



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:34 AM UTC

PDB ID : 8YM4 / pdb_00008ym4
Title : Structure of Caspase-8/cFLIP death effector domain assembly
Authors : Lin, S.-C.; Yang, C.-Y.
Deposited on : 2024-03-08
Resolution : 2.34 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
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
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

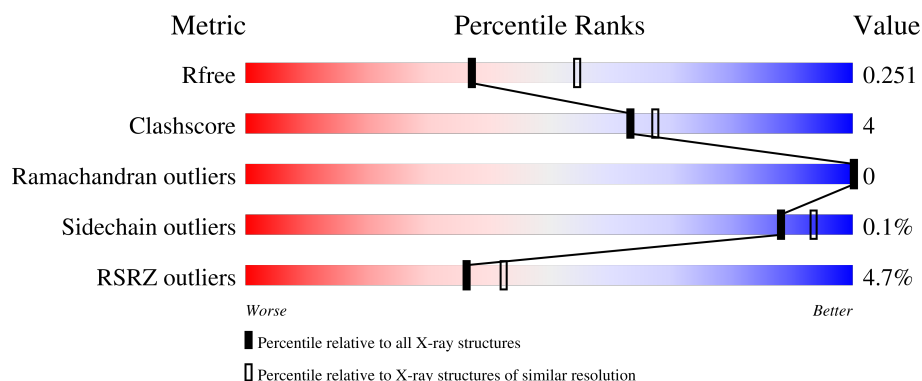
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	185	5% 86% 12%
1	B	185	5% 91% 8%
1	C	185	2% 94% 5%
1	D	185	4% 91% 9%
2	F	184	8% 84% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	184	4% 79% 16% 5%
2	H	184	3% 83% 12% 5%
2	I	184	5% 83% 8% 9%
2	J	184	5% 83% 12% 5%
2	K	184	3% 85% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14567 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 Caspase-8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	184	Total	C	N	O	S	Se	0	0	0
			1528	967	258	294	2	7			
1	B	182	Total	C	N	O	S	Se	0	0	0
			1510	956	255	290	2	7			
1	D	184	Total	C	N	O	S	Se	0	0	0
			1531	968	261	294	2	6			
1	A	182	Total	C	N	O	S	Se	0	0	0
			1510	956	255	290	2	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	122	GLY	PHE	engineered mutation	UNP Q14790
C	123	GLY	LEU	engineered mutation	UNP Q14790
B	122	GLY	PHE	engineered mutation	UNP Q14790
B	123	GLY	LEU	engineered mutation	UNP Q14790
D	122	GLY	PHE	engineered mutation	UNP Q14790
D	123	GLY	LEU	engineered mutation	UNP Q14790
A	122	GLY	PHE	engineered mutation	UNP Q14790
A	123	GLY	LEU	engineered mutation	UNP Q14790

- Molecule 2 is a protein called CASP8 and FADD-like apoptosis regulator subunit p43.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	175	Total	C	N	O	S	Se	0	0	0
			1418	902	245	263	2	6			
2	G	175	Total	C	N	O	S	Se	0	0	0
			1418	902	245	263	2	6			
2	F	169	Total	C	N	O	S	Se	0	0	0
			1373	873	239	254	2	5			
2	K	179	Total	C	N	O	S	Se	0	0	0
			1446	918	252	268	2	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	I	168	Total	C	N	O	S	Se	0	0	0
			1369	871	236	254	2	6			
2	J	174	Total	C	N	O	S	Se	0	0	0
			1412	898	244	262	2	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	GLY	-	expression tag	UNP O15519
H	-1	SER	-	expression tag	UNP O15519
H	0	HIS	-	expression tag	UNP O15519
H	7	GLY	HIS	engineered mutation	UNP O15519
G	-2	GLY	-	expression tag	UNP O15519
G	-1	SER	-	expression tag	UNP O15519
G	0	HIS	-	expression tag	UNP O15519
G	7	GLY	HIS	engineered mutation	UNP O15519
F	-2	GLY	-	expression tag	UNP O15519
F	-1	SER	-	expression tag	UNP O15519
F	0	HIS	-	expression tag	UNP O15519
F	7	GLY	HIS	engineered mutation	UNP O15519
K	-2	GLY	-	expression tag	UNP O15519
K	-1	SER	-	expression tag	UNP O15519
K	0	HIS	-	expression tag	UNP O15519
K	7	GLY	HIS	engineered mutation	UNP O15519
I	-2	GLY	-	expression tag	UNP O15519
I	-1	SER	-	expression tag	UNP O15519
I	0	HIS	-	expression tag	UNP O15519
I	7	GLY	HIS	engineered mutation	UNP O15519
J	-2	GLY	-	expression tag	UNP O15519
J	-1	SER	-	expression tag	UNP O15519
J	0	HIS	-	expression tag	UNP O15519
J	7	GLY	HIS	engineered mutation	UNP O15519

