



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 08:14 PM UTC

PDB ID : 6LRB / pdb_00006lrp
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 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

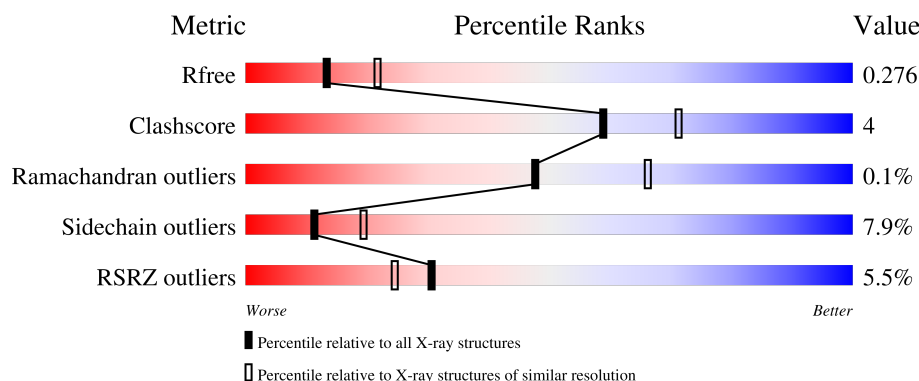
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	416	3% 84% 13% ..
1	B	416	6% 83% 12% ..
1	C	416	6% 83% 14% ..
1	D	416	6% 83% 14% ..
1	E	416	6% 84% 13% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	416	6% 83% 13% ••

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 (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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		

Continued on next page...

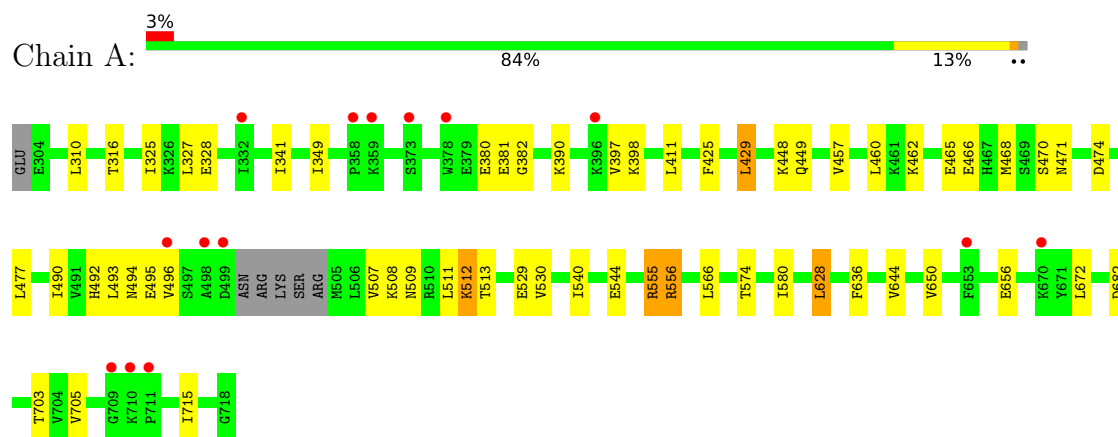
Continued from previous page...

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

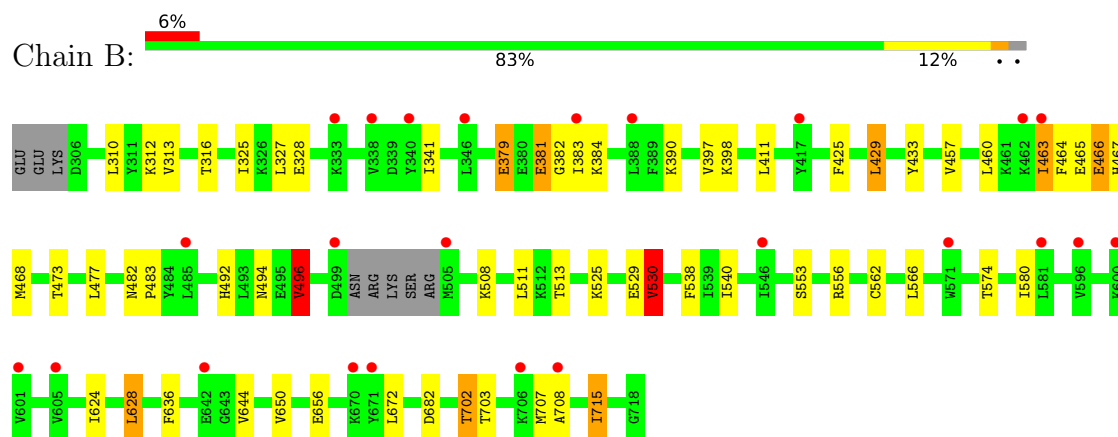
3 Residue-property plots [i](#)

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.

