



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:20 AM BST

PDB ID : 6LRB
Title : The A form apo structure of NrS-1 C terminal region-CTR
Authors : Chen, X.; Gan, J.
Deposited on : 2020-01-15
Resolution : 2.65 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

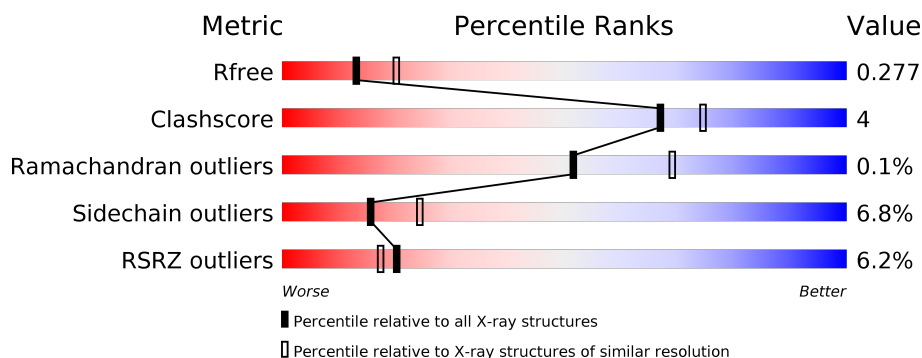
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 on 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	416	<div> <div>6%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	B	416	<div> <div>6%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	C	416	<div> <div>5%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>
1	D	416	<div> <div>6%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	E	416	<div> <div>6%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	F	416	<div> <div>7%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 19863 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 Primase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3316	2152	535	618	11			
1	B	408	Total	C	N	O	S	0	0	0
			3297	2141	535	610	11			
1	C	410	Total	C	N	O	S	0	0	0
			3315	2152	538	614	11			
1	D	409	Total	C	N	O	S	0	0	0
			3304	2145	533	615	11			
1	E	409	Total	C	N	O	S	0	0	0
			3308	2148	534	615	11			
1	F	408	Total	C	N	O	S	0	0	0
			3301	2144	536	610	11			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	4	Total	O	0	0
			4	4		
3	C	5	Total	O	0	0
			5	5		
3	D	3	Total	O	0	0
			3	3		

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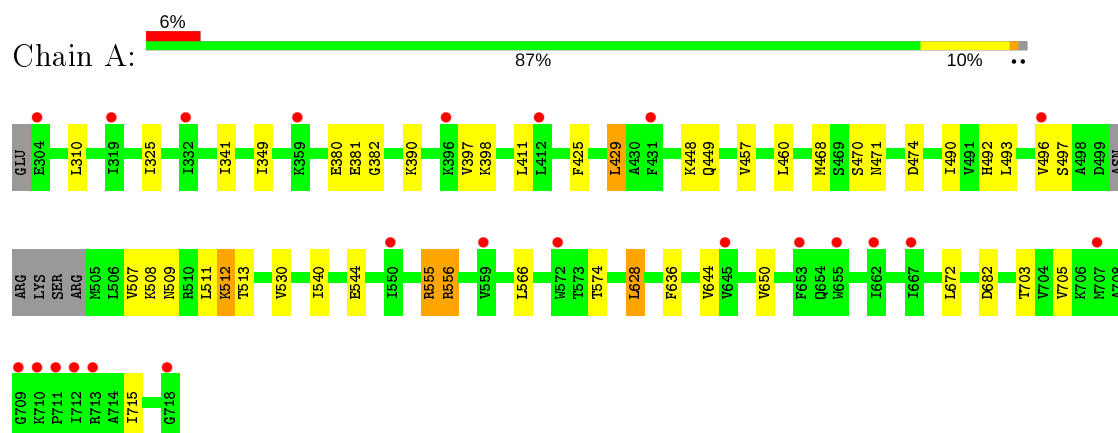
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total	O	0	0
			2	2		
3	F	5	Total	O	0	0
			5	5		

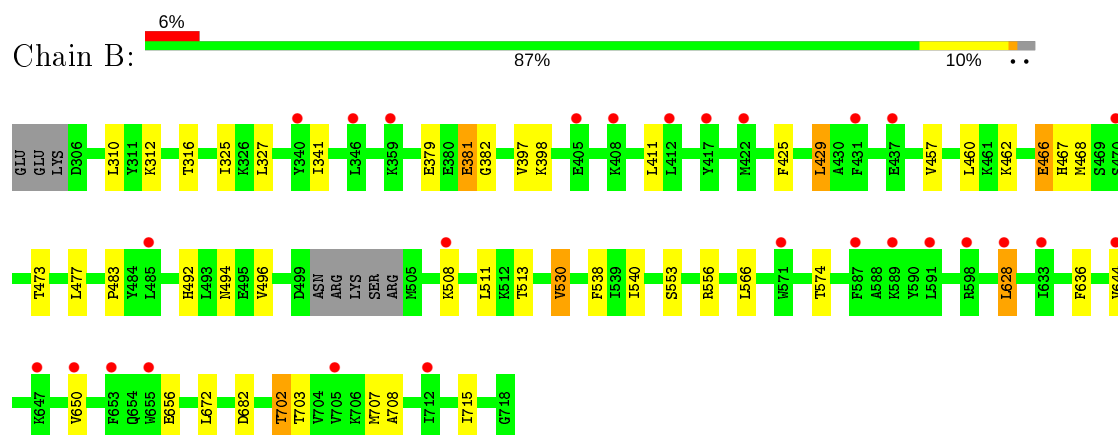
3 Residue-property plots

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.

