Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 11:19 AM EDT

PDB ID	:	6WS6
Title	:	Structural and functional analysis of a potent sarbecovirus neutralizing antibody
Authors	:	Pinto, D.; Park, Y.J.; Beltramello, M.; Walls, A.C.; Tortorici, M.A.; Bianchi, S.; Jaconi, S.; Culap, K.; Zatta, F.; Marco, A.D.; Peter, A.; Guarino, B.; Spreafico, R.; Cameroni, E.; Case, J.B.; Chen, R.E.; Havenar-Daughton, C.; Snell, G.; Telenti, A.; Virgin, H.W.; Lanzavecchia, A.; Diamond, M.S.; Fink, K.; Veesler, D.; Corti, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2020-04-30
Resolution	:	3.30 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

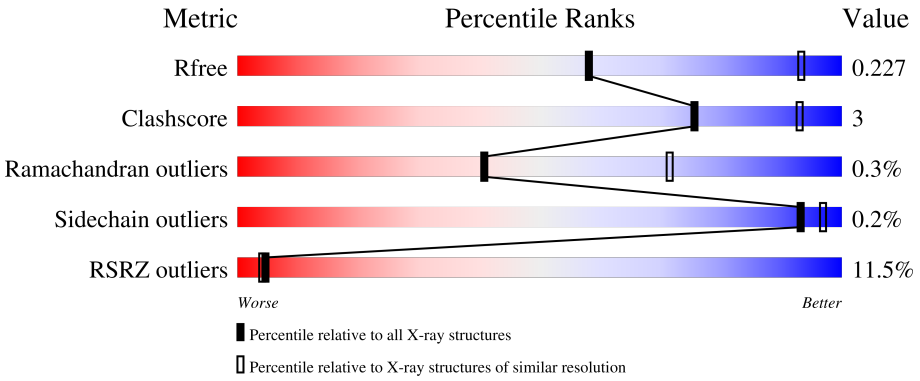
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	230	5% 88% 11%
1	C	230	29% 82% 10% 8%

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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

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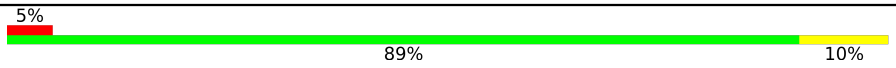
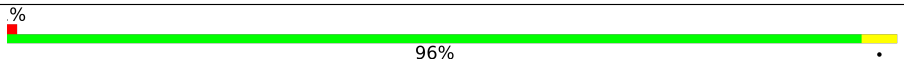
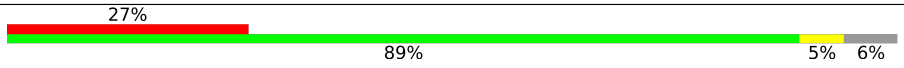
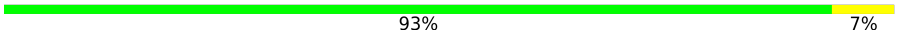
Mol	Chain	Length	Quality of chain
1	E	230	
2	B	214	
2	D	214	
2	F	214	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9671 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.

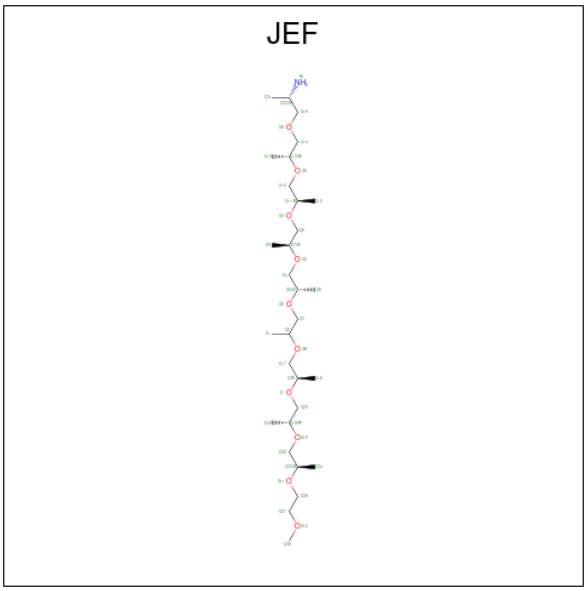
- Molecule 1 is a protein called S309 antigen-binding (Fab) fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1713	1078	289	339	7			
1	C	212	Total	C	N	O	S	0	0	0
			1534	965	261	301	7			
1	E	229	Total	C	N	O	S	0	0	0
			1710	1076	290	337	7			

