Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 01:04 AM EDT

PDB ID	:	4GIP
Title	:	Structure of the cleavage-activated prefusion form of the parainfluenza virus 5 (PIV5) fusion protein
Authors	:	Welch, B.D.; Liu, Y.; Kors, C.A.; Leser, G.P.; Jardetzky, T.S.; Lamb, R.A.
Deposited on	:	2012-08-08
Resolution	:	2.00 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

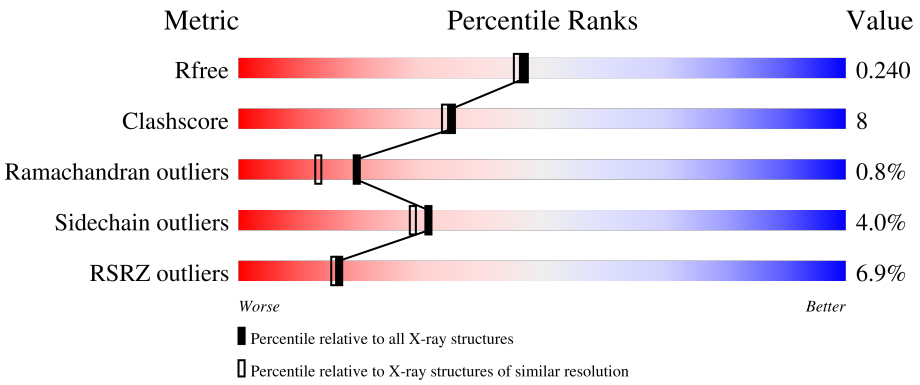
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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 <=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	81	12%, 80%, 15%
1	B	81	14%, 75%, 21%
1	C	81	10%, 74%, 22%
2	D	409	6%, 79%, 11%, 8%
2	E	409	4%, 76%, 15%, 8%

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Mol	Chain	Length	Quality of chain
2	F	409	5% 78% 13% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	201	-	-	X	-
3	NAG	E	603	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11335 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 Fusion glycoprotein F2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	81	625	396	107	118	4	0	0	0
1	B	81	625	396	107	118	4	0	0	0
1	C	81	625	396	107	118	4	0	0	0

- Molecule 2 is a protein called Fusion glycoprotein F1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	375	2785	1763	462	543	17	0	0	0
2	E	375	2785	1763	462	543	17	0	0	0
2	F	375	2785	1763	462	543	17	0	0	0

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	478	GLU	-	expression tag	UNP P04849
D	479	ASP	-	expression tag	UNP P04849
D	480	LYS	-	expression tag	UNP P04849
D	481	ILE	-	expression tag	UNP P04849
D	482	GLU	-	expression tag	UNP P04849
D	483	GLU	-	expression tag	UNP P04849
D	484	ILE	-	expression tag	UNP P04849
D	485	LEU	-	expression tag	UNP P04849
D	486	SER	-	expression tag	UNP P04849
D	487	LYS	-	expression tag	UNP P04849
D	488	ILE	-	expression tag	UNP P04849
D	489	TYR	-	expression tag	UNP P04849

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Chain	Residue	Modelled	Actual	Comment	Reference
D	490	HIS	-	expression tag	UNP P04849
D	491	ILE	-	expression tag	UNP P04849
D	492	GLU	-	expression tag	UNP P04849
D	493	ASN	-	expression tag	UNP P04849
D	494	GLU	-	expression tag	UNP P04849
D	495	ILE	-	expression tag	UNP P04849
D	496	ALA	-	expression tag	UNP P04849
D	497	ARG	-	expression tag	UNP P04849
D	498	ILE	-	expression tag	UNP P04849
D	499	LYS	-	expression tag	UNP P04849
D	500	LYS	-	expression tag	UNP P04849
D	501	LEU	-	expression tag	UNP P04849
D	502	ILE	-	expression tag	UNP P04849
D	503	GLY	-	expression tag	UNP P04849
D	504	GLU	-	expression tag	UNP P04849
D	505	ALA	-	expression tag	UNP P04849
D	506	HIS	-	expression tag	UNP P04849
D	507	HIS	-	expression tag	UNP P04849
D	508	HIS	-	expression tag	UNP P04849
D	509	HIS	-	expression tag	UNP P04849
D	510	HIS	-	expression tag	UNP P04849
D	511	HIS	-	expression tag	UNP P04849
E	478	GLU	-	expression tag	UNP P04849
E	479	ASP	-	expression tag	UNP P04849
E	480	LYS	-	expression tag	UNP P04849
E	481	ILE	-	expression tag	UNP P04849
E	482	GLU	-	expression tag	UNP P04849
E	483	GLU	-	expression tag	UNP P04849
E	484	ILE	-	expression tag	UNP P04849
E	485	LEU	-	expression tag	UNP P04849
E	486	SER	-	expression tag	UNP P04849
E	487	LYS	-	expression tag	UNP P04849
E	488	ILE	-	expression tag	UNP P04849
E	489	TYR	-	expression tag	UNP P04849
E	490	HIS	-	expression tag	UNP P04849
E	491	ILE	-	expression tag	UNP P04849
E	492	GLU	-	expression tag	UNP P04849
E	493	ASN	-	expression tag	UNP P04849
E	494	GLU	-	expression tag	UNP P04849
E	495	ILE	-	expression tag	UNP P04849
E	496	ALA	-	expression tag	UNP P04849
E	497	ARG	-	expression tag	UNP P04849