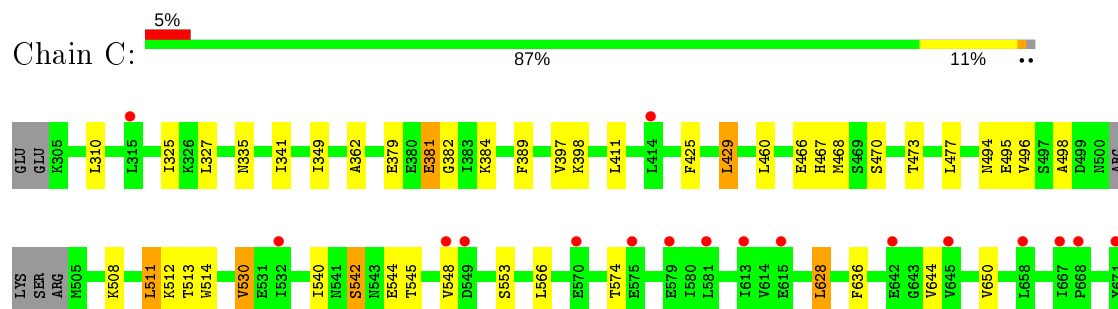
• Molecule 1: Primase



• Molecule 1: Primase

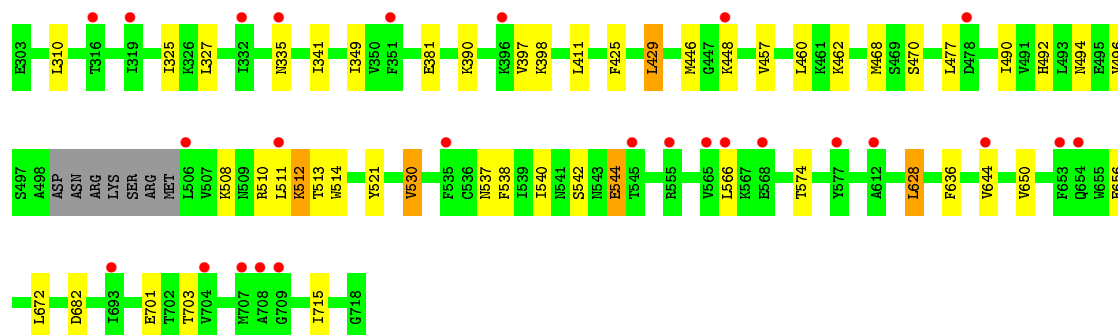
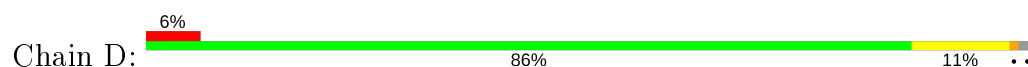


• Molecule 1: Primase

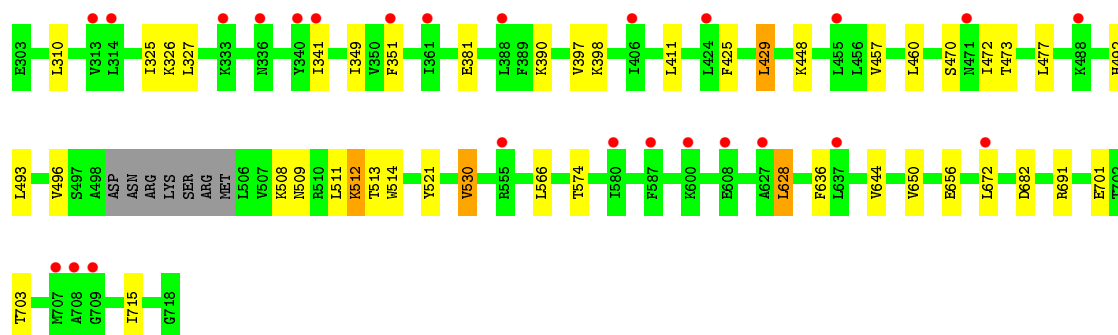
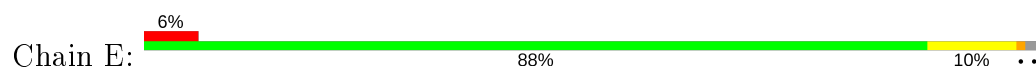




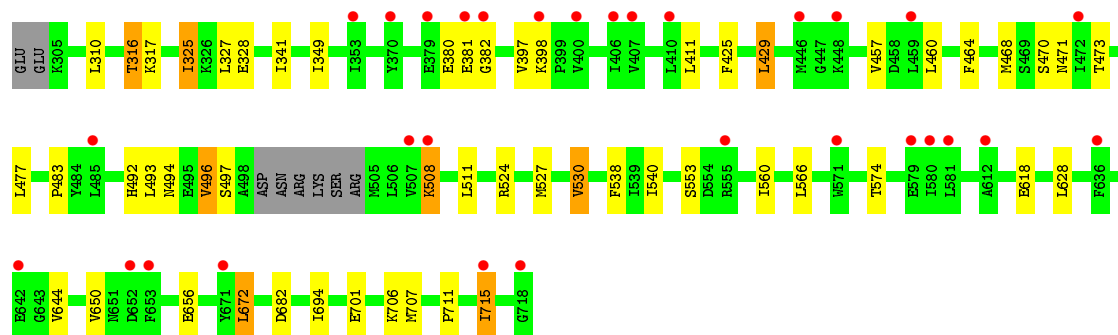
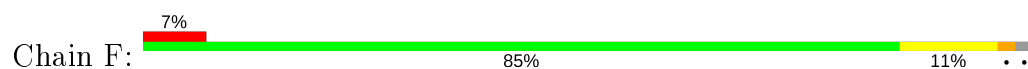
• Molecule 1: Primase