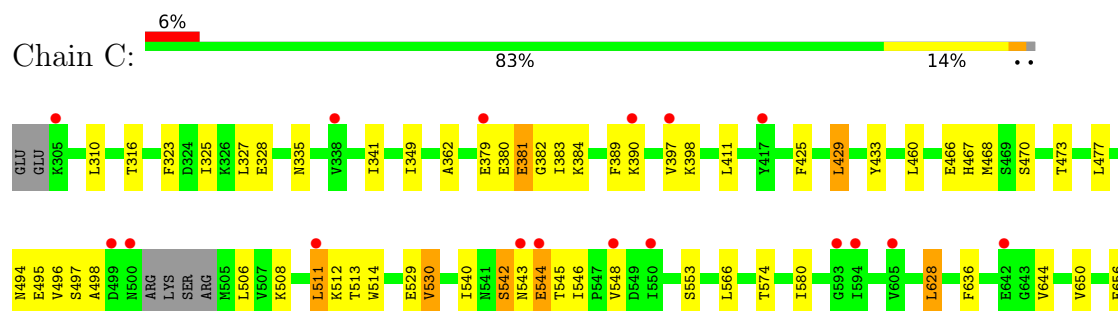
• Molecule 1: Primase

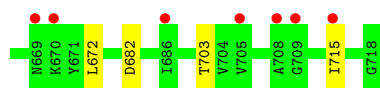


• Molecule 1: Primase

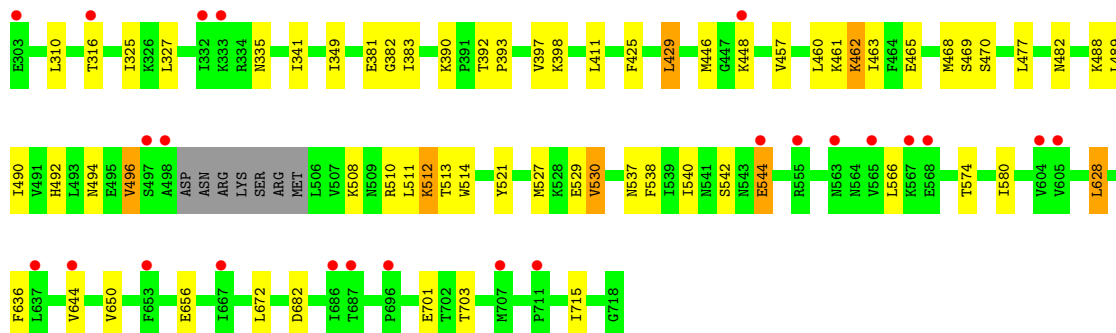
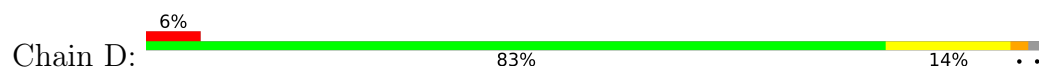


• Molecule 1: Primase

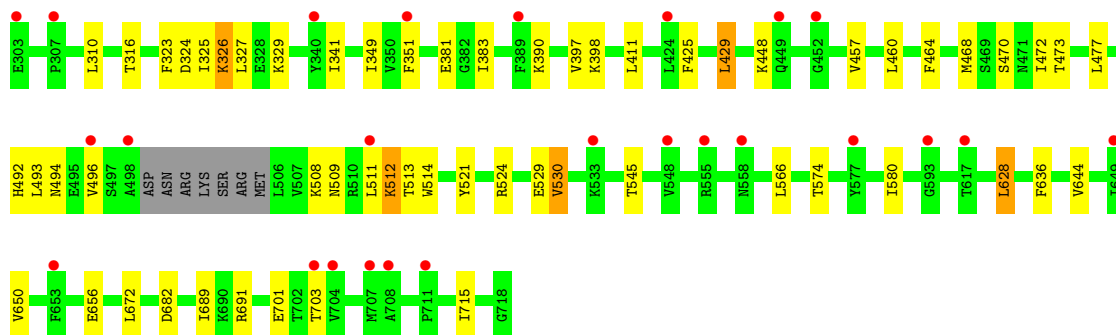
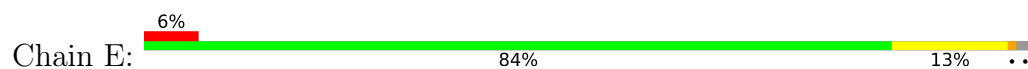




