



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2024 – 10:05 AM EDT

PDB ID : 8TV5  
Title : Structure of the EphA2 LBDCRD bound to FabS1CE\_L1 in a 2:1 (EphA2 to Fab) ratio  
Authors : Singer, A.U.; Bruce, H.A.; Blazer, L.; Adams, J.J.; Sicheri, F.; Sidhu, S.S.  
Deposited on : 2023-08-17  
Resolution : 4.60 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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.002 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.3

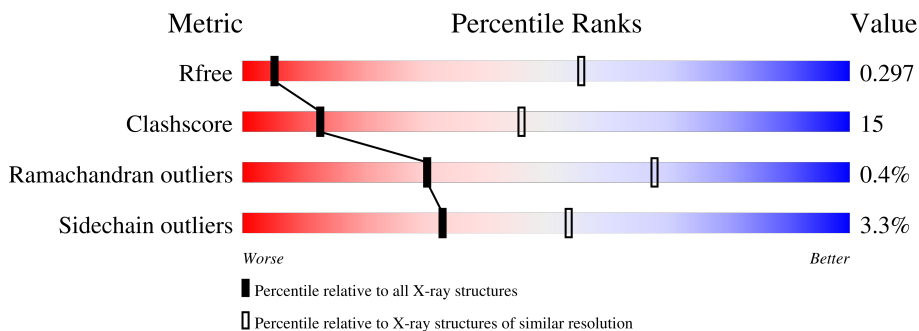
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1068 (5.30-3.90)
Clashscore	180529	1123 (5.30-3.90)
Ramachandran outliers	177936	1015 (5.30-3.90)
Sidechain outliers	177891	1016 (5.32-3.88)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	236	
2	B	211	
3	C	308	
3	F	308	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7736 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 S1CE variant of Fab\_L1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	231	1723	1097	283	337	6	0	0	0

- Molecule 2 is a protein called S1CE variant of Fab\_L1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	210	1557	970	256	325	6	0	0	0

- Molecule 3 is a protein called Ephrin type-A receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	F	299	2246	1423	363	438	22	0	0	0
3	C	294	2208	1401	360	426	21	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	327	LEU	-	expression tag	UNP P29317
F	328	VAL	-	expression tag	UNP P29317
F	329	PRO	-	expression tag	UNP P29317
F	330	ARG	-	expression tag	UNP P29317
C	327	LEU	-	expression tag	UNP P29317
C	328	VAL	-	expression tag	UNP P29317
C	329	PRO	-	expression tag	UNP P29317
C	330	ARG	-	expression tag	UNP P29317

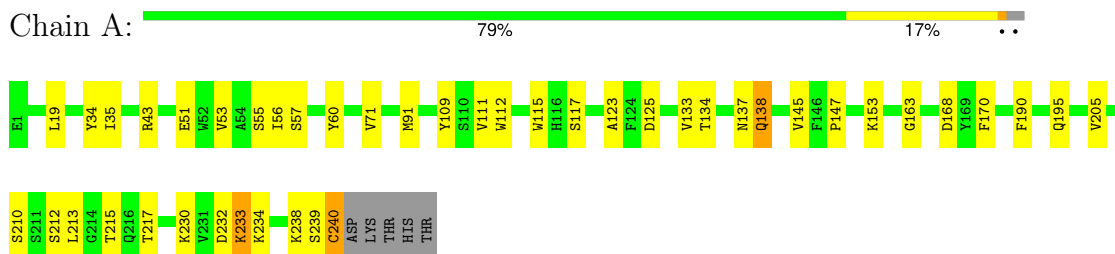
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	C	2	Total	Mg	0	0
			2	2		

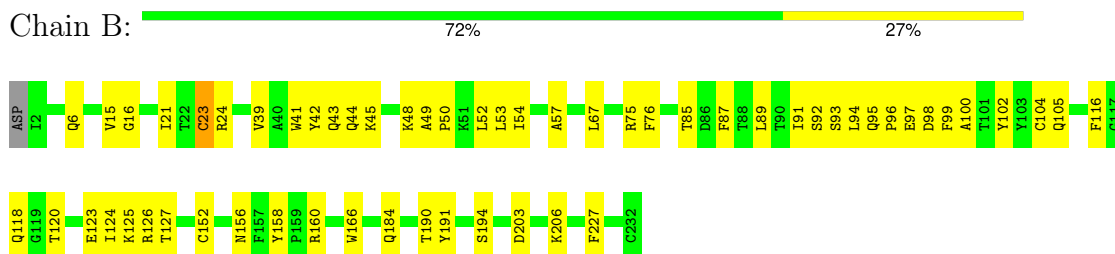
### 3 Residue-property plots

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. 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. 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.