- Molecule 3 is SELENIUM ATOM (CCD ID: SE) (formula: Se) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total	Se	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	11	Total 11	O 11	0	0
4	B	7	Total 7	O 7	0	0
4	D	12	Total 12	O 12	0	0
4	G	1	Total 1	O 1	0	0
4	K	10	Total 10	O 10	0	0
4	I	2	Total 2	O 2	0	0
4	J	7	Total 7	O 7	0	0
4	A	1	Total 1	O 1	0	0

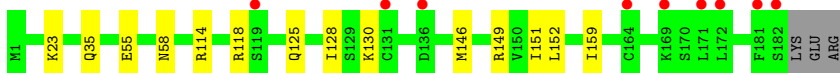
3 Residue-property plots [i](#)

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: Caspase-8



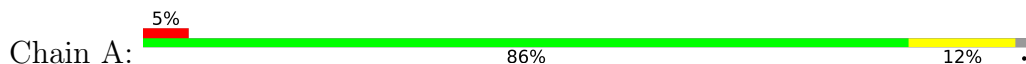
- Molecule 1: Caspase-8



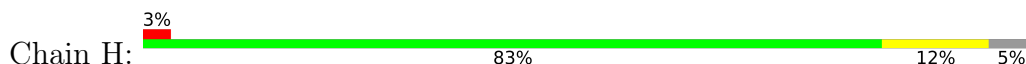
- Molecule 1: Caspase-8



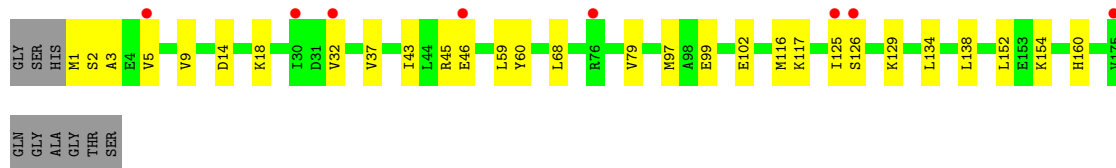
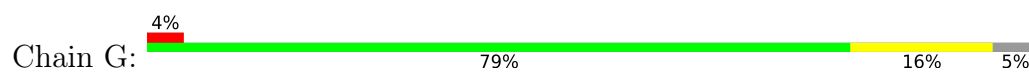
- Molecule 1: Caspase-8



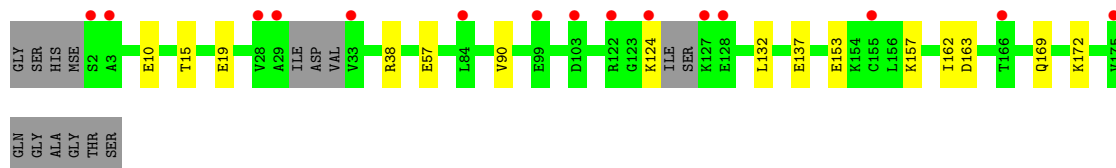
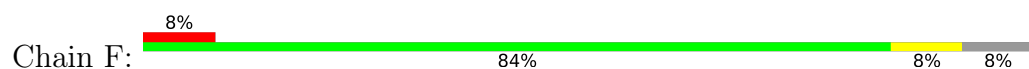
- Molecule 2: CASP8 and FADD-like apoptosis regulator subunit p43



