Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 11:46 PM EDT

PDB ID	:	4MMU
Title	:	Crystal Structure of Prefusion-stabilized RSV F Variant DS-Cav1 at pH 5.5
Authors	:	Joyce, M.G.; Mclellan, J.S.; Stewart-Jones, G.B.E.; Sastry, M.; Yang, Y.; Graham, B.S.; Kwong, P.D.
Deposited on	:	2013-09-09
Resolution	:	3.00 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:

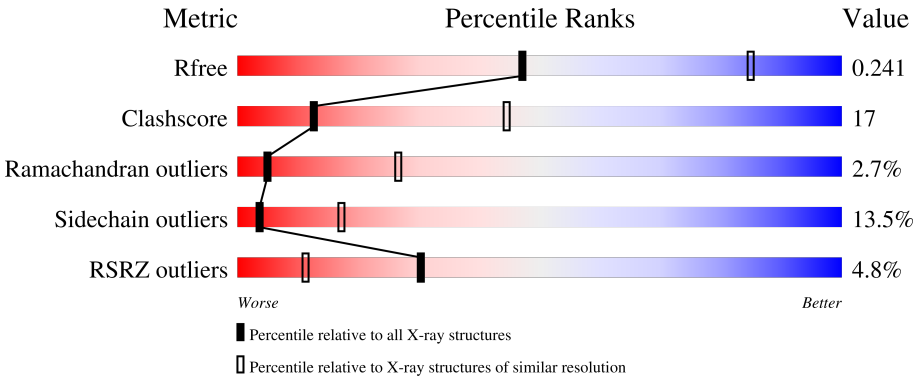
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	82	11% 60% 28% 11%
2	B	414	3% 66% 21% 10%

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	SO4	B	601	-	-	-	X
3	SO4	B	605	-	-	X	-
4	NAG	B	602	-	-	X	X
5	PO4	B	606	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3642 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
1	A	82	Total	C	N	O	S	0	0	0
			644	402	109	130	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	PRO	engineered mutation	UNP P03420

- Molecule 2 is a protein called Fusion glycoprotein F1 fused with Fibritin trimerization domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	373	Total	C	N	O	S	0	0	0
			2878	1820	476	562	20			

There are 17 discrepancies between the modelled and reference sequences:

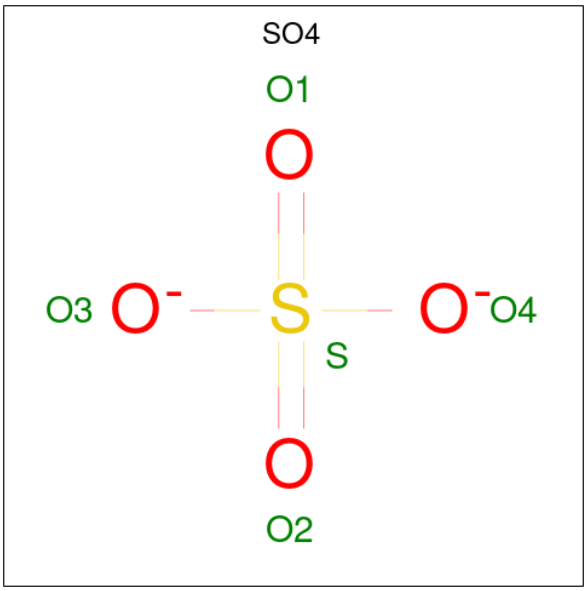
Chain	Residue	Modelled	Actual	Comment	Reference
B	155	CYS	SER	engineered mutation	UNP P03420
B	190	PHE	SER	engineered mutation	UNP P03420
B	207	LEU	VAL	engineered mutation	UNP P03420
B	290	CYS	SER	engineered mutation	UNP P03420
B	379	VAL	ILE	engineered mutation	UNP P03420
B	447	VAL	MET	engineered mutation	UNP P03420
B	514	SER	-	linker	UNP P03420
B	515	ALA	-	linker	UNP P03420
B	516	ILE	-	linker	UNP P03420
B	517	GLY	-	linker	UNP P03420
B	539	LEU	PHE	variant	UNP P10104
B	545	GLY	-	expression tag	UNP P10104
B	546	GLY	-	expression tag	UNP P10104
B	547	LEU	-	expression tag	UNP P10104

Continued on next page...

