



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:11 PM UTC

PDB ID : 7PHW / pdb_00007phw
Title : PfCyRPA bound to monoclonal antibody Cy.004 Fab fragment
Authors : Ragotte, R.J.; Higgins, M.K.
Deposited on : 2021-08-18
Resolution : 2.79 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

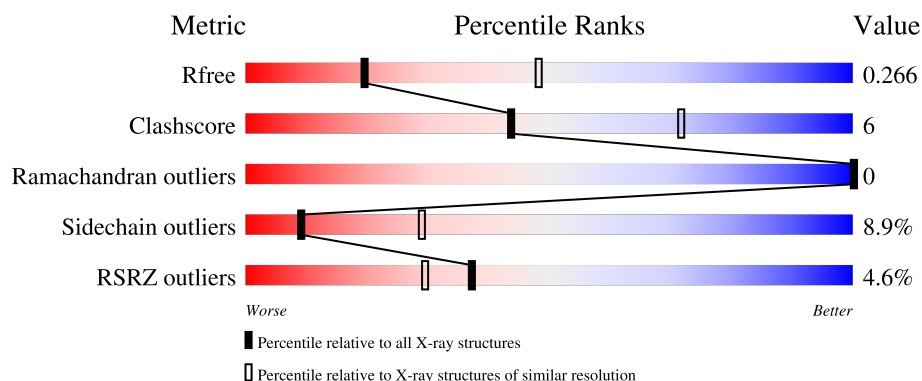
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	343	5% 70% 20% 8%
1	D	343	8% 70% 19% 9%
2	B	321	2% 61% 7% 31%
2	E	321	2% 60% 8% 30%
3	C	209	% 83% 15% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	209	3% 83% 14% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11683 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 Cysteine-rich protective antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2648	1708	424	503	13			
1	D	312	Total	C	N	O	S	0	0	0
			2599	1677	415	494	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ALA	SER	conflict	UNP Q8IFM8
A	324	ALA	THR	conflict	UNP Q8IFM8
A	340	ALA	THR	conflict	UNP Q8IFM8
A	363	GLY	-	expression tag	UNP Q8IFM8
A	364	GLY	-	expression tag	UNP Q8IFM8
A	365	GLY	-	expression tag	UNP Q8IFM8
A	366	GLY	-	expression tag	UNP Q8IFM8
A	367	SER	-	expression tag	UNP Q8IFM8
A	368	GLU	-	expression tag	UNP Q8IFM8
A	369	PRO	-	expression tag	UNP Q8IFM8
A	370	GLU	-	expression tag	UNP Q8IFM8
A	371	ALA	-	expression tag	UNP Q8IFM8
D	147	ALA	SER	conflict	UNP Q8IFM8
D	324	ALA	THR	conflict	UNP Q8IFM8
D	340	ALA	THR	conflict	UNP Q8IFM8
D	363	GLY	-	expression tag	UNP Q8IFM8
D	364	GLY	-	expression tag	UNP Q8IFM8
D	365	GLY	-	expression tag	UNP Q8IFM8
D	366	GLY	-	expression tag	UNP Q8IFM8
D	367	SER	-	expression tag	UNP Q8IFM8
D	368	GLU	-	expression tag	UNP Q8IFM8
D	369	PRO	-	expression tag	UNP Q8IFM8
D	370	GLU	-	expression tag	UNP Q8IFM8
D	371	ALA	-	expression tag	UNP Q8IFM8

- Molecule 2 is a protein called Monoclonal antibody Cy.004 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	223	Total	C	N	O	S	0	0	0
			1634	1023	277	329	5			
2	E	226	Total	C	N	O	S	0	1	0
			1655	1034	280	335	6			

- Molecule 3 is a protein called Monoclonal antibody Cy.004 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	209	Total	C	N	O	S	0	0	0
			1577	978	265	329	5			
3	F	207	Total	C	N	O	S	0	0	0
			1566	972	263	327	4			

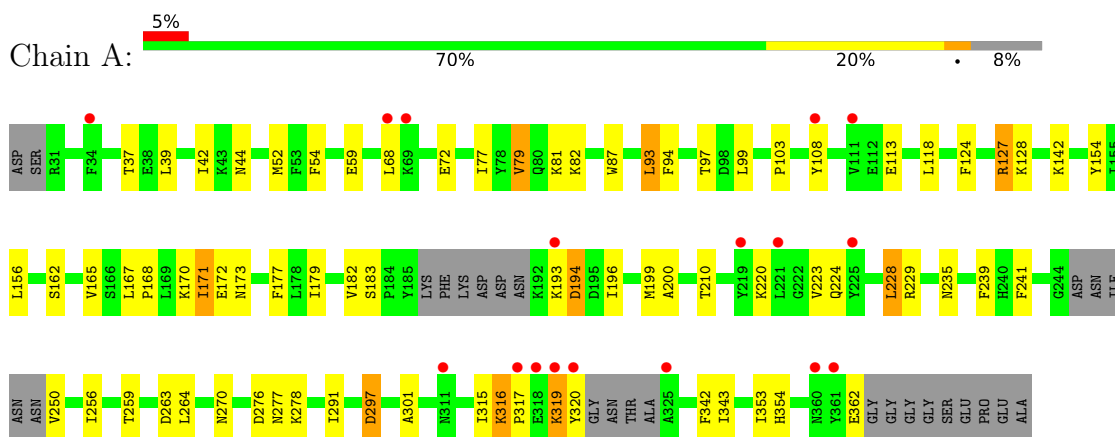
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	E	1	Total	Ca	0	0
			1	1		