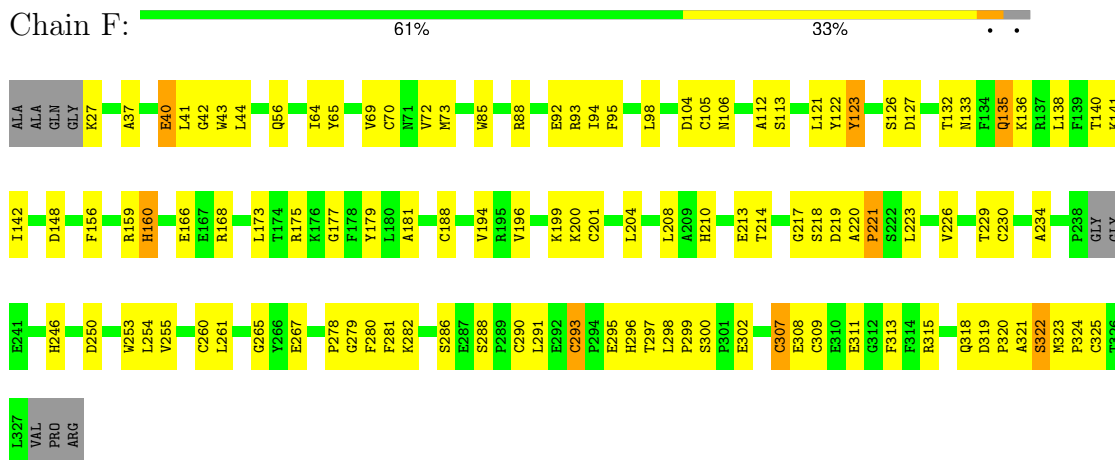
- Molecule 1: S1CE variant of Fab\_L1 heavy chain



- Molecule 2: S1CE variant of Fab\_L1 light chain



- Molecule 3: Ephrin type-A receptor 2



- Molecule 3: Ephrin type-A receptor 2



ALA	ALA	GLN	GLY	K27	A37	G38	L41	G42	W43	L44	H45	H46	P47	Y48	G49	L54	M55	Q56	N57	I58	Y65	M66	Y67	C70	N71	V72	M73	Q77	D78	N79	W80	L81	R82	T83	N84	R83	I94	F95	L98	K99	F100	T101	V102	R103	D104	C105	N106	S107	A112	K116	Y122	D127	L128	D129	L138	K141	L145	F156	E157	V161	K162	L163	E166	E167	R168	R175	Y179	L180	A181	V189	A190	L191	V194	K199	K200	C201	P202	E203	L204	H210	E213	T214	I215	A216	G217	S218	D219	A220	P221	S222	L223	A224	T225	V226	D232	H233	P237	R244	M245	V249	W253	L254	V255	P256	I257	L261	C262	G265	C273	F280	F281	K282	F283	S286	E287	S288	P289	C290	T297	L298	A304	T305	S306	C309	E310	E311	G312	F313	F314	R315	ALA	PRO	GLN	ASP	PRO	ALA	SER	W223	L327	VAL	PRO	ARG
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## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.88Å 72.89Å 241.96Å 90.00° 89.04° 90.00°	Depositor
Resolution (Å)	120.96 – 4.60 120.96 – 4.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (120.96-4.60) 98.8 (120.96-4.60)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 4.66Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.265 , 0.298 0.265 , 0.297	Depositor DCC
$R_{free}$ test set	8308 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	160.0	Xtrriage
Anisotropy	0.493	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 216.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	7736	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	267.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG

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	0.28	0/1773	0.49	0/2427
2	B	0.26	0/1590	0.51	0/2169
3	C	0.28	0/2266	0.62	3/3090 (0.1%)
3	F	0.28	0/2306	0.64	3/3150 (0.1%)
All	All	0.27	0/7935	0.58	6/10836 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	F	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	C	41	LEU	CB-CG-CD1	9.03	126.35	111.00
3	C	41	LEU	CA-CB-CG	7.24	131.95	115.30
3	F	135	GLN	C-N-CA	5.64	135.79	121.70
3	F	159	ARG	C-N-CA	5.56	135.59	121.70
3	C	298	LEU	CA-CB-CG	5.35	127.61	115.30
3	F	223	LEU	CA-CB-CG	5.25	127.39	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
3	C	222	SER	Peptide
3	F	220	ALA	Peptide

## 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	1723	0	1634	41	0
2	B	1557	0	1454	45	0
3	C	2208	0	2019	78	0
3	F	2246	0	2038	73	0
4	C	2	0	0	0	0
All	All	7736	0	7145	221	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 15.