• Molecule 1: Primase



• Molecule 1: Primase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	150.72Å 150.39Å 149.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.56 – 2.65 29.56 – 2.59	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.56-2.65) 95.6 (29.56-2.59)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.57Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.233 , 0.278 0.233 , 0.277	Depositor DCC
R_{free} test set	5168 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 23.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l 0.055 for -l,-k,-h 0.055 for -h,l,k 0.467 for l,h,k 0.467 for k,l,h	Xtriage
Reported twinning fraction	0.382 for H, K, L 0.354 for -L, -H, K 0.264 for K, -L, -H	Depositor
Outliers	0 of 103455 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	19863	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: 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	0.65	0/3383	0.75	0/4583
1	B	0.65	0/3364	0.75	0/4558
1	C	0.63	0/3382	0.75	1/4581 (0.0%)
1	D	0.67	0/3371	0.76	0/4568
1	E	0.65	0/3375	0.75	0/4572
1	F	0.60	0/3368	0.75	0/4562
All	All	0.64	0/20243	0.75	1/27424 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	498	ALA	N-CA-C	-5.54	96.03	111.00

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	3316	0	3346	32	0
1	B	3297	0	3332	27	0
1	C	3315	0	3351	34	0
1	D	3304	0	3331	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3308	0	3342	31	0
1	F	3301	0	3343	44	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	1	0	0	0	0
3	B	4	0	0	0	0
3	C	5	0	0	0	0
3	D	3	0	0	1	0
3	E	2	0	0	0	0
3	F	5	0	0	3	0
All	All	19863	0	20045	155	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 (155) 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:E:493:LEU:HD11	1:E:511:LEU:HD21	1.49	0.94
1:E:325:ILE:HD13	1:F:349:ILE:HD11	1.51	0.91
1:F:511:LEU:HD21	1:F:540:ILE:HD11	1.52	0.91
1:F:327:LEU:HD13	1:F:527:MET:CE	2.02	0.88
1:A:512:LYS:HD3	1:C:496:VAL:HG21	1.56	0.88
1:C:325:ILE:HD13	1:E:349:ILE:HD11	1.55	0.86
1:D:468:MET:HG3	1:D:490:ILE:HB	1.60	0.84
1:F:493:LEU:HD13	1:F:508:LYS:HD3	1.61	0.82
1:A:512:LYS:HD3	1:C:496:VAL:CG2	2.09	0.80
1:A:508:LYS:O	1:A:511:LEU:HB3	1.82	0.80
1:E:511:LEU:HD23	1:E:514:TRP:CE3	2.17	0.80
1:B:341:ILE:HG21	1:D:325:ILE:HD11	1.67	0.77
1:D:511:LEU:HD21	1:D:540:ILE:HD11	1.67	0.77
1:D:349:ILE:HD11	1:F:325:ILE:HD13	1.66	0.76
1:F:672:LEU:HD12	1:F:715:ILE:HG13	1.64	0.76
1:B:511:LEU:HD21	1:B:540:ILE:HD11	1.67	0.75
1:F:524:ARG:HD3	3:F:802:HOH:O	1.85	0.75
1:A:511:LEU:HD21	1:A:540:ILE:HD11	1.69	0.75
1:A:349:ILE:HD11	1:B:325:ILE:HD13	1.71	0.72
1:F:325:ILE:HG13	1:F:325:ILE:O	1.87	0.72
1:D:510:ARG:HD3	1:D:514:TRP:CZ2	2.25	0.72
1:A:325:ILE:HD11	1:C:341:ILE:HG21	1.71	0.71
1:B:341:ILE:HG21	1:D:325:ILE:CD1	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:327:LEU:HD13	1:F:527:MET:HE1	1.75	0.67
1:A:325:ILE:CD1	1:C:341:ILE:HG21	2.25	0.67
1:E:511:LEU:HD23	1:E:514:TRP:HE3	1.60	0.66
1:D:460:LEU:HB2	1:D:468:MET:HE1	1.77	0.66
1:A:493:LEU:CD1	1:A:511:LEU:HD13	2.26	0.65