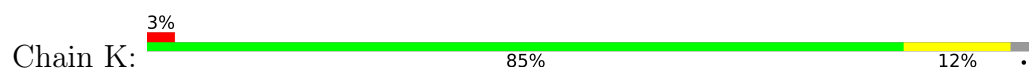
- Molecule 2: CASP8 and FADD-like apoptosis regulator subunit p43



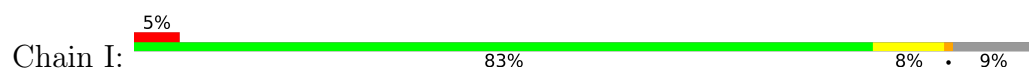
- Molecule 2: CASP8 and FADD-like apoptosis regulator subunit p43



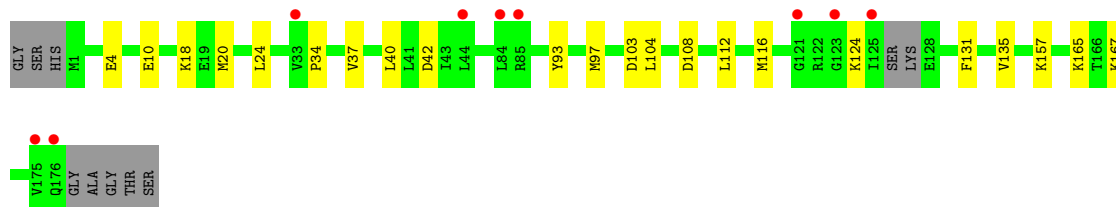
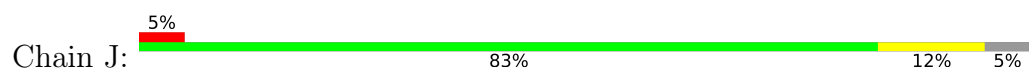
- Molecule 2: CASP8 and FADD-like apoptosis regulator subunit p43



- Molecule 2: CASP8 and FADD-like apoptosis regulator subunit p43



- Molecule 2: CASP8 and FADD-like apoptosis regulator subunit p43



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.27Å 167.45Å 179.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 2.34 29.84 – 2.34	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.84-2.34) 97.7 (29.84-2.34)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.79 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.206 , 0.253 0.205 , 0.251	Depositor DCC
R_{free} test set	5080 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14567	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SE

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	0.22	0/1520	0.43	0/2021
1	B	0.24	0/1520	0.43	0/2021
1	C	0.29	0/1538	0.48	0/2044
1	D	0.26	0/1541	0.44	0/2048
2	F	0.21	0/1380	0.37	0/1839
2	G	0.21	0/1427	0.36	0/1906
2	H	0.23	0/1427	0.37	0/1906
2	I	0.24	0/1376	0.38	0/1834
2	J	0.26	0/1420	0.41	0/1896
2	K	0.25	0/1455	0.40	0/1942
All	All	0.24	0/14604	0.41	0/19457

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1510	0	1551	18	0
1	B	1510	0	1551	9	0
1	C	1528	0	1570	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1531	0	1571	10	0
2	F	1373	0	1449	10	0
2	G	1418	0	1503	23	0
2	H	1418	0	1503	15	0
2	I	1369	0	1441	10	0
2	J	1412	0	1492	15	0
2	K	1446	0	1526	14	0
3	F	1	0	0	0	0
4	A	1	0	0	0	0
4	B	7	0	0	0	0
4	C	11	0	0	0	0
4	D	12	0	0	0	0
4	G	1	0	0	0	0
4	I	2	0	0	0	0
4	J	7	0	0	0	0
4	K	10	0	0	0	0
All	All	14567	0	15157	119	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 4.