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Chain	Residue	Modelled	Actual	Comment	Reference
E	498	ILE	-	expression tag	UNP P04849
E	499	LYS	-	expression tag	UNP P04849
E	500	LYS	-	expression tag	UNP P04849
E	501	LEU	-	expression tag	UNP P04849
E	502	ILE	-	expression tag	UNP P04849
E	503	GLY	-	expression tag	UNP P04849
E	504	GLU	-	expression tag	UNP P04849
E	505	ALA	-	expression tag	UNP P04849
E	506	HIS	-	expression tag	UNP P04849
E	507	HIS	-	expression tag	UNP P04849
E	508	HIS	-	expression tag	UNP P04849
E	509	HIS	-	expression tag	UNP P04849
E	510	HIS	-	expression tag	UNP P04849
E	511	HIS	-	expression tag	UNP P04849
F	478	GLU	-	expression tag	UNP P04849
F	479	ASP	-	expression tag	UNP P04849
F	480	LYS	-	expression tag	UNP P04849
F	481	ILE	-	expression tag	UNP P04849
F	482	GLU	-	expression tag	UNP P04849
F	483	GLU	-	expression tag	UNP P04849
F	484	ILE	-	expression tag	UNP P04849
F	485	LEU	-	expression tag	UNP P04849
F	486	SER	-	expression tag	UNP P04849
F	487	LYS	-	expression tag	UNP P04849
F	488	ILE	-	expression tag	UNP P04849
F	489	TYR	-	expression tag	UNP P04849
F	490	HIS	-	expression tag	UNP P04849
F	491	ILE	-	expression tag	UNP P04849
F	492	GLU	-	expression tag	UNP P04849
F	493	ASN	-	expression tag	UNP P04849
F	494	GLU	-	expression tag	UNP P04849
F	495	ILE	-	expression tag	UNP P04849
F	496	ALA	-	expression tag	UNP P04849
F	497	ARG	-	expression tag	UNP P04849
F	498	ILE	-	expression tag	UNP P04849
F	499	LYS	-	expression tag	UNP P04849
F	500	LYS	-	expression tag	UNP P04849
F	501	LEU	-	expression tag	UNP P04849
F	502	ILE	-	expression tag	UNP P04849
F	503	GLY	-	expression tag	UNP P04849
F	504	GLU	-	expression tag	UNP P04849
F	505	ALA	-	expression tag	UNP P04849

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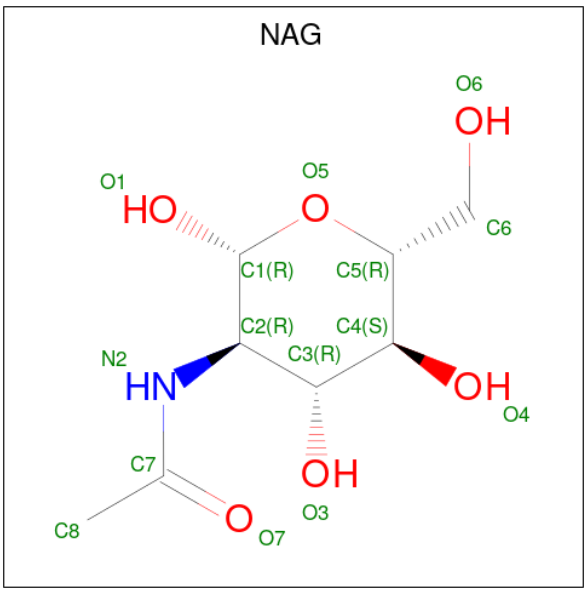
Chain	Residue	Modelled	Actual	Comment	Reference
F	506	HIS	-	expression tag	UNP P04849
F	507	HIS	-	expression tag	UNP P04849
F	508	HIS	-	expression tag	UNP P04849
F	509	HIS	-	expression tag	UNP P04849
F	510	HIS	-	expression tag	UNP P04849
F	511	HIS	-	expression tag	UNP P04849

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
3	D	1	14	8	1	5	0	0
3	D	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	E	1	14	8	1	5	0	0
3	E	1	14	8	1	5	0	0
3	E	1	14	8	1	5	0	0
3	C	1	14	8	1	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	C	1	14	8	1	5	0	0
			Total	C	N	O		
3	F	1	14	8	1	5	0	0
			Total	C	N	O		
3	F	1	14	8	1	5	0	0

- Molecule 4 is water.

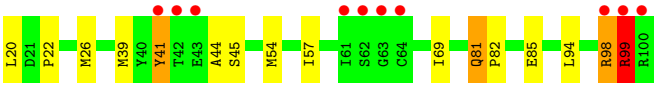
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	39	39	39	0	0
			Total	O		
4	D	287	287	287	0	0
			Total	O		
4	B	21	21	21	0	0
			Total	O		
4	E	279	279	279	0	0
			Total	O		
4	C	46	46	46	0	0
			Total	O		
4	F	279	279	279	0	0

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.

