



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:46 PM UTC

PDB ID : 6WS6 / pdb_00006ws6
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)

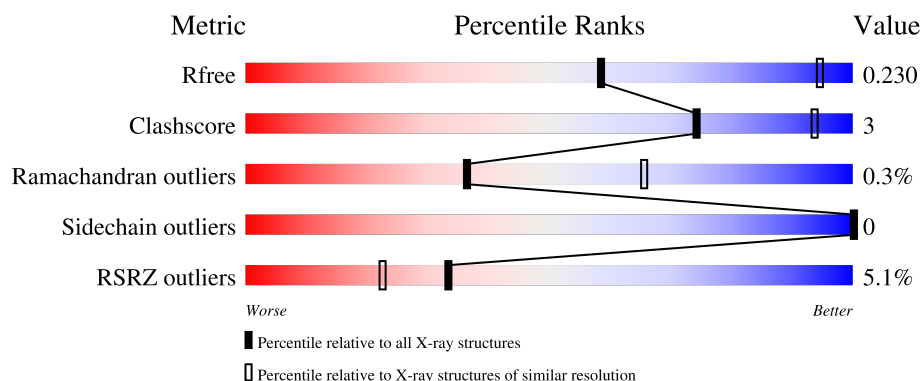
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	230	
1	C	230	

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Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	E	230	% 89% 10%
2	B	214	% 96%
2	D	214	14% 90% 6%
2	F	214	93% 7%

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	JEF	A	401	-	X	-	-

2 Entry composition

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.

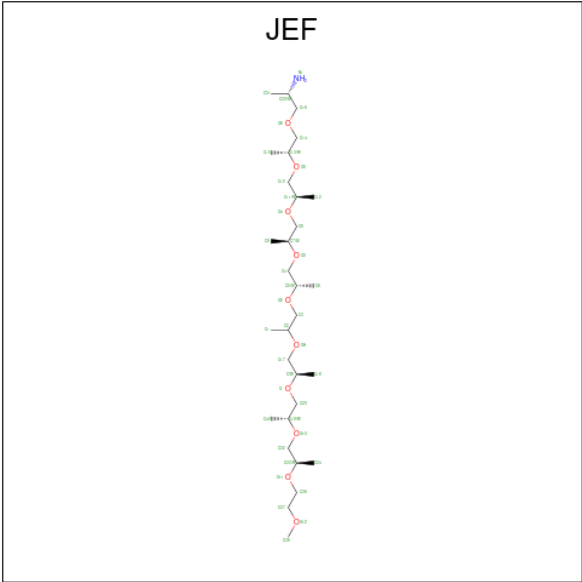
- Molecule 1 is a protein called S309 antigen-binding (Fab) fragment, heavy chain.

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) (CCD ID: JEF) (formula: C₃₀H₆₃NO₁₀).

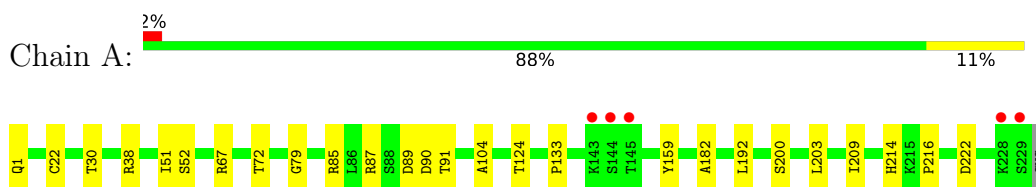


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	41	30	1	10	0	0

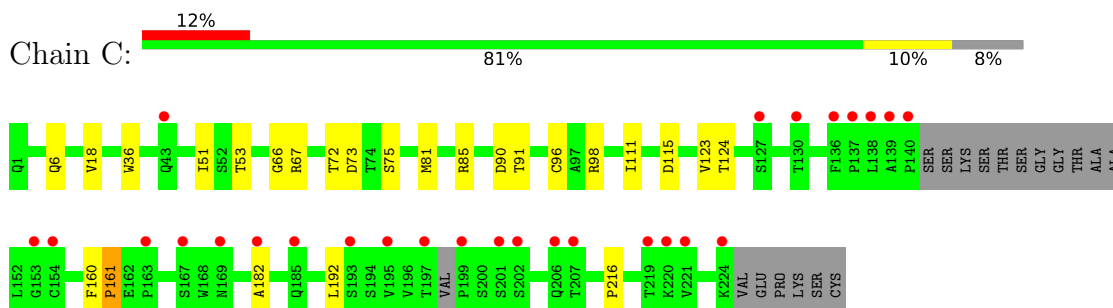
3 Residue-property plots [i](#)

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.

