



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 09:51 PM UTC

PDB ID : 9BFA / pdb\_00009bfa  
Title : BCAT mutant  
Authors : Dong, M.  
Deposited on : 2024-04-17  
Resolution : 1.79 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

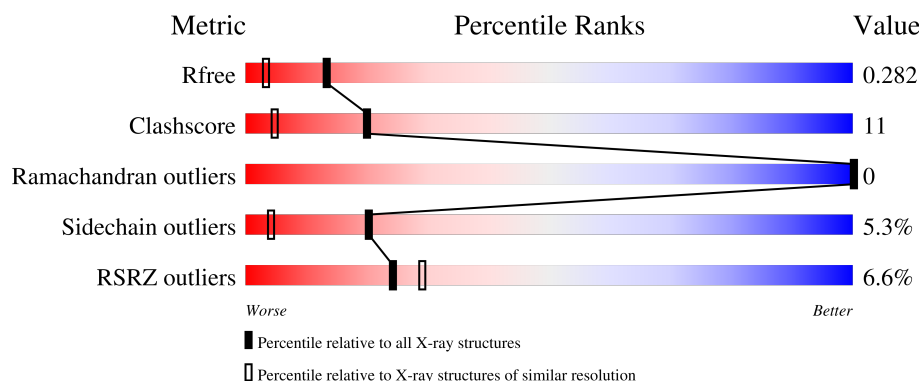
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	364	<div> <div>5%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	B	364	<div> <div>5%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	E	364	<div> <div>8%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>
1	F	364	<div> <div>8%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12375 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 Branched-chain-amino-acid aminotransferase, cytosolic.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	P	S	0	1	0
			2890	1857	476	541	1	15			
1	B	363	Total	C	N	O	P	S	0	0	0
			2885	1854	477	538	1	15			
1	E	364	Total	C	N	O	P	S	0	0	0
			2882	1853	474	539	1	15			
1	F	363	Total	C	N	O	P	S	0	0	0
			2885	1854	477	538	1	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLU	THR	conflict	UNP P54687
A	379	ARG	SER	conflict	UNP P54687
B	33	GLU	THR	conflict	UNP P54687
B	379	ARG	SER	conflict	UNP P54687
E	33	GLU	THR	conflict	UNP P54687
E	379	ARG	SER	conflict	UNP P54687
F	33	GLU	THR	conflict	UNP P54687
F	379	ARG	SER	conflict	UNP P54687

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Mg	0	0
			3	3		

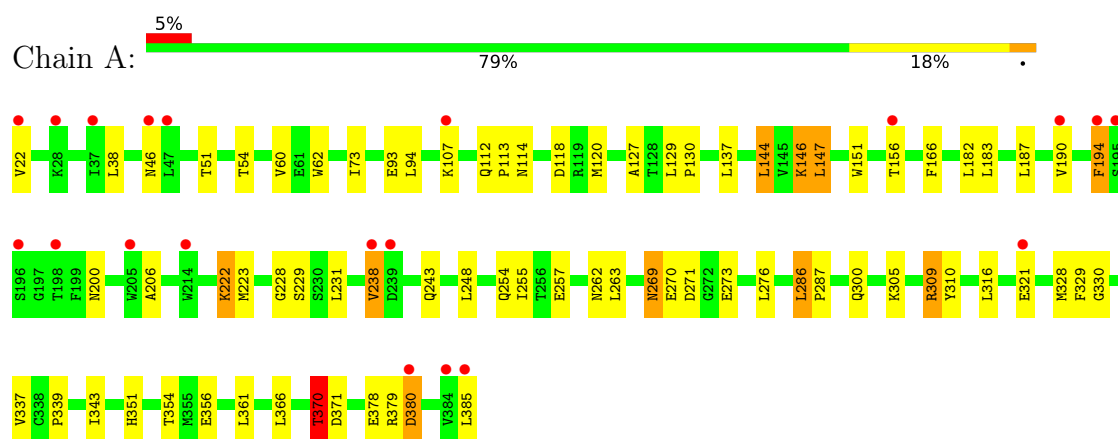
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	207	Total 207	O 207	0	0
3	B	183	Total 183	O 183	0	0
3	E	230	Total 230	O 230	0	0
3	F	210	Total 210	O 210	0	0