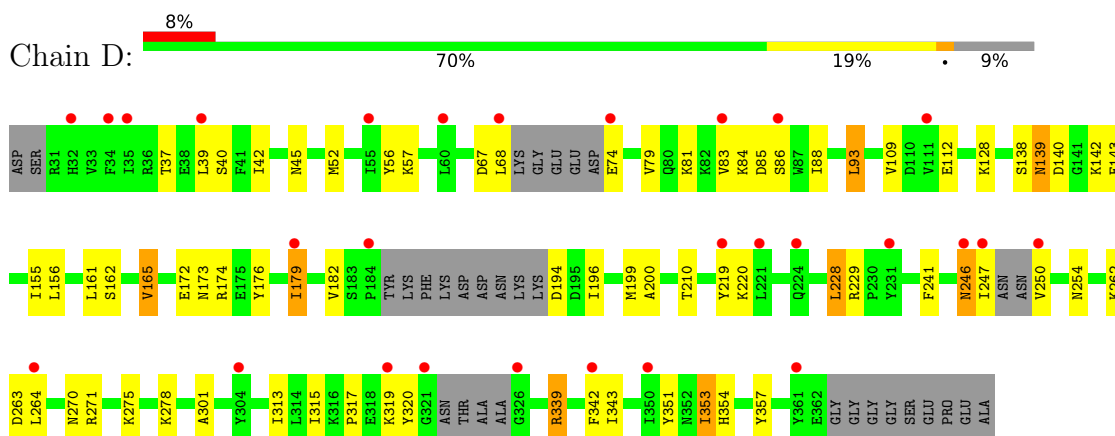
3 Residue-property plots [i](#)

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.

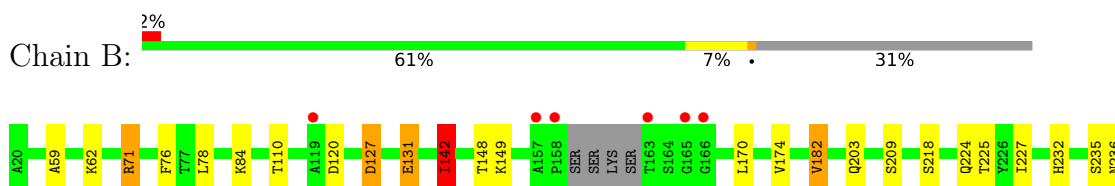
- Molecule 1: Cysteine-rich protective antigen

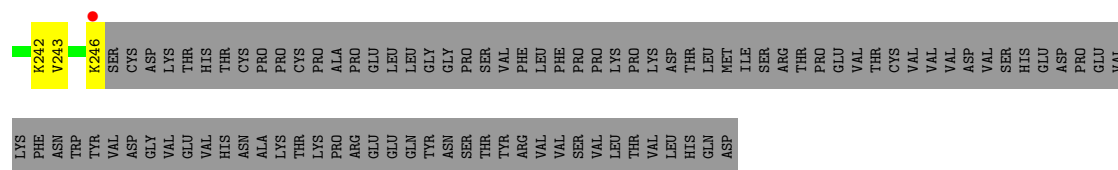


- Molecule 1: Cysteine-rich protective antigen

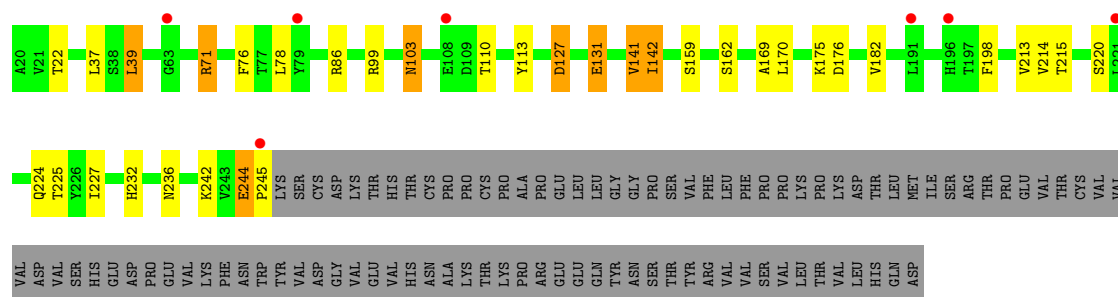


- Molecule 2: Monoclonal antibody Cy.004 heavy chain

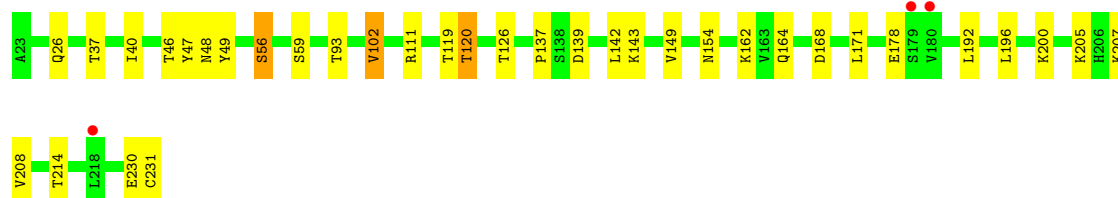
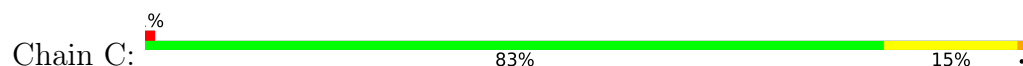




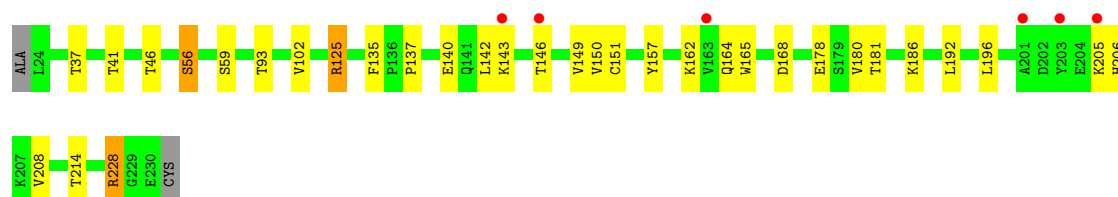
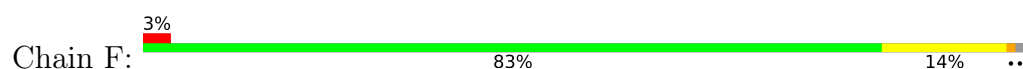
- Molecule 2: Monoclonal antibody Cy.004 heavy chain



- Molecule 3: Monoclonal antibody Cy.004 light chain



- Molecule 3: Monoclonal antibody Cy.004 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.06Å 80.32Å 114.91Å 90.00° 115.23° 90.00°	Depositor
Resolution (Å)	47.11 – 2.79 47.11 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.11-2.79) 99.0 (47.11-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.4 (24-FEB-2021)	Depositor
R, R_{free}	0.239 , 0.277 0.225 , 0.266	Depositor DCC
R_{free} test set	2164 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.628	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11683	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5323e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CA