- Molecule 2 is a protein called S309 antigen-binding (Fab) fragment, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1616	1005	275	332	4			
2	D	201	Total	C	N	O	S	0	0	0
			1441	890	247	300	4			
2	F	213	Total	C	N	O	S	0	0	0
			1616	1005	275	332	4			

- Molecule 3 is O-(O-(2-AMINOPROPYL)-O'-(2-METHOXYETHYL)POLYPROPYLENE GLYCOL 500) (three-letter code: JEF) (formula: $C_{30}H_{63}NO_{10}$).



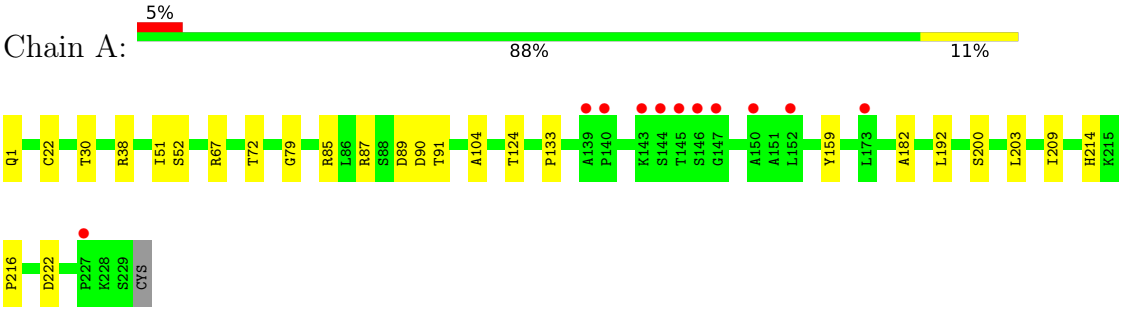
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	41	30	1	10	0	0

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.

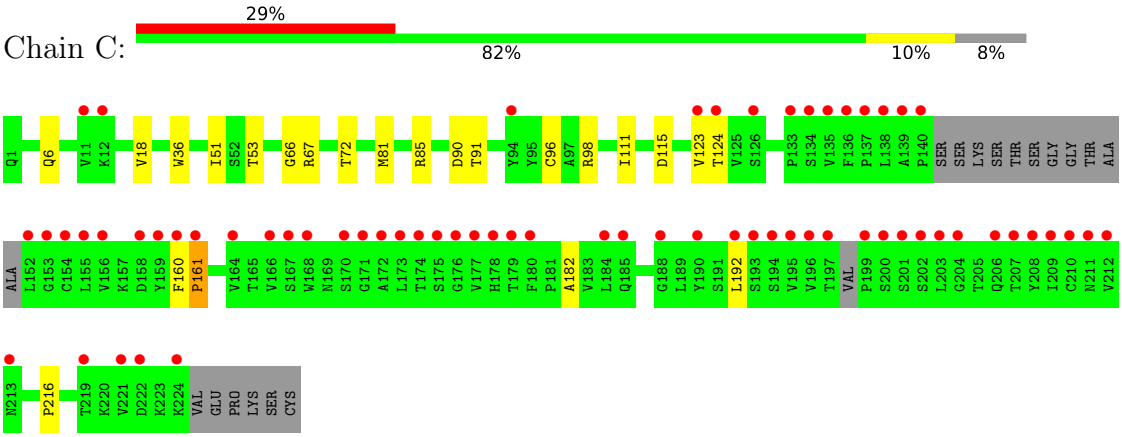
• Molecule 1: S309 antigen-binding (Fab) fragment, heavy chain

Chain A:



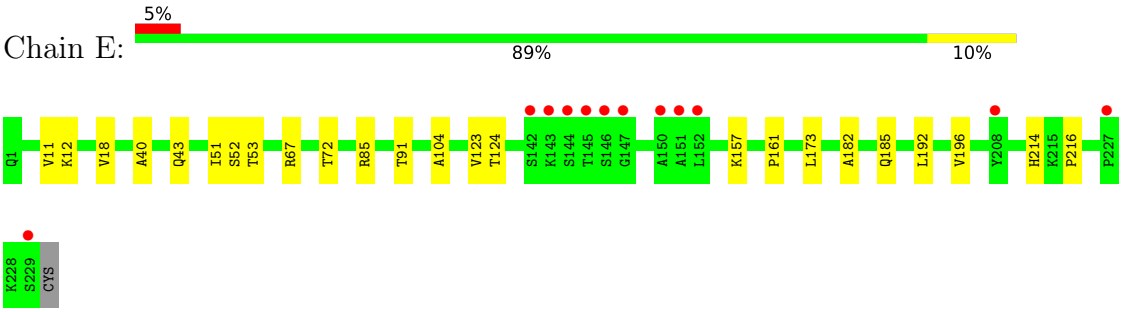
• Molecule 1: S309 antigen-binding (Fab) fragment, heavy chain

Chain C:



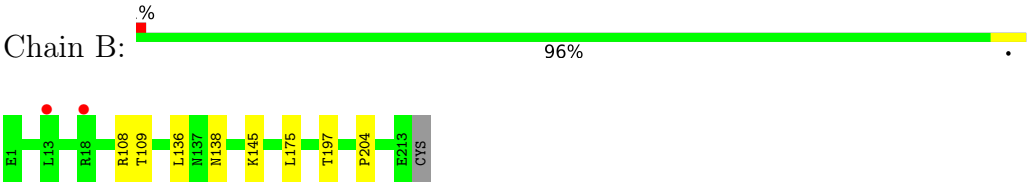
• Molecule 1: S309 antigen-binding (Fab) fragment, heavy chain

Chain E:



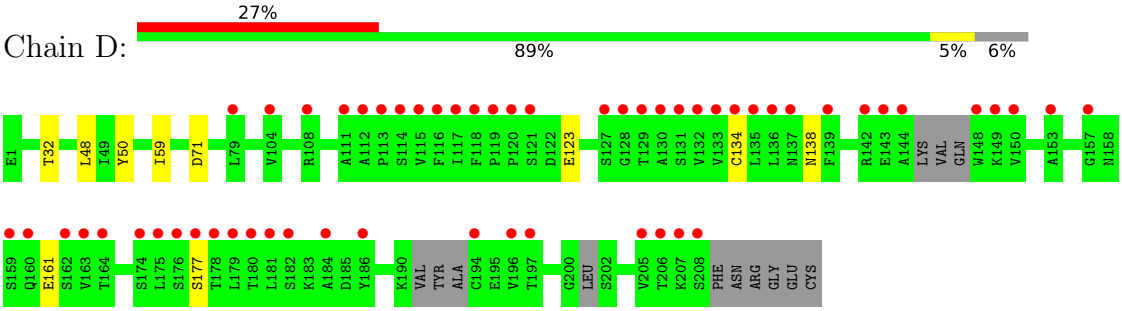
• Molecule 2: S309 antigen-binding (Fab) fragment, light chain

Chain B:



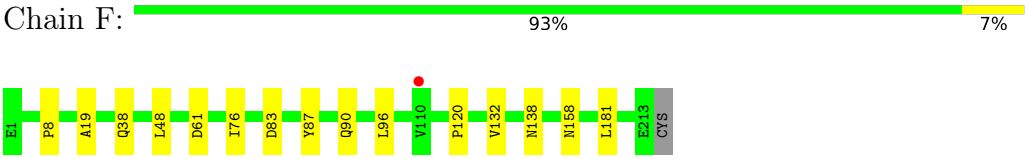
• Molecule 2: S309 antigen-binding (Fab) fragment, light chain

Chain D:



• Molecule 2: S309 antigen-binding (Fab) fragment, light chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	132.59Å 132.59Å 301.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.76 – 3.30 93.76 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (93.76-3.30) 100.0 (93.76-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.18rc4-3812	Depositor
R, R_{free}	0.188 , 0.227 0.188 , 0.227	Depositor DCC
R_{free} test set	2073 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	75.2	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9671	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: JEF

