



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:21 AM UTC

PDB ID : 8TV5 / pdb_00008tv5
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

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
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

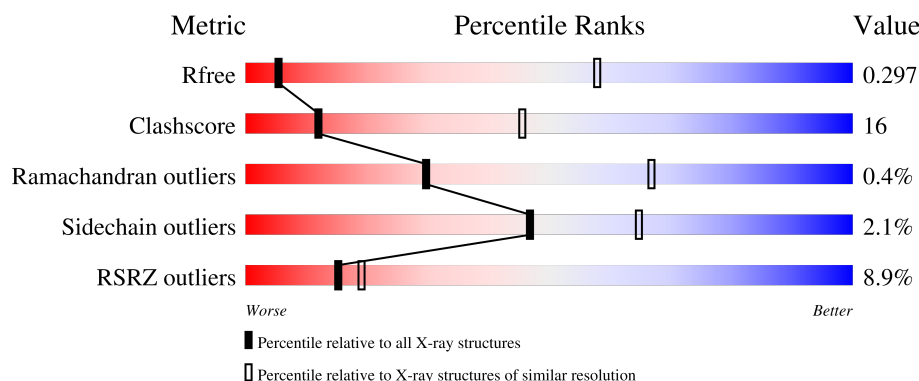
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1007 (5.28-3.92)
Clashscore	190562	1022 (5.26-3.94)
Ramachandran outliers	187476	1069 (5.30-3.90)
Sidechain outliers	187428	1051 (5.30-3.90)
RSRZ outliers	180081	1002 (5.28-3.92)

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	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
1	A	231	Total	C	N	O	S	0	0	0
			1723	1097	283	337	6			

- Molecule 2 is a protein called S1CE variant of Fab_L1 light chain.

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

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

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

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

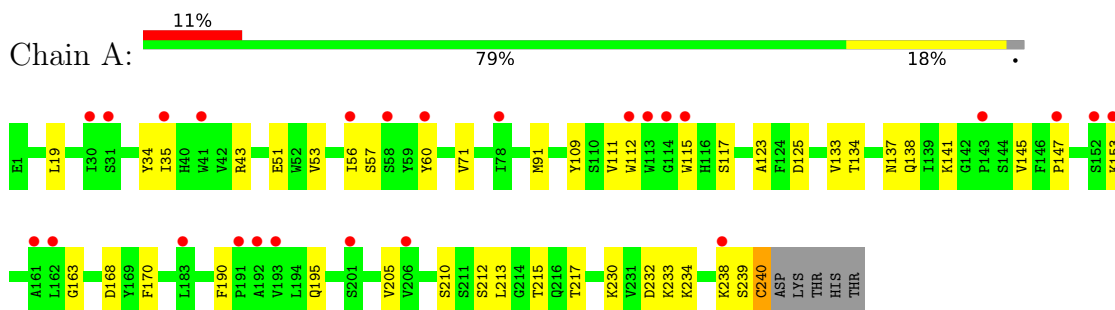
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	Mg	0	0
			2	2		

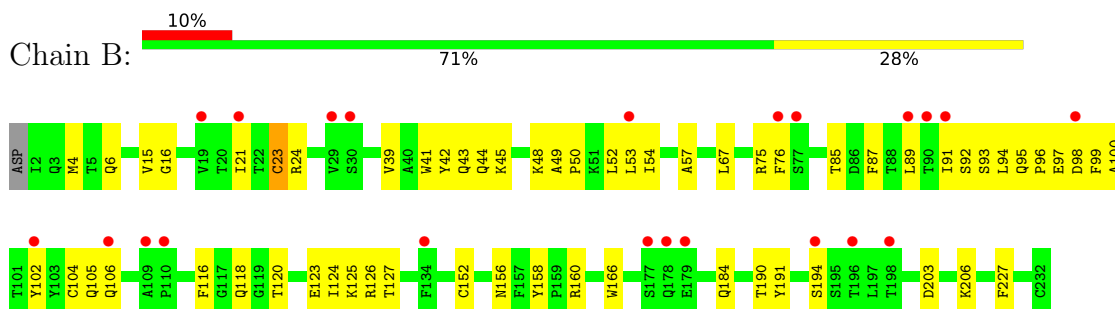
3 Residue-property plots

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 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.