1:F:493:LEU:HB3	1:F:508:LYS:HE3	1.78	0.65
1:A:555:ARG:HH21	1:A:556:ARG:NH2	1.95	0.64
1:B:473:THR:HG22	1:D:513:THR:HG21	1.79	0.64
1:D:429:LEU:HD11	1:D:460:LEU:HD21	1.79	0.64
1:F:429:LEU:HD11	1:F:460:LEU:HD21	1.81	0.63
1:B:429:LEU:HD11	1:B:460:LEU:HD21	1.81	0.63
1:C:379:GLU:HG2	1:C:379:GLU:O	1.98	0.62
1:A:468:MET:HG3	1:A:490:ILE:HB	1.82	0.62
1:F:560:ILE:HA	3:F:803:HOH:O	1.98	0.62
1:E:429:LEU:HD11	1:E:460:LEU:HD21	1.81	0.62
1:A:493:LEU:HD11	1:A:511:LEU:HD13	1.82	0.61
1:C:429:LEU:HD11	1:C:460:LEU:HD21	1.80	0.61
1:A:429:LEU:HD11	1:A:460:LEU:HD21	1.80	0.61
1:E:512:LYS:HD3	1:F:496:VAL:HG21	1.82	0.61
1:E:325:ILE:CD1	1:F:341:ILE:HG21	2.31	0.60
1:A:555:ARG:HH21	1:A:556:ARG:HH22	1.48	0.60
1:E:472:ILE:HB	1:E:493:LEU:HD23	1.84	0.60
1:C:496:VAL:HG13	1:C:496:VAL:O	2.02	0.60
1:C:513:THR:HG21	1:E:473:THR:CG2	2.32	0.60
1:D:460:LEU:CB	1:D:468:MET:HE1	2.32	0.59
1:E:325:ILE:HD11	1:F:341:ILE:HG21	1.84	0.59
1:F:511:LEU:CD2	1:F:540:ILE:HD11	2.29	0.59
1:F:471:ASN:HA	1:F:494:ASN:HD22	1.68	0.58
1:F:327:LEU:HD13	1:F:527:MET:HE3	1.86	0.58
1:A:448:LYS:HB2	1:B:553:SER:OG	2.04	0.58
1:F:694:ILE:HG13	1:F:715:ILE:HD12	1.86	0.57
1:F:327:LEU:CD2	1:F:530:VAL:HG21	2.35	0.56
1:E:512:LYS:HD3	1:F:496:VAL:CG2	2.36	0.55
1:B:379:GLU:HG2	1:B:379:GLU:O	2.06	0.54
1:F:706:LYS:HG3	1:F:706:LYS:O	2.07	0.54
1:A:460:LEU:HB3	1:A:468:MET:HE1	1.89	0.53
1:B:473:THR:CG2	1:D:513:THR:HG21	2.38	0.53
1:B:425:PHE:CE2	1:B:429:LEU:HD12	2.44	0.53
1:E:493:LEU:HD11	1:E:511:LEU:CD2	2.31	0.53
1:E:425:PHE:CE2	1:E:429:LEU:HD12	2.44	0.53
1:B:702:THR:HA	1:B:715:ILE:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:508:LYS:O	1:F:511:LEU:HB3	2.10	0.53
1:A:513:THR:HG21	1:C:473:THR:HG22	1.90	0.52
1:D:425:PHE:CE2	1:D:429:LEU:HD12	2.44	0.52
1:F:327:LEU:HD21	1:F:530:VAL:HG21	1.91	0.52
1:A:341:ILE:HG21	1:B:325:ILE:HD11	1.90	0.52
1:A:425:PHE:CE2	1:A:429:LEU:HD12	2.45	0.52
1:C:425:PHE:CE2	1:C:429:LEU:HD12	2.45	0.52
1:C:495:GLU:OE1	1:C:495:GLU:HA	2.09	0.52
1:B:496:VAL:CG1	1:D:512:LYS:HD3	2.40	0.51
1:C:508:LYS:O	1:C:511:LEU:HB3	2.10	0.51
1:C:511:LEU:CD2	1:C:540:ILE:HD11	2.41	0.51
1:E:513:THR:HG21	1:F:473:THR:CG2	2.41	0.51
1:F:425:PHE:CE2	1:F:429:LEU:HD12	2.46	0.51
1:E:513:THR:HG21	1:F:473:THR:HG22	1.94	0.50
1:A:460:LEU:HB3	1:A:468:MET:CE	2.41	0.50
1:B:483:PRO:HG2	1:D:521:TYR:CE1	2.47	0.50
1:C:325:ILE:CD1	1:E:349:ILE:HD11	2.34	0.49
1:F:460:LEU:HB3	1:F:468:MET:HE1	1.95	0.49
1:A:508:LYS:O	1:A:511:LEU:CB	2.58	0.49
1:B:312:LYS:O	1:B:316:THR:HG23	2.13	0.49
1:C:460:LEU:HB3	1:C:468:MET:HE1	1.94	0.49
1:E:509:ASN:HB3	1:F:496:VAL:HG22	1.95	0.48
1:C:512:LYS:HE3	1:C:548:VAL:HG12	1.94	0.48
1:D:544:GLU:HA	1:D:544:GLU:OE1	2.14	0.48
1:E:325:ILE:HD13	1:F:349:ILE:CD1	2.35	0.48
1:D:349:ILE:HD11	1:F:325:ILE:CD1	2.38	0.48
1:C:362:ALA:HA	1:E:351:PHE:HE2	1.78	0.48
1:D:511:LEU:CD2	1:D:540:ILE:HD11	2.41	0.48
1:B:511:LEU:CD2	1:B:540:ILE:HD11	2.41	0.48
1:A:382:GLY:HA3	1:C:335:ASN:OD1	2.13	0.48
1:B:508:LYS:O	1:B:511:LEU:HB3	2.14	0.47
1:D:508:LYS:O	1:D:511:LEU:HB3	2.14	0.47
1:A:460:LEU:CB	1:A:468:MET:HE1	2.44	0.47