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	0.78	1/2708 (0.0%)	1.08	10/3652 (0.3%)
1	D	0.72	0/2657	1.08	7/3585 (0.2%)
2	B	0.78	1/1670 (0.1%)	1.03	1/2273 (0.0%)
2	E	0.72	0/1695	1.04	3/2308 (0.1%)
3	C	0.73	0/1610	1.05	6/2192 (0.3%)
3	F	0.71	0/1599	1.05	0/2177
All	All	0.74	2/11939 (0.0%)	1.06	27/16187 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	GLU	CA-C	-8.08	1.42	1.52
2	B	142	ILE	CG1-CD1	5.59	1.73	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ASN	CA-CB-CG	8.56	121.16	112.60
2	E	103	ASN	CA-CB-CG	6.72	119.33	112.60
1	A	316	LYS	N-CA-C	-6.52	98.97	109.40
1	A	297	ASP	CA-CB-CG	6.39	118.99	112.60
1	D	86	SER	N-CA-C	6.30	118.65	108.32
1	A	154	TYR	CA-C-N	6.11	130.31	120.30
1	A	154	TYR	C-N-CA	6.11	130.31	120.30
2	B	127	ASP	CA-CB-CG	6.10	118.70	112.60
2	E	127	ASP	CA-CB-CG	6.10	118.70	112.60
3	C	48	ASN	N-CA-C	5.89	118.73	109.96
1	A	171	ILE	CA-C-O	-5.88	113.43	120.78
1	A	113	GLU	N-CA-C	5.85	119.59	110.17
3	C	154	ASN	N-CA-C	5.79	118.83	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	176	ASP	N-CA-C	5.64	118.07	111.02
1	D	139	ASN	N-CA-C	-5.51	107.56	114.56
1	D	67	ASP	CA-C-N	5.46	131.53	121.70
1	D	67	ASP	C-N-CA	5.46	131.53	121.70
1	D	246	ASN	N-CA-C	-5.46	105.66	112.93
3	C	47	TYR	CA-C-N	5.35	128.93	121.02
3	C	47	TYR	C-N-CA	5.35	128.93	121.02
1	D	74	GLU	CA-C-N	5.21	129.81	122.09
1	D	74	GLU	C-N-CA	5.21	129.81	122.09
3	C	49	TYR	CA-C-N	5.16	125.74	122.18
3	C	49	TYR	C-N-CA	5.16	125.74	122.18
1	A	194	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	291	ILE	N-CA-CB	5.13	118.31	111.64
1	A	79	VAL	N-CA-CB	5.05	116.76	111.00

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	2648	0	2548	35	0
1	D	2599	0	2494	57	0
2	B	1634	0	1582	11	0
2	E	1655	0	1602	15	0
3	C	1577	0	1513	16	0
3	F	1566	0	1503	13	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
All	All	11683	0	11242	139	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 6.