All (221) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLN:OE1	1:A:170:PHE:HB3	1.23	1.37
1:A:138:GLN:NE2	1:A:170:PHE:CG	2.05	1.25
1:A:138:GLN:NE2	1:A:170:PHE:CD1	2.25	1.05
1:A:138:GLN:OE1	1:A:170:PHE:CB	2.14	0.94
3:C:37:ALA:HB1	3:C:41:LEU:HD23	1.50	0.92
1:A:138:GLN:CD	1:A:170:PHE:HB3	2.02	0.79
1:A:138:GLN:HE22	1:A:170:PHE:CB	1.97	0.77
3:F:113:SER:O	3:C:106:ASN:ND2	2.17	0.76
2:B:16:GLY:HA2	2:B:93:SER:HB3	1.69	0.73
3:C:203:GLU:OE2	3:C:210:HIS:NE2	2.22	0.72
3:F:214:THR:HG21	3:F:226:VAL:HG11	1.69	0.72
3:F:295:GLU:HB3	3:F:324:PRO:HB3	1.70	0.72
2:B:75:ARG:NH2	2:B:97:GLU:OE2	2.23	0.71
3:F:148:ASP:O	3:C:141:LYS:NZ	2.23	0.71
3:C:166:GLU:HB3	3:C:168:ARG:HH12	1.55	0.70
3:F:93:ARG:NE	3:F:218:SER:O	2.25	0.70
3:C:127:ASP:OD2	3:C:175:ARG:HD2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:122:TYR:HB2	3:C:181:ALA:HB3	1.73	0.68
3:F:122:TYR:HB2	3:F:181:ALA:HB3	1.74	0.68
3:F:265:GLY:H	3:F:282:LYS:HB3	1.59	0.68
1:A:19:LEU:HD12	1:A:133:VAL:HG13	1.74	0.67
3:C:282:LYS:HG2	3:C:290:CYS:HA	1.77	0.67
2:B:21:ILE:HG12	2:B:120:THR:HG21	1.76	0.67
3:C:191:LEU:HD21	3:C:194:VAL:HG23	1.77	0.67
2:B:75:ARG:HB2	2:B:92:SER:H	1.60	0.66
3:C:99:LYS:HB3	3:C:163:LEU:HD11	1.77	0.66
2:B:75:ARG:HD2	2:B:91:ILE:HG23	1.78	0.66
2:B:54:ILE:HG13	2:B:67:LEU:HA	1.78	0.65
3:F:315:ARG:NH1	3:F:321:ALA:HA	2.12	0.65
1:A:138:GLN:NE2	1:A:170:PHE:CB	2.56	0.65
3:C:297:THR:HA	3:C:310:GLU:HB2	1.79	0.64
2:B:203:ASP:HA	2:B:206:LYS:HD2	1.79	0.64
3:C:38:GLY:HA2	3:C:65:TYR:CD2	2.34	0.63
3:C:27:LYS:N	3:C:200:LYS:O	2.32	0.62
3:F:261:LEU:HD13	3:F:286:SER:HA	1.80	0.62
3:F:255:VAL:HG21	3:C:255:VAL:HG21	1.82	0.61
3:C:46:HIS:HB3	3:C:80:TRP:HB2	1.83	0.61
3:F:282:LYS:NZ	3:F:288:SER:O	2.34	0.61
3:F:166:GLU:HB3	3:F:168:ARG:HH12	1.66	0.61
3:C:101:THR:HG21	3:C:161:VAL:HG22	1.83	0.61
2:B:45:LYS:HD2	2:B:100:ALA:HB2	1.82	0.61
3:C:44:LEU:HB2	3:C:82:ARG:HH21	1.64	0.61
1:A:138:GLN:CD	1:A:170:PHE:CB	2.67	0.60
3:C:214:THR:HG22	3:C:215:ILE:H	1.67	0.60
2:B:94:LEU:HD11	2:B:124:ILE:HG12	1.82	0.60
1:A:57:SER:O	1:A:60:TYR:N	2.35	0.59
2:B:98:ASP:HB2	2:B:102:TYR:OH	2.02	0.59
3:F:44:LEU:HD22	3:F:132:THR:HA	1.85	0.59
3:F:293:CYS:SG	3:F:300:SER:OG	2.60	0.59
1:A:53:VAL:HG13	1:A:71:VAL:HG21	1.84	0.59
2:B:43:GLN:HB3	2:B:53:LEU:HD11	1.85	0.58
3:C:280:PHE:HB3	3:C:290:CYS:HB3	1.85	0.58
3:C:282:LYS:NZ	3:C:288:SER:OG	2.37	0.58
2:B:15:VAL:HA	2:B:94:LEU:HD13	1.85	0.58
3:F:27:LYS:N	3:F:200:LYS:O	2.36	0.58
3:F:297:THR:OG1	3:F:308:GLU:O	2.20	0.57
3:C:93:ARG:NE	3:C:218:SER:O	2.36	0.57