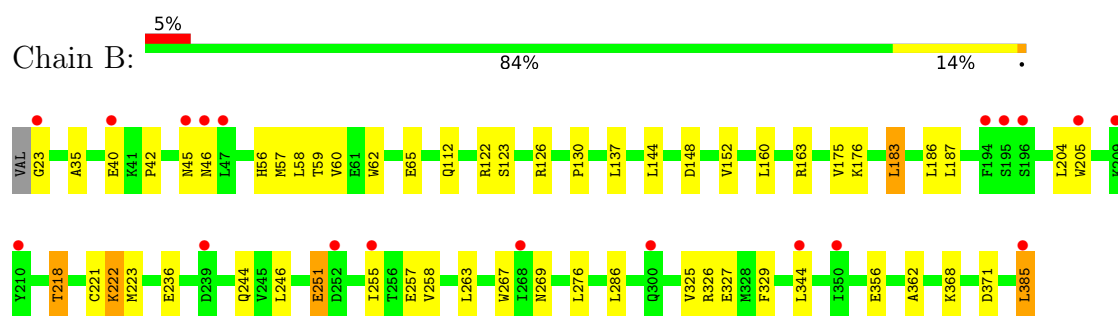
### 3 Residue-property plots

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.

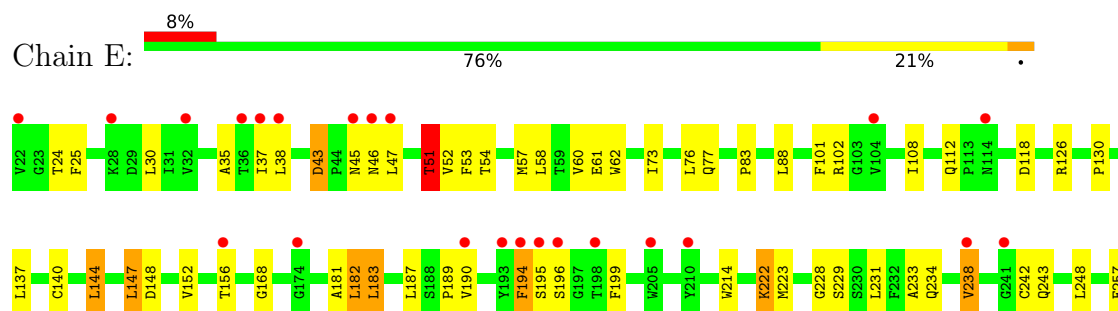
- Molecule 1: Branched-chain-amino-acid aminotransferase, cytosolic



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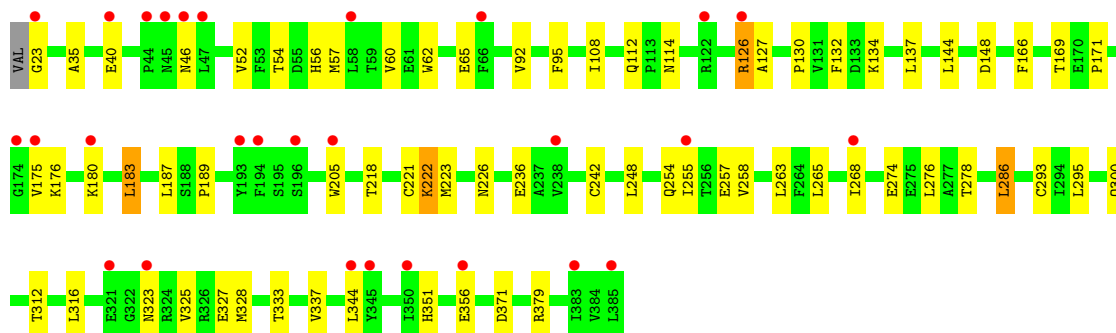
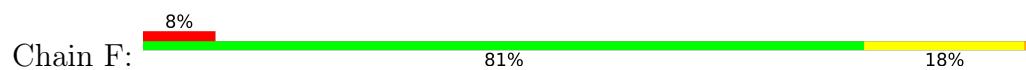


- Molecule 1: Branched-chain-amino-acid aminotransferase, cytosolic





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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.28Å 115.63Å 149.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.44 – 1.79 91.44 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.4 (91.44-1.79) 99.4 (91.44-1.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.232 , 0.268 0.245 , 0.282	Depositor DCC
$R_{free}$ test set	8936 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 25.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12375	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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 52.53 % 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 4.7992e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, LLP

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	0.59	0/2939	1.09	10/3999 (0.3%)
1	B	0.59	0/2934	1.07	5/3989 (0.1%)
1	E	0.59	0/2931	1.07	7/3988 (0.2%)
1	F	0.60	0/2934	1.06	7/3989 (0.2%)
All	All	0.59	0/11738	1.07	29/15965 (0.2%)

