Full wwPDB X-ray Structure Validation Report (i)

Jan 9, 2025 – 12:09 PM EST

PDB ID	:	8W3J
Title	:	Crystal structure of prefusion-stabilized RSV F protein UFCR2-iSS
Authors	:	Lee, Y.Z.; Stanfield, R.L.; Wilson, I.A.; Zhu, J.
Deposited on	:	2024-02-22
Resolution	:	2.83 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 (1)) were used in the production of this report:

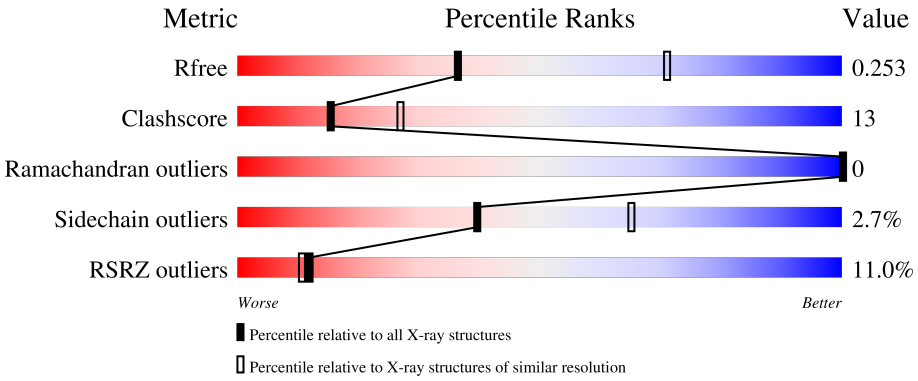
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.83 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}	164625	1367 (2.86-2.82)
Clashscore	180529	1455 (2.86-2.82)
Ramachandran outliers	177936	1422 (2.86-2.82)
Sidechain outliers	177891	1423 (2.86-2.82)
RSRZ outliers	164620	1368 (2.86-2.82)

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	F	507	10% 66% 21% • 12%

2 Entry composition

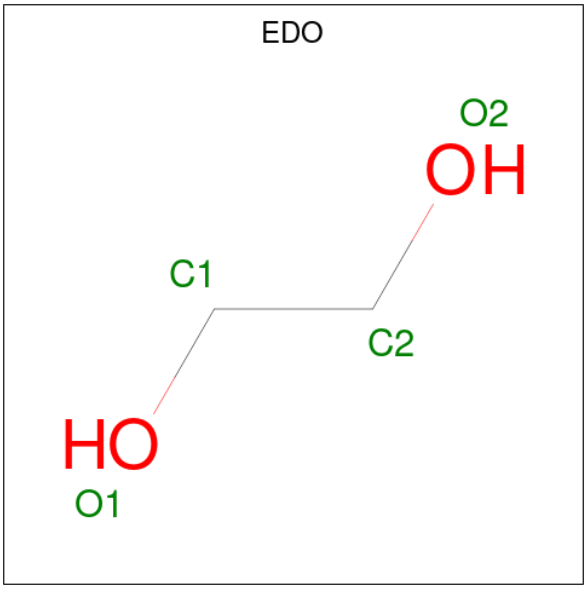
There are 4 unique types of molecules in this entry. The entry contains 3462 atoms, of which 6 are hydrogens and 0 are deuteriums.

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 Prefusion-stabilized RSV F protein UFCR2-iSS.

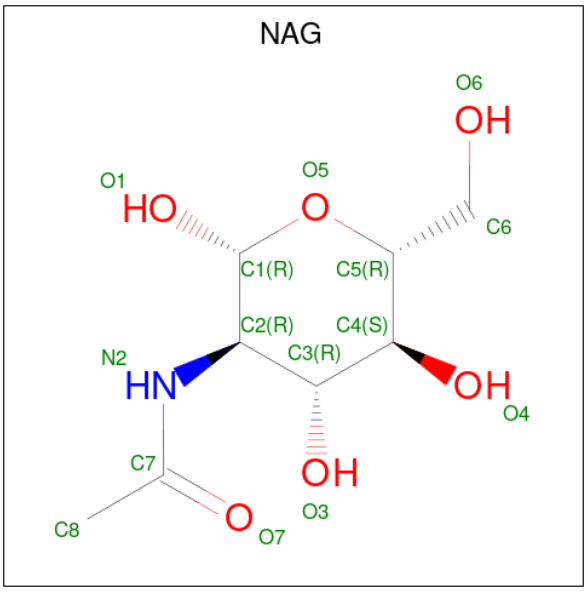
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	F	445	3426	2151	570	680	25	0	0	0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	F	1	10	2	6	2	0	0

- 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
3	F	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is water.

