALA	4.0
1	A	134	GLN	3.9
3	C	108	ARG	3.9
2	B	170	SER	3.8
3	C	112	GLU	3.7
3	C	110	LEU	3.6
3	C	240	SER	3.6
2	B	162	PRO	3.6
2	B	171	ILE	3.5
2	B	385	TRP	3.5
1	A	183	LYS	3.5
2	E	161	ILE	3.5
1	A	141	ARG	3.4
3	C	113	ILE	3.4
2	E	175	LEU	3.4
2	E	391	ARG	3.4
3	F	108	ARG	3.3
1	D	179	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	135	LEU	3.2
1	A	135	LEU	3.2
2	B	391	ARG	3.1
2	E	164	ASN	3.1
1	D	145	VAL	3.0
1	D	144	LEU	3.0
1	A	136	LEU	2.9
1	A	186	GLU	2.9
2	E	163	THR	2.8
2	B	173	GLU	2.8
2	E	172	LEU	2.7
3	C	172	LEU	2.7
2	E	388	SER	2.7
3	F	241	ALA	2.7
1	A	138	LYS	2.7
2	E	166	ARG	2.6
2	E	233	VAL	2.6
2	B	175	LEU	2.5
2	B	389	ASP	2.5
1	D	183	LYS	2.5
3	F	112	GLU	2.5
1	A	184	GLN	2.5
2	B	164	ASN	2.5
3	C	241	ALA	2.5
1	A	182	GLN	2.5
2	B	172	LEU	2.4
3	C	119	GLN	2.4
1	A	144	LEU	2.4
3	C	120	LYS	2.3
2	E	230	ASP	2.3
2	B	174	ASN	2.3
1	D	184	GLN	2.3
2	B	386	LEU	2.3
2	B	384	GLY	2.3
2	E	169	ARG	2.3
1	D	138	LYS	2.3
2	E	387	THR	2.2
2	B	281	ASP	2.2
3	F	393	THR	2.2
2	E	425	ASP	2.2
3	C	114	TYR	2.1
3	C	126	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	140	VAL	2.1
1	A	175	LEU	2.0
2	E	170	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](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
5	NAG	B	501	15/15	0.60	0.29	124,124,125,125	0
5	NAG	E	501	15/15	0.66	0.25	104,105,105,105	0
6	CA	F	501	1/1	0.93	0.13	26,26,26,26	0
6	CA	E	503	1/1	0.94	0.12	42,42,42,42	0
6	CA	B	502	1/1	0.94	0.05	60,60,60,60	0
6	CA	B	503	1/1	0.96	0.10	43,43,43,43	0
6	CA	E	502	1/1	0.96	0.11	70,70,70,70	0
6	CA	C	502	1/1	0.98	0.12	30,30,30,30	0
6	CA	C	501	1/1	0.99	0.09	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.