3:C:104:ASP:OD2	3:C:106:ASN:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:GLN:HG2	2:B:100:ALA:HB3	1.85	0.56
3:C:43:TRP:H	3:C:84:ASN:HD21	1.52	0.56
3:F:296:HIS:HB3	3:F:313:PHE:CD2	2.40	0.56
3:C:77:GLN:HB3	3:C:79:ASN:ND2	2.21	0.56
3:C:282:LYS:NZ	3:C:286:SER:OG	2.37	0.56
3:C:200:LYS:HG2	3:C:215:ILE:HA	1.88	0.55
3:C:313:PHE:HE1	3:C:327:LEU:HG	1.69	0.55
1:A:168:ASP:OD1	1:A:195:GLN:NE2	2.39	0.55
3:F:219:ASP:OD1	3:F:219:ASP:N	2.37	0.55
3:C:82:ARG:NH1	3:C:83:THR:O	2.39	0.55
3:F:218:SER:N	3:F:221:PRO:HG3	2.21	0.55
3:C:102:VAL:HG22	3:C:189:VAL:HG13	1.89	0.55
1:A:138:GLN:CD	1:A:170:PHE:CG	2.78	0.55
2:B:24:ARG:NH2	2:B:85:THR:OG1	2.36	0.54
2:B:75:ARG:CZ	2:B:95:GLN:HB2	2.38	0.54
3:F:254:LEU:HB3	3:F:255:VAL:HG22	1.87	0.54
3:F:300:SER:OG	3:F:307:CYS:SG	2.65	0.54
3:F:200:LYS:HE2	3:F:213:GLU:HG2	1.89	0.54
3:C:98:LEU:HD22	3:C:194:VAL:HG22	1.90	0.54
3:C:72:VAL:HG23	3:C:73:MET:HG2	1.88	0.53
3:C:77:GLN:HB3	3:C:79:ASN:HD21	1.72	0.53
2:B:48:LYS:HD3	2:B:49:ALA:H	1.73	0.53
3:C:66:MET:HE3	3:C:190:ALA:HB1	1.91	0.53
1:A:34:TYR:CE2	1:A:109:TYR:HA	2.44	0.53
3:C:55:MET:HB3	3:C:66:MET:HG3	1.91	0.53
3:C:245:MET:HG2	3:C:256:PRO:HA	1.90	0.53
3:F:280:PHE:HB3	3:F:290:CYS:HB3	1.91	0.53
1:A:210:SER:HA	1:A:213:LEU:HG	1.91	0.52
3:C:55:MET:N	3:C:66:MET:O	2.30	0.52
3:F:210:HIS:HB3	3:F:229:THR:HB	1.92	0.52
2:B:41:TRP:HB2	2:B:54:ILE:HG22	1.92	0.52
1:A:112:TRP:CZ2	3:C:190:ALA:HB2	2.45	0.51
3:C:223:LEU:HD13	3:C:224:ALA:HB3	1.92	0.51
1:A:115:TRP:HB3	3:C:55:MET:HG3	1.92	0.51
1:A:43:ARG:NE	1:A:51:GLU:OE1	2.44	0.51
1:A:138:GLN:CD	1:A:170:PHE:CD1	2.83	0.51
1:A:147:PRO:HD3	1:A:233:LYS:HD3	1.93	0.51
1:A:230:LYS:NZ	1:A:232:ASP:OD1	2.43	0.50
1:A:238:LYS:O	1:A:240:CYS:N	2.44	0.50
3:C:310:GLU:HG2	3:C:311:GLU:N	2.26	0.50
3:F:72:VAL:HG23	3:F:73:MET:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:281:PHE:HZ	3:F:322:SER:HA	1.76	0.50
3:C:48:TYR:CG	3:C:49:GLY:N	2.79	0.50
1:A:91:MET:SD	1:A:91:MET:N	2.84	0.50
3:C:237:PRO:HG3	3:C:261:LEU:HD12	1.92	0.50
3:F:201:CYS:HB3	3:F:253:TRP:CE2	2.47	0.50
3:C:298:LEU:HG	3:C:310:GLU:HG3	1.94	0.50
3:C:204:LEU:HG	3:C:253:TRP:CD1	2.47	0.50
3:F:133:ASN:OD1	3:F:133:ASN:O	2.30	0.50
3:C:199:LYS:HB2	3:C:216:ALA:HB2	1.93	0.49
3:F:219:ASP:C	3:F:221:PRO:HD3	2.32	0.49
3:F:315:ARG:HA	3:F:325:CYS:HA	1.94	0.49
2:B:44:GLN:HG3	2:B:50:PRO:HG3	1.95	0.49
1:A:57:SER:OG	1:A:60:TYR:HB2	2.13	0.49
2:B:53:LEU:HD13	2:B:76:PHE:CE2	2.48	0.49
3:C:201:CYS:HB3	3:C:253:TRP:CE2	2.47	0.49
2:B:99:PHE:CG	2:B:99:PHE:O	2.66	0.49
2:B:41:TRP:HB3	2:B:89:LEU:HD22	1.95	0.49
3:F:112:ALA:HA	3:C:112:ALA:HA	1.95	0.49