All (119) 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:H:103:ASP:OD2	2:H:167:LYS:NZ	2.22	0.71
2:G:154:LYS:NZ	2:J:4:GLU:OE2	2.23	0.70
2:I:153:GLU:HG3	2:I:165:LYS:HG3	1.75	0.69
2:H:63:ARG:HH22	1:A:31:PRO:HG3	1.57	0.69
2:I:153:GLU:OE2	2:I:165:LYS:NZ	2.25	0.68
2:G:68:LEU:HD21	2:G:79:VAL:HG21	1.76	0.68
2:J:103:ASP:OD2	2:J:167:LYS:NZ	2.25	0.68
1:B:151:ILE:HB	1:B:159:ILE:HD12	1.77	0.67
1:A:146:MSE:HE2	1:A:152:LEU:HB2	1.78	0.64
2:G:117:LYS:NZ	2:J:42:ASP:OD2	2.31	0.64
2:G:3:ALA:HB2	2:G:45:ARG:HH12	1.63	0.64
2:J:20:MSE:HE2	2:J:24:LEU:HD11	1.79	0.64
1:C:89:GLU:OE2	1:C:95:ARG:HD2	2.00	0.62
2:J:157:LYS:HB2	2:J:165:LYS:HD2	1.82	0.61
1:A:151:ILE:HB	1:A:159:ILE:HD12	1.81	0.61
2:K:1:MSE:HE1	2:K:52:VAL:HA	1.82	0.60
2:F:57:GLU:OE2	2:F:90:VAL:HG22	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLY:O	1:A:126:GLU:HB2	2.02	0.60
2:K:20:MSE:HE2	2:K:24:LEU:HD11	1.84	0.59
2:J:131:PHE:O	2:J:135:VAL:HG23	2.03	0.58
2:F:124:LYS:HG2	2:F:137:GLU:OE2	2.03	0.58
2:G:116:MSE:HG3	2:G:134:LEU:HD11	1.87	0.57
2:K:56:ALA:HB2	2:K:74:MSE:HE1	1.87	0.56
2:G:160:HIS:NE2	2:K:31:ASP:OD2	2.38	0.56
2:G:126:SER:H	2:G:129:LYS:HE2	1.71	0.55
1:B:146:MSE:HE2	1:B:152:LEU:HB2	1.90	0.54
2:K:112:LEU:HD22	2:K:116:MSE:HE2	1.89	0.54
2:H:22:LEU:HD23	2:H:40:LEU:HD22	1.89	0.54
2:F:15:THR:HG22	2:F:19:GLU:OE2	2.08	0.54
2:G:32:VAL:HG21	2:G:43:ILE:HD13	1.90	0.53
2:F:169:GLN:HA	2:F:172:LYS:HE2	1.91	0.52
2:F:153:GLU:OE2	2:F:172:LYS:NZ	2.33	0.52
1:C:40:ASP:OD2	1:C:43:MSE:HE2	2.10	0.52
2:G:18:LYS:HG2	2:G:37:VAL:HG11	1.92	0.51
1:B:55:GLU:HG2	1:B:58:ASN:HB3	1.91	0.51
2:H:24:LEU:HD22	2:H:90:VAL:HG11	1.92	0.51
2:I:20:MSE:HE2	2:I:62:VAL:HG12	1.93	0.51
2:G:5:VAL:O	2:G:9:VAL:HG23	2.10	0.51
2:H:132:LEU:HA	2:H:135:VAL:HG22	1.92	0.50
2:J:10:GLU:HG2	2:J:37:VAL:HG13	1.92	0.50
1:A:124:LEU:O	1:A:128:ILE:HG12	2.12	0.50
2:F:163:ASP:N	2:F:163:ASP:OD1	2.45	0.50
1:A:8:TYR:HA	1:A:42:LEU:HD21	1.93	0.50
2:J:104:LEU:HD22	2:J:108:ASP:HB3	1.92	0.50
2:I:20:MSE:CE	2:I:62:VAL:HA	2.42	0.49
1:B:125:GLN:O	1:B:130:LYS:NZ	2.38	0.49
1:D:109:SER:HA	1:D:139:LEU:HD23	1.95	0.48