Continued from previous page...

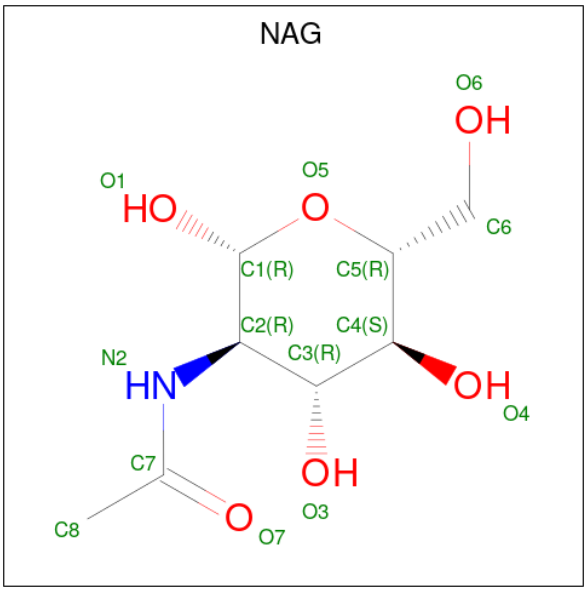
Chain	Residue	Modelled	Actual	Comment	Reference
B	548	VAL	-	expression tag	UNP P10104
B	549	PRO	-	expression tag	UNP P10104
B	550	ARG	-	expression tag	UNP P10104

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



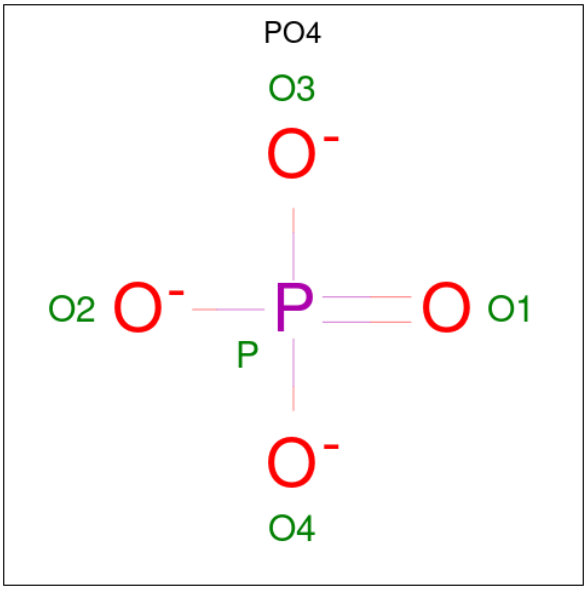
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O P 5 4 1	0	0

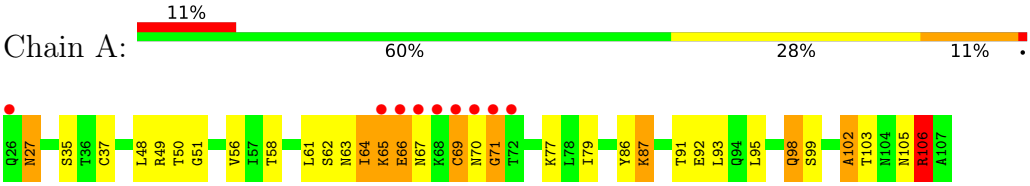
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	12	Total O 12 12	0	0
6	B	69	Total O 69 69	0	0