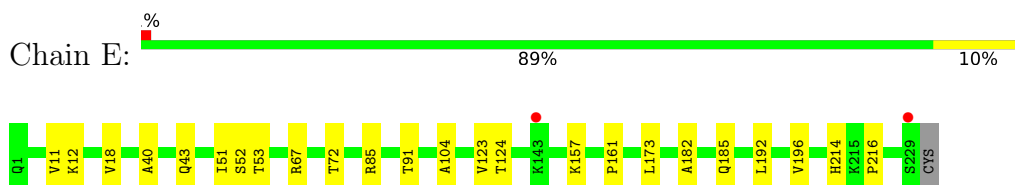
- Molecule 1: S309 antigen-binding (Fab) fragment, heavy chain



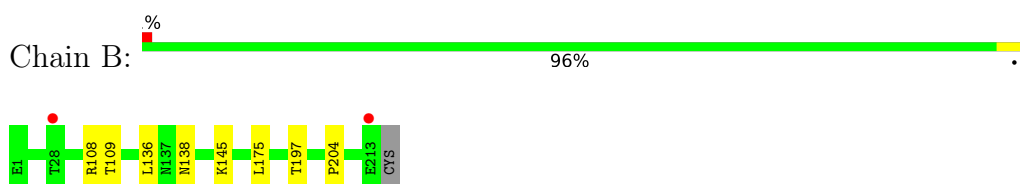
- Molecule 1: S309 antigen-binding (Fab) fragment, heavy chain



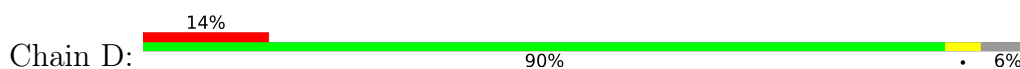
- Molecule 1: S309 antigen-binding (Fab) fragment, heavy chain

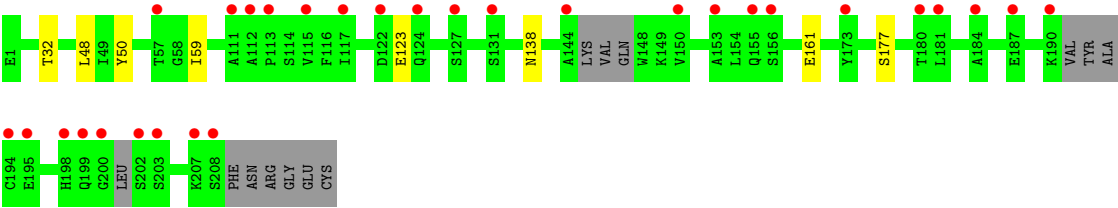


- Molecule 2: S309 antigen-binding (Fab) fragment, light chain

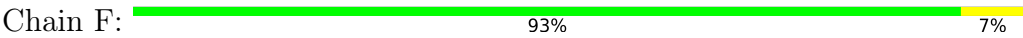


- Molecule 2: S309 antigen-binding (Fab) fragment, light chain





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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.18rc4-3812	Depositor
R, R_{free}	0.188 , 0.227 0.191 , 0.230	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 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.08	0/1756	0.24	0/2395
1	C	0.08	0/1573	0.22	0/2153
1	E	0.08	0/1753	0.23	0/2390
2	B	0.07	0/1649	0.25	0/2242
2	D	0.08	0/1467	0.25	0/2002
2	F	0.07	0/1649	0.24	0/2242
All	All	0.08	0/9847	0.24	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	15	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	59	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 (59) 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:C:73:ASP:OD2	1:C:75:SER:OG	2.34	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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/230 (99%)	218 (96%)	9 (4%)	0	100	100
1	C	206/230 (90%)	195 (95%)	10 (5%)	1 (0%)	24	55
1	E	227/230 (99%)	218 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	211/214 (99%)	201 (95%)	9 (4%)	1 (0%)	24	55
2	D	193/214 (90%)	183 (95%)	9 (5%)	1 (0%)	24	55
2	F	211/214 (99%)	200 (95%)	10 (5%)	1 (0%)	24	55
All	All	1275/1332 (96%)	1215 (95%)	56 (4%)	4 (0%)	36	65

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 ⓘ

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%)	148 (100%)	0	100	100
2	F	182/185 (98%)	182 (100%)	0	100	100
All	All	1042/1131 (92%)	1042 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	HIS
2	B	137	ASN

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Mol	Chain	Res	Type
2	B	189	HIS
1	C	65	GLN
1	C	211	ASN
2	D	138	ASN
2	D	160	GLN
2	D	189	HIS
1	E	178	HIS
2	F	152	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](#)