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	0.25	0/1756	0.45	0/2395
1	C	0.24	0/1573	0.45	0/2153
1	E	0.24	0/1753	0.44	0/2390
2	B	0.24	0/1649	0.44	0/2242
2	D	0.24	0/1467	0.43	0/2002
2	F	0.24	0/1649	0.43	0/2242
All	All	0.24	0/9847	0.44	0/13424

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

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	1713	0	1656	15	0
1	C	1534	0	1380	14	0
1	E	1710	0	1654	15	0
2	B	1616	0	1560	4	0
2	D	1441	0	1298	5	0
2	F	1616	0	1560	8	0
3	A	41	0	63	1	0
All	All	9671	0	9171	58	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 3.

All (58) 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:F:90:GLN:HE21	2:F:96:LEU:HD21	1.57	0.68
1:A:209:ILE:HD11	1:A:222:ASP:HB3	1.79	0.65
1:E:11:VAL:HG21	1:E:161:PRO:HG3	1.79	0.64
1:C:182:ALA:HB2	1:C:192:LEU:HD23	1.79	0.64
1:A:182:ALA:HB2	1:A:192:LEU:HD23	1.79	0.64
2:F:120:PRO:HD3	2:F:132:VAL:HG22	1.84	0.59
1:E:182:ALA:HB2	1:E:192:LEU:HD23	1.86	0.57
1:E:52:SER:OG	1:E:104:ALA:O	2.21	0.56
1:C:182:ALA:HA	1:C:192:LEU:HB3	1.89	0.54
1:C:53:THR:HG22	1:C:72:THR:HG21	1.89	0.54
1:E:91:THR:HG23	1:E:124:THR:HA	1.90	0.53
1:E:51:ILE:HD13	1:E:72:THR:HG23	1.90	0.53
1:A:91:THR:HG23	1:A:124:THR:HA	1.89	0.53
1:A:51:ILE:HD13	1:A:72:THR:HG23	1.92	0.52
2:F:19:ALA:HB3	2:F:76:ILE:HB	1.91	0.51
2:D:48:LEU:HD12	2:D:59:ILE:HD12	1.92	0.50
1:C:67:ARG:NH2	1:C:90:ASP:OD2	2.41	0.49
1:E:12:LYS:HG3	1:E:18:VAL:HB	1.94	0.49
1:A:1:GLN:HG3	2:D:50:TYR:CZ	2.48	0.49
1:E:18:VAL:HG11	1:E:123:VAL:HG11	1.95	0.48
2:B:136:LEU:HB2	2:B:175:LEU:HB3	1.96	0.48
1:C:98:ARG:NH2	1:C:115:ASP:OD2	2.42	0.48
1:A:182:ALA:HA	1:A:192:LEU:HB3	1.95	0.48
1:A:200:SER:HA	1:A:203:LEU:HD13	1.95	0.47
1:C:66:GLY:O	1:C:85:ARG:NH2	2.44	0.47
1:C:91:THR:HG23	1:C:124:THR:HA	1.96	0.47
1:C:51:ILE:HD13	1:C:72:THR:HG23	1.97	0.47
1:E:182:ALA:HA	1:E:192:LEU:HB3	1.97	0.47
1:A:30:THR:HG21	3:A:401:JEF:H201	1.96	0.47
1:C:6:GLN:OE1	1:C:96:CYS:N	2.47	0.47
2:F:38:GLN:HB2	2:F:48:LEU:HD11	1.98	0.46
2:D:161:GLU:HA	2:D:177:SER:HA	1.96	0.46
1:E:214:HIS:CD2	1:E:216:PRO:HD2	2.51	0.46
1:A:87:ARG:NH2	1:A:89:ASP:OD2	2.47	0.45
1:A:67:ARG:HG2	1:A:85:ARG:NH2	2.33	0.44
1:E:173:LEU:HD21	1:E:196:VAL:HG11	1.99	0.44
2:B:108:ARG:HG2	2:B:109:THR:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:123:GLU:OE2	2:D:123:GLU:N	2.46	0.44
2:B:145:LYS:HB3	2:B:197:THR:HB	2.01	0.43
2:F:158:ASN:HD22	2:F:181:LEU:HD21	1.83	0.43
1:E:53:THR:HG22	1:E:72:THR:HG21	1.99	0.43
1:C:36:TRP:CE2	1:C:81:MET:HB2	2.53	0.43
2:B:204:PRO:HG2	2:F:8:PRO:HB2	2.01	0.42
1:E:67:ARG:HG2	1:E:85:ARG:HH21	1.84	0.42
1:C:18:VAL:HG11	1:C:123:VAL:HG11	2.00	0.42
1:A:38:ARG:NH1	1:A:90:ASP:OD2	2.48	0.42
1:C:161:PRO:HD2	1:C:216:PRO:HG2	2.02	0.42
1:E:157:LYS:NZ	1:E:185:GLN:OE1	2.53	0.42
1:E:67:ARG:HG2	1:E:85:ARG:NH2	2.34	0.41
1:A:22:CYS:N	1:A:79:GLY:O	2.54	0.41
1:C:111:ILE:HG12	2:D:32:THR:HB	2.03	0.41
1:C:160:PHE:HA	1:C:161:PRO:HA	1.76	0.41
1:E:40:ALA:HB3	1:E:43:GLN:HB2	2.01	0.41
2:F:61:ASP:OD1	2:F:61:ASP:N	2.53	0.41
1:A:52:SER:OG	1:A:104:ALA:O	2.30	0.41
2:F:83:ASP:O	2:F:87:TYR:OH	2.23	0.40
1:A:133:PRO:HB3	1:A:159:TYR:HB3	2.02	0.40
1:A:214:HIS:CD2	1:A:216:PRO:HD2	2.57	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	227/230 (99%)	218 (96%)	9 (4%)	0	100 100
1	C	206/230 (90%)	195 (95%)	10 (5%)	1 (0%)	29 61
1	E	227/230 (99%)	218 (96%)	9 (4%)	0	100 100
2	B	211/214 (99%)	201 (95%)	9 (4%)	1 (0%)	29 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	193/214 (90%)	183 (95%)	9 (5%)	1 (0%)	29 61
2	F	211/214 (99%)	200 (95%)	10 (5%)	1 (0%)	29 61
All	All	1275/1332 (96%)	1215 (95%)	56 (4%)	4 (0%)	41 71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	138	ASN
2	F	138	ASN
2	B	138	ASN
1	C	161	PRO