1:A:153:LYS:HD3	2:B:227:PHE:HB3	1.93	0.48
2:B:39:VAL:HG22	2:B:57:ALA:HB2	1.95	0.48
3:F:122:TYR:HA	3:F:141:LYS:HA	1.96	0.48
3:F:37:ALA:HB1	3:F:41:LEU:HD23	1.95	0.48
3:F:319:ASP:HA	3:F:323:MET:HE3	1.95	0.48
3:C:129:ASP:OD1	3:C:179:TYR:OH	2.31	0.48
3:C:283:PHE:CD2	3:C:306:SER:HB3	2.47	0.48
1:A:145:VAL:HG12	1:A:233:LYS:HD2	1.96	0.48
2:B:160:ARG:HD3	2:B:191:TYR:CE2	2.49	0.48
3:F:296:HIS:HB3	3:F:313:PHE:HD2	1.79	0.48
3:F:246:HIS:ND1	3:F:255:VAL:HG23	2.28	0.48
3:F:166:GLU:CB	3:F:168:ARG:HH12	2.27	0.48
3:C:203:GLU:HB2	3:C:213:GLU:HB3	1.96	0.48
3:F:217:GLY:HA3	3:F:221:PRO:CG	2.43	0.47
1:A:117:SER:HA	3:C:55:MET:SD	2.54	0.47
2:B:156:ASN:HA	2:B:190:THR:HB	1.96	0.47
3:F:204:LEU:HG	3:F:253:TRP:CD1	2.48	0.47
1:A:60:TYR:OH	3:C:70:CYS:HB3	2.14	0.47
3:F:127:ASP:OD2	3:F:175:ARG:HD2	2.14	0.47
1:A:35:ILE:HB	1:A:56:ILE:HG22	1.97	0.47
3:F:255:VAL:HG21	3:C:255:VAL:HG11	1.97	0.47
3:F:85:TRP:HB2	3:F:179:TYR:CZ	2.50	0.47
3:F:295:GLU:HG3	3:F:296:HIS:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:315:ARG:NH2	3:F:325:CYS:SG	2.88	0.47
2:B:100:ALA:H	2:B:102:TYR:HE1	1.62	0.47
1:A:111:VAL:HG21	3:C:70:CYS:SG	2.56	0.46
1:A:112:TRP:CE2	3:C:190:ALA:HB2	2.49	0.46
2:B:99:PHE:CE1	2:B:123:GLU:HA	2.50	0.46
2:B:94:LEU:HD23	2:B:95:GLN:N	2.30	0.46
3:C:54:LEU:HB3	3:C:67:TYR:CZ	2.50	0.46
3:C:138:LEU:HD12	3:C:138:LEU:O	2.15	0.46
3:C:298:LEU:HG	3:C:310:GLU:HA	1.97	0.46
3:F:104:ASP:O	3:C:116:LYS:NZ	2.49	0.45
2:B:97:GLU:CD	2:B:97:GLU:H	2.19	0.45
3:F:208:LEU:HB2	3:F:260:CYS:HB2	1.98	0.45
3:F:104:ASP:OD2	3:F:106:ASN:HB3	2.16	0.45
3:F:234:ALA:HB1	3:F:260:CYS:HB3	1.98	0.45
3:F:318:GLN:CD	3:F:318:GLN:H	2.20	0.45
3:F:298:LEU:HD11	3:F:308:GLU:OE1	2.17	0.45
3:F:315:ARG:HD3	3:F:319:ASP:HB3	1.98	0.45
1:A:34:TYR:O	1:A:35:ILE:HD13	2.17	0.45
3:C:232:ASP:O	3:C:273:CYS:HB2	2.16	0.45
3:F:278:PRO:HD3	3:F:302:GLU:OE1	2.17	0.45
3:F:279:GLY:HA2	3:F:299:PRO:HB3	1.99	0.45
3:F:64:ILE:HG13	3:F:65:TYR:CD2	2.52	0.44
3:F:265:GLY:N	3:F:282:LYS:HB3	2.29	0.44
1:A:212:SER:HA	1:A:215:THR:HG22	1.98	0.44
2:B:23:CYS:HB2	2:B:41:TRP:CZ2	2.53	0.44
3:F:309:CYS:SG	3:F:315:ARG:N	2.90	0.44
3:C:217:GLY:H	3:C:249:VAL:HA	1.82	0.44
3:F:42:GLY:O	3:F:43:TRP:HB2	2.18	0.44
3:F:135:GLN:HE21	3:F:138:LEU:CD2	2.31	0.44
3:C:145:ILE:HG23	3:C:168:ARG:NH2	2.33	0.44
3:F:37:ALA:HB3	3:F:40:GLU:HA	2.00	0.44
3:F:69:VAL:O	3:F:188:CYS:HA	2.18	0.43
2:B:126:ARG:NH1	2:B:127:THR:HB	2.33	0.43
3:C:220:ALA:N	3:C:221:PRO:HD3	2.34	0.43
3:F:98:LEU:HD22	3:F:194:VAL:HG22	1.99	0.43
2:B:39:VAL:HG21	2:B:87:PHE:HB3	2.00	0.43
1:A:111:VAL:HG23	1:A:112:TRP:CD1	2.53	0.43