All (139) 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:D:83:VAL:HG21	1:D:88:ILE:CD1	1.66	1.23
2:E:127:ASP:HA	2:E:131:GLU:HG3	1.29	1.10
2:B:127:ASP:HA	2:B:131:GLU:HG3	1.29	1.10
1:D:83:VAL:HG21	1:D:88:ILE:HD12	1.11	1.09
3:C:40:ILE:HG21	3:C:119:THR:HG21	1.43	1.00
1:D:83:VAL:CG2	1:D:88:ILE:HD12	1.97	0.93
1:D:57:LYS:NZ	1:D:112:GLU:HG2	1.88	0.88
1:D:57:LYS:HZ1	1:D:112:GLU:HG2	1.37	0.87
1:D:81:LYS:NZ	1:D:142:LYS:HE2	1.89	0.87
1:A:42:ILE:HD13	1:A:353:ILE:HD12	1.55	0.85
1:D:83:VAL:CG2	1:D:88:ILE:CD1	2.53	0.84
1:A:316:LYS:O	1:A:319:LYS:HE2	1.77	0.83
1:D:83:VAL:HG12	1:D:84:LYS:H	1.43	0.81
1:D:81:LYS:HZ1	1:D:142:LYS:HE2	1.49	0.75
1:D:83:VAL:HG12	1:D:84:LYS:N	2.03	0.73
1:A:52:MET:HG2	1:A:165:VAL:HG23	1.70	0.73
3:F:125:ARG:HD2	3:F:157:TYR:CG	2.26	0.70
1:A:39:LEU:HD13	1:A:354:HIS:CE1	2.28	0.69
1:A:301:ALA:O	1:A:317:PRO:HD2	1.93	0.69
1:D:39:LEU:HD13	1:D:354:HIS:CE1	2.28	0.69
1:A:277:ASN:HD21	1:D:57:LYS:NZ	1.92	0.67
1:D:83:VAL:HG21	1:D:88:ILE:HD11	1.71	0.67
2:B:71:ARG:HG3	2:B:76:PHE:HB3	1.75	0.67
3:C:40:ILE:CG2	3:C:119:THR:HG21	2.21	0.66
1:D:52:MET:HG2	1:D:165:VAL:HG13	1.79	0.64
1:D:56:TYR:OH	1:D:139:ASN:O	2.16	0.63
2:E:71:ARG:HG3	2:E:76:PHE:HB3	1.81	0.63
1:A:170:LYS:HB2	1:A:235:ASN:HD21	1.64	0.62
1:D:81:LYS:HZ3	1:D:142:LYS:HE2	1.63	0.61
1:D:52:MET:HG2	1:D:165:VAL:CG1	2.30	0.61
1:D:179:ILE:HG23	1:D:199:MET:HG3	1.83	0.61
1:A:200:ALA:HB3	1:A:210:THR:HB	1.84	0.59
3:F:137:PRO:HD3	3:F:149:VAL:HG22	1.84	0.59
1:D:93:LEU:HD23	1:D:93:LEU:N	2.17	0.59
1:A:167:LEU:HB2	1:A:168:PRO:HD2	1.84	0.58
1:A:316:LYS:O	1:A:319:LYS:CE	2.49	0.57
2:E:127:ASP:CA	2:E:131:GLU:HG3	2.19	0.57
1:D:219:TYR:CE2	1:D:220:LYS:NZ	2.73	0.57
1:D:83:VAL:CG1	1:D:84:LYS:H	2.16	0.57
1:D:40:SER:HB3	1:D:353:ILE:HD11	1.87	0.56
1:D:81:LYS:NZ	1:D:142:LYS:CE	2.68	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:ASP:CA	2:B:131:GLU:HG3	2.20	0.56
2:E:110:THR:HG23	2:E:142:ILE:HA	1.88	0.56
1:D:140:ASP:OD1	1:D:143:GLU:N	2.36	0.54
2:B:110:THR:HG23	2:B:142:ILE:HA	1.90	0.54
1:A:124:PHE:HA	1:A:127:ARG:HD3	1.90	0.54
1:A:79:VAL:HG23	1:A:93:LEU:HD11	1.90	0.53
3:C:137:PRO:HD3	3:C:149:VAL:HG22	1.90	0.53
1:D:138:SER:HB2	1:D:143:GLU:O	2.09	0.52
2:E:113:TYR:CD1	2:E:141:VAL:HG13	2.44	0.52
2:E:182:VAL:HG12	2:E:232:HIS:CD2	2.44	0.52
1:D:37:THR:HG21	1:D:313:ILE:HD13	1.91	0.52
3:C:139:ASP:O	3:C:143:LYS:HG2	2.11	0.51
1:A:108:TYR:OH	1:A:179:ILE:HG13	2.10	0.51
2:E:227:ILE:HG12	2:E:242:LYS:HA	1.93	0.51
3:F:140:GLU:HA	3:F:143:LYS:HZ2	1.76	0.50
3:F:140:GLU:HA	3:F:143:LYS:NZ	2.26	0.50
1:A:77:ILE:HG22	1:A:93:LEU:HD12	1.93	0.50
2:B:227:ILE:HG12	2:B:242:LYS:HA	1.93	0.49
1:A:59:GLU:OE1	1:A:81:LYS:HE2	2.11	0.49
3:C:142:LEU:O	3:C:200:LYS:HD2	2.12	0.49
1:A:277:ASN:ND2	1:D:57:LYS:NZ	2.60	0.49
1:D:81:LYS:HZ1	1:D:142:LYS:CE	2.22	0.49
1:D:339:ARG:HD2	1:D:357:TYR:CE2	2.48	0.48
3:F:162:LYS:HB3	3:F:214:THR:HB	1.95	0.48
2:B:182:VAL:HG23	2:B:232:HIS:HD2	1.78	0.48
2:E:244:GLU:HG2	2:E:245:PRO:HD2	1.95	0.48
1:D:93:LEU:HD23	1:D:93:LEU:H	1.78	0.48
1:D:57:LYS:HZ3	1:D:112:GLU:HG2	1.75	0.47
1:D:343:ILE:HG12	1:D:353:ILE:HG22	1.96	0.47
1:D:138:SER:CB	1:D:143:GLU:O	2.62	0.47
1:A:343:ILE:HG12	1:A:353:ILE:HG12	1.96	0.47
2:B:174:VAL:HG11	2:B:182:VAL:HG11	1.95	0.47
1:A:156:LEU:HG	1:A:199:MET:HG3	1.97	0.47
3:C:119:THR:O	3:C:119:THR:HG23	2.14	0.47
3:C:168:ASP:HA	3:C:208:VAL:HG13	1.97	0.47
3:C:162:LYS:HB3	3:C:214:THR:HB	1.96	0.47
1:D:83:VAL:CG1	1:D:84:LYS:N	2.72	0.47
1:A:277:ASN:ND2	1:D:57:LYS:HZ1	2.12	0.46
2:E:162:SER:OG	2:E:169:ALA:O	2.32	0.46
1:D:79:VAL:HG23	1:D:93:LEU:HD21	1.98	0.46
1:A:99:LEU:HD13	1:A:103:PRO:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:TYR:OH	1:A:179:ILE:CG1	2.64	0.46
1:D:156:LEU:HD13	1:D:161:LEU:HD11	1.98	0.46
1:D:319:LYS:HG3	1:D:320:TYR:CD2	2.51	0.45
2:E:159:SER:H	2:E:162:SER:HB3	1.81	0.45
2:B:182:VAL:HG23	2:B:232:HIS:CD2	2.50	0.45
1:D:140:ASP:OD2	1:D:142:LYS:HB2	2.17	0.45
3:C:102:VAL:HA	3:C:120:THR:HA	1.99	0.45
3:F:168:ASP:HA	3:F:208:VAL:HG13	1.97	0.45
2:E:37:LEU:CD1	2:E:39:LEU:HD22	2.46	0.45
1:A:108:TYR:HB3	1:A:177:PHE:CE1	2.53	0.44
3:C:230:GLU:O	3:C:231:CYS:HB3	2.18	0.44
1:D:83:VAL:CG2	1:D:88:ILE:CG1	2.95	0.44
2:E:182:VAL:CG1	2:E:232:HIS:CD2	2.99	0.44
1:A:228:LEU:HA	1:A:241:PHE:HB3	1.99	0.44
1:D:42:ILE:HB	1:D:351:TYR:HB2	2.00	0.44
1:A:54:PHE:HB3	1:A:165:VAL:HG11	2.00	0.44
1:D:155:ILE:HD11	1:D:199:MET:HB3	2.00	0.44
1:D:200:ALA:HB3	1:D:210:THR:HB	1.99	0.44
1:A:94:PHE:CE2	3:C:111:ARG:NH2	2.86	0.44
3:F:206:HIS:O	3:F:228:ARG:HD2	2.18	0.44
1:D:219:TYR:HE2	1:D:220:LYS:NZ	2.15	0.44
3:F:56:SER:O	3:F:59:SER:HB3	2.18	0.44
1:A:342:PHE:HB3	1:A:354:HIS:HB2	1.99	0.43
1:A:42:ILE:HG22	1:A:87:TRP:CD1	2.52	0.43
1:D:228:LEU:HA	1:D:241:PHE:HB3	1.99	0.43
3:F:178:GLU:HB2	3:F:192:LEU:HD21	2.01	0.43
1:A:276:ASP:HB3	1:D:112:GLU:OE1	2.18	0.43
2:E:198:PHE:CD2	3:F:181:THR:HG23	2.54	0.43
1:D:40:SER:HB3	1:D:353:ILE:CD1	2.48	0.43
3:C:56:SER:O	3:C:59:SER:HB3	2.19	0.42
1:D:246:ASN:HB2	1:D:247:ILE:HD12	2.01	0.42
3:C:26:GLN:NE2	3:C:119:THR:HG22	2.35	0.42
2:B:59:ALA:HB3	2:B:62:LYS:HB2	2.00	0.42
1:D:179:ILE:HG23	1:D:199:MET:CG	2.49	0.42
1:D:83:VAL:CG2	1:D:88:ILE:HG13	2.50	0.42
3:C:37:THR:HG23	3:C:93:THR:HG22	2.02	0.42
1:D:342:PHE:HB3	1:D:354:HIS:HB2	2.01	0.42
1:D:301:ALA:O	1:D:317:PRO:HD2	2.20	0.41
3:F:151:CYS:HB2	3:F:165:TRP:CZ2	2.55	0.41
1:D:339:ARG:HD2	1:D:357:TYR:HE2	1.84	0.41
1:A:277:ASN:HD21	1:D:57:LYS:CE	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:THR:HG22	2:B:235:SER:HB3	2.01	0.41
2:E:182:VAL:CG1	2:E:232:HIS:HD2	2.33	0.41
1:A:97:THR:HG21	1:A:118:LEU:HD12	2.01	0.41
1:D:93:LEU:N	1:D:93:LEU:CD2	2.82	0.41
1:D:174:ARG:HD2	1:D:176:TYR:OH	2.21	0.41
1:A:171:ILE:HG22	1:A:172:GLU:HG3	2.03	0.41
3:C:178:GLU:HB2	3:C:192:LEU:HD21	2.03	0.41
3:F:37:THR:HG23	3:F:93:THR:HG22	2.03	0.41
1:A:44:ASN:HB2	1:A:87:TRP:HD1	1.86	0.41
3:F:135:PHE:HB2	3:F:150:VAL:HB	2.02	0.41
1:A:170:LYS:HB2	1:A:235:ASN:ND2	2.33	0.40
2:E:182:VAL:HG12	2:E:232:HIS:HD2	1.86	0.40
1:A:239:PHE:HB2	1:A:256:ILE:HG12	2.04	0.40
2:B:203:GLN:OE1	2:B:209:SER:HB2	2.21	0.40
1:D:319:LYS:H	1:D:319:LYS:HG2	1.66	0.40
1:A:99:LEU:O	3:C:111:ARG:NH1	2.53	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	309/343 (90%)	288 (93%)	21 (7%)	0	100	100
1	D	302/343 (88%)	283 (94%)	19 (6%)	0	100	100
2	B	219/321 (68%)	210 (96%)	9 (4%)	0	100	100
2	E	225/321 (70%)	214 (95%)	11 (5%)	0	100	100
3	C	207/209 (99%)	200 (97%)	7 (3%)	0	100	100
3	F	205/209 (98%)	197 (96%)	8 (4%)	0	100	100
All	All	1467/1746 (84%)	1392 (95%)	75 (5%)	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	297/316 (94%)	267 (90%)	30 (10%)	7	23
1	D	292/316 (92%)	264 (90%)	28 (10%)	8	26
2	B	179/272 (66%)	164 (92%)	15 (8%)	10	32
2	E	183/272 (67%)	163 (89%)	20 (11%)	6	21
3	C	180/180 (100%)	170 (94%)	10 (6%)	19	50
3	F	179/180 (99%)	166 (93%)	13 (7%)	13	38
All	All	1310/1536 (85%)	1194 (91%)	116 (9%)	9	29