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
1	E	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	THR	CA-CB-OG1	-10.31	94.14	109.60
1	E	156	THR	CA-CB-OG1	-7.38	98.53	109.60
1	E	194	PHE	CB-CA-C	7.03	123.17	109.33
1	A	370	THR	CA-CB-OG1	-7.01	99.09	109.60
1	A	194	PHE	CB-CA-C	6.84	122.81	109.33
1	F	40	GLU	CB-CA-C	6.66	121.04	109.65
1	A	194	PHE	N-CA-CB	-6.59	99.80	111.08
1	B	40	GLU	CB-CA-C	6.38	121.21	109.46
1	F	371	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	118	ASP	CA-CB-CG	6.05	118.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	238	VAL	N-CA-CB	6.01	121.65	110.77
1	B	371	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	238	VAL	N-CA-CB	5.89	121.43	110.77
1	E	51	THR	CA-CB-OG1	-5.75	100.97	109.60
1	A	51	THR	CA-CB-OG1	-5.74	101.00	109.60
1	B	218	THR	N-CA-CB	-5.73	101.97	111.49
1	E	118	ASP	CA-CB-CG	5.61	118.21	112.60
1	E	43	ASP	CA-CB-CG	5.54	118.14	112.60
1	F	166	PHE	CA-CB-CG	5.43	119.23	113.80
1	F	54	THR	CA-CB-OG1	-5.33	101.60	109.60
1	A	370	THR	N-CA-CB	-5.26	102.11	109.94
1	F	333	THR	CA-CB-OG1	-5.25	101.72	109.60
1	F	169	THR	CA-CB-OG1	-5.24	101.73	109.60
1	F	65	GLU	CB-CG-CD	5.22	121.47	112.60
1	B	385	LEU	N-CA-CB	5.20	119.33	110.50
1	A	321	GLU	CB-CG-CD	5.12	121.30	112.60
1	B	251	GLU	CB-CG-CD	5.12	121.30	112.60
1	A	371	ASP	CA-CB-CG	5.07	117.67	112.60
1	E	194	PHE	N-CA-CB	-5.07	102.42	111.08

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	126	ARG	Sidechain
1	F	126	ARG	Sidechain

## 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	2890	0	2840	64	0
1	B	2885	0	2847	50	0
1	E	2882	0	2835	84	0
1	F	2885	0	2846	63	0
2	B	3	0	0	0	0
3	A	207	0	0	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	183	0	0	29	0
3	E	230	0	0	56	0
3	F	210	0	0	41	0
All	All	12375	0	11368	261	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 11.