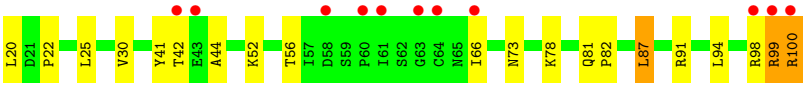
• Molecule 1: Fusion glycoprotein F2

Chain A:



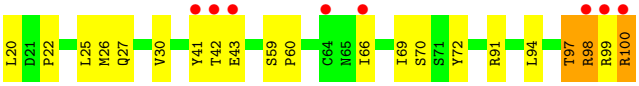
• Molecule 1: Fusion glycoprotein F2

Chain B:



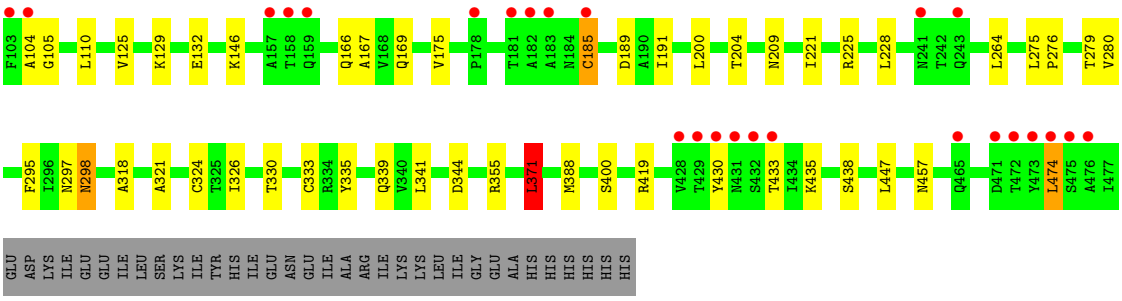
• Molecule 1: Fusion glycoprotein F2

Chain C:



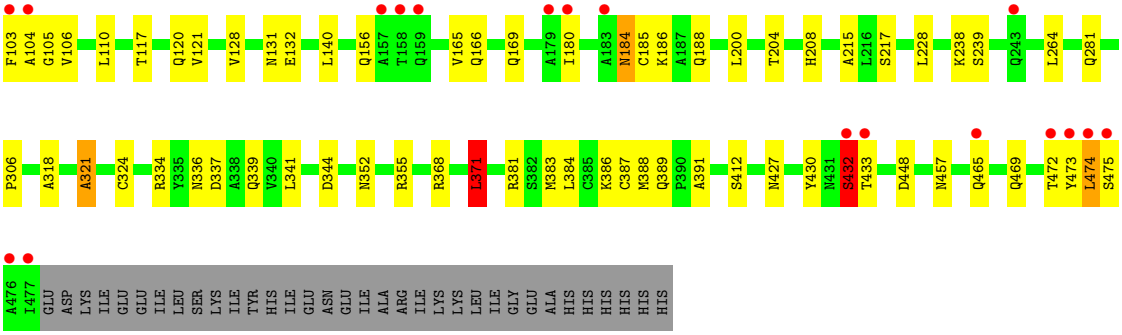
• Molecule 2: Fusion glycoprotein F1

Chain D:



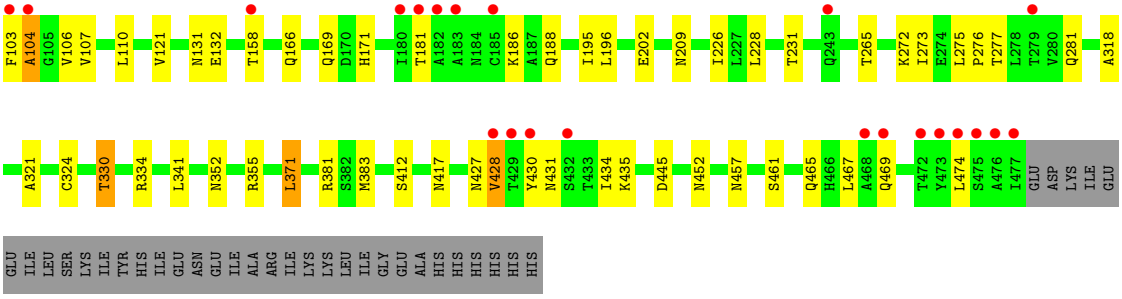
• Molecule 2: Fusion glycoprotein F1

Chain E:



- Molecule 2: Fusion glycoprotein F1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	250.93Å 140.52Å 84.60Å 90.00° 99.84° 90.00°	Depositor
Resolution (Å)	35.54 – 2.00 35.54 – 2.00	Depositor EDS
% Data completeness (in resolution range)	59.8 (35.54-2.00) 59.7 (35.54-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.96 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.220 , 0.243 0.216 , 0.240	Depositor DCC
R_{free} test set	5831 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11335	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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, 0.333 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: 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	0.34	0/634	0.55	0/864
1	B	0.32	0/634	0.56	0/864
1	C	0.33	0/634	0.55	0/864
2	D	0.37	0/2819	0.57	1/3857 (0.0%)
2	E	0.35	0/2819	0.56	1/3857 (0.0%)
2	F	0.38	0/2819	0.57	1/3857 (0.0%)
All	All	0.36	0/10359	0.57	3/14163 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	371	LEU	CA-CB-CG	-5.79	101.98	115.30
2	D	371	LEU	CA-CB-CG	-5.32	103.07	115.30
2	E	371	LEU	CA-CB-CG	-5.12	103.53	115.30

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	625	0	654	14	0
1	B	625	0	654	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	625	0	654	17	0
2	D	2785	0	2873	37	0
2	E	2785	0	2875	50	0
2	F	2785	0	2875	47	0
3	A	14	0	13	1	0
3	B	14	0	13	7	0
3	C	28	0	25	1	0
3	D	28	0	26	6	0
3	E	42	0	39	15	0
3	F	28	0	26	10	0
4	A	39	0	0	2	0
4	B	21	0	0	2	0
4	C	46	0	0	3	0
4	D	287	0	0	7	0
4	E	279	0	0	10	0
4	F	279	0	0	18	0
All	All	11335	0	10727	174	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 8.