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	189/192 (98%)	189 (100%)	0	100 100
1	C	153/192 (80%)	153 (100%)	0	100 100
1	E	188/192 (98%)	188 (100%)	0	100 100
2	B	182/185 (98%)	182 (100%)	0	100 100
2	D	148/185 (80%)	146 (99%)	2 (1%)	67 82
2	F	182/185 (98%)	182 (100%)	0	100 100
All	All	1042/1131 (92%)	1040 (100%)	2 (0%)	93 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	71	ASP
2	D	134	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

1 ligand is 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	JEF	A	401	-	32,40,40	3.16	19 (59%)	40,48,48	1.83	11 (27%)

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	JEF	A	401	-	-	18/46/46/46	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	JEF	O-C20	5.46	1.53	1.43
3	A	401	JEF	C32-C33	5.09	1.62	1.50
3	A	401	JEF	O2-C3	4.93	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	JEF	C4-C5	4.91	1.62	1.50
3	A	401	JEF	C14-C13	4.73	1.61	1.50
3	A	401	JEF	C17-C	4.68	1.61	1.50
3	A	401	JEF	C10-C11	4.47	1.61	1.50
3	A	401	JEF	C16-C30	4.19	1.60	1.51
3	A	401	JEF	O4-C8	4.13	1.51	1.43
3	A	401	JEF	C20-C19	4.11	1.60	1.50
3	A	401	JEF	C8-C7	4.09	1.60	1.50
3	A	401	JEF	OH-C17	3.76	1.50	1.43
3	A	401	JEF	C3-C2	3.72	1.59	1.50
3	A	401	JEF	O5-C10	3.60	1.50	1.43
3	A	401	JEF	O6-C16	3.00	1.50	1.42
3	A	401	JEF	O11-C36	2.24	1.49	1.43
3	A	401	JEF	O3-C4	2.23	1.47	1.43
3	A	401	JEF	C36-C37	2.21	1.60	1.49
3	A	401	JEF	O6-C14	2.05	1.47	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	JEF	O4-C8-C7	-3.44	102.59	110.90
3	A	401	JEF	C4-O3-C7	-3.28	110.14	115.02
3	A	401	JEF	C17-OH-C2	-3.21	110.23	115.02
3	A	401	JEF	O-C20-C19	-3.14	103.32	110.90
3	A	401	JEF	O2-C3-C2	-2.97	103.73	110.90
3	A	401	JEF	C20-O-C	-2.90	110.70	115.02
3	A	401	JEF	C8-O4-C11	-2.67	111.04	115.02
3	A	401	JEF	C3-O2-C5	-2.54	111.24	115.02
3	A	401	JEF	O10-C19-C20	-2.38	101.31	108.89
3	A	401	JEF	C32-O10-C19	-2.19	111.75	115.02
3	A	401	JEF	O5-C10-C11	-2.19	105.62	110.90