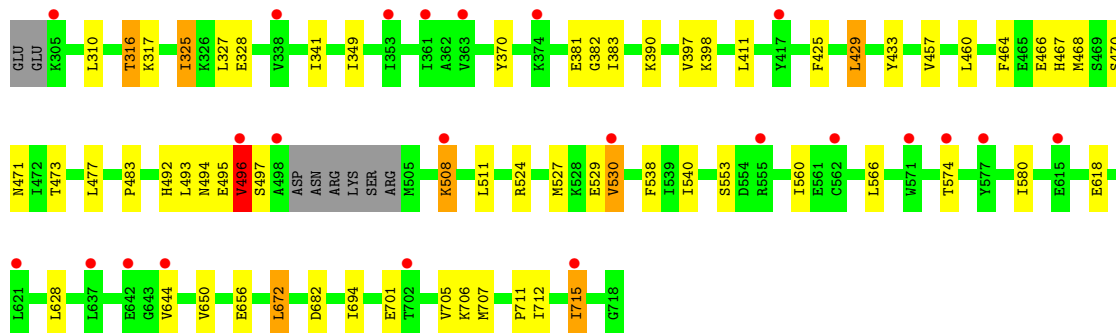
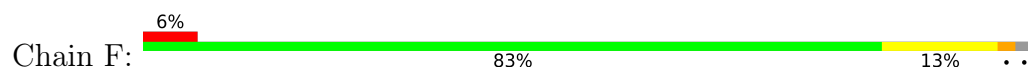
● Molecule 1: Primase



● 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 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.56-2.65) 98.1 (29.56-2.65)	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 0.230 , 0.276	Depositor DCC
R_{free} test set	5168 reflections (4.87%)	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)	0.30 , 21.2	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	0.88	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	0.89	1/3383 (0.0%)	1.00	3/4583 (0.1%)
1	B	0.90	3/3364 (0.1%)	1.02	8/4558 (0.2%)
1	C	0.86	3/3382 (0.1%)	1.02	9/4581 (0.2%)
1	D	0.94	7/3371 (0.2%)	1.02	6/4568 (0.1%)
1	E	0.90	6/3375 (0.2%)	0.99	4/4572 (0.1%)
1	F	0.86	0/3368	1.01	5/4562 (0.1%)
All	All	0.89	20/20243 (0.1%)	1.01	35/27424 (0.1%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	465	GLU	C-O	-7.85	1.17	1.24
1	D	488	LYS	CA-C	-7.41	1.43	1.52
1	D	392	THR	CA-CB	5.97	1.60	1.53
1	C	328	GLU	CA-C	-5.69	1.46	1.53
1	D	393	PRO	N-CA	5.58	1.54	1.47
1	E	324	ASP	C-O	-5.54	1.17	1.24
1	C	323	PHE	CA-CB	-5.36	1.46	1.53
1	E	324	ASP	CA-C	-5.32	1.46	1.52
1	C	497	SER	C-O	-5.32	1.19	1.24
1	E	524	ARG	CA-C	-5.29	1.46	1.52
1	D	383	ILE	C-O	-5.29	1.18	1.24
1	D	465	GLU	C-O	-5.22	1.19	1.24
1	B	383	ILE	C-O	-5.18	1.18	1.24
1	B	715	ILE	CA-CB	5.17	1.60	1.54
1	B	530	VAL	N-CA	-5.16	1.40	1.46
1	D	469	SER	CA-C	-5.07	1.46	1.52
1	E	323	PHE	C-O	-5.06	1.18	1.24
1	E	689	ILE	CA-CB	5.06	1.60	1.54
1	D	382	GLY	C-O	-5.04	1.20	1.24
1	E	326	LYS	C-O	-5.04	1.18	1.24