All (174) 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)
2:E:352:ASN:HD21	3:E:602:NAG:C1	1.06	1.60
2:E:457:ASN:HD21	3:E:603:NAG:C1	0.94	1.53
2:F:457:ASN:HD21	3:F:602:NAG:C1	1.12	1.52
2:F:352:ASN:HD21	3:F:601:NAG:C1	0.92	1.51
2:D:457:ASN:HD21	3:D:602:NAG:C1	0.87	1.50
1:B:73:ASN:ND2	3:B:201:NAG:C1	1.72	1.48
2:D:457:ASN:ND2	3:D:602:NAG:C1	1.73	1.47
2:F:457:ASN:ND2	3:F:602:NAG:C1	1.75	1.41
2:F:352:ASN:ND2	3:F:601:NAG:C1	1.77	1.40
2:E:457:ASN:ND2	3:E:603:NAG:C1	1.78	1.40
3:B:201:NAG:O4	3:E:601:NAG:C1	1.71	1.37
2:E:352:ASN:ND2	3:E:602:NAG:C1	1.85	1.37
2:E:352:ASN:HD21	3:E:602:NAG:C2	1.73	1.01
2:F:430:TYR:HB3	2:F:431:ASN:HA	1.51	0.93
2:F:272:LYS:NZ	4:F:906:HOH:O	2.00	0.91
3:B:201:NAG:HO4	3:E:601:NAG:C1	1.82	0.90
2:D:457:ASN:HD21	3:D:602:NAG:C2	1.85	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:334:ARG:NE	4:F:935:HOH:O	2.06	0.88
2:F:457:ASN:CG	3:F:602:NAG:C1	2.41	0.88
2:E:457:ASN:HD21	3:E:603:NAG:C2	1.92	0.82
1:B:94:LEU:HD11	2:E:110:LEU:HD23	1.61	0.81
3:D:601:NAG:O3	4:D:966:HOH:O	1.97	0.81
3:E:603:NAG:O7	4:E:841:HOH:O	1.98	0.81
2:D:388:MET:HG3	4:D:864:HOH:O	1.82	0.79
1:C:27:GLN:OE1	4:C:339:HOH:O	2.01	0.78
2:F:352:ASN:HD21	3:F:601:NAG:C2	1.94	0.78
2:D:457:ASN:ND2	3:D:602:NAG:C2	2.47	0.76
1:B:73:ASN:CG	3:B:201:NAG:C1	2.55	0.75
2:F:334:ARG:NH2	4:F:916:HOH:O	2.20	0.73
2:F:445:ASP:OD2	4:F:851:HOH:O	2.07	0.71
2:D:209:ASN:OD1	4:D:893:HOH:O	2.07	0.71
2:E:457:ASN:CG	3:E:603:NAG:C1	2.59	0.71
1:B:56:THR:N	4:E:844:HOH:O	2.24	0.69
1:B:99:ARG:NH1	2:E:132:GLU:OE2	2.26	0.68
2:E:169:GLN:OE1	4:E:844:HOH:O	2.11	0.68
2:E:184:ASN:HB3	2:E:188:GLN:HG2	1.76	0.68
2:E:430:TYR:HD1	2:E:432:SER:HB2	1.60	0.67
2:F:188:GLN:NE2	4:F:910:HOH:O	2.27	0.67
2:E:156:GLN:OE1	4:E:899:HOH:O	2.14	0.66
1:B:73:ASN:HD22	3:B:201:NAG:C1	2.01	0.65
1:C:100:ARG:NH2	4:C:342:HOH:O	2.26	0.65
2:F:275:LEU:HD12	2:F:276:PRO:HD2	1.78	0.65
2:E:427:ASN:ND2	4:E:979:HOH:O	2.06	0.65
2:E:384:LEU:O	4:E:887:HOH:O	2.15	0.64
1:B:94:LEU:HB3	2:E:128:VAL:HG11	1.78	0.64
2:F:181:THR:OG1	4:F:974:HOH:O	2.16	0.62
1:C:94:LEU:HD11	2:F:110:LEU:HD23	1.82	0.61
2:E:457:ASN:ND2	3:E:603:NAG:C2	2.59	0.61
2:E:386:LYS:HE3	2:E:388:MET:HE1	1.83	0.60
2:F:277:THR:HA	4:F:751:HOH:O	1.99	0.60
2:F:318:ALA:HB2	2:F:341:LEU:HD21	1.84	0.59
2:F:352:ASN:CG	3:F:601:NAG:C1	2.67	0.59
2:D:355:ARG:NH2	4:D:891:HOH:O	2.35	0.59
1:A:94:LEU:HD11	2:D:110:LEU:HD23	1.84	0.58
2:F:186:LYS:O	4:F:901:HOH:O	2.17	0.58
2:E:430:TYR:CD1	2:E:432:SER:HB2	2.39	0.57
2:F:352:ASN:ND2	3:F:601:NAG:C2	2.62	0.56
2:E:465:GLN:O	2:E:469:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:344:ASP:OD1	2:E:355:ARG:NH1	2.32	0.55