All (261) 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:337:VAL:HB	3:A:623:HOH:O	1.48	1.13
1:F:268:ILE:HG13	3:F:672:HOH:O	1.61	0.99
1:B:152:VAL:HG13	3:B:503:HOH:O	1.60	0.99
1:E:102:ARG:HG3	3:E:511:HOH:O	1.66	0.96
1:E:339:PRO:HD3	3:E:505:HOH:O	1.69	0.92
1:F:126:ARG:HB3	1:F:223:MET:HE1	1.53	0.90
1:B:126:ARG:HB3	1:B:223:MET:HE1	1.56	0.87
1:E:242:CYS:SG	3:E:688:HOH:O	2.34	0.85
1:B:58:LEU:HG	3:B:658:HOH:O	1.77	0.84
1:F:323:ASN:HB3	3:F:624:HOH:O	1.80	0.81
1:E:152:VAL:HG11	3:E:519:HOH:O	1.81	0.80
1:F:293:CYS:SG	3:F:512:HOH:O	2.39	0.80
1:F:108:ILE:HG12	3:F:640:HOH:O	1.80	0.79
1:F:95:PHE:CE1	3:F:665:HOH:O	2.35	0.79
1:E:54:THR:HG21	3:E:633:HOH:O	1.83	0.78
1:E:168:GLY:HA2	3:E:650:HOH:O	1.82	0.78
1:E:47:LEU:HB2	3:E:649:HOH:O	1.83	0.77
1:F:278:THR:HG21	3:F:634:HOH:O	1.85	0.77
1:B:385:LEU:C	3:B:560:HOH:O	2.28	0.77
1:B:56:HIS:HD2	1:B:148:ASP:OD1	1.68	0.76
1:E:148:ASP:HB3	3:E:633:HOH:O	1.85	0.76
1:F:218:THR:HG23	1:F:226:ASN:OD1	1.87	0.75
1:F:274:GLU:HA	3:F:672:HOH:O	1.86	0.75
1:B:35:ALA:H	1:B:56:HIS:HE1	1.35	0.74
1:E:152:VAL:HG23	3:E:503:HOH:O	1.86	0.74
1:A:380:ASP:C	3:A:507:HOH:O	2.30	0.74
1:E:300:GLN:NE2	1:E:379:ARG:HH22	1.85	0.74
1:F:57:MET:SD	3:F:506:HOH:O	2.45	0.73
3:E:682:HOH:O	1:F:126:ARG:HD2	1.89	0.72
1:E:47:LEU:CB	3:E:649:HOH:O	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LEU:HD13	3:B:533:HOH:O	1.89	0.72
1:F:56:HIS:HD2	1:F:148:ASP:OD1	1.72	0.72
1:F:175:VAL:HG12	3:F:682:HOH:O	1.89	0.72
1:B:57:MET:SD	3:B:507:HOH:O	2.48	0.72
1:F:327:GLU:HB2	3:F:565:HOH:O	1.90	0.72
1:F:127:ALA:HB2	3:F:502:HOH:O	1.90	0.71
1:F:295:LEU:HD11	3:F:634:HOH:O	1.89	0.71
1:E:52:VAL:HG12	3:E:524:HOH:O	1.90	0.71
1:A:337:VAL:CB	3:A:623:HOH:O	2.21	0.71
1:A:223:MET:HE3	3:A:654:HOH:O	1.88	0.70
1:B:126:ARG:CB	1:B:223:MET:HE1	2.21	0.70
1:E:61:GLU:HA	3:E:509:HOH:O	1.91	0.70
1:A:166:PHE:CD2	3:A:687:HOH:O	2.44	0.70
1:E:140:CYS:SG	3:E:720:HOH:O	2.49	0.70
1:E:234:GLN:NE2	3:E:502:HOH:O	2.26	0.69
1:B:325:VAL:HG22	3:B:673:HOH:O	1.91	0.69
1:A:146:LYS:HD3	3:A:680:HOH:O	1.92	0.69
1:F:312:THR:HA	3:F:504:HOH:O	1.93	0.69
1:E:195:SER:HB3	3:E:647:HOH:O	1.93	0.68
1:A:129:LEU:HB2	3:A:687:HOH:O	1.93	0.68
1:F:222:LLP:HG3	3:F:665:HOH:O	1.92	0.67
1:E:57:MET:SD	3:E:506:HOH:O	2.52	0.67
1:E:269:ASN:C	1:E:269:ASN:HD22	2.03	0.67
1:A:194:PHE:CE2	3:A:539:HOH:O	2.47	0.66
1:A:270:GLU:O	3:A:501:HOH:O	2.12	0.66
1:F:35:ALA:H	1:F:56:HIS:HE1	1.43	0.66
1:F:327:GLU:HB3	3:F:529:HOH:O	1.94	0.66
1:E:25:PHE:CE1	3:E:715:HOH:O	2.49	0.65
1:F:126:ARG:CB	1:F:223:MET:HE1	2.24	0.65
1:E:190:VAL:HG13	3:E:548:HOH:O	1.97	0.65
1:B:126:ARG:HB3	1:B:223:MET:CE	2.27	0.65
1:A:269:ASN:C	1:A:269:ASN:HD22	2.04	0.65
1:A:114[B]:ASN:ND2	1:A:114[B]:ASN:H	1.96	0.64
1:A:351:HIS:HE1	1:A:356:GLU:OE1	1.81	0.64
1:B:258:VAL:HG13	3:B:533:HOH:O	1.97	0.64