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	-	40,40,40	3.26	25 (62%)	48,48,48	1.76	14 (29%)

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	-	-	17/46/46/46	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	JEF	O-C20	5.72	1.53	1.43
3	A	401	JEF	C32-C33	5.23	1.62	1.50
3	A	401	JEF	O2-C3	5.16	1.52	1.43
3	A	401	JEF	O10-C19	5.11	1.51	1.44
3	A	401	JEF	C4-C5	5.04	1.62	1.50
3	A	401	JEF	C14-C13	4.85	1.61	1.50
3	A	401	JEF	C17-C	4.81	1.61	1.50
3	A	401	JEF	C10-C11	4.59	1.61	1.50
3	A	401	JEF	O3-C7	4.43	1.50	1.44
3	A	401	JEF	O4-C8	4.33	1.51	1.43
3	A	401	JEF	C16-C30	4.32	1.60	1.51
3	A	401	JEF	C20-C19	4.21	1.60	1.50
3	A	401	JEF	C8-C7	4.20	1.60	1.50
3	A	401	JEF	OH-C17	3.93	1.50	1.43
3	A	401	JEF	C3-C2	3.82	1.59	1.50
3	A	401	JEF	O5-C10	3.76	1.50	1.43
3	A	401	JEF	O4-C11	3.42	1.49	1.44
3	A	401	JEF	O5-C13	3.17	1.48	1.44
3	A	401	JEF	O6-C16	3.02	1.50	1.42
3	A	401	JEF	O11-C33	2.47	1.47	1.44
3	A	401	JEF	O3-C4	2.33	1.47	1.43
3	A	401	JEF	OH-C2	2.33	1.47	1.44
3	A	401	JEF	O11-C36	2.28	1.49	1.43
3	A	401	JEF	C36-C37	2.26	1.60	1.49
3	A	401	JEF	O6-C14	2.07	1.47	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	JEF	O4-C8-C7	-3.38	102.59	110.82
3	A	401	JEF	C4-O3-C7	-3.33	110.14	115.05
3	A	401	JEF	C17-OH-C2	-3.26	110.23	115.05
3	A	401	JEF	O-C20-C19	-3.08	103.32	110.82
3	A	401	JEF	C20-O-C	-2.94	110.70	115.05
3	A	401	JEF	O2-C3-C2	-2.91	103.73	110.82
3	A	401	JEF	C8-O4-C11	-2.71	111.04	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	JEF	C3-O2-C5	-2.58	111.24	115.05
3	A	401	JEF	O3-C7-C9	-2.37	101.64	110.22
3	A	401	JEF	O10-C19-C20	-2.35	101.31	108.90
3	A	401	JEF	C32-O10-C19	-2.23	111.75	115.05
3	A	401	JEF	O5-C10-C11	-2.14	105.62	110.82
3	A	401	JEF	C1-C2-C3	-2.03	106.98	112.69
3	A	401	JEF	C10-O5-C13	-2.01	112.09	115.05

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
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	O10-C19-C20-O
3	A	401	JEF	O5-C10-C11-O4
3	A	401	JEF	C2-C3-O2-C5
3	A	401	JEF	C37-C36-O11-C33

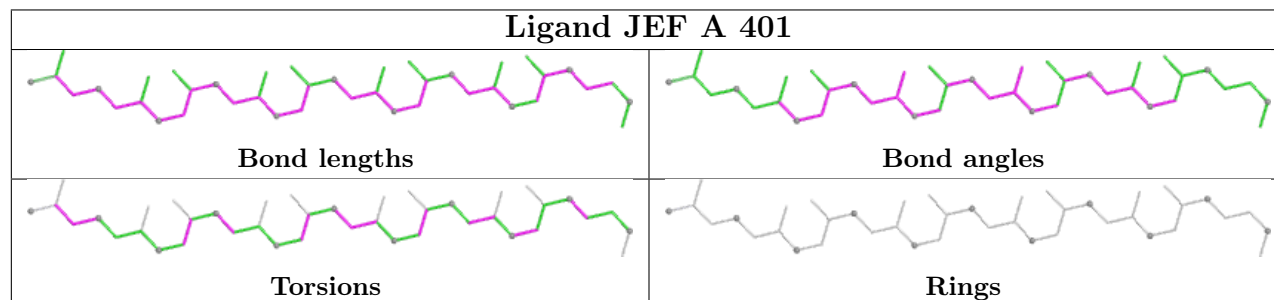
There are no ring outliers.