2:G:126:SER:HB3	2:G:129:LYS:HG3	1.94	0.48
2:K:22:LEU:HD23	2:K:40:LEU:HD22	1.94	0.48
2:J:97:MSE:HE2	2:J:135:VAL:CG1	2.44	0.48
2:H:10:GLU:CD	2:H:38:ARG:HB2	2.39	0.48
1:C:163:VAL:O	1:C:166:GLN:HG2	2.14	0.48
1:D:134:ASP:OD1	1:D:135:ASP:N	2.43	0.48
1:C:55:GLU:HG2	1:C:58:ASN:HB3	1.97	0.47
2:I:34:PRO:HG2	2:I:40:LEU:HD13	1.95	0.47
2:K:97:MSE:HE3	2:K:135:VAL:HG13	1.97	0.47
1:D:83:LYS:HE3	1:D:87:GLU:OE2	2.14	0.47
2:H:20:MSE:HE3	2:H:98:ALA:HB1	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:116:MSE:HE3	2:G:138:LEU:HD11	1.98	0.46
1:D:134:ASP:HB3	1:D:136:ASP:OD1	2.16	0.46
2:H:10:GLU:OE1	2:H:38:ARG:HB2	2.16	0.46
1:C:134:ASP:OD2	1:B:114:ARG:NE	2.49	0.46
2:H:32:VAL:HG11	2:H:43:ILE:HD13	1.98	0.45
2:G:3:ALA:HB2	2:G:45:ARG:NH1	2.29	0.45
1:B:23:LYS:HB3	1:B:35:GLN:OE1	2.17	0.45
2:F:157:LYS:HG3	2:F:162:ILE:HD11	1.98	0.45
2:G:2:SER:OG	2:G:3:ALA:N	2.50	0.45
2:F:10:GLU:OE1	2:F:38:ARG:HB2	2.17	0.44
1:A:118:ARG:HH12	1:A:121:LYS:NZ	2.15	0.44
1:A:118:ARG:HH12	1:A:121:LYS:HZ2	1.65	0.44
2:G:99:GLU:HA	2:G:102:GLU:HG2	2.00	0.43
1:A:23:LYS:HB3	1:A:35:GLN:OE1	2.19	0.43
2:K:116:MSE:HE3	2:K:134:LEU:HD21	1.99	0.43
2:H:57:GLU:O	2:H:61:ARG:HG2	2.19	0.43
2:K:170:LYS:HA	2:K:170:LYS:HD3	1.86	0.43
2:I:119:TYR:OH	2:I:154:LYS:NZ	2.49	0.43
2:G:125:ILE:HA	2:G:129:LYS:NZ	2.34	0.43
2:J:18:LYS:HG2	2:J:37:VAL:HG11	2.01	0.43
2:H:126:SER:HB3	2:H:129:LYS:HG2	2.01	0.43
2:G:43:ILE:O	2:G:46:GLU:HG2	2.19	0.43
2:G:97:MSE:HE1	2:G:152:LEU:HD22	2.00	0.43
1:D:168:ASN:OD1	1:D:169:LYS:N	2.52	0.42
2:F:132:LEU:HD23	2:F:132:LEU:HA	1.90	0.42
2:H:102:GLU:O	1:A:31:PRO:HB2	2.19	0.42
2:J:112:LEU:O	2:J:116:MSE:HG3	2.19	0.42
1:A:165:ALA:N	1:A:172:LEU:HD11	2.34	0.42
1:D:8:TYR:O	1:D:12:GLU:HG2	2.20	0.42
1:A:125:GLN:CD	1:A:133:LEU:HD13	2.44	0.42
2:H:63:ARG:NH2	1:A:31:PRO:HG3	2.31	0.42
2:G:117:LYS:HB2	2:G:117:LYS:HE3	1.86	0.42
2:J:93:TYR:O	2:J:97:MSE:HG2	2.19	0.42
2:G:1:MSE:HE2	2:G:5:VAL:HG21	2.01	0.41
2:K:21:LEU:HD23	2:K:21:LEU:HA	1.94	0.41
1:D:146:MSE:HE2	1:D:152:LEU:HB2	2.02	0.41
1:B:128:ILE:HD13	1:B:149:ARG:HD2	2.01	0.41
1:B:130:LYS:HA	1:B:130:LYS:HD3	1.82	0.41