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	496	VAL	N-CA-C	10.12	119.61	111.62
1	C	543	ASN	N-CA-C	10.04	122.30	111.36
1	B	496	VAL	N-CA-C	8.83	119.05	111.90
1	D	463	ILE	N-CA-C	7.81	118.61	110.72
1	D	529	GLU	N-CA-C	-6.37	100.13	110.20
1	D	489	LEU	N-CA-C	-6.33	105.68	113.41
1	B	715	ILE	N-CA-CB	6.23	118.47	110.99
1	C	498	ALA	N-CA-C	-6.04	96.03	108.53
1	B	463	ILE	CB-CA-C	-5.98	103.97	112.22
1	A	495	GLU	N-CA-C	-5.94	99.05	108.73
1	F	496	VAL	N-CA-C	5.93	116.31	111.62
1	C	529	GLU	N-CA-C	-5.89	101.13	109.96
1	C	506	LEU	N-CA-C	-5.83	98.42	108.56
1	B	496	VAL	CB-CA-C	-5.80	105.73	111.30
1	C	383	ILE	N-CA-C	5.72	116.34	107.99
1	A	529	GLU	N-CA-C	-5.71	101.83	110.28
1	E	329	LYS	N-CA-C	-5.62	99.45	108.55
1	D	383	ILE	N-CA-C	5.59	116.36	108.36
1	C	546	ILE	CB-CA-C	-5.58	105.75	110.94
1	F	383	ILE	N-CA-C	5.46	116.17	108.36
1	C	497	SER	N-CA-C	5.45	115.43	108.24
1	B	379	GLU	N-CA-C	5.44	119.03	107.67
1	E	383	ILE	N-CA-C	5.36	115.81	107.99
1	F	495	GLU	N-CA-C	-5.35	100.58	109.46
1	F	529	GLU	N-CA-C	-5.34	101.95	109.96
1	C	543	ASN	CA-C-N	5.31	131.68	121.54
1	C	543	ASN	C-N-CA	5.31	131.68	121.54
1	B	624	ILE	N-CA-C	-5.20	105.53	110.42
1	D	462	LYS	N-CA-C	-5.19	105.70	111.36
1	E	689	ILE	CB-CA-C	-5.19	105.25	112.04
1	E	529	GLU	N-CA-C	-5.16	102.22	109.96
1	B	562	CYS	N-CA-CB	-5.14	103.02	110.84
1	A	466	GLU	N-CA-C	5.14	119.17	113.01
1	F	712	ILE	CB-CA-C	-5.09	103.03	110.62
1	B	529	GLU	N-CA-C	-5.04	102.41	109.96

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	3316	0	3346	35	0
1	B	3297	0	3332	34	0
1	C	3315	0	3351	37	0
1	D	3304	0	3331	32	0
1	E	3308	0	3342	32	0
1	F	3301	0	3343	47	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	174	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 (174) 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:A:460:LEU:CB	1:A:468:MET:HE1	2.06	0.85
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:460:LEU:HB3	1:A:468:MET:HE1	1.62	0.81
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:327:LEU:HD13	1:F:527:MET:HE1	1.69	0.73
1:A:349:ILE:HD11	1:B:325:ILE:HD13	1.71	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:F:325:ILE:HG13	1:F:325:ILE:O	1.87	0.70
1:B:341:ILE:HG21	1:D:325:ILE:CD1	2.22	0.69
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: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:460:LEU:HB2	1:A:468:MET:HE1	1.78	0.62
1:C:460:LEU:HB3	1:C:468:MET:HE1	1.80	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:B:460:LEU:HB3	1:B:468:MET:HE1	1.83	0.60
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:460:LEU:HB2	1:D:468:MET:HE1	1.89	0.55
1:B:379:GLU:O	1:B:379:GLU:HG2	2.06	0.54
1:F:706:LYS:O	1:F:706:LYS:HG3	2.07	0.54
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
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:HA	1:C:495:GLU:OE1	2.09	0.52
1:F:370:TYR:HH	1:F:467:HIS:HD1	1.56	0.52
1:B:496:VAL:CG1	1:D:512:LYS:HD3	2.40	0.51
1:D:460:LEU:CB	1:D:468:MET:HE1	2.39	0.51
1:B:525:LYS:NZ	1:D:527:MET:O	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:B:313:VAL:O	1:B:316:THR:OG1	2.26	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:C:460:LEU:CB	1:C:468:MET:HE1	2.41	0.49
1:A:508:LYS:O	1:A:511:LEU:CB	2.58	0.49
1:B:464:PHE:HB2	1:B:468:MET:HE3	1.95	0.49
1:B:312:LYS:O	1:B:316:THR:HG23	2.13	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:349:ILE:HD11	1:F:325:ILE:CD1	2.38	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:464:PHE:HB2	1:F:468:MET:HE3	1.94	0.48
1:C:362:ALA:HA	1:E:351:PHE:HE2	1.78	0.48
1:B:460:LEU:CB	1:B:468:MET:HE1	2.44	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:E:457:VAL:HG21	1:E:492:HIS:CE1	2.49	0.47
1:F:327:LEU:O	1:F:328:GLU:C	2.55	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:D:461:LYS:N	1:D:468:MET:HE1	2.30	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
1:A:460:LEU:HB3	1:A:468:MET:CE	2.41	0.46
1:C:511:LEU:HD21	1:C:540:ILE:HD11	1.98	0.45
1:C:513:THR:O	1:C:514:TRP:C	2.58	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:O	1:F:711:PRO:HG2	2.16	0.45
1:E:327:LEU:HD23	1:E:530:VAL:HG21	1.99	0.44
1:F:327:LEU:HD13	1:F:527:MET:HE3	1.93	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:F:370:TYR:OH	1:F:467:HIS:ND1	2.41	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:A:382:GLY:HA3	1:C:335:ASN:CG	2.42	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:C:433:TYR:C	1:C:433:TYR:CD1	2.97	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:468:MET:HA	1:D:490:ILE:O	2.19	0.43
1:F:460:LEU:HB3	1:F:468:MET:HE1	2.01	0.43
1:E:508:LYS:HB3	1:E:511:LEU:HD12	2.01	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:433:TYR:CD1	1:F:433:TYR:C	2.97	0.42
1:E:521:TYR:CE1	1:F:483:PRO:HG2	2.55	0.42
1:F:457:VAL:HG21	1:F:492:HIS:CE1	2.54	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:D:460:LEU:C	1:D:468:MET:HE1	2.44	0.41
1:B:433:TYR:CD1	1:B:433:TYR:C	2.98	0.41
1:E:464:PHE:HB2	1:E:468:MET:HE3	2.02	0.41
1:F:511:LEU:HD11	1:F:538:PHE:CG	2.55	0.41
1:B:482:ASN:O	1:B:482:ASN:CG	2.63	0.41
1:A:327:LEU:O	1:A:328:GLU:C	2.64	0.41
1:B:511:LEU:HD11	1:B:538:PHE:CD1	2.55	0.41
1:D:482:ASN:CG	1:D:482:ASN:O	2.62	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:O	1:C:511:LEU:HD12	2.21	0.41
1:A:474:ASP:OD1	1:A:508:LYS:NZ	2.46	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
1:B:327:LEU:O	1:B:328:GLU:C	2.63	0.40
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