1:B:100:ARG:HG3	4:B:313:HOH:O	2.06	0.55
2:D:457:ASN:CG	3:D:602:NAG:C1	2.66	0.55
2:F:166:GLN:HB3	2:F:169:GLN:HB2	1.89	0.55
2:F:381:ARG:NH2	4:F:863:HOH:O	2.37	0.55
2:F:457:ASN:OD1	3:F:602:NAG:C1	2.55	0.55
2:E:352:ASN:ND2	3:E:602:NAG:C2	2.49	0.54
1:B:52:LYS:HB2	2:E:166:GLN:HG2	1.90	0.54
2:D:419:ARG:H	1:B:100:ARG:HH22	1.54	0.54
1:A:85:GLU:OE1	4:A:323:HOH:O	2.18	0.54
1:C:43:GLU:HG2	4:F:847:HOH:O	2.08	0.54
1:C:27:GLN:HB3	2:F:434:ILE:HD11	1.89	0.54
2:D:318:ALA:HB2	2:D:341:LEU:HD21	1.91	0.53
1:C:98:ARG:CZ	1:C:98:ARG:HB2	2.38	0.53
3:B:201:NAG:O4	3:E:601:NAG:O5	2.06	0.53
1:B:91:ARG:NE	2:E:131:ASN:OD1	2.42	0.53
2:F:321:ALA:HB1	2:F:324:CYS:HB2	1.91	0.53
2:D:167:ALA:O	4:D:835:HOH:O	2.18	0.53
2:D:200:LEU:O	2:D:204:THR:HG23	2.09	0.52
1:C:100:ARG:HG2	2:F:104:ALA:O	2.09	0.52
2:E:371:LEU:HD13	2:F:121:VAL:HG21	1.92	0.51
2:D:297:ASN:HB3	4:D:873:HOH:O	2.11	0.51
2:E:368:ARG:HD3	2:E:383:MET:HB2	1.92	0.51
2:D:419:ARG:N	1:B:100:ARG:HH22	2.09	0.50
1:A:41:TYR:HE1	1:A:44:ALA:HB2	1.76	0.50
2:D:371:LEU:HD13	2:E:121:VAL:HG21	1.94	0.50
2:D:275:LEU:HD12	2:D:276:PRO:HD2	1.94	0.49
1:A:81:GLN:HB3	1:A:82:PRO:HD3	1.94	0.49
1:A:99:ARG:HD3	2:D:129:LYS:HA	1.95	0.49
1:B:78:LYS:HA	1:B:81:GLN:HG2	1.95	0.49
2:E:336:ASN:OD1	2:E:337:ASP:N	2.45	0.49
2:F:435:LYS:N	4:F:893:HOH:O	2.23	0.49
1:B:81:GLN:HB2	1:B:82:PRO:HD3	1.95	0.48
1:A:39:MET:SD	2:D:280:VAL:HG22	2.54	0.48
2:E:103:PHE:HD1	2:E:106:VAL:HG23	1.77	0.48
2:F:195:ILE:O	4:F:812:HOH:O	2.20	0.48
2:F:428:VAL:HG23	2:F:430:TYR:CD1	2.48	0.48
2:D:132:GLU:HG3	4:D:887:HOH:O	2.14	0.48
2:E:318:ALA:HB2	2:E:341:LEU:HD21	1.96	0.48
3:E:603:NAG:H81	2:F:452:ASN:HB3	1.96	0.48
2:E:238:LYS:HG3	2:E:239:SER:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:457:ASN:ND2	3:F:602:NAG:O5	2.20	0.47
1:B:100:ARG:C	1:B:100:ARG:HE	2.18	0.47
2:D:321:ALA:HB1	2:D:324:CYS:HB2	1.97	0.47
2:F:355:ARG:NH2	4:F:947:HOH:O	2.47	0.47
2:D:185:CYS:O	2:D:189:ASP:HB2	2.15	0.47
2:D:419:ARG:HD3	2:E:103:PHE:O	2.15	0.47
2:D:125:VAL:O	2:D:129:LYS:HD3	2.15	0.46
2:D:175:VAL:HG23	2:D:191:ILE:HD13	1.96	0.46
1:B:66:ILE:HD11	2:E:180:ILE:HG21	1.98	0.46
2:E:381:ARG:NH1	4:E:801:HOH:O	2.18	0.46
3:C:201:NAG:H2	4:C:317:HOH:O	2.15	0.46
1:B:87:LEU:HD13	2:E:215:ALA:HB1	1.97	0.46
1:C:20:LEU:HD23	1:C:22:PRO:HG3	1.98	0.46
2:F:383:MET:HG2	4:F:931:HOH:O	2.15	0.46
2:D:344:ASP:OD1	2:D:355:ARG:NH1	2.47	0.46
2:D:435:LYS:HD2	2:D:435:LYS:HA	1.73	0.46
2:E:103:PHE:O	2:E:105:GLY:N	2.49	0.46
2:E:166:GLN:HB3	2:E:169:GLN:HB2	1.97	0.46
2:E:474:LEU:HD23	2:E:475:SER:H	1.80	0.46
1:B:99:ARG:CG	1:B:100:ARG:HB2	2.45	0.46
2:F:202:GLU:HB3	2:F:226:ILE:HG23	1.98	0.46
3:B:201:NAG:C4	3:E:601:NAG:C1	2.84	0.45