2:I:103:ASP:HA	2:J:124:LYS:H	1.85	0.41
2:G:60:TYR:HB2	2:G:79:VAL:HG11	2.03	0.41
2:K:32:VAL:O	2:K:34:PRO:HD3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LYS:HG2	1:A:111:GLU:OE1	2.21	0.41
1:D:127:GLU:HG2	1:D:159:ILE:HD13	2.02	0.41
2:J:34:PRO:HG2	2:J:40:LEU:HD13	2.01	0.41
1:C:40:ASP:OD1	1:C:43:MSE:HG3	2.20	0.41
2:K:105:ASP:OD1	2:K:105:ASP:N	2.51	0.41
2:I:104:LEU:HD22	2:I:108:ASP:HB3	2.03	0.41
2:I:128:GLU:H	2:I:129:LYS:NZ	2.19	0.41
1:A:124:LEU:HD23	1:A:127:GLU:OE1	2.21	0.41
1:C:113:SER:HB2	1:D:134:ASP:OD2	2.21	0.41
2:F:169:GLN:HA	2:F:172:LYS:CE	2.51	0.41
2:K:104:LEU:HD22	2:K:108:ASP:HB3	2.03	0.41
1:A:165:ALA:HB2	1:A:172:LEU:HD21	2.03	0.41
2:J:97:MSE:HE2	2:J:135:VAL:HG13	2.02	0.40
2:H:160:HIS:HE2	2:K:11:GLU:CD	2.28	0.40
2:I:24:LEU:O	2:I:90:VAL:HG13	2.22	0.40
1:D:151:ILE:HB	1:D:159:ILE:HD12	2.03	0.40
2:H:140:LYS:NZ	2:G:14:ASP:OD2	2.54	0.40
1:A:124:LEU:HD23	1:A:124:LEU:HA	1.90	0.40
2:G:59:LEU:HB2	2:G:68:LEU:HD13	2.04	0.40
1:A:168:ASN:OD1	1:A:170:SER:OG	2.26	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	180/185 (97%)	176 (98%)	4 (2%)	0	100	100
1	B	180/185 (97%)	175 (97%)	5 (3%)	0	100	100
1	C	182/185 (98%)	178 (98%)	4 (2%)	0	100	100
1	D	182/185 (98%)	179 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	163/184 (89%)	159 (98%)	4 (2%)	0	100	100
2	G	173/184 (94%)	166 (96%)	7 (4%)	0	100	100
2	H	173/184 (94%)	168 (97%)	5 (3%)	0	100	100
2	I	162/184 (88%)	158 (98%)	4 (2%)	0	100	100
2	J	170/184 (92%)	165 (97%)	5 (3%)	0	100	100
2	K	177/184 (96%)	170 (96%)	7 (4%)	0	100	100
All	All	1742/1844 (94%)	1694 (97%)	48 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	171/167 (102%)	171 (100%)	0	100	100
1	B	171/167 (102%)	170 (99%)	1 (1%)	78	86
1	C	173/167 (104%)	173 (100%)	0	100	100
1	D	173/167 (104%)	173 (100%)	0	100	100
2	F	156/161 (97%)	156 (100%)	0	100	100
2	G	162/161 (101%)	162 (100%)	0	100	100
2	H	162/161 (101%)	162 (100%)	0	100	100
2	I	157/161 (98%)	156 (99%)	1 (1%)	78	86
2	J	161/161 (100%)	161 (100%)	0	100	100
2	K	164/161 (102%)	164 (100%)	0	100	100
All	All	1650/1634 (101%)	1648 (100%)	2 (0%)	88	93