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	JEF	O10-C19-C20-O
3	A	401	JEF	C40-C19-C20-O
3	A	401	JEF	O-C-C17-OH
3	A	401	JEF	C18-C-C17-OH
3	A	401	JEF	OH-C2-C3-O2
3	A	401	JEF	C1-C2-C3-O2

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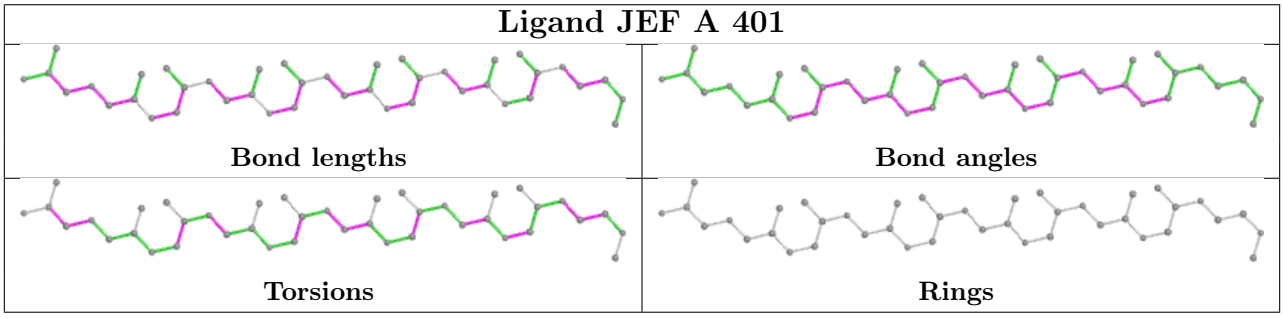
Mol	Chain	Res	Type	Atoms
3	A	401	JEF	O3-C4-C5-O2
3	A	401	JEF	O5-C10-C11-C12
3	A	401	JEF	O6-C16-C30-C31
3	A	401	JEF	O6-C16-C30-N1
3	A	401	JEF	C30-C16-O6-C14
3	A	401	JEF	C33-C32-O10-C19
3	A	401	JEF	C7-C8-O4-C11
3	A	401	JEF	O3-C4-C5-C6
3	A	401	JEF	O5-C10-C11-O4
3	A	401	JEF	C2-C3-O2-C5
3	A	401	JEF	C37-C36-O11-C33
3	A	401	JEF	O11-C36-C37-O12