2:F:465:GLN:O	2:F:469:GLN:HG2	2.17	0.45
1:B:20:LEU:O	1:B:22:PRO:HD3	2.17	0.45
2:F:330:THR:HB	4:F:955:HOH:O	2.16	0.45
2:E:318:ALA:HB3	2:E:339:GLN:HB2	1.99	0.45
1:B:98:ARG:HB2	2:E:103:PHE:CZ	2.52	0.45
1:B:99:ARG:HG3	1:B:100:ARG:HB2	1.98	0.45
1:A:99:ARG:HB2	1:A:99:ARG:HH11	1.81	0.44
1:B:94:LEU:HD12	1:B:94:LEU:HA	1.81	0.44
1:A:22:PRO:HD2	4:A:336:HOH:O	2.17	0.44
2:E:184:ASN:O	2:E:186:LYS:N	2.51	0.44
2:F:417:ASN:HB2	4:F:958:HOH:O	2.16	0.44
1:B:25:LEU:HB3	1:B:30:VAL:HB	2.00	0.44
1:C:91:ARG:NE	2:F:131:ASN:OD1	2.40	0.44
1:B:41:TYR:HE1	1:B:44:ALA:HB2	1.83	0.44
2:E:306:PRO:HB3	4:E:933:HOH:O	2.17	0.44
2:D:264:LEU:HD23	2:D:264:LEU:HA	1.89	0.44
1:C:94:LEU:HG	2:F:107:VAL:HG11	1.99	0.43
1:B:52:LYS:NZ	4:B:304:HOH:O	2.40	0.43
2:E:264:LEU:HD23	2:E:264:LEU:HA	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:387:CYS:O	2:E:391:ALA:HA	2.19	0.43
1:A:98:ARG:O	1:A:99:ARG:NH1	2.51	0.43
2:D:295:PHE:CE2	2:D:298:ASN:HA	2.54	0.43
2:E:389:GLN:HB3	2:E:412:SER:HB3	2.00	0.43
2:E:321:ALA:HB1	2:E:324:CYS:HB2	2.01	0.43
1:C:72:TYR:CD1	2:F:196:LEU:HB3	2.54	0.43
2:F:132:GLU:HG2	4:F:943:HOH:O	2.18	0.42
2:F:427:ASN:ND2	4:F:969:HOH:O	2.52	0.42
1:A:20:LEU:O	1:A:22:PRO:HD3	2.19	0.42
2:D:104:ALA:HA	2:D:105:GLY:HA2	1.52	0.42
2:D:474:LEU:HG	2:F:474:LEU:HD11	2.00	0.42
1:A:22:PRO:O	1:A:26:MET:HG3	2.20	0.42
1:A:57:ILE:HD12	1:A:69:ILE:HD11	2.00	0.42
2:F:228:LEU:HB3	2:F:231:THR:OG1	2.19	0.42
1:A:54:MET:HG2	3:A:201:NAG:H81	2.02	0.42
1:C:22:PRO:O	1:C:26:MET:HG3	2.20	0.42
1:C:97:THR:CG2	2:F:106:VAL:HB	2.49	0.42
2:D:221:ILE:O	2:D:225:ARG:HG3	2.20	0.41
1:C:59:SER:HA	1:C:60:PRO:HD3	1.87	0.41
2:E:165:VAL:HG21	2:E:228:LEU:HG	2.02	0.41
2:D:166:GLN:HB3	2:D:169:GLN:HB2	2.02	0.41
2:D:333:CYS:HB3	2:D:335:TYR:O	2.21	0.41
2:D:321:ALA:HB3	2:D:326:ILE:HD11	2.03	0.41
1:A:94:LEU:HD12	1:A:94:LEU:HA	1.94	0.41
2:E:448:ASP:OD2	4:E:811:HOH:O	2.22	0.41
2:F:467:LEU:HD23	2:F:467:LEU:HA	1.91	0.41
1:C:25:LEU:HB3	1:C:30:VAL:HB	2.03	0.41
2:D:447:LEU:HB2	4:E:952:HOH:O	2.21	0.41
2:D:146:LYS:HA	2:D:146:LYS:HD3	1.77	0.40
1:B:41:TYR:CE1	1:B:44:ALA:HB2	2.55	0.40
2:E:117:THR:H	2:E:120:GLN:NE2	2.20	0.40
1:C:66:ILE:HG22	1:C:69:ILE:HG13	2.03	0.40
1:C:94:LEU:HD12	1:C:94:LEU:HA	1.85	0.40
2:E:200:LEU:O	2:E:204:THR:HG23	2.22	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	79/81 (98%)	76 (96%)	2 (2%)	1 (1%)	12	6
1	B	79/81 (98%)	75 (95%)	3 (4%)	1 (1%)	12	6
1	C	79/81 (98%)	74 (94%)	5 (6%)	0	100	100
2	D	373/409 (91%)	358 (96%)	14 (4%)	1 (0%)	41	37
2	E	373/409 (91%)	351 (94%)	16 (4%)	6 (2%)	9	4
2	F	373/409 (91%)	361 (97%)	10 (3%)	2 (0%)	29	23
All	All	1356/1470 (92%)	1295 (96%)	50 (4%)	11 (1%)	19	13