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	406/416 (98%)	388 (96%)	18 (4%)	0	100	100
1	B	404/416 (97%)	384 (95%)	19 (5%)	1 (0%)	43	60
1	C	406/416 (98%)	383 (94%)	22 (5%)	1 (0%)	43	60
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%)	48	66

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%)	332 (92%)	31 (8%)	10	17
1	B	360/379 (95%)	333 (92%)	27 (8%)	12	21
1	C	362/379 (96%)	333 (92%)	29 (8%)	11	19
1	D	361/379 (95%)	333 (92%)	28 (8%)	11	20
1	E	362/379 (96%)	334 (92%)	28 (8%)	12	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	361/379 (95%)	332 (92%)	29 (8%)	11	19
All	All	2169/2274 (95%)	1997 (92%)	172 (8%)	11	19

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	LEU
1	A	316	THR
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	462	LYS
1	A	470	SER
1	A	477	LEU
1	A	494	ASN
1	A	496	VAL
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	580	ILE
1	A	628	LEU
1	A	644	VAL
1	A	650	VAL
1	A	656	GLU
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	384	LYS
1	B	390	LYS
1	B	397	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	398	LYS
1	B	411	LEU
1	B	429	LEU
1	B	463	ILE
1	B	465	GLU
1	B	466	GLU
1	B	477	LEU
1	B	494	ASN
1	B	496	VAL
1	B	530	VAL
1	B	566	LEU
1	B	574	THR
1	B	580	ILE
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	316	THR
1	C	380	GLU
1	C	381	GLU
1	C	384	LYS
1	C	390	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	544	GLU
1	C	545	THR
1	C	566	LEU
1	C	574	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	580	ILE
1	C	628	LEU
1	C	644	VAL
1	C	650	VAL
1	C	656	GLU
1	C	672	LEU
1	C	682	ASP
1	C	703	THR
1	C	715	ILE
1	D	310	LEU
1	D	316	THR
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	580	ILE
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	316	THR
1	E	326	LYS
1	E	381	GLU
1	E	390	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	397	VAL
1	E	398	LYS
1	E	411	LEU
1	E	429	LEU
1	E	470	SER
1	E	477	LEU
1	E	494	ASN
1	E	496	VAL
1	E	512	LYS
1	E	530	VAL
1	E	545	THR
1	E	566	LEU
1	E	574	THR
1	E	580	ILE
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	381	GLU
1	F	390	LYS
1	F	397	VAL
1	F	398	LYS
1	F	411	LEU
1	F	429	LEU
1	F	466	GLU
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	580	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	705	VAL
1	F	707	MET
1	F	715	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	GLN
1	A	413	ASN
1	A	449	GLN
1	A	537	ASN
1	A	564	ASN
1	A	583	ASN
1	A	623	GLN
1	B	413	ASN
1	B	471	ASN
1	B	537	ASN
1	B	564	ASN
1	B	583	ASN
1	C	413	ASN
1	C	537	ASN
1	C	564	ASN
1	C	583	ASN
1	D	413	ASN
1	D	449	GLN
1	D	537	ASN
1	D	564	ASN
1	D	583	ASN
1	D	623	GLN
1	E	413	ASN
1	E	537	ASN
1	E	564	ASN
1	E	583	ASN
1	F	413	ASN
1	F	471	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	494	ASN
1	F	537	ASN
1	F	564	ASN
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 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