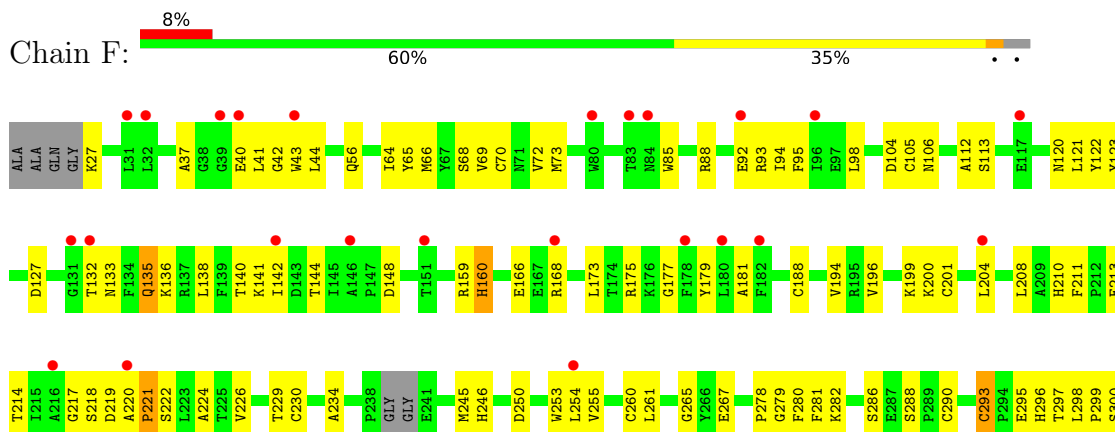
- Molecule 1: S1CE variant of Fab_L1 heavy chain



- Molecule 2: S1CE variant of Fab_L1 light chain



- Molecule 3: Ephrin type-A receptor 2





● Molecule 3: Ephrin type-A receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 4.66Å)	Xtriage
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	912 reflections (9.27%)	wwPDB-VP
Wilson B-factor (Å ²)	160.0	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 576.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	7736	wwPDB-VP
Average B, all atoms (Å ²)	267.0	wwPDB-VP

Xtriage'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.*

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: 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	0.21	0/1773	0.38	0/2427
2	B	0.13	0/1590	0.34	0/2169
3	C	0.19	0/2266	0.54	5/3090 (0.2%)
3	F	0.20	0/2306	0.64	5/3150 (0.2%)
All	All	0.19	0/7935	0.51	10/10836 (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 (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	135	GLN	CA-C-N	7.46	135.79	121.54
3	F	135	GLN	C-N-CA	7.46	135.79	121.54
3	F	159	ARG	CA-C-N	7.36	135.59	121.54
3	F	159	ARG	C-N-CA	7.36	135.59	121.54
3	C	160	HIS	CA-C-N	-5.87	114.82	122.51
3	C	160	HIS	C-N-CA	-5.87	114.82	122.51
3	F	160	HIS	N-CA-C	-5.66	98.75	110.80
3	C	159	ARG	CA-C-N	-5.42	115.00	122.16
3	C	159	ARG	C-N-CA	-5.42	115.00	122.16
3	C	41	LEU	CB-CG-CD1	5.22	126.35	110.70

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

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	47	0
3	C	2208	0	2019	84	0
3	F	2246	0	2038	78	0
4	C	2	0	0	0	0
All	All	7736	0	7145	234	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 16.