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	68	LEU
1	A	72	GLU
1	A	82	LYS
1	A	93	LEU
1	A	127	ARG
1	A	128	LYS
1	A	142	LYS
1	A	162	SER
1	A	182	VAL
1	A	183	SER
1	A	193	LYS
1	A	194	ASP
1	A	196	ILE
1	A	220	LYS
1	A	223	VAL
1	A	224	GLN
1	A	228	LEU
1	A	229	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	250	VAL
1	A	259	THR
1	A	263	ASP
1	A	264	LEU
1	A	270	ASN
1	A	278	LYS
1	A	297	ASP
1	A	315	ILE
1	A	319	LYS
1	A	320	TYR
1	A	362	GLU
2	B	71	ARG
2	B	78	LEU
2	B	84	LYS
2	B	120	ASP
2	B	131	GLU
2	B	142	ILE
2	B	149	LYS
2	B	170	LEU
2	B	182	VAL
2	B	218	SER
2	B	224	GLN
2	B	225	THR
2	B	236	ASN
2	B	243	VAL
2	B	246	LYS
3	C	46	THR
3	C	56	SER
3	C	102	VAL
3	C	120	THR
3	C	126	THR
3	C	164	GLN
3	C	171	LEU
3	C	196	LEU
3	C	205	LYS
3	C	207	LYS
1	D	45	ASN
1	D	68	LEU
1	D	85	ASP
1	D	93	LEU
1	D	109	VAL
1	D	128	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	162	SER
1	D	165	VAL
1	D	172	GLU
1	D	173	ASN
1	D	179	ILE
1	D	182	VAL
1	D	194	ASP
1	D	196	ILE
1	D	228	LEU
1	D	229	ARG
1	D	250	VAL
1	D	254	ASN
1	D	262	LYS
1	D	263	ASP
1	D	264	LEU
1	D	270	ASN
1	D	271	ARG
1	D	275	LYS
1	D	278	LYS
1	D	315	ILE
1	D	339	ARG
1	D	353	ILE
2	E	22	THR
2	E	39	LEU
2	E	71	ARG
2	E	78	LEU
2	E	86	ARG
2	E	99	ARG
2	E	103	ASN
2	E	131	GLU
2	E	141	VAL
2	E	142	ILE
2	E	170	LEU
2	E	175	LYS
2	E	213	VAL
2	E	214	VAL
2	E	215	THR
2	E	220	SER
2	E	224	GLN
2	E	225	THR
2	E	236	ASN
2	E	244	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	41	THR
3	F	46	THR
3	F	56	SER
3	F	102	VAL
3	F	125	ARG
3	F	142	LEU
3	F	146	THR
3	F	164	GLN
3	F	180	VAL
3	F	186	LYS
3	F	196	LEU
3	F	205	LYS
3	F	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	76	HIS
1	A	91	ASN
1	A	277	ASN
1	A	287	ASN
1	A	338	ASN
1	A	348	GLN
2	B	101	GLN
3	C	33	ASN
3	C	216	GLN
3	C	227	ASN
1	D	76	HIS
1	D	91	ASN
1	D	145	ASN
1	D	224	GLN
1	D	287	ASN
1	D	338	ASN
2	E	236	ASN
3	F	33	ASN
3	F	53	GLN
3	F	216	GLN
3	F	227	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 4 ligands modelled in this entry, 4 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