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%)	0.50	14 (3%)	48	40	30, 73, 107, 163	0
1	B	408/416 (98%)	0.69	24 (5%)	28	21	28, 81, 115, 138	0
1	C	410/416 (98%)	0.61	24 (5%)	28	21	25, 81, 112, 152	0
1	D	409/416 (98%)	0.59	24 (5%)	28	21	12, 77, 116, 146	0
1	E	409/416 (98%)	0.70	25 (6%)	27	20	18, 79, 112, 156	0
1	F	408/416 (98%)	0.70	23 (5%)	30	24	31, 81, 118, 163	0
All	All	2454/2496 (98%)	0.63	134 (5%)	30	24	12, 79, 114, 163	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	498	ALA	6.2
1	D	303	GLU	4.3
1	C	642	GLU	4.2
1	A	499	ASP	4.0
1	E	707	MET	3.9
1	F	642	GLU	3.8
1	D	605	VAL	3.7
1	F	305	LYS	3.6
1	D	316	THR	3.6
1	F	508	LYS	3.5
1	B	642	GLU	3.5
1	A	709	GLY	3.3
1	F	715	ILE	3.3
1	B	340	TYR	3.2
1	E	498	ALA	3.2
1	F	637	LEU	3.2
1	D	498	ALA	3.2
1	B	499	ASP	3.1
1	B	601	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	565	VAL	3.1
1	B	417	TYR	3.0
1	D	567	LYS	3.0
1	B	708	ALA	3.0
1	B	333	LYS	3.0
1	A	498	ALA	3.0
1	B	671	TYR	2.9
1	E	617	THR	2.9
1	E	496	VAL	2.9
1	C	500	ASN	2.9
1	C	379	GLU	2.9
1	C	390	LYS	2.9
1	D	707	MET	2.9
1	F	571	TRP	2.9
1	A	378	TRP	2.8
1	D	497	SER	2.8
1	E	424	LEU	2.8
1	D	448	LYS	2.8
1	E	303	GLU	2.8
1	E	703	THR	2.8
1	A	496	VAL	2.7
1	D	686	ILE	2.7
1	E	653	PHE	2.7
1	B	462	LYS	2.7
1	E	351	PHE	2.7
1	C	548	VAL	2.6
1	C	715	ILE	2.6
1	A	670	LYS	2.6
1	B	605	VAL	2.6
1	A	653	PHE	2.6
1	D	637	LEU	2.5
1	B	600	LYS	2.5
1	A	711	PRO	2.5
1	D	711	PRO	2.5
1	C	705	VAL	2.5
1	C	499	ASP	2.5
1	D	555	ARG	2.5
1	C	605	VAL	2.5
1	B	571	TRP	2.5
1	B	505	MET	2.5
1	A	359	LYS	2.4
1	D	687	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	604	VAL	2.4
1	E	511	LEU	2.4
1	E	533	LYS	2.4
1	D	653	PHE	2.4
1	A	358	PRO	2.4
1	E	548	VAL	2.4
1	B	463	ILE	2.4
1	B	546	ILE	2.4
1	F	353	ILE	2.4
1	A	373	SER	2.4
1	A	332	ILE	2.3
1	A	710	LYS	2.3
1	B	706	LYS	2.3
1	E	340	TYR	2.3
1	E	449	GLN	2.3
1	C	594	ILE	2.3
1	D	333	LYS	2.3
1	E	558	ASN	2.3
1	E	555	ARG	2.3
1	C	338	VAL	2.3
1	F	644	VAL	2.3
1	B	346	LEU	2.3
1	C	708	ALA	2.3
1	D	544	GLU	2.3
1	D	568	GLU	2.3
1	C	686	ILE	2.2
1	E	708	ALA	2.2
1	F	702	THR	2.2
1	E	577	TYR	2.2
1	F	417	TYR	2.2
1	B	596	VAL	2.2
1	F	361	ILE	2.2
1	F	562	CYS	2.2
1	E	307	PRO	2.2
1	F	374	LYS	2.2
1	C	417	TYR	2.2
1	F	577	TYR	2.2
1	C	593	GLY	2.2
1	D	644	VAL	2.2
1	B	670	LYS	2.2
1	E	704	VAL	2.2
1	E	389	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	709	GLY	2.1
1	B	338	VAL	2.1
1	F	363	VAL	2.1
1	F	615	GLU	2.1
1	A	396	LYS	2.1
1	C	305	LYS	2.1
1	E	711	PRO	2.1
1	B	388	LEU	2.1
1	C	543	ASN	2.1
1	E	452	GLY	2.1
1	F	621	LEU	2.1
1	E	593	GLY	2.1
1	C	550	ILE	2.1
1	C	544	GLU	2.1
1	C	670	LYS	2.1
1	F	574	THR	2.1
1	C	669	ASN	2.1
1	D	563	ASN	2.1
1	B	383	ILE	2.1
1	F	338	VAL	2.1
1	F	496	VAL	2.1
1	F	530	VAL	2.1
1	D	696	PRO	2.0
1	C	511	LEU	2.0
1	D	332	ILE	2.0
1	E	649	ILE	2.0
1	C	397	VAL	2.0
1	B	485	LEU	2.0
1	B	581	LEU	2.0
1	D	667	ILE	2.0
1	F	555	ARG	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