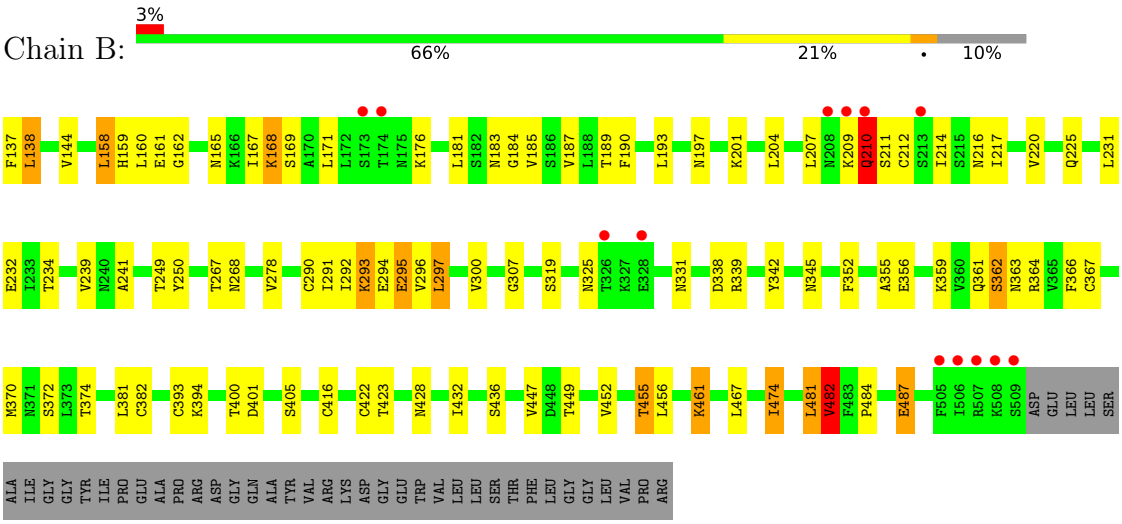
3 Residue-property plots (i)

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



• Molecule 2: Fusion glycoprotein F1 fused with Fibritin trimerization domain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	168.59Å 168.59Å 168.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.50 – 3.00 28.50 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.50-3.00) 99.8 (28.50-3.00)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	0.22	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 3.00Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.178 , 0.228 0.192 , 0.241	Depositor DCC
R_{free} test set	859 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	66.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 72.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3642	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: NAG, PO4, SO4

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	0.45	0/651	0.74	0/879
2	B	0.50	0/2922	0.79	1/3962 (0.0%)
All	All	0.49	0/3573	0.78	1/4841 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	400	THR	C-N-CA	5.08	134.41	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	644	0	650	32	0
2	B	2878	0	2923	84	0
3	B	20	0	0	3	0
4	B	14	0	13	8	0
5	B	5	0	0	0	0
6	A	12	0	0	0	0
6	B	69	0	0	0	0
All	All	3642	0	3586	113	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 17.