1:E:457:VAL:HG21	1:E:492:HIS:CE1	2.49	0.47
1:A:513:THR:HG21	1:C:473:THR:CG2	2.45	0.47
1:F:706:LYS:HA	1:F:711:PRO:HA	1.96	0.47
1:D:457:VAL:HG21	1:D:492:HIS:CE1	2.49	0.47
1:B:466:GLU:HG2	1:B:467:HIS:CD2	2.49	0.46
1:A:705:VAL:O	1:A:705:VAL:HG23	2.15	0.46
1:C:513:THR:OG1	1:C:514:TRP:N	2.48	0.46
1:A:511:LEU:CD2	1:A:540:ILE:HD11	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:LEU:HD21	1:C:540:ILE:HD11	1.98	0.45
1:C:553:SER:OG	1:E:448:LYS:HB2	2.17	0.45
1:B:457:VAL:HG21	1:B:492:HIS:CE1	2.52	0.45
1:C:325:ILE:CD1	1:E:341:ILE:HG21	2.47	0.45
1:D:335:ASN:OD1	1:F:382:GLY:HA3	2.17	0.45
1:A:449:GLN:HE22	1:B:556:ARG:HD2	1.81	0.45
1:F:711:PRO:HG2	1:F:711:PRO:O	2.16	0.45
1:E:327:LEU:HD23	1:E:530:VAL:HG21	1.99	0.44
1:F:464:PHE:HB2	1:F:468:MET:HE3	1.99	0.44
1:A:457:VAL:HG21	1:A:492:HIS:CE1	2.53	0.44
1:D:448:LYS:HB2	1:F:553:SER:OG	2.18	0.44
1:C:466:GLU:HG2	1:C:467:HIS:CD2	2.53	0.44
1:D:537:ASN:HA	3:D:901:HOH:O	2.18	0.44
1:C:325:ILE:HD11	1:E:341:ILE:HG21	2.00	0.43
1:B:381:GLU:HB3	1:B:382:GLY:H	1.59	0.43
1:A:325:ILE:HD13	1:C:349:ILE:HD11	2.00	0.43
1:D:341:ILE:HA	3:F:801:HOH:O	2.18	0.43
1:E:493:LEU:HD13	1:E:511:LEU:HD11	2.01	0.43
1:D:468:MET:HA	1:D:490:ILE:O	2.19	0.43
1:B:460:LEU:HB3	1:B:468:MET:HE1	2.01	0.43
1:E:508:LYS:HB3	1:E:511:LEU:HD12	2.01	0.42
1:F:327:LEU:O	1:F:328:GLU:C	2.55	0.42
1:F:316:THR:HG22	1:F:317:LYS:HG3	2.01	0.42
1:E:691:ARG:NH2	1:F:618:GLU:O	2.40	0.42
1:C:327:LEU:HD23	1:C:530:VAL:HG21	2.01	0.42
1:D:628:LEU:HD13	1:D:636:PHE:CZ	2.54	0.42
1:F:457:VAL:HG21	1:F:492:HIS:CE1	2.54	0.42
1:E:521:TYR:CE1	1:F:483:PRO:HG2	2.55	0.42
1:B:511:LEU:CD1	1:B:538:PHE:CD1	3.03	0.42
1:F:511:LEU:CD1	1:F:538:PHE:CD1	3.03	0.42
1:F:511:LEU:HD11	1:F:538:PHE:CD1	2.54	0.42
1:D:327:LEU:HD23	1:D:530:VAL:HG21	2.01	0.41
1:F:511:LEU:HD11	1:F:538:PHE:CG	2.55	0.41
1:B:511:LEU:HD11	1:B:538:PHE:CD1	2.55	0.41
1:A:471:ASN:HB3	1:B:513:THR:HB	2.02	0.41
1:A:628:LEU:HD13	1:A:636:PHE:CZ	2.56	0.41
1:C:511:LEU:HD12	1:C:511:LEU:O	2.21	0.41
1:D:446:MET:HA	1:D:542:SER:O	2.21	0.41
1:E:493:LEU:CD1	1:E:511:LEU:HD21	2.36	0.41
1:C:389:PHE:CD1	1:C:467:HIS:CE1	3.09	0.41
1:C:495:GLU:HB3	1:C:542:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:THR:O	1:C:514:TRP:C	2.58	0.41
1:A:460:LEU:C	1:A:468:MET:HE3	2.42	0.41
1:D:511:LEU:HD11	1:D:538:PHE:CD1	2.55	0.40
1:A:509:ASN:O	1:A:512:LYS:HB2	2.21	0.40
1:B:327:LEU:HD23	1:B:530:VAL:HG21	2.03	0.40
1:E:628:LEU:HD13	1:E:636:PHE:CZ	2.57	0.40
1:C:628:LEU:HD13	1:C:636:PHE:CZ	2.56	0.40
1:B:628:LEU:HD13	1:B:636:PHE:CZ	2.56	0.40
1:C:381:GLU:HB3	1:C:382:GLY:H	1.60	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	406/416 (98%)	388 (96%)	18 (4%)	0	100	100
1	B	404/416 (97%)	384 (95%)	19 (5%)	1 (0%)	47	64
1	C	406/416 (98%)	383 (94%)	22 (5%)	1 (0%)	47	64
1	D	405/416 (97%)	388 (96%)	17 (4%)	0	100	100
1	E	405/416 (97%)	387 (96%)	18 (4%)	0	100	100
1	F	404/416 (97%)	389 (96%)	15 (4%)	0	100	100
All	All	2430/2496 (97%)	2319 (95%)	109 (4%)	2 (0%)	51	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	544	GLU
1	B	708	ALA