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	JEF	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	229/230 (99%)	0.66	11 (4%) 30 28	41, 61, 100, 176	0
1	C	212/230 (92%)	1.45	66 (31%) 0 0	45, 103, 155, 172	0
1	E	229/230 (99%)	0.69	12 (5%) 27 25	45, 62, 116, 150	0
2	B	213/214 (99%)	0.71	2 (0%) 84 84	44, 62, 87, 104	0
2	D	201/214 (93%)	1.39	57 (28%) 0 0	54, 107, 165, 218	0
2	F	213/214 (99%)	0.61	1 (0%) 91 91	49, 64, 84, 111	0
All	All	1297/1332 (97%)	0.91	149 (11%) 4 4	41, 68, 146, 218	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	144	ALA	6.4
1	C	137	PRO	6.3
2	D	135	LEU	6.3
1	C	195	VAL	5.9
1	C	139	ALA	5.8
1	C	152	LEU	5.7
1	A	146	SER	5.7
1	C	197	THR	5.4
2	D	136	LEU	5.2
2	D	134	CYS	5.0
1	C	194	SER	4.9
1	C	188	GLY	4.9
1	C	140	PRO	4.8
1	C	136	PHE	4.8
1	C	174	THR	4.7
1	A	144	SER	4.6
1	C	168	TRP	4.5
2	D	116	PHE	4.5
1	C	153	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
2	D	114	SER	4.4
2	D	196	VAL	4.4
1	C	154	CYS	4.3
1	C	204	GLY	4.2
2	D	133	VAL	4.2
1	C	207	THR	4.1
2	D	118	PHE	4.0
1	C	196	VAL	4.0
2	D	148	TRP	3.9
1	C	212	VAL	3.9
1	C	156	VAL	3.9
1	A	145	THR	3.9
2	D	119	PRO	3.7
1	C	161	PRO	3.7
2	D	181	LEU	3.6
2	D	175	LEU	3.6
2	D	163	VAL	3.6
2	D	197	THR	3.5
1	C	192	LEU	3.5
1	A	147	GLY	3.5
1	C	221	VAL	3.5
1	E	144	SER	3.5
1	C	208	TYR	3.5
1	C	135	VAL	3.5
1	E	147	GLY	3.4
1	C	210	CYS	3.4
2	D	121	SER	3.4
2	D	131	SER	3.4
1	C	178	HIS	3.4
1	C	199	PRO	3.3
1	C	134	SER	3.3
2	D	115	VAL	3.3
1	C	158	ASP	3.2
2	D	177	SER	3.2
2	B	13	LEU	3.1
2	D	164	THR	3.1
1	C	180	PHE	3.1
1	C	160	PHE	3.1
1	C	159	TYR	3.1
1	C	219	THR	3.1
2	D	174	SER	3.1
2	D	120	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	179	LEU	3.0
2	D	142	ARG	3.0
2	D	132	VAL	3.0
1	C	123	VAL	3.0
2	D	113	PRO	3.0
1	C	224	LYS	2.9
2	D	129	THR	2.9
2	D	137	ASN	2.9
1	C	213	ASN	2.9
1	E	146	SER	2.9
2	D	128	GLY	2.9
2	D	162	SER	2.9
2	D	160	GLN	2.9
1	A	150	ALA	2.9
1	C	184	LEU	2.9
1	E	208	TYR	2.9
2	D	180	THR	2.8
1	C	171	GLY	2.8
2	D	149	LYS	2.8
2	D	139	PHE	2.7
1	A	227	PRO	2.7
2	D	206	THR	2.7
2	D	153	ALA	2.7
1	E	143	LYS	2.7
1	C	155	LEU	2.7
2	D	178	THR	2.7
2	D	205	VAL	2.7
2	D	182	SER	2.7
1	C	222	ASP	2.7
1	C	211	ASN	2.6
1	C	124	THR	2.6
2	D	117	ILE	2.6
1	C	170	SER	2.6
1	C	173	LEU	2.6
2	D	111	ALA	2.6
1	E	145	THR	2.6
1	C	126	SER	2.6
2	D	207	LYS	2.6
1	C	209	ILE	2.6
2	D	130	ALA	2.5
2	D	157	GLY	2.5
1	E	150	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	167	SER	2.5
2	D	159	SER	2.5
2	D	104	VAL	2.4
1	C	185	GLN	2.4
2	D	127	SER	2.4
1	C	206	GLN	2.4
2	D	186	TYR	2.4
1	C	202	SER	2.4
1	C	179	THR	2.4
1	C	166	VAL	2.4
1	C	172	ALA	2.4
1	C	193	SER	2.3
1	C	164	VAL	2.3
1	C	200	SER	2.3
2	D	143	GLU	2.3
1	E	151	ALA	2.3
2	D	208	SER	2.3
1	C	11	VAL	2.3
2	D	194	CYS	2.3
1	A	143	LYS	2.3
1	A	140	PRO	2.2
2	D	108	ARG	2.2
1	C	203	LEU	2.2
1	C	177	VAL	2.2
1	C	94	TYR	2.2
1	C	133	PRO	2.2
1	C	190	TYR	2.2
1	E	152	LEU	2.2
2	D	112	ALA	2.2
1	C	176	GLY	2.2
1	C	201	SER	2.1
2	D	176	SER	2.1
1	E	227	PRO	2.1
1	C	138	LEU	2.1
2	D	79	LEU	2.1
1	C	175	SER	2.1
1	E	142	SER	2.1
2	D	184	ALA	2.1
1	C	12	LYS	2.1
1	E	229	SER	2.1
2	D	150	VAL	2.1
1	A	152	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	139	ALA	2.0
2	F	110	VAL	2.0
1	A	173	LEU	2.0
2	B	18	ARG	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)