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 than 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, 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	229/230 (99%)	-0.14	5 (2%) 62 43	41, 61, 100, 176	0
1	C	212/230 (92%)	0.67	27 (12%) 8 6	45, 103, 155, 172	0
1	E	229/230 (99%)	-0.14	2 (0%) 81 65	45, 62, 116, 150	0
2	B	213/214 (99%)	-0.19	2 (0%) 81 65	44, 62, 87, 104	0
2	D	201/214 (93%)	0.78	30 (14%) 5 5	54, 107, 165, 218	0
2	F	213/214 (99%)	-0.27	0 100 100	49, 64, 84, 111	0
All	All	1297/1332 (97%)	0.10	66 (5%) 33 22	41, 68, 146, 218	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	199	PRO	5.9
1	C	140	PRO	5.6
2	D	200	GLY	5.5
1	A	229	SER	4.9
2	D	155	GLN	4.6
1	C	197	THR	3.9
1	C	169	ASN	3.6
2	D	150	VAL	3.6
2	D	187	GLU	3.5
1	C	221	VAL	3.5
1	C	139	ALA	3.5
2	D	181	LEU	3.5
2	D	124	GLN	3.4
2	D	208	SER	3.4
1	C	130	THR	3.3
1	A	143	LYS	3.3
2	D	115	VAL	3.3
2	D	199	GLN	3.3
2	D	131	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	206	GLN	3.2
1	C	207	THR	3.2
1	A	228	LYS	3.1
2	D	194	CYS	3.1
1	C	219	THR	3.0
1	A	145	THR	3.0
1	C	185	GLN	3.0
1	C	136	PHE	2.9
2	D	113	PRO	2.9
1	C	224	LYS	2.9
1	C	153	GLY	2.8
2	D	156	SER	2.8
2	D	184	ALA	2.8
2	D	203	SER	2.8
2	D	207	LYS	2.8
2	D	180	THR	2.8
1	E	229	SER	2.7
2	D	195	GLU	2.7
2	D	122	ASP	2.7
2	D	190	LYS	2.6
1	C	138	LEU	2.5
1	C	193	SER	2.5
2	D	173	TYR	2.5
1	C	154	CYS	2.4
2	D	117	ILE	2.4
2	B	28	THR	2.4
1	C	137	PRO	2.4
1	C	202	SER	2.3
2	D	202	SER	2.3
1	C	43	GLN	2.3
2	D	127	SER	2.3
1	C	220	LYS	2.3
1	A	144	SER	2.2
1	C	163	PRO	2.2
1	E	143	LYS	2.2
2	D	57	THR	2.2
1	C	127	SER	2.2
1	C	182	ALA	2.2
1	C	195	VAL	2.1
2	D	112	ALA	2.1
2	D	144	ALA	2.1
1	C	201	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	213	GLU	2.1
1	C	167	SER	2.1
2	D	198	HIS	2.1
2	D	111	ALA	2.1
2	D	153	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

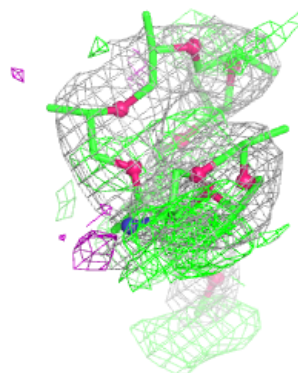
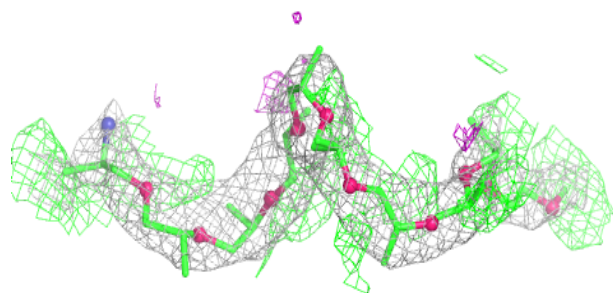
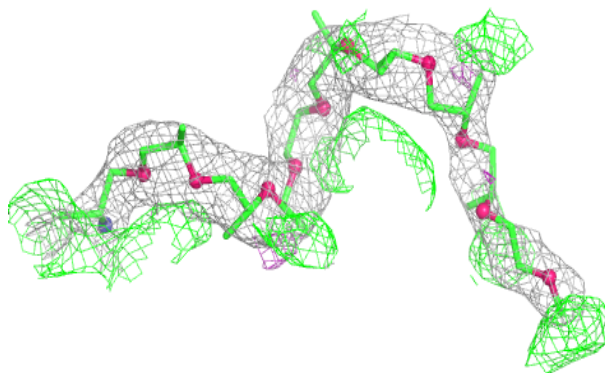
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	JEF	A	401	41/41	0.88	0.24	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.