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	363/379 (96%)	336 (93%)	27 (7%)	13	21
1	B	360/379 (95%)	338 (94%)	22 (6%)	18	29
1	C	362/379 (96%)	339 (94%)	23 (6%)	17	27
1	D	361/379 (95%)	335 (93%)	26 (7%)	14	22
1	E	362/379 (96%)	338 (93%)	24 (7%)	16	25
1	F	361/379 (95%)	335 (93%)	26 (7%)	14	22
All	All	2169/2274 (95%)	2021 (93%)	148 (7%)	16	24

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	LEU
1	A	380	GLU
1	A	381	GLU
1	A	390	LYS
1	A	397	VAL
1	A	398	LYS
1	A	411	LEU
1	A	429	LEU
1	A	470	SER
1	A	474	ASP
1	A	496	VAL
1	A	497	SER
1	A	507	VAL
1	A	512	LYS
1	A	530	VAL
1	A	544	GLU
1	A	555	ARG
1	A	556	ARG
1	A	566	LEU
1	A	574	THR
1	A	628	LEU
1	A	644	VAL

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Mol	Chain	Res	Type
1	A	650	VAL
1	A	672	LEU
1	A	682	ASP
1	A	703	THR
1	A	715	ILE
1	B	310	LEU
1	B	381	GLU
1	B	397	VAL
1	B	398	LYS
1	B	411	LEU
1	B	429	LEU
1	B	462	LYS
1	B	466	GLU
1	B	477	LEU
1	B	494	ASN
1	B	530	VAL
1	B	566	LEU
1	B	574	THR
1	B	628	LEU
1	B	644	VAL
1	B	650	VAL
1	B	656	GLU
1	B	672	LEU
1	B	682	ASP
1	B	702	THR
1	B	703	THR
1	B	707	MET
1	C	310	LEU
1	C	381	GLU
1	C	384	LYS
1	C	397	VAL
1	C	398	LYS
1	C	411	LEU
1	C	429	LEU
1	C	470	SER
1	C	477	LEU
1	C	494	ASN
1	C	511	LEU
1	C	530	VAL
1	C	542	SER
1	C	545	THR
1	C	566	LEU

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Mol	Chain	Res	Type
1	C	574	THR
1	C	628	LEU
1	C	644	VAL
1	C	650	VAL
1	C	672	LEU
1	C	682	ASP
1	C	703	THR
1	C	715	ILE
1	D	310	LEU
1	D	381	GLU
1	D	390	LYS
1	D	397	VAL
1	D	398	LYS
1	D	411	LEU
1	D	429	LEU
1	D	462	LYS
1	D	470	SER
1	D	477	LEU
1	D	494	ASN
1	D	496	VAL
1	D	512	LYS
1	D	530	VAL
1	D	544	GLU
1	D	566	LEU
1	D	574	THR
1	D	628	LEU
1	D	644	VAL
1	D	650	VAL
1	D	656	GLU
1	D	672	LEU
1	D	682	ASP
1	D	701	GLU
1	D	703	THR
1	D	715	ILE
1	E	310	LEU
1	E	326	LYS
1	E	381	GLU
1	E	390	LYS
1	E	397	VAL
1	E	398	LYS
1	E	411	LEU
1	E	429	LEU

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Mol	Chain	Res	Type
1	E	470	SER
1	E	477	LEU
1	E	496	VAL
1	E	512	LYS
1	E	530	VAL
1	E	566	LEU
1	E	574	THR
1	E	628	LEU
1	E	644	VAL
1	E	650	VAL
1	E	656	GLU
1	E	672	LEU
1	E	682	ASP
1	E	701	GLU
1	E	703	THR
1	E	715	ILE
1	F	310	LEU
1	F	316	THR
1	F	325	ILE
1	F	380	GLU
1	F	381	GLU
1	F	397	VAL
1	F	398	LYS
1	F	411	LEU
1	F	429	LEU
1	F	470	SER
1	F	477	LEU
1	F	496	VAL
1	F	497	SER
1	F	508	LYS
1	F	530	VAL
1	F	566	LEU
1	F	574	THR
1	F	628	LEU
1	F	644	VAL
1	F	650	VAL
1	F	656	GLU
1	F	672	LEU
1	F	682	ASP
1	F	701	GLU
1	F	707	MET
1	F	715	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	GLN
1	A	449	GLN
1	A	471	ASN
1	A	537	ASN
1	A	564	ASN
1	A	578	GLN
1	A	583	ASN
1	B	434	GLN
1	B	471	ASN
1	B	537	ASN
1	B	564	ASN
1	B	578	GLN
1	B	583	ASN
1	C	434	GLN
1	C	471	ASN
1	C	537	ASN
1	C	564	ASN
1	C	578	GLN
1	C	583	ASN
1	D	434	GLN
1	D	471	ASN
1	D	537	ASN
1	D	564	ASN
1	D	578	GLN
1	D	583	ASN
1	D	659	GLN
1	E	348	GLN
1	E	434	GLN
1	E	471	ASN
1	E	537	ASN
1	E	564	ASN
1	E	578	GLN
1	E	583	ASN
1	F	434	GLN
1	F	471	ASN
1	F	494	ASN
1	F	537	ASN
1	F	564	ASN
1	F	578	GLN
1	F	583	ASN
1	F	623	GLN

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 monosaccharides 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