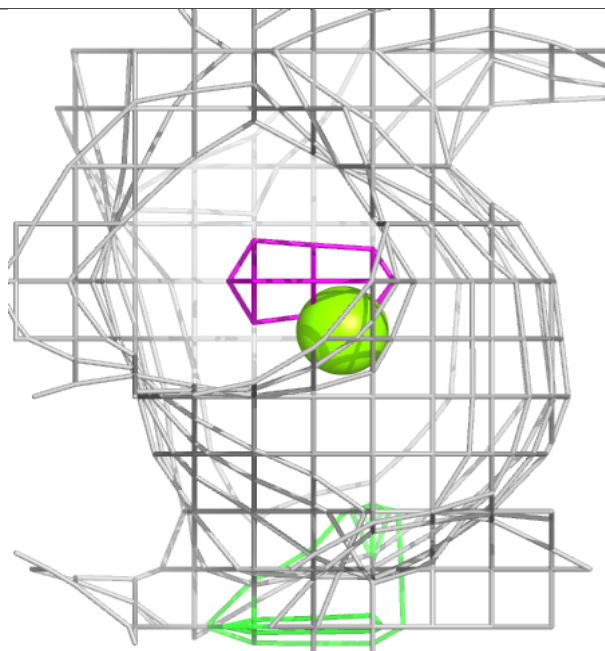
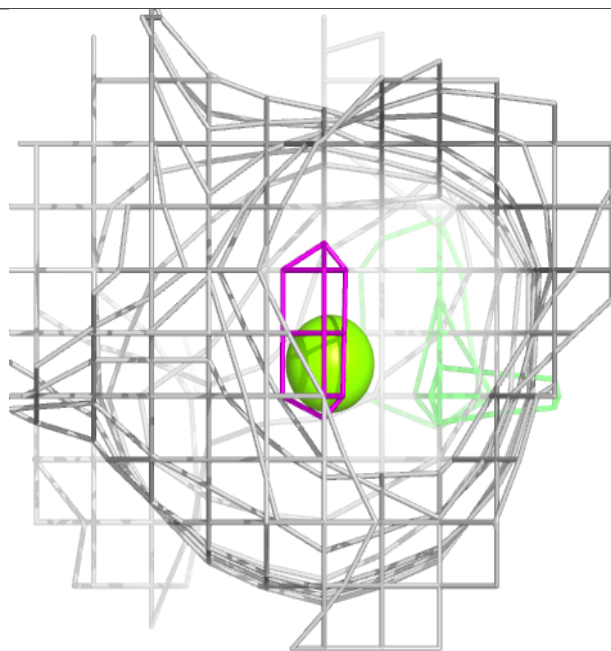
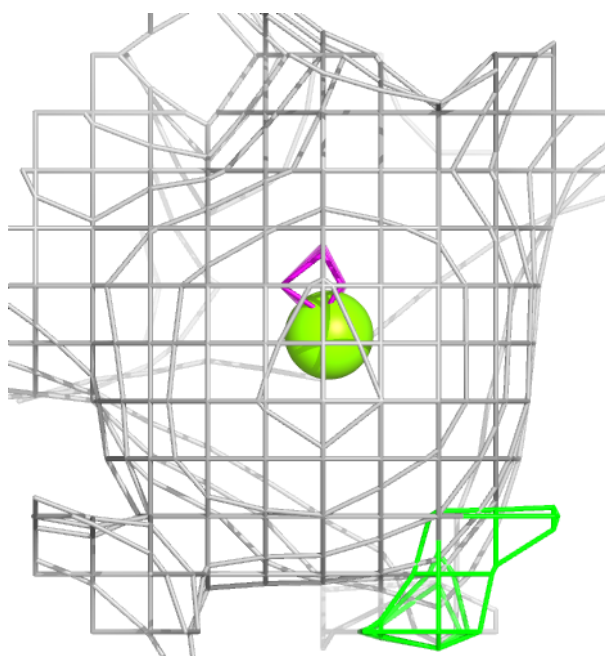
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	E	801	1/1	0.96	0.08	30,30,30,30	0
2	MG	D	801	1/1	0.97	0.12	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.