1:A:190:PHE:CE2	2:B:194:SER:HB3	2.53	0.43
3:F:309:CYS:HB3	3:F:313:PHE:O	2.19	0.43
1:A:125:ASP:N	1:A:125:ASP:OD1	2.51	0.43
2:B:105:GLN:HG3	2:B:116:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:298:LEU:H	3:C:310:GLU:HB2	1.83	0.43
3:F:121:LEU:HG	3:F:142:ILE:HD12	2.00	0.43
3:F:323:MET:CG	3:F:324:PRO:HD2	2.49	0.43
3:C:156:PHE:CE2	3:C:157:GLU:OE2	2.72	0.42
3:F:92:GLU:O	3:F:173:LEU:HD12	2.20	0.42
1:A:123:ALA:O	2:B:42:TYR:OH	2.27	0.42
3:F:95:PHE:O	3:F:196:VAL:HA	2.18	0.42
3:C:43:TRP:HB3	3:C:81:LEU:HD11	2.01	0.42
2:B:152:CYS:HB2	2:B:166:TRP:CZ2	2.54	0.42
3:F:315:ARG:HD2	3:F:320:PRO:O	2.19	0.42
2:B:125:LYS:HA	2:B:158:TYR:OH	2.18	0.42
3:C:262:CYS:HB2	3:C:287:GLU:HA	2.01	0.42
3:C:38:GLY:HA2	3:C:65:TYR:CG	2.55	0.42
3:C:214:THR:HG22	3:C:215:ILE:N	2.32	0.42
1:A:115:TRP:NE1	3:C:66:MET:HG2	2.34	0.41
3:F:88:ARG:HB2	3:F:177:GLY:HA2	2.02	0.41
3:C:265:GLY:HA2	3:C:304:ALA:O	2.20	0.41
2:B:15:VAL:HG13	2:B:94:LEU:HD22	2.03	0.41
3:F:199:LYS:HZ3	3:F:250:ASP:HA	1.85	0.41
3:F:94:ILE:HG23	3:F:173:LEU:HD11	2.02	0.41
3:C:104:ASP:C	3:C:106:ASN:H	2.23	0.41
3:C:101:THR:HG21	3:C:161:VAL:CG2	2.50	0.41
2:B:95:GLN:HB3	2:B:96:PRO:HD2	2.02	0.41
3:C:104:ASP:HB3	3:C:107:SER:H	1.85	0.41
2:B:6:GLN:HB2	2:B:118:GLN:HG3	2.01	0.41
2:B:45:LYS:HD2	2:B:45:LYS:HA	1.84	0.41
3:F:123:TYR:N	3:F:140:THR:O	2.48	0.41
1:A:56:ILE:HG12	1:A:57:SER:H	1.86	0.41
3:C:244:ARG:N	3:C:257:ILE:O	2.47	0.41
1:A:163:GLY:HA3	1:A:205:VAL:HG12	2.02	0.40
1:A:217:THR:HB	1:A:234:LYS:HE3	2.04	0.40
2:B:123:GLU:OE2	2:B:184:GLN:HG3	2.22	0.40
2:B:93:SER:O	2:B:94:LEU:HB2	2.21	0.40
3:F:267:GLU:HB3	3:F:290:CYS:SG	2.61	0.40
3:C:93:ARG:HG2	3:C:95:PHE:CE1	2.57	0.40
3:C:224:ALA:O	3:C:226:VAL:N	2.54	0.40
3:C:233:HIS:HB2	3:C:273:CYS:HB2	2.04	0.40
2:B:43:GLN:CG	2:B:100:ALA:HB3	2.50	0.40
2:B:52:LEU:HD12	2:B:53:LEU:N	2.36	0.40
3:F:56:GLN:HG3	3:F:64:ILE:HB	2.03	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	229/236 (97%)	215 (94%)	13 (6%)	1 (0%)	30	68
2	B	208/211 (99%)	190 (91%)	18 (9%)	0	100	100
3	C	290/308 (94%)	248 (86%)	42 (14%)	0	100	100
3	F	295/308 (96%)	250 (85%)	42 (14%)	3 (1%)	13	48
All	All	1022/1063 (96%)	903 (88%)	115 (11%)	4 (0%)	30	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	SER
3	F	160	HIS
3	F	136	LYS
3	F	221	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	188/198 (95%)	182 (97%)	6 (3%)	34	54
2	B	173/184 (94%)	171 (99%)	2 (1%)	67	79
3	C	229/256 (90%)	223 (97%)	6 (3%)	41	60
3	F	234/256 (91%)	221 (94%)	13 (6%)	17	39
All	All	824/894 (92%)	797 (97%)	27 (3%)	33	54