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	185	CYS
1	B	99	ARG
2	E	184	ASN
2	E	185	CYS
2	E	433	THR
2	E	104	ALA
2	E	321	ALA
1	A	99	ARG
2	E	432	SER
2	F	428	VAL
2	F	104	ALA

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	73/73 (100%)	68 (93%)	5 (7%)	16	11
1	B	73/73 (100%)	70 (96%)	3 (4%)	30	28
1	C	73/73 (100%)	66 (90%)	7 (10%)	8	5
2	D	316/347 (91%)	305 (96%)	11 (4%)	36	35
2	E	316/347 (91%)	306 (97%)	10 (3%)	39	38
2	F	316/347 (91%)	305 (96%)	11 (4%)	36	35
All	All	1167/1260 (93%)	1120 (96%)	47 (4%)	31	29

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	TYR
1	A	45	SER
1	A	81	GLN
1	A	98	ARG
1	A	99	ARG
2	D	228	LEU
2	D	279	THR
2	D	298	ASN
2	D	330	THR
2	D	339	GLN
2	D	371	LEU
2	D	400	SER
2	D	430	TYR
2	D	433	THR
2	D	438	SER
2	D	474	LEU
1	B	42	THR
1	B	87	LEU
1	B	100	ARG
2	E	140	LEU
2	E	208	HIS
2	E	217	SER
2	E	281	GLN
2	E	334	ARG
2	E	371	LEU
2	E	432	SER
2	E	472	THR
2	E	473	TYR
2	E	474	LEU
1	C	41	TYR

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Mol	Chain	Res	Type
1	C	42	THR
1	C	70	SER
1	C	97	THR
1	C	98	ARG
1	C	99	ARG
1	C	100	ARG
2	F	103	PHE
2	F	158	THR
2	F	171	HIS
2	F	209	ASN
2	F	265	THR
2	F	273	ILE
2	F	281	GLN
2	F	330	THR
2	F	371	LEU
2	F	412	SER
2	F	461	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	457	ASN
2	E	352	ASN
2	E	457	ASN
2	F	352	ASN
2	F	457	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)

11 ligands 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	E	602	-	14,14,15	0.49	0	17,19,21	0.88	1 (5%)
3	NAG	C	202	-	14,14,15	0.49	0	17,19,21	1.46	1 (5%)
3	NAG	F	601	-	14,14,15	0.47	0	17,19,21	1.53	3 (17%)
3	NAG	E	601	-	14,14,15	0.48	0	17,19,21	0.80	1 (5%)
3	NAG	A	201	1	14,14,15	0.54	0	17,19,21	1.09	2 (11%)
3	NAG	C	201	-	14,14,15	0.51	0	17,19,21	0.92	1 (5%)
3	NAG	E	603	-	14,14,15	0.51	0	17,19,21	0.82	1 (5%)
3	NAG	F	602	-	14,14,15	0.55	0	17,19,21	0.99	0
3	NAG	D	602	-	14,14,15	0.46	0	17,19,21	0.83	1 (5%)
3	NAG	B	201	-	14,14,15	0.54	0	17,19,21	0.79	0
3	NAG	D	601	-	14,14,15	0.53	0	17,19,21	0.71	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
3	NAG	E	602	-	-	2/6/23/26	0/1/1/1
3	NAG	C	202	-	-	3/6/23/26	0/1/1/1
3	NAG	F	601	-	-	4/6/23/26	0/1/1/1
3	NAG	E	601	-	-	2/6/23/26	0/1/1/1
3	NAG	A	201	1	-	2/6/23/26	0/1/1/1
3	NAG	C	201	-	-	0/6/23/26	0/1/1/1
3	NAG	E	603	-	-	3/6/23/26	0/1/1/1
3	NAG	F	602	-	-	2/6/23/26	0/1/1/1
3	NAG	D	602	-	-	0/6/23/26	0/1/1/1
3	NAG	B	201	-	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	601	-	-	4/6/23/26	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(^{o})	Ideal(^{o})
3	F	601	NAG	C1-O5-C5	4.59	118.42	112.19
3	C	202	NAG	C1-O5-C5	4.26	117.97	112.19
3	C	201	NAG	C1-O5-C5	2.81	116.00	112.19
3	E	601	NAG	C1-O5-C5	2.53	115.62	112.19
3	F	601	NAG	C4-C3-C2	-2.38	107.53	111.02
3	A	201	NAG	C2-N2-C7	-2.33	119.58	122.90
3	E	602	NAG	O5-C5-C6	2.29	110.80	107.20
3	D	602	NAG	C1-O5-C5	2.28	115.28	112.19
3	E	603	NAG	C1-O5-C5	2.15	115.11	112.19
3	F	601	NAG	C2-N2-C7	-2.14	119.85	122.90
3	A	201	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	601	NAG	C1-C2-N2-C7
3	D	601	NAG	C8-C7-N2-C2
3	D	601	NAG	O7-C7-N2-C2
3	C	202	NAG	C1-C2-N2-C7
3	C	202	NAG	C8-C7-N2-C2
3	C	202	NAG	O7-C7-N2-C2
3	F	602	NAG	C8-C7-N2-C2
3	F	602	NAG	O7-C7-N2-C2
3	F	601	NAG	C4-C5-C6-O6
3	E	602	NAG	C4-C5-C6-O6
3	D	601	NAG	O5-C5-C6-O6
3	E	602	NAG	O5-C5-C6-O6
3	B	201	NAG	C8-C7-N2-C2
3	E	601	NAG	C4-C5-C6-O6
3	E	601	NAG	O5-C5-C6-O6
3	F	601	NAG	C8-C7-N2-C2
3	B	201	NAG	O7-C7-N2-C2
3	A	201	NAG	C4-C5-C6-O6
3	E	603	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	F	601	NAG	O5-C5-C6-O6
3	F	601	NAG	O7-C7-N2-C2
3	A	201	NAG	O5-C5-C6-O6
3	E	603	NAG	O7-C7-N2-C2
3	B	201	NAG	C4-C5-C6-O6
3	E	603	NAG	C4-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	602	NAG	4	0
3	F	601	NAG	5	0
3	E	601	NAG	4	0
3	A	201	NAG	1	0
3	C	201	NAG	1	0
3	E	603	NAG	7	0
3	F	602	NAG	5	0
3	D	602	NAG	5	0
3	B	201	NAG	7	0
3	D	601	NAG	1	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)