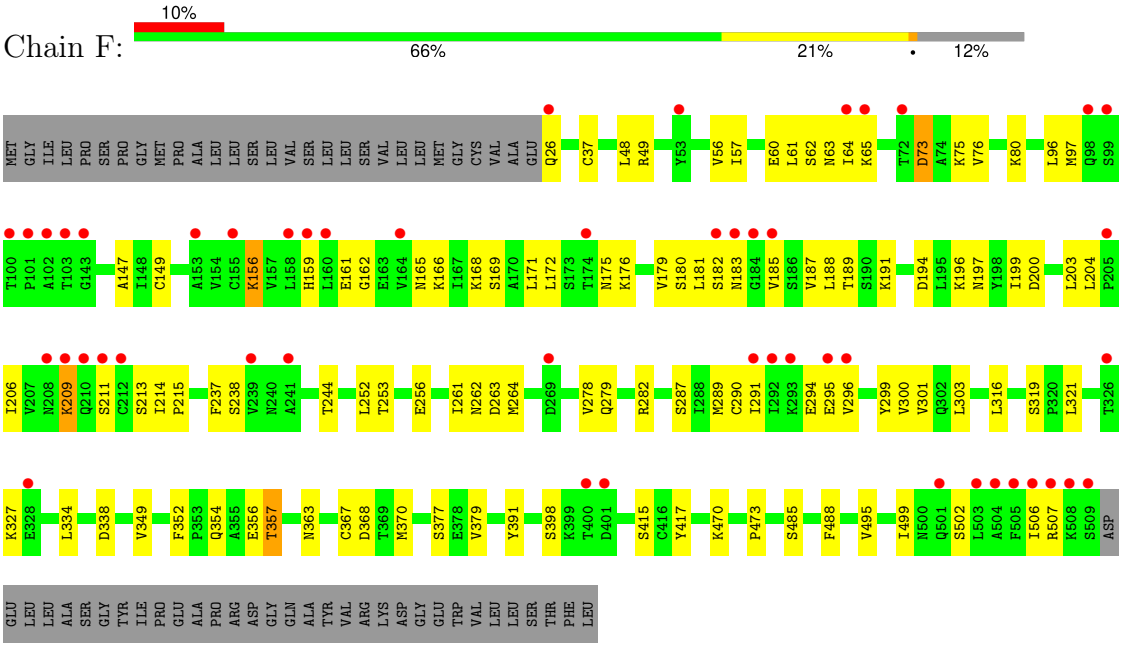
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	12	Total O 12 12	0	0

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: Prefusion-stabilized RSV F protein UFCR2-iSS

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	169.22Å 169.22Å 169.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.84 – 2.83 37.84 – 2.83	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.84-2.83) 99.8 (37.84-2.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.224 , 0.258 0.223 , 0.253	Depositor DCC
R_{free} test set	1026 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	50.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3462	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 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	F	0.56	1/3475 (0.0%)	0.82	0/4712

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	263	ASP	C-N	5.24	1.46	1.34

There are no bond angle outliers.