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	SER
1	A	134	THR
1	A	137	ASN
1	A	138	GLN
1	A	233	LYS
1	A	240	CYS
2	B	23	CYS
2	B	104	CYS
3	F	40	GLU
3	F	70	CYS
3	F	105	CYS
3	F	123	TYR
3	F	126	SER
3	F	156	PHE
3	F	160	HIS
3	F	230	CYS
3	F	291	LEU
3	F	293	CYS
3	F	307	CYS
3	F	311	GLU
3	F	322	SER
3	C	56	GLN
3	C	57	ASN
3	C	58	ILE
3	C	70	CYS
3	C	105	CYS
3	C	309	CYS

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

Mol	Chain	Res	Type
3	F	79	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](#)

Of 2 ligands modelled in this entry, 2 are 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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

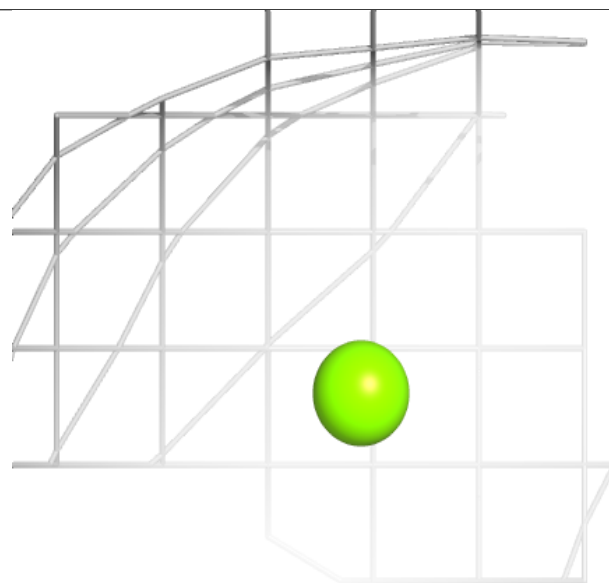
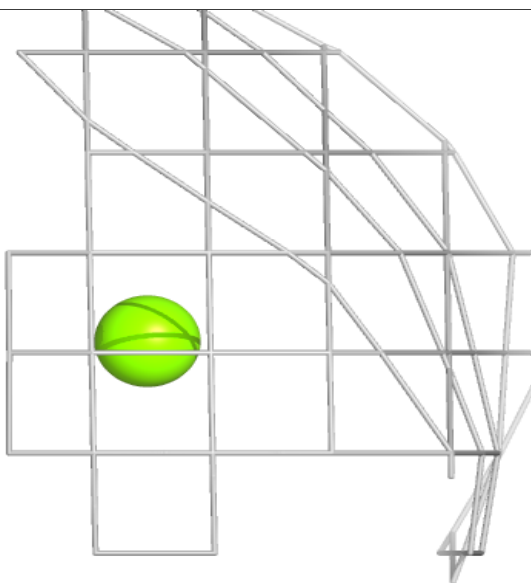
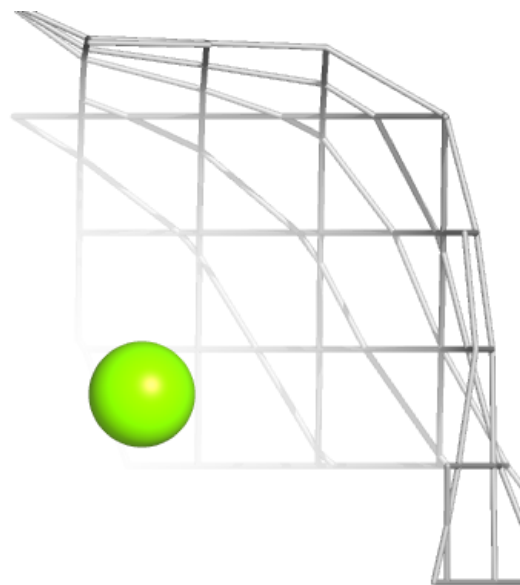
### 6.4 Ligands