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	317/343 (92%)	0.63	17 (5%) 31 24	52, 84, 125, 146	0
1	D	312/343 (90%)	1.04	28 (8%) 15 11	66, 103, 143, 159	0
2	B	223/321 (69%)	0.45	7 (3%) 51 41	53, 79, 102, 109	0
2	E	226/321 (70%)	0.52	7 (3%) 51 41	46, 89, 131, 138	1 (0%)
3	C	209/209 (100%)	0.37	3 (1%) 73 64	58, 77, 107, 115	0
3	F	207/209 (99%)	0.55	6 (2%) 53 43	53, 81, 137, 151	0
All	All	1494/1746 (85%)	0.63	68 (4%) 37 29	46, 85, 132, 159	1 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	68	LEU	5.8
1	D	321	GLY	5.8
1	A	325	ALA	4.5
1	A	320	TYR	4.5
1	A	361	TYR	4.4
1	D	34	PHE	4.0
3	F	163	VAL	3.7
1	D	250	VAL	3.6
1	D	221	LEU	3.5
1	D	219	TYR	3.4
1	D	247	ILE	3.4
1	D	350	ILE	3.3
2	B	119	ALA	3.3
1	D	246	ASN	3.3
1	D	231	TYR	3.0
3	C	180	VAL	3.0
2	E	245	PRO	3.0
2	B	158	PRO	2.9
1	A	319	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	317	PRO	2.9
1	D	319	LYS	2.7
3	F	203	TYR	2.7
1	A	111	VAL	2.7
3	F	205	LYS	2.7
1	D	179	ILE	2.7
1	D	264	LEU	2.6
2	E	63	GLY	2.6
1	D	32	HIS	2.6
1	D	74	GLU	2.6
2	B	165	GLY	2.6
2	E	79	TYR	2.5
1	D	326	GLY	2.5
2	E	196	HIS	2.4
1	D	361	TYR	2.4
1	D	83	VAL	2.4
1	D	304	TYR	2.4
1	D	342	PHE	2.4
2	B	163	THR	2.4
2	B	246	LYS	2.3
1	D	35	ILE	2.3
1	D	86	SER	2.3
1	D	55	ILE	2.3
1	D	224	GLN	2.3
1	D	39	LEU	2.3
2	E	191	LEU	2.3
2	B	157	ALA	2.2
1	A	318	GLU	2.2
1	A	311	ASN	2.2
1	D	184	PRO	2.2
1	A	193	LYS	2.2
1	A	221	LEU	2.2
1	A	225	TYR	2.2
1	A	69	LYS	2.1
1	D	60	LEU	2.1
2	E	221	LEU	2.1
3	C	179	SER	2.1
1	A	34	PHE	2.1
1	D	111	VAL	2.1
2	E	108	GLU	2.1
3	F	143	LYS	2.1
1	A	108	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	219	TYR	2.1
1	A	68	LEU	2.1
3	F	201	ALA	2.0
3	F	146	THR	2.0
1	A	360	ASN	2.0
3	C	218	LEU	2.0
2	B	166	GLY	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](#)

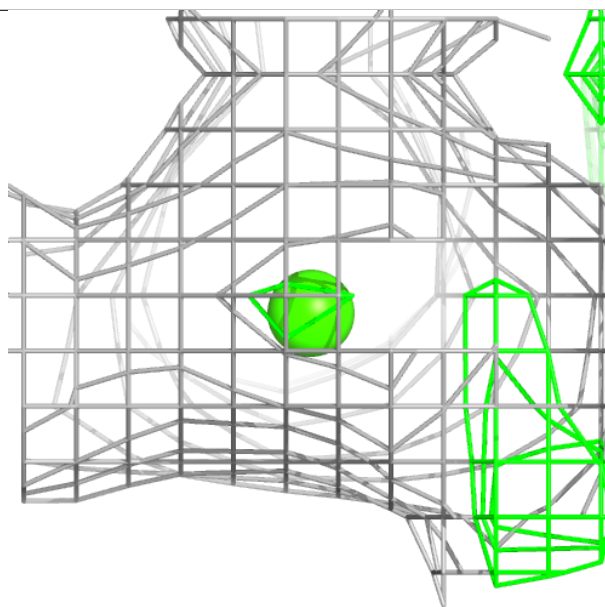
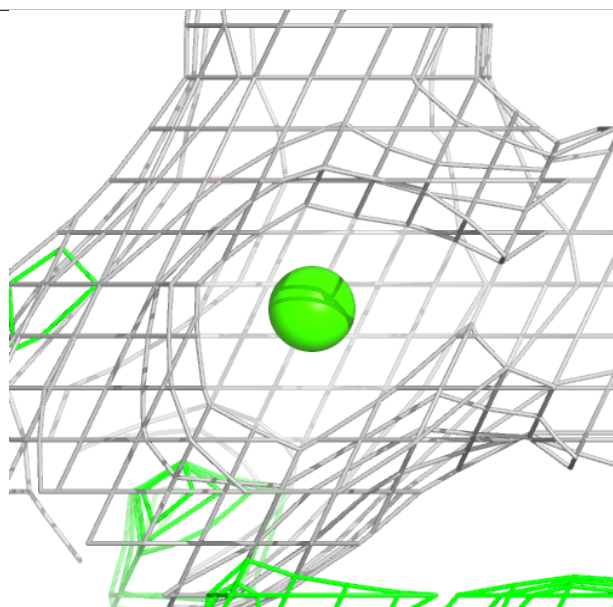
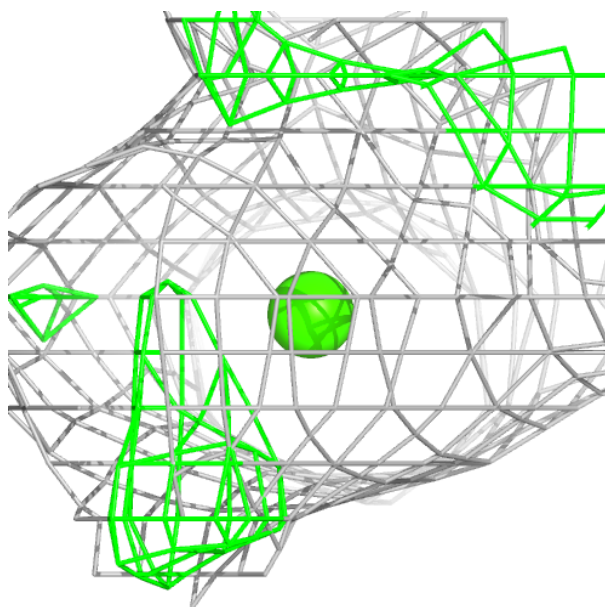
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	B	401	1/1	0.89	0.16	100,100,100,100	0
4	CA	E	401	1/1	0.91	0.14	98,98,98,98	0
4	CA	D	401	1/1	0.96	0.12	67,67,67,67	0
4	CA	A	401	1/1	0.96	0.10	63,63,63,63	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.