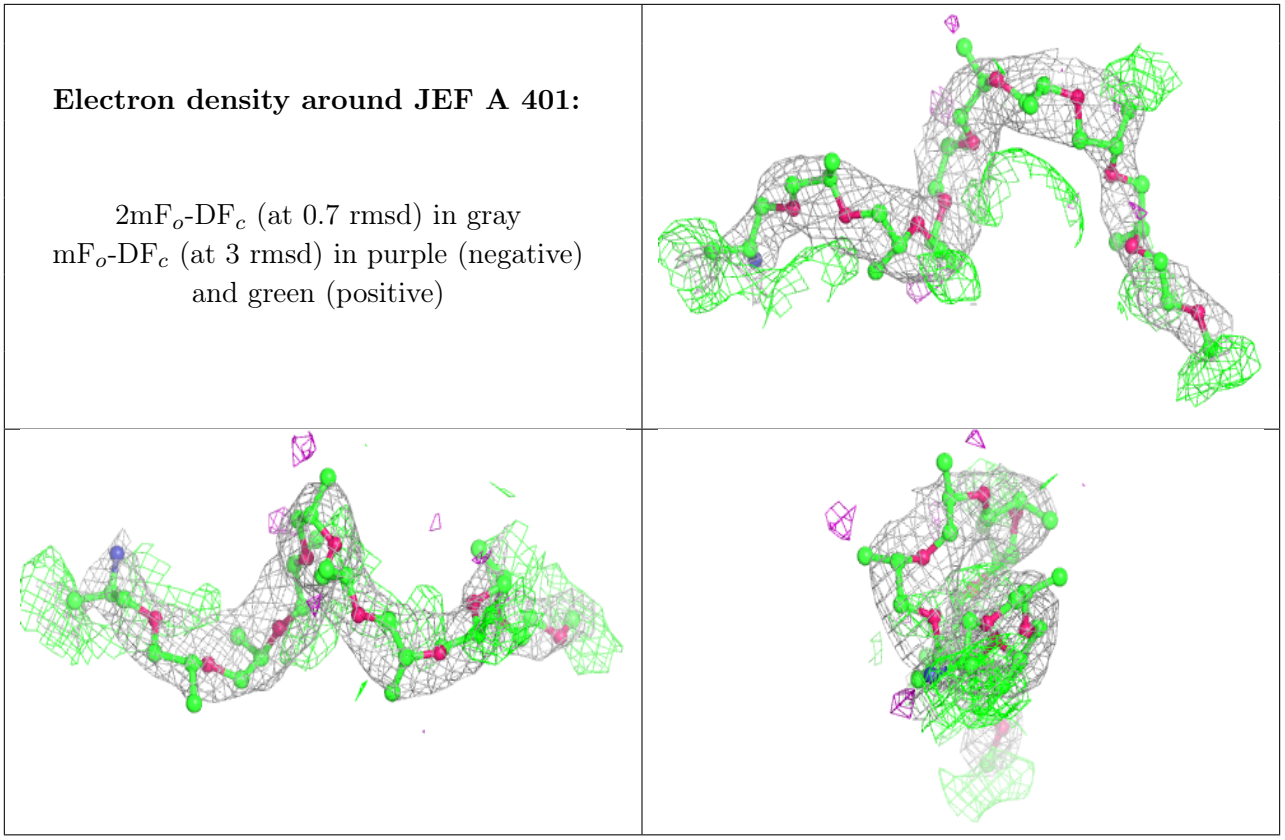
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	JEF	A	401	41/41	0.88	0.40	63,81,109,129	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around JEF A 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.