All (113) 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)
4:B:602:NAG:O3	4:B:602:NAG:H83	1.47	1.12
2:B:292:ILE:CD1	2:B:297:LEU:HD12	1.80	1.11
2:B:292:ILE:HD11	2:B:297:LEU:HD12	1.30	1.09
2:B:209:LYS:CA	2:B:210:GLN:HB2	1.81	1.08
2:B:294:GLU:C	2:B:295:GLU:HG3	1.70	1.06
2:B:290:CYS:SG	2:B:300:VAL:HG23	1.95	1.06
2:B:209:LYS:HA	2:B:210:GLN:HB2	1.38	1.05
2:B:209:LYS:HB3	2:B:210:GLN:CB	1.93	0.99
2:B:160:LEU:HB2	2:B:161:GLU:HG2	1.44	0.98
2:B:452:VAL:O	2:B:455:THR:HG23	1.62	0.97
2:B:209:LYS:HB3	2:B:210:GLN:HB3	1.41	0.97
4:B:602:NAG:H83	4:B:602:NAG:C3	1.93	0.97
1:A:102:ALA:HB3	1:A:103:THR:HA	1.44	0.96
2:B:294:GLU:O	2:B:295:GLU:HG3	1.69	0.92
2:B:416:CYS:HG	2:B:422:CYS:HG	0.96	0.88
2:B:159:HIS:CE1	2:B:291:ILE:HG21	2.09	0.88
2:B:209:LYS:CB	2:B:210:GLN:CB	2.52	0.88
2:B:159:HIS:CE1	2:B:291:ILE:CG2	2.58	0.87
2:B:382:CYS:HG	2:B:393:CYS:HG	0.88	0.87
4:B:602:NAG:H83	4:B:602:NAG:HO3	1.40	0.86
2:B:292:ILE:HG22	2:B:292:ILE:O	1.74	0.85
1:A:102:ALA:CB	1:A:103:THR:HA	2.07	0.84
2:B:209:LYS:CB	2:B:210:GLN:HB2	2.08	0.83
2:B:292:ILE:HD13	2:B:297:LEU:HD12	1.65	0.79
2:B:165:ASN:OD1	2:B:168:LYS:HE3	1.82	0.79
2:B:294:GLU:O	2:B:295:GLU:CG	2.30	0.79
2:B:290:CYS:O	2:B:291:ILE:HG22	1.83	0.78
2:B:294:GLU:C	2:B:295:GLU:CG	2.54	0.75
2:B:209:LYS:CA	2:B:210:GLN:CB	2.63	0.75
4:B:602:NAG:O3	4:B:602:NAG:C8	2.30	0.74
1:A:105:ASN:O	1:A:106:ARG:HB2	1.88	0.74
2:B:209:LYS:CB	2:B:210:GLN:HB3	2.17	0.74
2:B:292:ILE:HD11	2:B:297:LEU:CD1	2.14	0.73
2:B:482:VAL:HG13	2:B:482:VAL:O	1.88	0.73
4:B:602:NAG:C3	4:B:602:NAG:C8	2.62	0.72
2:B:452:VAL:O	2:B:455:THR:CG2	2.36	0.71
2:B:137:PHE:N	3:B:601:SO4:O1	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:CYS:C	2:B:291:ILE:CG2	2.61	0.69
2:B:181:LEU:O	2:B:184:GLY:N	2.24	0.69
2:B:181:LEU:HD13	2:B:185:VAL:O	1.93	0.68
2:B:290:CYS:O	2:B:291:ILE:CG2	2.41	0.68
4:B:602:NAG:H83	4:B:602:NAG:H3	1.76	0.66
1:A:64:ILE:HD12	1:A:87:LYS:HE2	1.78	0.66
2:B:290:CYS:C	2:B:291:ILE:HG23	2.15	0.66
2:B:161:GLU:N	2:B:162:GLY:HA2	2.12	0.65
1:A:63:ASN:O	1:A:63:ASN:ND2	2.30	0.64
2:B:432:ILE:HD11	2:B:447:VAL:HG22	1.78	0.64
1:A:35:SER:HB2	2:B:474:ILE:HD13	1.79	0.63
2:B:209:LYS:HB3	2:B:211:SER:H	1.64	0.63
1:A:65:LYS:O	1:A:67:ASN:N	2.35	0.59
2:B:361:GLN:C	2:B:362:SER:OG	2.42	0.57
2:B:482:VAL:O	2:B:482:VAL:CG1	2.54	0.56
2:B:209:LYS:HA	2:B:210:GLN:HE21	1.71	0.56
4:B:602:NAG:C8	4:B:602:NAG:H3	2.33	0.56
2:B:293:LYS:O	3:B:605:SO4:O4	2.25	0.55
2:B:422:CYS:SG	2:B:452:VAL:HG13	2.47	0.54
1:A:69:CYS:SG	1:A:71:GLY:N	2.79	0.54
2:B:294:GLU:HA	3:B:605:SO4:O2	2.08	0.54