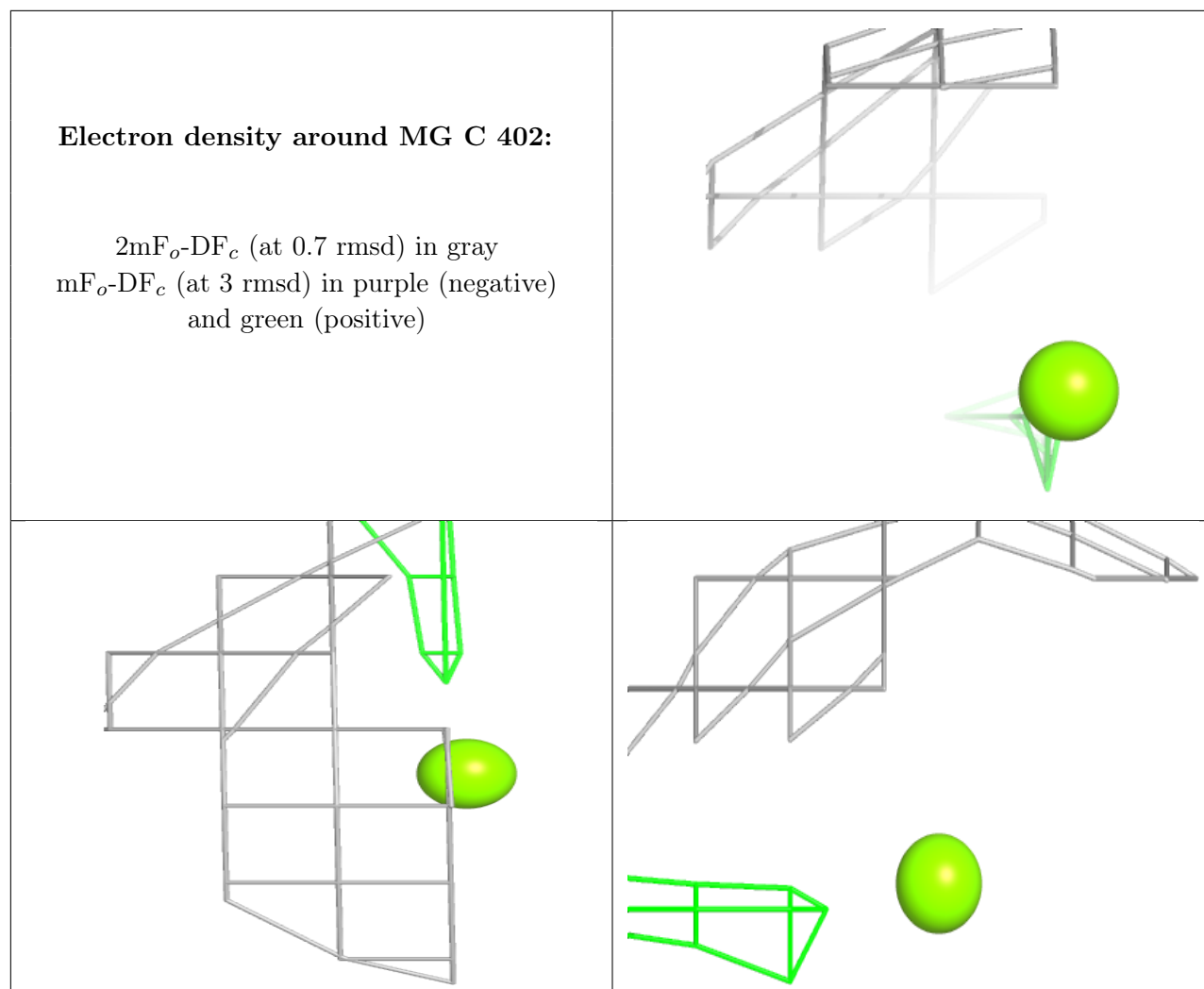
Unable to reproduce the depositors R factor - this section is therefore empty.

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 MG C 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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.