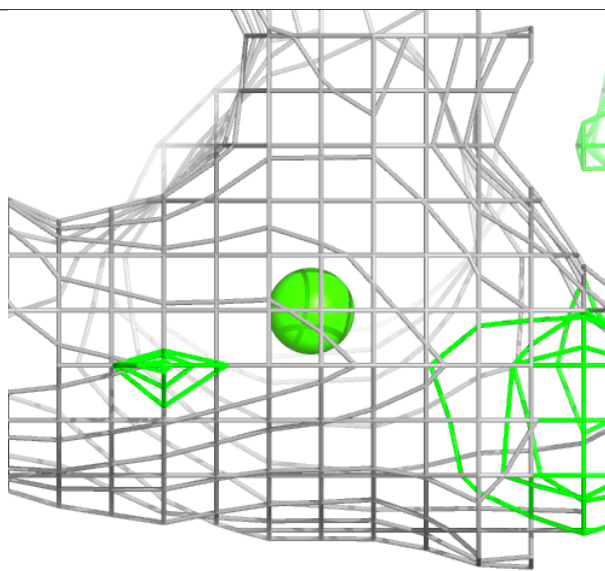
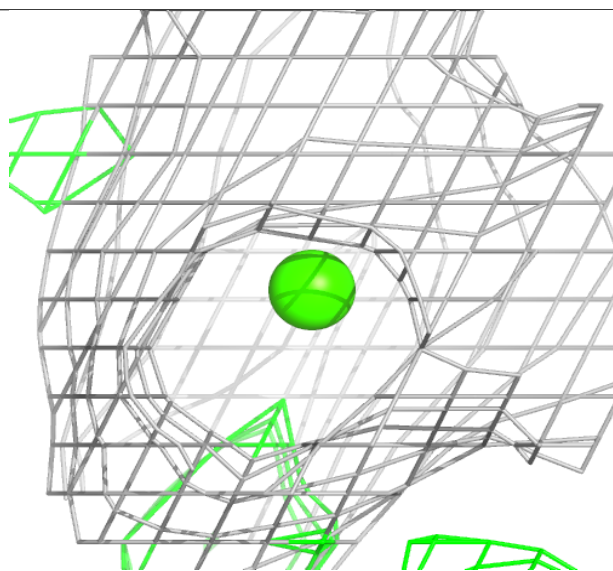
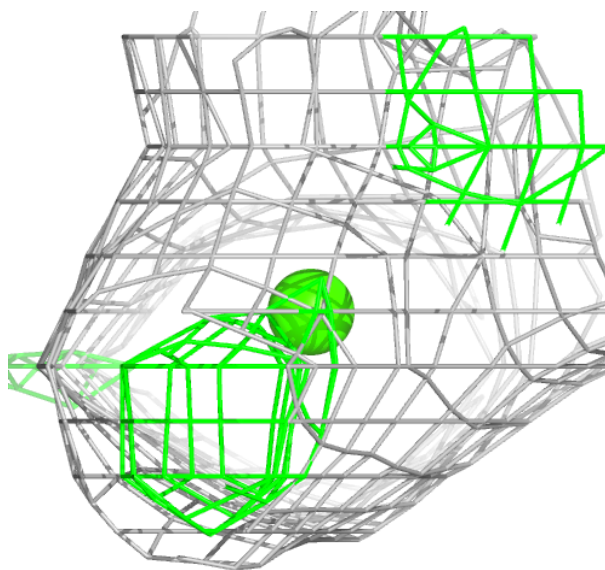
Electron density around CA B 401:

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



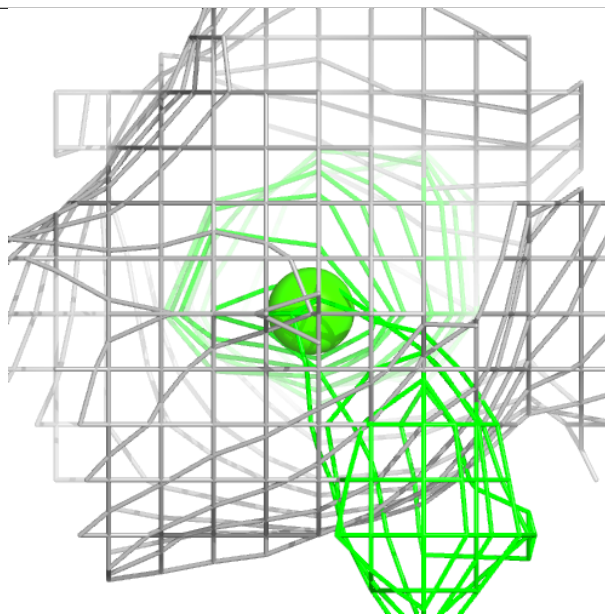
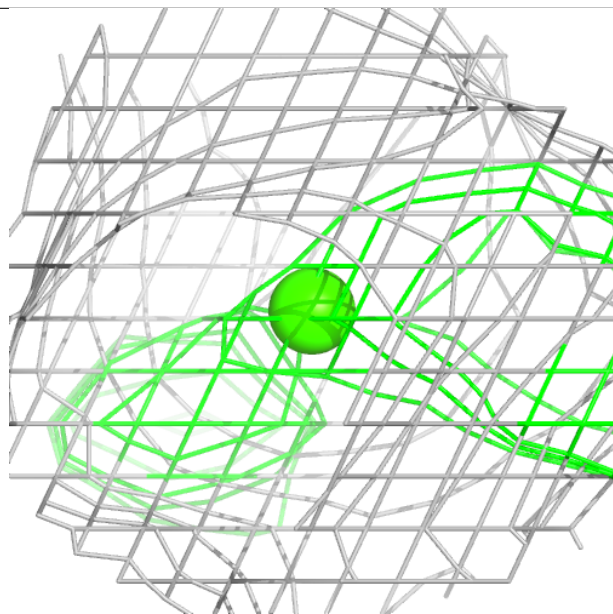
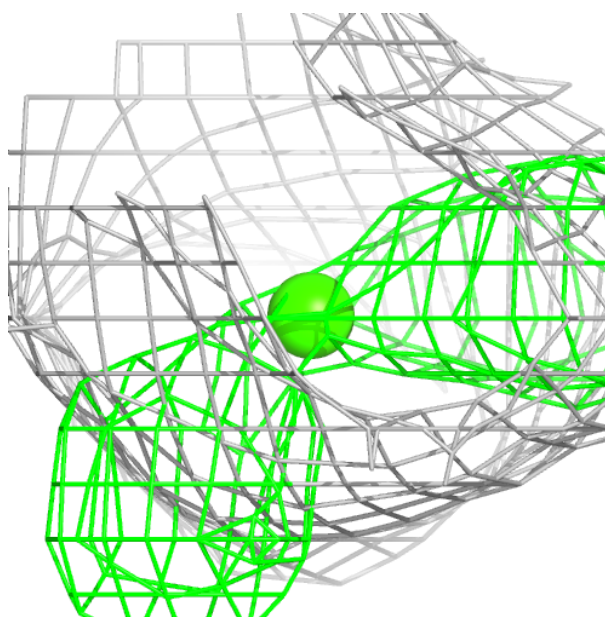
Electron density around CA E 401:

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



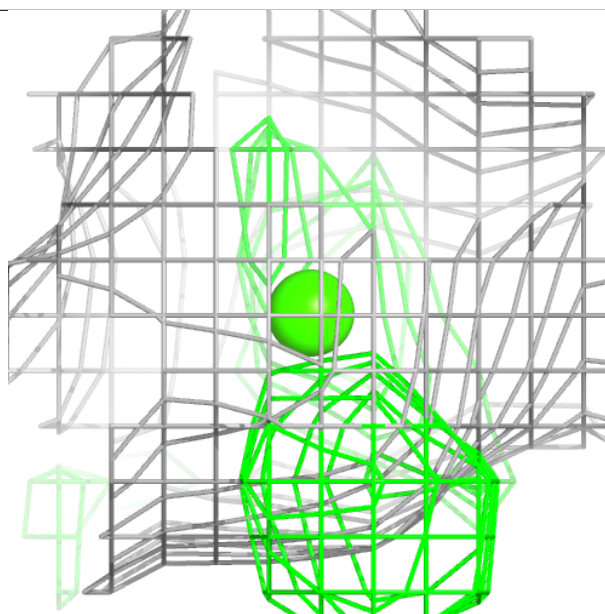
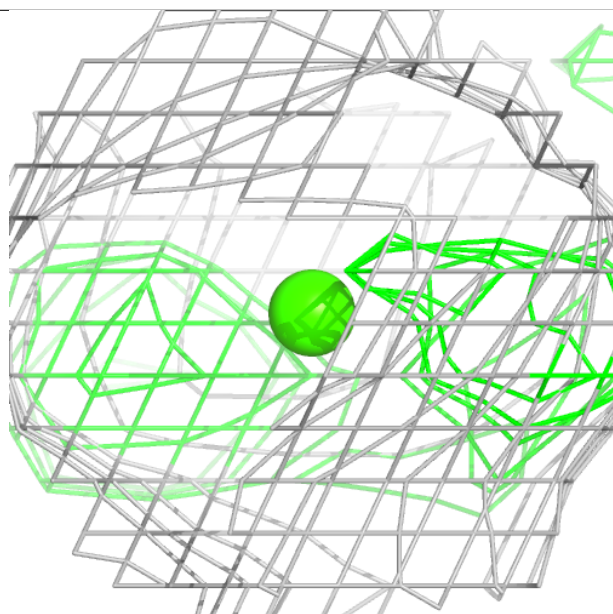
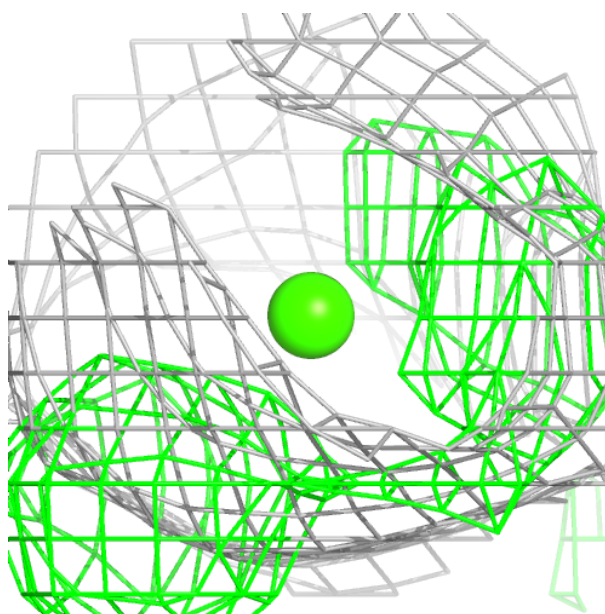
Electron density around CA D 401:

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



Electron density around CA 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 ⓘ

There are no such residues in this entry.