2:B:290:CYS:SG	2:B:300:VAL:CG2	2.84	0.53
2:B:292:ILE:O	2:B:292:ILE:CG2	2.47	0.52
2:B:294:GLU:O	2:B:295:GLU:CD	2.47	0.52
1:A:102:ALA:CB	1:A:103:THR:CA	2.83	0.52
2:B:159:HIS:CE1	2:B:291:ILE:HG22	2.41	0.52
1:A:56:VAL:HG23	2:B:187:VAL:HG11	1.93	0.51
2:B:325:ASN:H	2:B:331:ASN:HD21	1.59	0.51
2:B:161:GLU:N	2:B:162:GLY:CA	2.73	0.51
1:A:105:ASN:O	1:A:106:ARG:CB	2.56	0.50
2:B:481:LEU:O	2:B:482:VAL:HB	2.11	0.50
1:A:63:ASN:O	1:A:63:ASN:CG	2.49	0.50
1:A:50:THR:HB	2:B:307:GLY:H	1.77	0.50
2:B:292:ILE:O	2:B:293:LYS:O	2.30	0.50
2:B:352:PHE:CE2	2:B:372:SER:HB3	2.47	0.50
2:B:294:GLU:O	2:B:295:GLU:OE2	2.30	0.49
1:A:50:THR:HG22	1:A:51:GLY:N	2.27	0.49
2:B:292:ILE:HA	2:B:296:VAL:O	2.11	0.49
2:B:209:LYS:HB3	2:B:211:SER:N	2.26	0.49
2:B:338:ASP:HB2	2:B:342:TYR:OH	2.12	0.49
2:B:171:LEU:HD21	2:B:189:THR:HB	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:O	1:A:66:GLU:C	2.50	0.49
1:A:67:ASN:HB2	2:B:207:LEU:HD23	1.94	0.49
1:A:48:LEU:HD22	2:B:367:CYS:HB2	1.96	0.48
1:A:64:ILE:O	1:A:87:LYS:NZ	2.31	0.47
2:B:181:LEU:HD12	2:B:181:LEU:N	2.29	0.47
2:B:217:ILE:HA	2:B:220:VAL:HG13	1.97	0.47
1:A:93:LEU:HD13	2:B:297:LEU:HD11	1.97	0.47
1:A:70:ASN:O	1:A:71:GLY:C	2.53	0.47
1:A:98:GLN:HA	1:A:99:SER:HA	1.65	0.46
2:B:481:LEU:O	2:B:482:VAL:CB	2.64	0.46
2:B:232:GLU:HG2	2:B:250:TYR:CZ	2.52	0.45
1:A:37:CYS:SG	2:B:319:SER:HB3	2.57	0.45
2:B:361:GLN:O	2:B:364:ARG:N	2.49	0.45
1:A:79:ILE:HG13	2:B:220:VAL:HG12	1.99	0.45
2:B:231:LEU:HA	2:B:234:THR:HG22	2.01	0.43
1:A:61:LEU:HB2	1:A:86:TYR:OH	2.17	0.42
2:B:484:PRO:HB2	2:B:487:GLU:OE2	2.19	0.42
1:A:106:ARG:HA	1:A:106:ARG:HD2	1.57	0.42
1:A:27:ASN:HD22	1:A:27:ASN:HA	1.68	0.42
2:B:181:LEU:C	2:B:184:GLY:H	2.19	0.42
2:B:447:VAL:O	2:B:461:LYS:HE3	2.20	0.41
2:B:209:LYS:HA	2:B:210:GLN:NE2	2.35	0.41
2:B:364:ARG:HG2	2:B:366:PHE:CE1	2.55	0.41
2:B:197:ASN:O	2:B:201:LYS:HB2	2.21	0.41
2:B:405:SER:HB2	2:B:452:VAL:HG21	2.02	0.41
1:A:65:LYS:CB	1:A:65:LYS:NZ	2.83	0.41
1:A:65:LYS:HB3	1:A:65:LYS:HZ3	1.86	0.40
1:A:58:THR:HA	2:B:297:LEU:O	2.21	0.40
2:B:158:LEU:HD12	2:B:158:LEU:HA	1.93	0.40
2:B:382:CYS:HG	2:B:393:CYS:CB	2.28	0.40
4:B:602:NAG:O3	4:B:602:NAG:C7	2.68	0.40
1:A:79:ILE:CD1	2:B:220:VAL:HG12	2.52	0.40
1:A:64:ILE:H	1:A:64:ILE:HG13	1.38	0.40
1:A:93:LEU:HD13	2:B:297:LEU:CD1	2.50	0.40
2:B:362:SER:HB2	2:B:363:ASN:H	1.49	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	80/82 (98%)	69 (86%)	7 (9%)	4 (5%)	2 12
2	B	371/414 (90%)	343 (92%)	20 (5%)	8 (2%)	6 31
All	All	451/496 (91%)	412 (91%)	27 (6%)	12 (3%)	5 26