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	410/416 (98%)	0.31	23 (5%) 24 21	30, 73, 107, 163	0
1	B	408/416 (98%)	0.37	27 (6%) 18 15	28, 81, 115, 138	0
1	C	410/416 (98%)	0.43	20 (4%) 29 26	25, 81, 112, 152	0
1	D	409/416 (98%)	0.42	26 (6%) 19 16	12, 77, 116, 146	0
1	E	409/416 (98%)	0.40	25 (6%) 21 18	18, 79, 112, 156	0
1	F	408/416 (98%)	0.39	30 (7%) 14 12	31, 81, 118, 163	0
All	All	2454/2496 (98%)	0.39	151 (6%) 20 17	12, 79, 114, 163	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	381	GLU	8.1
1	C	671	TYR	7.1
1	B	571	TRP	6.2
1	F	580	ILE	5.4
1	A	711	PRO	5.4
1	E	336	ASN	5.3
1	D	565	VAL	4.8
1	F	652	ASP	4.6
1	D	707	MET	4.5
1	E	707	MET	4.4
1	E	608	GLU	4.1
1	C	642	GLU	4.0
1	D	708	ALA	4.0
1	C	581	LEU	4.0
1	F	353	ILE	4.0
1	B	340	TYR	4.0
1	D	316	THR	4.0
1	F	485	LEU	3.9
1	F	379	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	555	ARG	3.8
1	E	314	LEU	3.8
1	E	361	ILE	3.8
1	A	304	GLU	3.7
1	F	507	VAL	3.6
1	B	589	LYS	3.6
1	E	637	LEU	3.5
1	F	581	LEU	3.5
1	B	346	LEU	3.5
1	E	313	VAL	3.5
1	B	417	TYR	3.5
1	C	548	VAL	3.5
1	E	580	ILE	3.4
1	A	359	LYS	3.4
1	B	633	ILE	3.4
1	C	579	GLU	3.3
1	C	697	TYR	3.3
1	F	612	ALA	3.3
1	D	577	TYR	3.3
1	F	571	TRP	3.2
1	D	478	ASP	3.2
1	C	658	LEU	3.2
1	B	412	LEU	3.1
1	B	655	TRP	3.1
1	D	644	VAL	3.1
1	A	319	ILE	3.0
1	D	709	GLY	3.0
1	C	615	GLU	3.0
1	D	654	GLN	3.0
1	B	437	GLU	3.0
1	C	686	ILE	3.0
1	F	555	ARG	2.9
1	F	653	PHE	2.9
1	F	715	ILE	2.9
1	B	653	PHE	2.9
1	E	709	GLY	2.9
1	B	644	VAL	2.9
1	F	636	PHE	2.9
1	F	508	LYS	2.8
1	D	566	LEU	2.8
1	D	535	PHE	2.8
1	F	400	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	448	LYS	2.8
1	B	705	VAL	2.7
1	D	568	GLU	2.7
1	D	653	PHE	2.7
1	F	446	MET	2.7
1	A	396	LYS	2.7
1	C	645	VAL	2.7
1	A	496	VAL	2.7
1	A	707	MET	2.7
1	D	335	ASN	2.7
1	D	612	ALA	2.7
1	E	600	LYS	2.7
1	C	712	ILE	2.7
1	D	351	PHE	2.6
1	A	713	ARG	2.6
1	B	359	LYS	2.6
1	C	575	GLU	2.6
1	F	410	LEU	2.6
1	C	532	ILE	2.6
1	D	332	ILE	2.6
1	B	647	LYS	2.6
1	A	709	GLY	2.6
1	E	587	PHE	2.5
1	B	650	VAL	2.5
1	D	506	LEU	2.5
1	F	671	TYR	2.5
1	C	667	ILE	2.5
1	D	396	LYS	2.5
1	E	406	ILE	2.5
1	D	545	THR	2.5
1	C	613	ILE	2.5
1	E	708	ALA	2.5
1	C	549	ASP	2.5
1	F	472	ILE	2.4
1	C	570	GLU	2.4
1	A	662	ILE	2.4
1	E	424	LEU	2.4
1	A	431	PHE	2.4
1	B	587	PHE	2.4
1	F	718	GLY	2.4
1	B	508	LYS	2.4
1	E	351	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	653	PHE	2.4
1	A	572	TRP	2.4
1	A	718	GLY	2.3
1	A	712	ILE	2.3
1	E	341	ILE	2.3
1	A	645	VAL	2.3
1	E	340	TYR	2.3
1	E	672	LEU	2.3
1	D	704	VAL	2.3
1	D	319	ILE	2.3
1	B	408	LYS	2.3
1	A	550	ILE	2.3
1	B	598	ARG	2.3
1	D	448	LYS	2.3
1	A	412	LEU	2.3
1	A	332	ILE	2.3
1	F	398	LYS	2.2
1	B	628	LEU	2.2
1	B	405	GLU	2.2
1	B	431	PHE	2.2
1	C	315	LEU	2.2
1	D	511	LEU	2.2
1	A	559	VAL	2.2
1	E	488	LYS	2.2
1	E	555	ARG	2.1
1	E	627	ALA	2.1
1	F	579	GLU	2.1
1	F	370	TYR	2.1
1	F	382	GLY	2.1
1	F	459	LEU	2.1
1	E	333	LYS	2.1
1	B	712	ILE	2.1
1	D	693	ILE	2.1
1	E	471	ASN	2.1
1	E	455	LEU	2.1
1	F	642	GLU	2.1
1	B	485	LEU	2.1
1	A	667	ILE	2.1
1	C	668	PRO	2.1
1	F	406	ILE	2.1
1	B	470	SER	2.1
1	C	414	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	655	TRP	2.0
1	A	710	LYS	2.0
1	B	422	MET	2.0
1	B	591	LEU	2.0
1	F	407	VAL	2.0
1	E	388	LEU	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 monosaccharides in this entry.