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	F	3426	0	3458	92	0
2	F	4	6	6	0	0
3	F	14	0	13	0	0
4	F	12	0	0	0	0
All	All	3456	6	3477	92	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 13.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:LYS:NZ	1:F:180:SER:O	2.01	0.92
1:F:76:VAL:HG12	1:F:80:LYS:HE2	1.57	0.86
1:F:507:ARG:O	1:F:507:ARG:NH1	2.11	0.83
1:F:162:GLY:HA2	1:F:165:ASN:HD22	1.49	0.77
1:F:206:ILE:HD13	1:F:213:SER:HB3	1.71	0.72
1:F:64:ILE:O	1:F:64:ILE:HG13	1.88	0.72
1:F:301:VAL:HG12	1:F:303:LEU:HD13	1.71	0.72
1:F:182:SER:O	1:F:183:ASN:HB2	1.88	0.71
1:F:156:LYS:HA	1:F:156:LYS:HE2	1.73	0.69
1:F:56:VAL:HB	1:F:189:THR:HG22	1.75	0.69
1:F:97:MET:HE1	1:F:290:CYS:O	1.94	0.68
1:F:194:ASP:OD2	1:F:197:ASN:HB2	1.92	0.68
1:F:162:GLY:CA	1:F:165:ASN:HD22	2.07	0.67
1:F:156:LYS:HE2	1:F:156:LYS:CA	2.24	0.67
1:F:97:MET:CE	1:F:290:CYS:O	2.44	0.66
1:F:159:HIS:CE1	1:F:291:ILE:HD13	2.33	0.64
1:F:502:SER:O	1:F:506:ILE:HG23	1.98	0.64
1:F:237:PHE:CE2	1:F:289:MET:HG2	2.35	0.62
1:F:49:ARG:HG2	1:F:49:ARG:HH11	1.65	0.61
1:F:61:LEU:O	1:F:295:GLU:HB3	2.01	0.61
1:F:76:VAL:CG1	1:F:80:LYS:HE2	2.30	0.61
1:F:237:PHE:CD2	1:F:289:MET:HG2	2.36	0.60
1:F:156:LYS:HA	1:F:156:LYS:CE	2.29	0.60
1:F:301:VAL:HG12	1:F:303:LEU:CD1	2.32	0.59
1:F:64:ILE:HG21	1:F:204:LEU:HD21	1.84	0.59
1:F:60:GLU:OE1	1:F:191:LYS:HE2	2.03	0.59
1:F:278:VAL:O	1:F:282:ARG:HG3	2.02	0.59
1:F:253:THR:OG1	1:F:256:GLU:HG3	2.03	0.58
1:F:147:ALA:HA	1:F:370:MET:HE1	1.86	0.58
1:F:57:ILE:HB	1:F:299:TYR:CE1	2.39	0.57
1:F:171:LEU:HD12	1:F:175:ASN:O	2.05	0.57
1:F:209:LYS:HG3	1:F:211:SER:O	2.04	0.57
1:F:181:LEU:HB2	1:F:185:VAL:HG23	1.86	0.57
1:F:181:LEU:HD11	1:F:187:VAL:HG11	1.89	0.55
1:F:156:LYS:HE2	1:F:156:LYS:N	2.22	0.54
1:F:62:SER:HB2	1:F:196:LYS:HA	1.90	0.53
1:F:181:LEU:N	1:F:181:LEU:HD23	2.23	0.53
1:F:398:SER:HA	1:F:485:SER:O	2.08	0.52
1:F:290:CYS:SG	1:F:300:VAL:HG23	2.50	0.52
1:F:415:SER:HB3	1:F:417:TYR:CE2	2.45	0.52
1:F:49:ARG:NE	1:F:368:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:64:ILE:CG2	1:F:204:LEU:HD21	2.41	0.51
1:F:179:VAL:HG12	1:F:181:LEU:HD23	1.93	0.50
1:F:97:MET:HE1	1:F:289:MET:O	2.11	0.50
1:F:96:LEU:HD11	1:F:237:PHE:O	2.12	0.50
1:F:37:CYS:SG	1:F:319:SER:HB3	2.52	0.50
1:F:168:LYS:HE2	1:F:296:VAL:CG2	2.42	0.49
1:F:96:LEU:HD12	1:F:238:SER:HA	1.95	0.48
1:F:352:PHE:CE2	1:F:367:CYS:HB3	2.48	0.48
1:F:75:LYS:HD3	1:F:215:PRO:O	2.13	0.48
1:F:252:LEU:O	1:F:282:ARG:NH2	2.33	0.48
1:F:290:CYS:SG	1:F:300:VAL:CG2	3.01	0.48
1:F:354:GLN:HB2	1:F:357:THR:HG22	1.95	0.48
1:F:188:LEU:C	1:F:188:LEU:HD23	2.34	0.47
1:F:203:LEU:O	1:F:206:ILE:HB	2.14	0.47
1:F:356:GLU:H	1:F:356:GLU:CD	2.17	0.47
1:F:96:LEU:O	1:F:96:LEU:HD23	2.15	0.47
1:F:181:LEU:HD11	1:F:187:VAL:CG1	2.45	0.47
1:F:415:SER:HB3	1:F:417:TYR:HE2	1.78	0.47
1:F:379:VAL:HG23	1:F:391:TYR:CZ	2.49	0.46
1:F:354:GLN:O	1:F:357:THR:HG22	2.16	0.46
1:F:356:GLU:OE1	1:F:356:GLU:N	2.43	0.46
1:F:96:LEU:HD23	1:F:96:LEU:C	2.36	0.45
1:F:349:VAL:HG23	1:F:377:SER:HA	1.98	0.45
1:F:354:GLN:O	1:F:357:THR:CG2	2.65	0.44
1:F:172:LEU:HD23	1:F:172:LEU:HA	1.83	0.44
1:F:165:ASN:OD1	1:F:294:GLU:OE1	2.35	0.44
1:F:162:GLY:HA2	1:F:165:ASN:ND2	2.24	0.44
1:F:48:LEU:HD22	1:F:367:CYS:HB2	2.00	0.44
1:F:279:GLN:H	1:F:279:GLN:CD	2.22	0.44
1:F:176:LYS:HB2	1:F:176:LYS:HE2	1.49	0.43
1:F:168:LYS:O	1:F:172:LEU:HG	2.18	0.43
1:F:63:ASN:HB2	1:F:295:GLU:OE2	2.17	0.43
1:F:244:THR:OG1	1:F:287:SER:HB3	2.19	0.42
1:F:321:LEU:HD11	1:F:473:PRO:HB3	2.00	0.42
1:F:73:ASP:OD2	1:F:214:ILE:HD12	2.19	0.42
1:F:65:LYS:HA	1:F:65:LYS:HD3	1.86	0.42
1:F:179:VAL:HG12	1:F:181:LEU:CD2	2.49	0.42
1:F:168:LYS:HE2	1:F:296:VAL:HG23	2.02	0.42
1:F:200:ASP:HA	1:F:204:LEU:HG	2.01	0.42
1:F:209:LYS:HB3	1:F:209:LYS:HE3	1.58	0.41
1:F:61:LEU:O	1:F:196:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:316:LEU:HD23	1:F:338:ASP:O	2.20	0.41
1:F:161:GLU:OE1	1:F:161:GLU:N	2.53	0.41
1:F:199:ILE:HG12	1:F:203:LEU:HD12	2.03	0.41
1:F:182:SER:O	1:F:183:ASN:CB	2.56	0.41
1:F:60:GLU:CD	1:F:191:LYS:HE2	2.41	0.41
1:F:495:VAL:O	1:F:499:ILE:HG13	2.20	0.41
1:F:49:ARG:HH11	1:F:49:ARG:CG	2.34	0.40
1:F:171:LEU:HD21	1:F:189:THR:OG1	2.21	0.40
1:F:261:ILE:HA	1:F:264:MET:SD	2.61	0.40
1:F:26:GLN:N	1:F:363:ASN:HD22	2.19	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	F	443/507 (87%)	426 (96%)	17 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	F	406/457 (89%)	395 (97%)	11 (3%)	40 65