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

Mol	Chain	Res	Type
1	B	118	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	90	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	13	GLN
1	C	166	GLN
1	B	13	GLN
1	D	49	GLN
1	D	97	GLN
1	D	125	GLN
2	H	86	ASN
2	F	82	HIS
2	F	86	ASN
2	K	160	HIS
2	K	173	GLN
2	I	160	HIS
2	I	169	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 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	175/185 (94%)	0.62	9 (5%)	33 39	33, 54, 97, 106	0
1	B	175/185 (94%)	0.29	9 (5%)	33 39	22, 44, 84, 98	0
1	C	177/185 (95%)	-0.02	4 (2%)	61 66	21, 35, 66, 89	0
1	D	178/185 (96%)	0.19	7 (3%)	43 49	24, 43, 71, 83	0
2	F	164/184 (89%)	0.70	15 (9%)	15 18	33, 54, 84, 103	0
2	G	169/184 (91%)	0.43	8 (4%)	36 42	30, 48, 85, 102	0
2	H	169/184 (91%)	0.45	6 (3%)	46 52	32, 51, 80, 108	0
2	I	162/184 (88%)	0.34	9 (5%)	30 35	31, 47, 77, 89	0
2	J	168/184 (91%)	0.33	9 (5%)	31 37	24, 43, 76, 94	0
2	K	173/184 (94%)	0.07	5 (2%)	53 60	25, 41, 69, 85	0
All	All	1710/1844 (92%)	0.34	81 (4%)	36 42	21, 47, 83, 108	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	175	VAL	5.1
2	J	125	ILE	5.0
2	K	178	ALA	4.5
2	I	29	ALA	4.4
1	A	127	GLU	4.2
2	F	2	SER	4.2
2	F	155	CYS	3.8
2	I	33	VAL	3.8
2	F	33	VAL	3.7
2	F	29	ALA	3.7
1	A	182	SER	3.6
1	B	182	SER	3.6
2	F	103	ASP	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	128	ILE	3.4
1	A	131	CYS	3.4
1	A	181	PHE	3.3
2	H	175	VAL	3.3
2	I	84	LEU	3.3
1	A	124	LEU	3.3
2	G	125	ILE	3.3
1	B	181	PHE	3.2
2	I	127	LYS	3.2
1	B	136	ASP	3.1
2	K	177	GLY	3.1
2	H	32	VAL	3.0
2	F	28	VAL	3.0
1	B	169	LYS	3.0
2	G	30	ILE	2.9
2	G	32	VAL	2.9
1	D	93	PRO	2.8
2	F	3	ALA	2.8
2	F	127	LYS	2.8
2	J	84	LEU	2.8
2	G	175	VAL	2.8
1	C	181	PHE	2.8
2	I	175	VAL	2.8
2	F	166	THR	2.7
1	D	3	PHE	2.7
1	A	130	LYS	2.7
1	C	184	GLU	2.7
1	B	131	CYS	2.7
2	H	33	VAL	2.6
1	D	92	THR	2.6
1	A	125	GLN	2.6
1	C	136	ASP	2.6
2	H	30	ILE	2.6
2	K	0	HIS	2.6
1	D	125	GLN	2.5
2	I	118	ASP	2.5
2	I	-1	SER	2.5
2	J	121	GLY	2.5
1	B	164	CYS	2.4
1	D	131	CYS	2.4
1	B	171	LEU	2.4
2	J	44	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	167	ILE	2.4
2	H	29	ALA	2.4
2	J	123	GLY	2.4
2	J	33	VAL	2.4
2	G	46	GLU	2.3
1	B	119	SER	2.3
1	A	129	SER	2.3
2	F	99	GLU	2.2
2	I	0	HIS	2.2
2	F	124	LYS	2.2
2	F	122	ARG	2.2
2	H	31	ASP	2.2
2	G	76	ARG	2.1
2	J	85	ARG	2.1
1	D	2	ASP	2.1
2	G	126	SER	2.1
1	D	114	ARG	2.1
2	F	128	GLU	2.1
2	K	85	ARG	2.1
2	F	84	LEU	2.1
2	J	176	GLN	2.1
2	J	175	VAL	2.1
2	G	5	VAL	2.1
2	I	82	HIS	2.0
1	B	172	LEU	2.0
2	K	33	VAL	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](#)