All (234) 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	0.83
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:CD	1:A:170:PHE:CB	2.67	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: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
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
1:A:138:GLN:CD	1:A:170:PHE:CG	2.78	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:F:282:LYS:NZ	3:F:288:SER:O	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:66:MET:HE3	3:F:68:SER:HB2	1.88	0.56
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:F:320:PRO:HD2	3:F:323:MET:HE3	1.88	0.55
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:138:GLN:CD	1:A:170:PHE:CD1	2.83	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
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:F:219:ASP:C	3:F:221:PRO:HD3	2.32	0.54
3:C:98:LEU:HD22	3:C:194:VAL:HG22	1.90	0.54
3:C:59:MET:HE2	3:C:59:MET:HA	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:NE	1:A:51:GLU:OE1	2.44	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:F:72:VAL:HG23	3:F:73:MET:HG2	1.93	0.50
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
2:B:97:GLU:CD	2:B:97:GLU:H	2.19	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:C:310:GLU:HG2	3:C:311:GLU:N	2.26	0.50
3:F:133:ASN:OD1	3:F:133:ASN:O	2.30	0.50
3:F:318:GLN:CD	3:F:318:GLN:H	2.20	0.49
3:C:199:LYS:HB2	3:C:216:ALA:HB2	1.93	0.49
3:F:315:ARG:HA	3:F:325:CYS:HA	1.94	0.49
2:B:4:MET:HE2	2:B:106:GLN:HB3	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:104:ASP:C	3:C:106:ASN:H	2.23	0.47
1:A:35:ILE:HB	1:A:56:ILE:HG22	1.97	0.47
2:B:45:LYS:HZ2	2:B:100:ALA:HB2	1.79	0.47
3:F:204:LEU:HB2	3:F:245:MET:HE1	1.95	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
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
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: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:120:ASN:OD1	3:F:144:THR:OG1	2.35	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:66:MET:HE1	3:C:190:ALA:HB1	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:199:LYS:HZ3	3:F:250:ASP:HA	1.83	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
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:222:SER:C	3:F:224:ALA:H	2.28	0.41
3:F:94:ILE:HG23	3:F:173:LEU:HD11	2.02	0.41
3:C:203:GLU:CD	3:C:212:PRO:HA	2.45	0.41
3:F:211:PHE:CD2	3:F:245:MET:HE2	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:305:THR:O	3:C:306:SER:C	2.64	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:104:ASP:C	3:C:106:ASN:N	2.78	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
3:C:66:MET:HE2	3:C:66:MET:HB2	2.00	0.40
3:C:126:SER:OG	3:C:128:LEU:O	2.39	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	67
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%)	12	47
All	All	1022/1063 (96%)	903 (88%)	115 (11%)	4 (0%)	30	67

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 ⓘ

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%)	184 (98%)	4 (2%)	47	65
2	B	173/184 (94%)	171 (99%)	2 (1%)	63	73
3	C	229/256 (90%)	223 (97%)	6 (3%)	40	60
3	F	234/256 (91%)	229 (98%)	5 (2%)	47	65
All	All	824/894 (92%)	807 (98%)	17 (2%)	47	65

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	THR
1	A	137	ASN
1	A	141	LYS
1	A	240	CYS
2	B	23	CYS
2	B	104	CYS
3	F	70	CYS
3	F	105	CYS
3	F	230	CYS
3	F	293	CYS
3	F	307	CYS
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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	129	GLN
2	B	118	GLN
3	F	77	GLN
3	F	135	GLN
3	C	56	GLN
3	C	60	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 ⓘ