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	73	ASP
1	F	149	CYS
1	F	156	LYS
1	F	169	SER
1	F	209	LYS
1	F	262	ASN
1	F	327	LYS
1	F	334	LEU
1	F	357	THR
1	F	470	LYS
1	F	488	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	165	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
2	EDO	F	601	-	3,3,3	0.79	0	2,2,2	0.24	0
3	NAG	F	602	1	14,14,15	0.85	1 (7%)	17,19,21	0.74	1 (5%)

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
2	EDO	F	601	-	-	0/1/1/1	-
3	NAG	F	602	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	602	NAG	C1-C2	2.63	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	602	NAG	C1-O5-C5	2.07	114.96	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	602	NAG	C4-C5-C6-O6
3	F	602	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	F	445/507 (87%)	0.39	49 (11%)	12	11	19, 51, 98, 134	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	505	PHE	7.2
1	F	101	PRO	5.3
1	F	211	SER	4.9
1	F	509	SER	4.8
1	F	506	ILE	4.8
1	F	212	CYS	4.7
1	F	504	ALA	4.3
1	F	210	GLN	4.0
1	F	508	LYS	3.9
1	F	182	SER	3.6
1	F	143	GLY	3.4
1	F	103	THR	3.4
1	F	155	CYS	3.3
1	F	183	ASN	3.2
1	F	100	THR	3.0
1	F	507	ARG	3.0
1	F	291	ILE	3.0
1	F	164	VAL	2.9
1	F	401	ASP	2.9
1	F	209	LYS	2.8
1	F	65	LYS	2.7
1	F	53	TYR	2.7
1	F	160	LEU	2.6
1	F	328	GLU	2.6
1	F	102	ALA	2.6
1	F	292	ILE	2.5
1	F	241	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	174	THR	2.4
1	F	184	GLY	2.3
1	F	153	ALA	2.3
1	F	158	LEU	2.3
1	F	72	THR	2.3
1	F	159	HIS	2.2
1	F	26	GLN	2.2
1	F	208	ASN	2.2
1	F	296	VAL	2.2
1	F	501	GLN	2.2
1	F	503	LEU	2.1
1	F	239	VAL	2.1
1	F	400	THR	2.1
1	F	64	ILE	2.1
1	F	185	VAL	2.1
1	F	269	ASP	2.1
1	F	205	PRO	2.1
1	F	99	SER	2.0
1	F	295	GLU	2.0
1	F	98	GLN	2.0
1	F	326	THR	2.0
1	F	293	LYS	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	F	602	14/15	0.45	0.18	63,100,106,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	F	601	4/4	0.93	0.14	36,44,48,51	0

6.5 Other polymers (i)

There are no such residues in this entry.