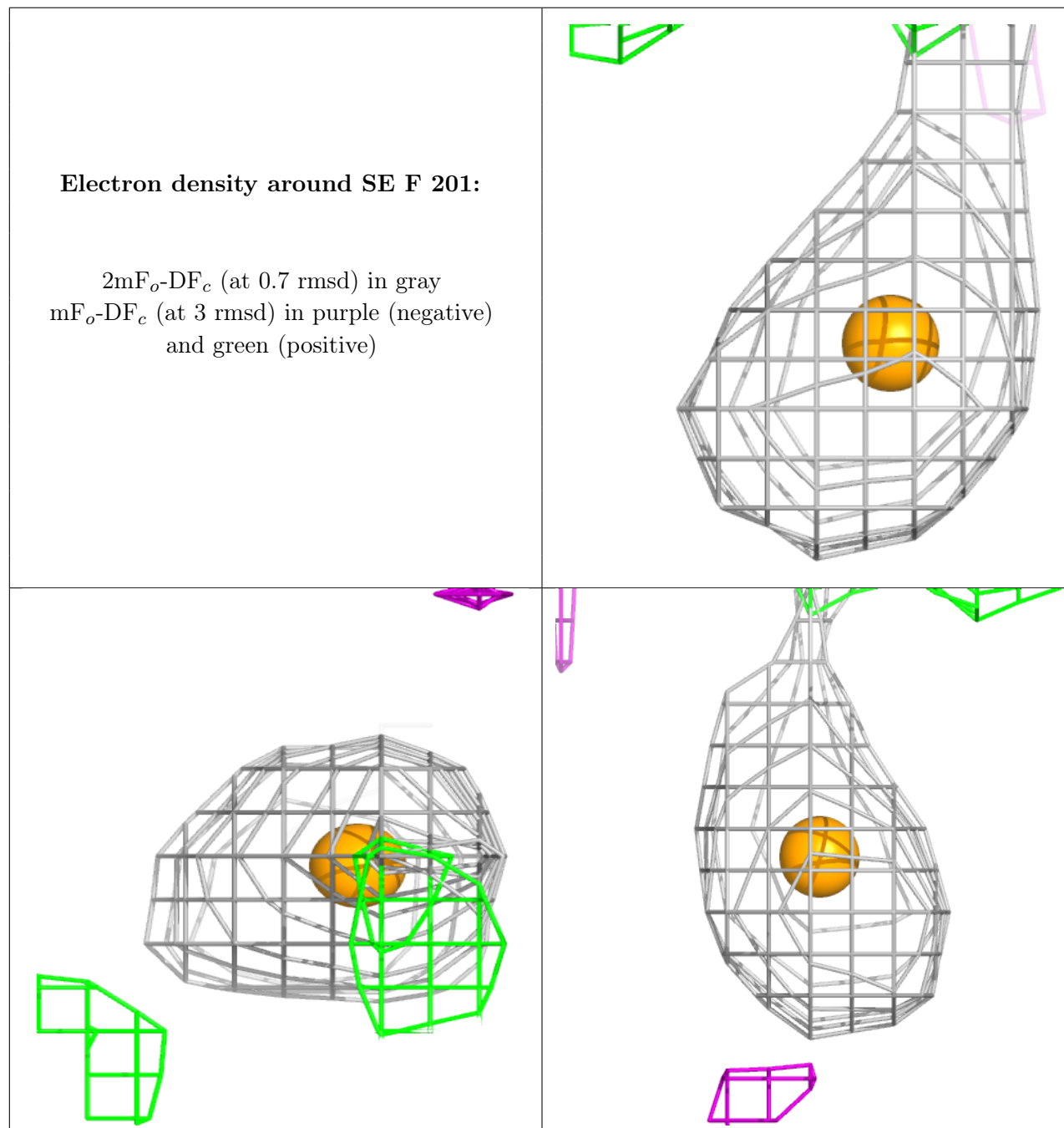
There are no oligosaccharides in this entry.

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	SE	F	201	1/1	0.91	0.18	112,112,112,112	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.