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	231/236 (97%)	0.56	25 (10%)	11 15	205, 249, 277, 314	0
2	B	210/211 (99%)	0.63	22 (10%)	11 16	208, 268, 333, 348	0
3	C	294/308 (95%)	0.46	19 (6%)	25 26	149, 241, 387, 404	0
3	F	299/308 (97%)	0.47	26 (8%)	16 19	175, 257, 435, 448	0
All	All	1034/1063 (97%)	0.52	92 (8%)	15 19	149, 253, 399, 448	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	40	GLU	7.4
2	B	76	PHE	5.9
1	A	152	SER	5.7
2	B	30	SER	5.3
1	A	113	TRP	5.2
3	C	39	GLY	5.2
3	C	40	GLU	5.0
1	A	143	PRO	4.6
3	C	315	ARG	4.5
3	F	39	GLY	4.5
2	B	110	PRO	4.5
3	C	257	ILE	4.3
3	C	271	ASP	4.3
1	A	147	PRO	4.0
2	B	90	THR	4.0
3	C	118	THR	4.0
3	F	180	LEU	3.9
1	A	114	GLY	3.8
1	A	206	VAL	3.7
2	B	29	VAL	3.6
3	F	80	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	255	VAL	3.5
3	F	182	PHE	3.5
2	B	102	TYR	3.5
2	B	178	GLN	3.4
2	B	198	THR	3.4
3	C	272	ALA	3.3
2	B	98	ASP	3.3
1	A	41	TRP	3.3
3	F	31	LEU	3.2
2	B	196	THR	3.1
3	C	119	PHE	3.1
2	B	177	SER	3.0
2	B	91	ILE	3.0
3	F	32	LEU	3.0
1	A	30	ILE	3.0
2	B	89	LEU	3.0
2	B	77	SER	2.9
3	F	305	THR	2.9
2	B	21	ILE	2.9
1	A	153	LYS	2.8
1	A	115	TRP	2.7
1	A	31	SER	2.7
1	A	201	SER	2.6
2	B	109	ALA	2.6
3	C	84	ASN	2.6
1	A	58	SER	2.6
1	A	35	ILE	2.6
3	C	43	TRP	2.6
3	F	117	GLU	2.6
2	B	19	VAL	2.6
3	F	309	CYS	2.5
3	F	84	ASN	2.5
3	C	74	SER	2.5
1	A	183	LEU	2.4
3	F	204	LEU	2.4
3	F	178	PHE	2.4
2	B	106	GLN	2.4
1	A	56	ILE	2.4
1	A	192	ALA	2.4
1	A	112	TRP	2.4
3	F	83	THR	2.4
3	F	142	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	60	TYR	2.3
3	C	192	LEU	2.3
3	F	254	LEU	2.3
1	A	161	ALA	2.3
3	C	117	GLU	2.3
3	C	213	GLU	2.3
3	C	59	MET	2.3
1	A	191	PRO	2.2
1	A	193	VAL	2.2
2	B	179	GLU	2.2
3	F	216	ALA	2.2
3	F	96	ILE	2.2
3	F	168	ARG	2.2
3	F	220	ALA	2.2
1	A	162	LEU	2.1
1	A	238	LYS	2.1
3	F	151	THR	2.1
3	C	68	SER	2.1
3	F	131	GLY	2.1
2	B	194	SER	2.1
3	F	132	THR	2.1
3	C	132	THR	2.1
2	B	53	LEU	2.0
1	A	78	ILE	2.0
3	F	146	ALA	2.0
3	F	92	GLU	2.0
3	C	254	LEU	2.0
3	F	43	TRP	2.0
2	B	134	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

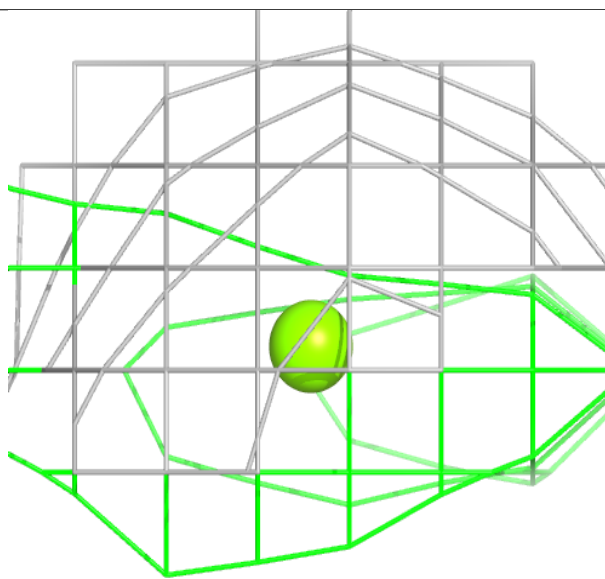
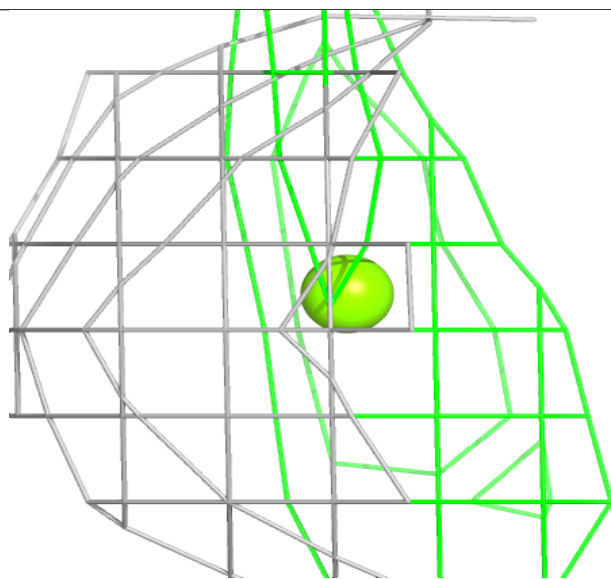
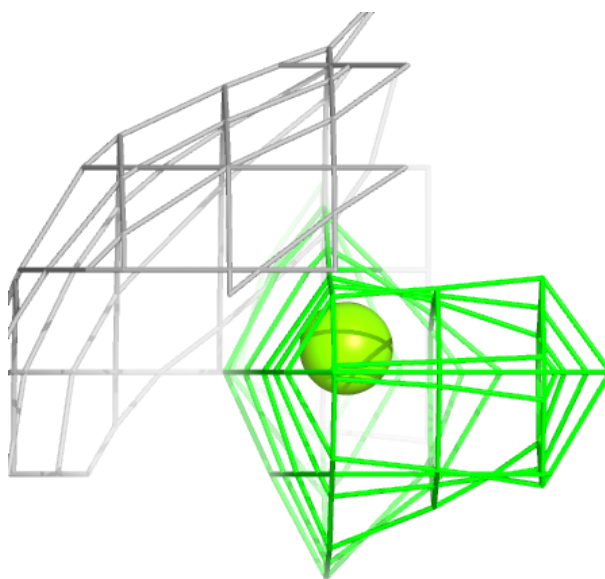
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	C	402	1/1	0.63	0.32	255,255,255,255	0
4	MG	C	401	1/1	0.81	0.13	224,224,224,224	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.