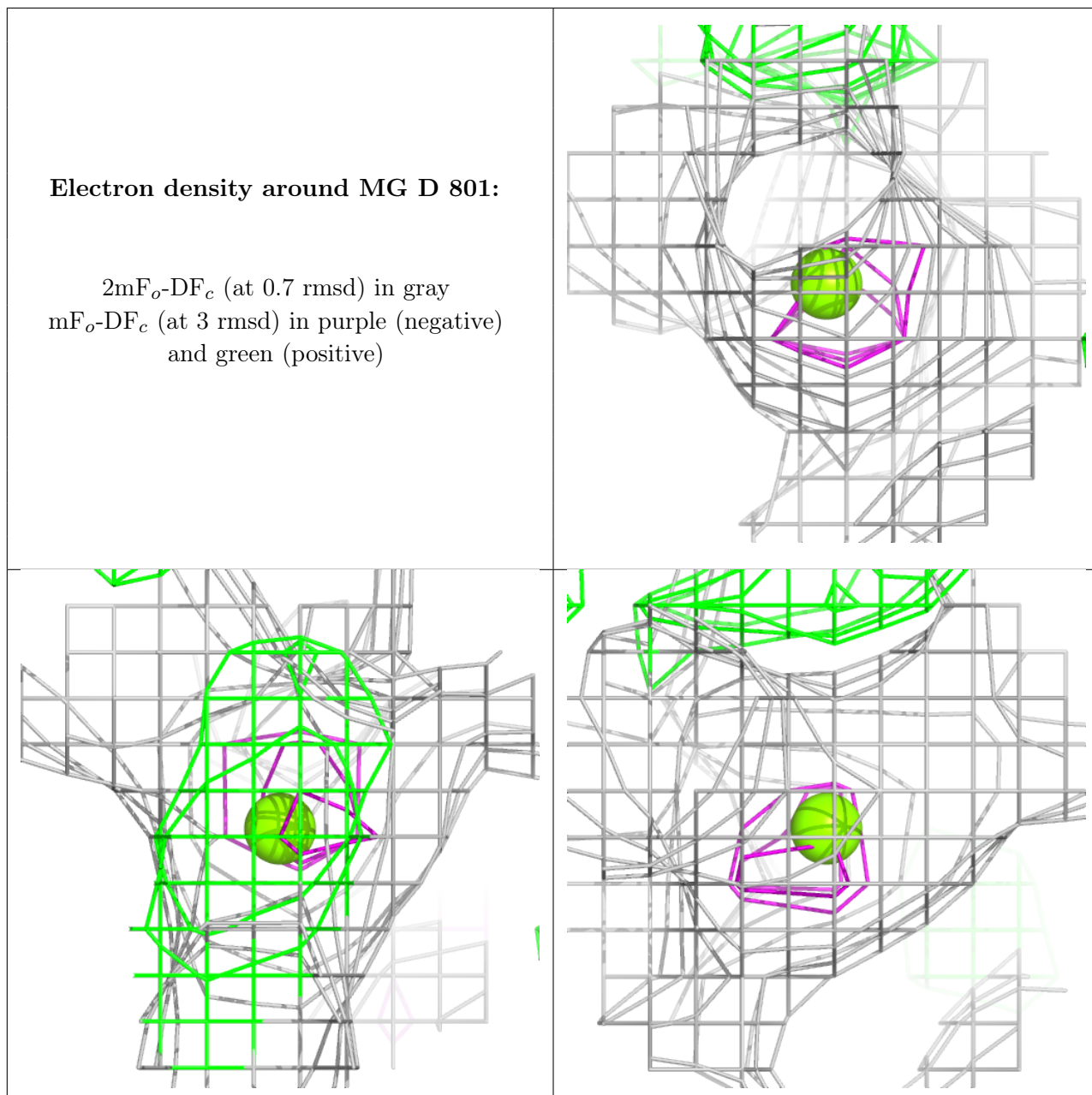
Electron density around MG E 801:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.