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	GLY
1	A	102	ALA
1	A	106	ARG
2	B	138	LEU
2	B	193	LEU
2	B	210	GLN
2	B	293	LYS
2	B	482	VAL
1	A	66	GLU
2	B	401	ASP
2	B	355	ALA
2	B	241	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%)	60 (82%)	13 (18%)	2 9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	341/373 (91%)	298 (87%)	43 (13%)	4 20
All	All	414/446 (93%)	358 (86%)	56 (14%)	4 17

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	49	ARG
1	A	62	SER
1	A	64	ILE
1	A	65	LYS
1	A	69	CYS
1	A	77	LYS
1	A	87	LYS
1	A	91	THR
1	A	92	GLU
1	A	95	LEU
1	A	98	GLN
1	A	106	ARG
2	B	138	LEU
2	B	144	VAL
2	B	158	LEU
2	B	167	ILE
2	B	168	LYS
2	B	169	SER
2	B	176	LYS
2	B	183	ASN
2	B	190	PHE
2	B	204	LEU
2	B	210	GLN
2	B	212	CYS
2	B	214	ILE
2	B	216	ASN
2	B	225	GLN
2	B	239	VAL
2	B	249	THR
2	B	267	THR
2	B	268	ASN
2	B	278	VAL
2	B	295	GLU
2	B	297	LEU
2	B	339	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	345	ASN
2	B	356	GLU
2	B	359	LYS
2	B	362	SER
2	B	370	MET
2	B	374	THR
2	B	381	LEU
2	B	394	LYS
2	B	423	THR
2	B	428	ASN
2	B	436	SER
2	B	449	THR
2	B	455	THR
2	B	456	LEU
2	B	461	LYS
2	B	467	LEU
2	B	474	ILE
2	B	481	LEU
2	B	482	VAL
2	B	487	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	63	ASN
1	A	88	ASN
2	B	210	GLN
2	B	224	GLN
2	B	240	ASN
2	B	276	ASN
2	B	331	ASN
2	B	345	ASN
2	B	354	GLN
2	B	437	ASN
2	B	496	ASN

5.3.3 RNA

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)

6 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	SO4	B	605	-	4,4,4	0.15	0	6,6,6	0.17	0
3	SO4	B	601	-	4,4,4	0.43	0	6,6,6	3.61	3 (50%)
3	SO4	B	603	-	4,4,4	0.16	0	6,6,6	0.23	0
5	PO4	B	606	-	4,4,4	1.21	1 (25%)	6,6,6	0.48	0
4	NAG	B	602	2	14,14,15	0.29	0	17,19,21	0.62	0
3	SO4	B	604	-	4,4,4	0.16	0	6,6,6	0.08	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
4	NAG	B	602	2	-	6/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	606	PO4	P-O1	2.26	1.56	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	SO4	O4-S-O3	-5.39	86.04	109.06
3	B	601	SO4	O4-S-O2	-4.46	86.05	109.31
3	B	601	SO4	O4-S-O1	-4.45	86.09	109.31

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	602	NAG	C3-C2-N2-C7
4	B	602	NAG	C8-C7-N2-C2
4	B	602	NAG	O7-C7-N2-C2
4	B	602	NAG	C4-C5-C6-O6
4	B	602	NAG	O5-C5-C6-O6
4	B	602	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	605	SO4	2	0
3	B	601	SO4	1	0
4	B	602	NAG	8	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

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	A	82/82 (100%)	0.11	9 (10%)	5	2	35, 81, 158, 171	0
2	B	373/414 (90%)	-0.42	13 (3%)	44	18	33, 63, 134, 180	0
All	All	455/496 (91%)	-0.32	22 (4%)	30	11	33, 67, 142, 180	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	208	ASN	5.4
1	A	68	LYS	5.3
2	B	210	GLN	5.3
1	A	70	ASN	4.8
1	A	69	CYS	4.5
2	B	509	SER	4.4
2	B	326	THR	4.1
2	B	505	PHE	4.0
1	A	71	GLY	3.8
2	B	173	SER	3.5
2	B	508	LYS	3.4
2	B	328	GLU	3.2
2	B	174	THR	3.0
2	B	209	LYS	2.8
2	B	213	SER	2.7
1	A	66	GLU	2.6
1	A	72	THR	2.5
2	B	507	ARG	2.4
2	B	506	ILE	2.4
1	A	67	ASN	2.2
1	A	65	LYS	2.1
1	A	26	GLN	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
5	PO4	B	606	5/5	0.28	0.67	298,298,298,299	0
4	NAG	B	602	14/15	0.38	0.55	141,146,147,148	0
3	SO4	B	601	5/5	0.48	0.59	233,233,234,234	0
3	SO4	B	605	5/5	0.76	0.26	163,163,164,165	0
3	SO4	B	604	5/5	0.85	0.19	170,170,171,171	0
3	SO4	B	603	5/5	0.93	0.31	102,105,106,107	0

6.5 Other polymers (i)

There are no such residues in this entry.