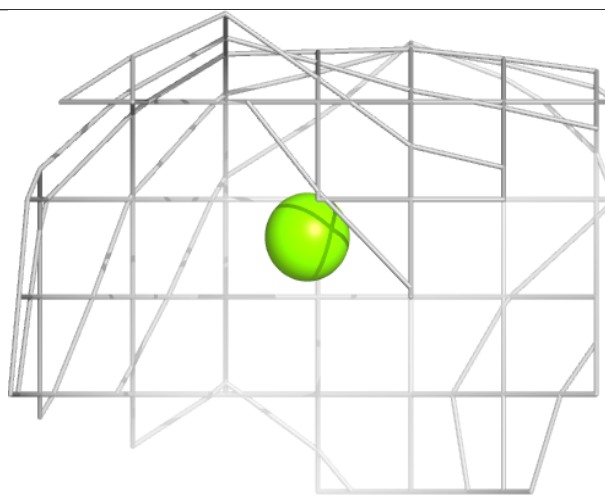
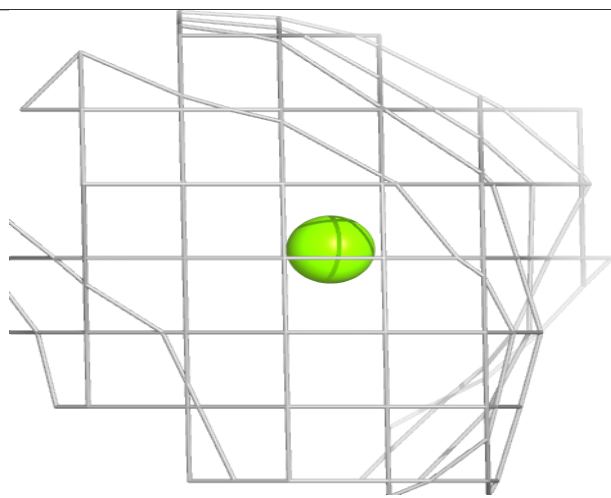
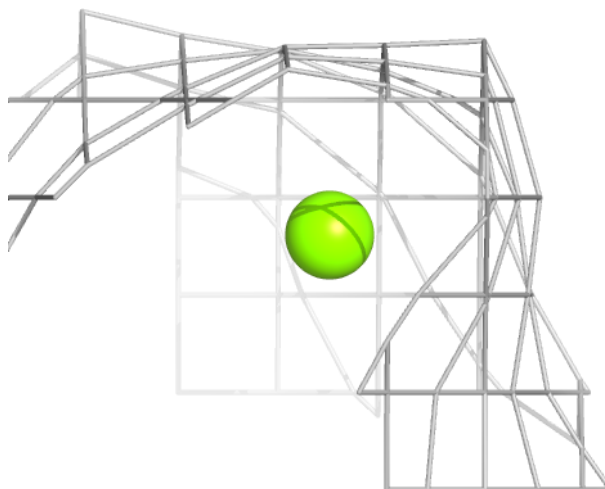
Electron density around MG C 402:

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



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](#)

There are no such residues in this entry.