6.4 Ligands [i](#)

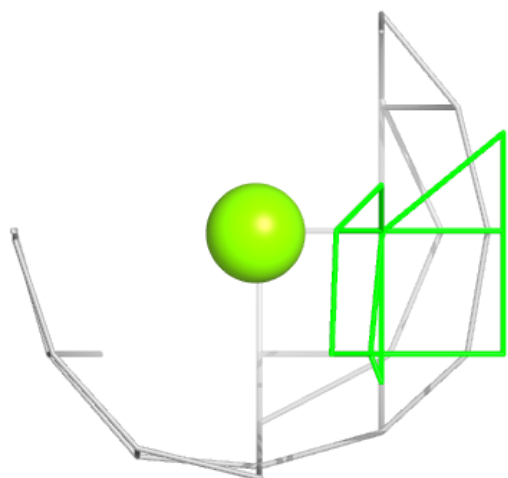
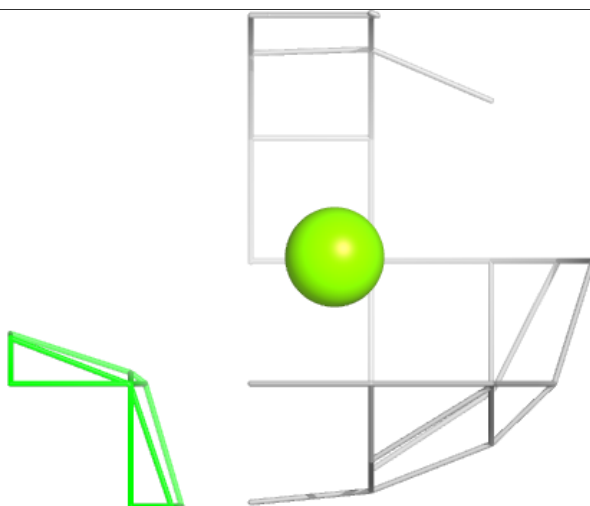
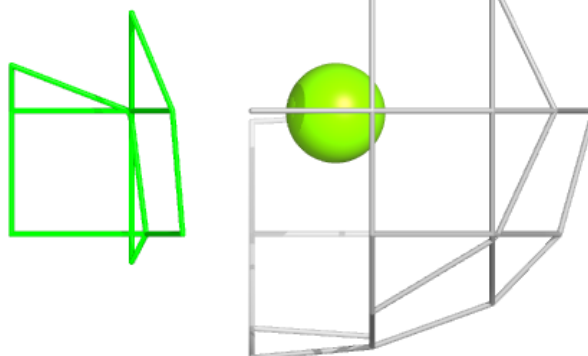
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	E	801	1/1	0.99	0.18	30,30,30,30	0
2	MG	D	801	1/1	1.00	0.19	26,26,26,26	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.

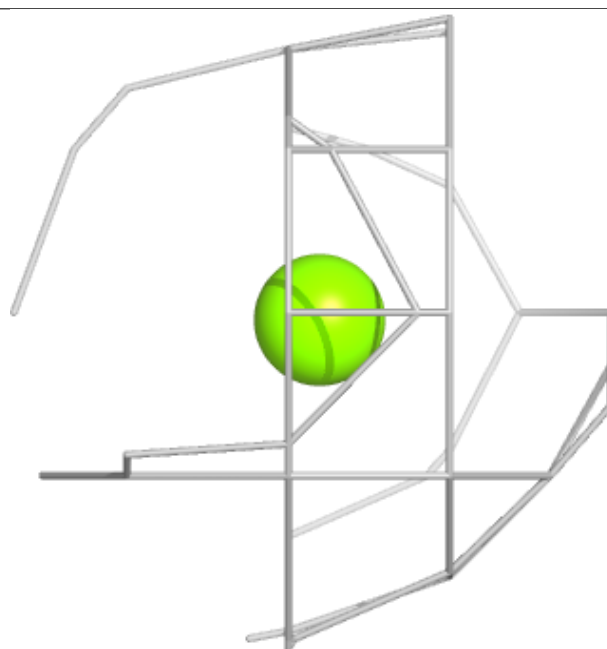
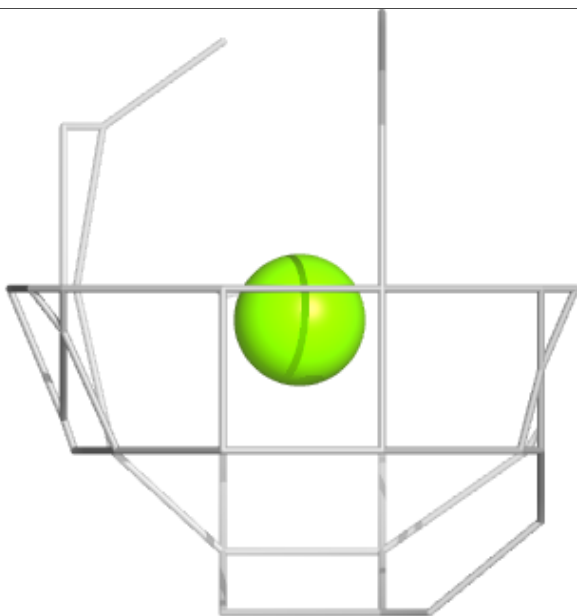
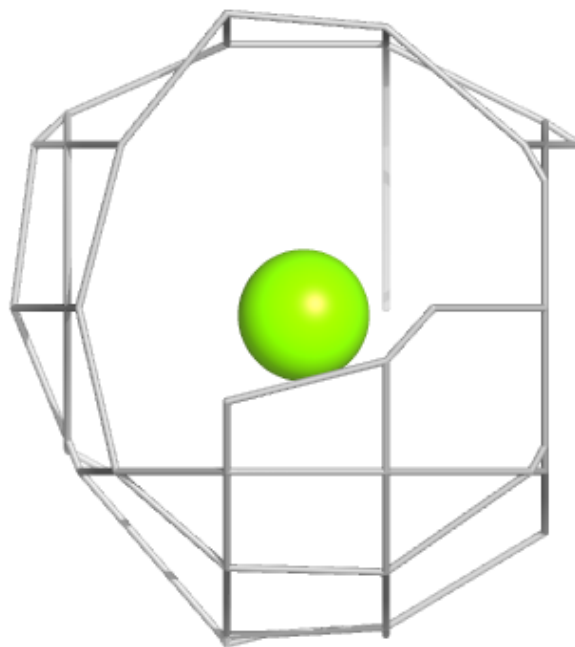
Electron density around MG E 801:

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



Electron density around MG D 801:

$2mF_o-DF_c$ (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.