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	81/81 (100%)	0.25	10 (12%)	4	3	18, 46, 105, 118	0
1	B	81/81 (100%)	0.30	11 (13%)	3	2	17, 46, 98, 136	0
1	C	81/81 (100%)	0.11	8 (9%)	7	6	16, 42, 94, 130	0
2	D	375/409 (91%)	0.03	25 (6%)	17	17	16, 38, 90, 141	0
2	E	375/409 (91%)	-0.08	18 (4%)	30	29	14, 39, 84, 143	0
2	F	375/409 (91%)	-0.00	22 (5%)	22	21	19, 37, 92, 127	0
All	All	1368/1470 (93%)	0.02	94 (6%)	16	16	14, 39, 93, 143	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	100	ARG	8.3
2	D	429	THR	8.0
2	E	104	ALA	7.3
2	D	474	LEU	7.0
2	E	103	PHE	6.9
1	B	100	ARG	6.9
2	E	473	TYR	6.6
2	F	473	TYR	6.6
1	B	98	ARG	5.8
1	A	64	CYS	5.4
2	F	476	ALA	5.1
1	A	100	ARG	5.1
1	C	42	THR	5.1
1	A	99	ARG	4.9
1	A	42	THR	4.9
2	E	476	ALA	4.8
2	D	431	ASN	4.7
1	C	99	ARG	4.5
2	D	432	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	99	ARG	4.5
1	B	61	ILE	4.4
2	D	103	PHE	4.3
2	D	433	THR	4.2
1	C	64	CYS	4.1
1	A	98	ARG	4.0
2	D	243	GLN	4.0
2	E	474	LEU	3.8
1	B	63	GLY	3.7
2	F	428	VAL	3.6
2	F	429	THR	3.6
2	D	476	ALA	3.5
2	F	104	ALA	3.5
2	F	477	ILE	3.5
2	F	182	ALA	3.5
2	D	241	ASN	3.5
1	A	43	GLU	3.4
1	A	41	TYR	3.3
2	E	180	ILE	3.3
2	F	430	TYR	3.2
1	B	42	THR	3.2
2	D	473	TYR	3.1
2	D	158	THR	3.1
2	E	183	ALA	3.1
1	B	43	GLU	3.1
1	C	43	GLU	3.1
2	F	183	ALA	3.1
1	A	63	GLY	3.1
2	D	181	THR	3.0
2	F	475	SER	3.0
2	D	104	ALA	2.8
2	F	469	GLN	2.8
2	F	472	THR	2.8
2	F	243	GLN	2.8
2	E	475	SER	2.8
2	F	158	THR	2.7
2	D	430	TYR	2.7
2	E	158	THR	2.7
2	E	243	GLN	2.6
2	E	157	ALA	2.6
2	F	279	THR	2.6
2	F	474	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	433	THR	2.6
2	D	471	ASP	2.5
2	E	432	SER	2.5
2	D	157	ALA	2.5
2	D	428	VAL	2.5
2	D	178	PRO	2.5
2	E	472	THR	2.5
2	F	185	CYS	2.5
2	F	468	ALA	2.5
2	E	179	ALA	2.5
1	B	58	ASP	2.4
1	A	61	ILE	2.4
1	B	60	PRO	2.4
1	A	62	SER	2.4
1	C	98	ARG	2.4
1	C	41	TYR	2.4
1	B	64	CYS	2.3
2	D	472	THR	2.3
2	E	465	GLN	2.3
2	F	432	SER	2.3
2	D	183	ALA	2.3
2	F	180	ILE	2.3
2	F	103	PHE	2.2
1	B	66	ILE	2.2
1	C	66	ILE	2.2
2	D	182	ALA	2.2
2	F	181	THR	2.2
2	E	159	GLN	2.2
2	E	477	ILE	2.1
2	D	159	GLN	2.1
2	D	475	SER	2.0
2	D	465	GLN	2.0
2	D	185	CYS	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
3	NAG	C	202	14/15	0.74	0.28	89,102,106,108	0
3	NAG	F	602	14/15	0.81	0.20	73,82,86,86	0
3	NAG	E	601	14/15	0.83	0.18	84,95,98,98	0
3	NAG	E	602	14/15	0.83	0.23	71,95,101,103	0
3	NAG	D	601	14/15	0.85	0.21	58,82,89,94	0
3	NAG	F	601	14/15	0.85	0.24	83,89,94,95	0
3	NAG	E	603	14/15	0.85	0.15	66,74,78,81	0
3	NAG	D	602	14/15	0.88	0.12	74,79,82,82	0
3	NAG	C	201	14/15	0.92	0.12	50,59,70,74	0
3	NAG	B	201	14/15	0.92	0.12	60,62,68,70	0
3	NAG	A	201	14/15	0.94	0.11	43,60,64,68	0

6.5 Other polymers (i)

There are no such residues in this entry.