1:A:190:VAL:HG13	3:A:591:HOH:O	1.97	0.63
1:E:108:ILE:HG12	3:E:519:HOH:O	1.98	0.63
1:E:182:LEU:HD23	3:E:509:HOH:O	1.99	0.62
1:A:146:LYS:CD	3:A:680:HOH:O	2.47	0.62
1:E:47:LEU:CD1	3:E:649:HOH:O	2.48	0.62
1:B:126:ARG:CG	1:B:223:MET:HE1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:337:VAL:HG12	3:E:505:HOH:O	1.99	0.62
1:B:205:TRP:CH2	1:B:236:GLU:OE2	2.54	0.61
1:A:366:LEU:O	1:A:370:THR:HB	2.01	0.61
1:A:127:ALA:HB1	3:A:510:HOH:O	2.01	0.60
1:A:194:PHE:CD2	3:A:539:HOH:O	2.54	0.60
1:E:300:GLN:HE21	1:E:379:ARG:HH22	1.49	0.60
1:A:146:LYS:HE2	3:A:680:HOH:O	2.01	0.60
1:B:221:CYS:HB3	1:B:223:MET:HE3	1.83	0.60
1:E:297:LEU:HD13	3:E:710:HOH:O	2.00	0.60
1:E:285:ILE:CD1	3:E:634:HOH:O	2.49	0.60
1:A:273:GLU:HB2	3:A:659:HOH:O	2.02	0.60
1:A:379:ARG:O	1:A:379:ARG:HG2	2.02	0.60
1:F:114:ASN:HB2	3:F:654:HOH:O	2.01	0.60
1:E:321:GLU:O	1:E:321:GLU:CG	2.50	0.59
1:F:255:ILE:N	3:F:504:HOH:O	2.35	0.59
1:E:47:LEU:HD12	3:E:649:HOH:O	2.02	0.59
1:B:35:ALA:H	1:B:56:HIS:CE1	2.19	0.59
1:A:46:ASN:HB3	3:A:672:HOH:O	2.03	0.58
1:F:218:THR:HG22	3:F:679:HOH:O	2.03	0.58
1:E:339:PRO:HD2	3:E:504:HOH:O	2.03	0.58
1:E:144:LEU:HD13	1:E:187:LEU:HD11	1.85	0.58
1:B:329:PHE:CE1	3:B:511:HOH:O	2.53	0.58
1:B:160:LEU:N	3:B:503:HOH:O	2.37	0.57
1:B:258:VAL:CG2	1:B:263:LEU:HD23	2.35	0.57
1:E:199:PHE:CE1	3:E:505:HOH:O	2.53	0.57
1:E:76:LEU:HD12	3:E:506:HOH:O	2.03	0.57
1:A:190:VAL:CG1	3:A:591:HOH:O	2.50	0.57
1:B:362:ALA:HA	3:B:511:HOH:O	2.03	0.56
1:E:24:THR:HA	3:E:527:HOH:O	2.04	0.56
1:F:221:CYS:HB3	1:F:223:MET:HE3	1.84	0.56
1:B:326:ARG:NH1	3:B:505:HOH:O	2.39	0.56
3:A:670:HOH:O	1:B:175:VAL:HG12	2.05	0.56
1:E:222:LLP:O3	1:E:222:LLP:NZ	2.34	0.56
1:F:95:PHE:CZ	3:F:665:HOH:O	2.56	0.56
1:E:30:LEU:HD22	3:E:600:HOH:O	2.05	0.56
1:F:316:LEU:HD11	3:F:705:HOH:O	2.05	0.55
1:B:246:LEU:HD11	1:B:255:ILE:HG23	1.88	0.55
1:F:222:LLP:N1	1:F:257:GLU:OE2	2.39	0.55
1:A:255:ILE:C	3:A:514:HOH:O	2.50	0.55
1:E:273:GLU:HB2	3:E:562:HOH:O	2.05	0.55
1:A:166:PHE:CE2	3:A:687:HOH:O	2.57	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LEU:HD12	1:B:183:LEU:C	2.32	0.54
1:E:58:LEU:HD22	3:E:693:HOH:O	2.07	0.54
1:A:329:PHE:CD2	1:A:337:VAL:CG2	2.91	0.54
1:B:368:LYS:HE2	3:B:567:HOH:O	2.07	0.54
1:E:231:LEU:HG	3:F:682:HOH:O	2.07	0.54
1:E:190:VAL:CG1	3:E:548:HOH:O	2.52	0.54
1:B:222:LLP:NZ	1:B:222:LLP:O3	2.39	0.53
1:F:35:ALA:H	1:F:56:HIS:CE1	2.23	0.53
1:A:222:LLP:O3	1:A:222:LLP:NZ	2.36	0.53
1:B:221:CYS:CB	1:B:223:MET:HE3	2.38	0.53
1:A:222:LLP:N1	1:A:257:GLU:OE1	2.41	0.53
1:A:337:VAL:CG2	3:A:623:HOH:O	2.55	0.53
1:F:183:LEU:HD12	1:F:183:LEU:C	2.33	0.53
1:A:339:PRO:HB3	1:A:354:THR:HG21	1.90	0.52
1:E:248:LEU:HG	3:E:516:HOH:O	2.08	0.52
1:A:129:LEU:CB	3:A:687:HOH:O	2.55	0.52
1:A:263:LEU:HD13	3:A:514:HOH:O	2.10	0.52
1:E:187:LEU:HD21	3:E:689:HOH:O	2.09	0.52
1:E:38:LEU:HD13	3:E:526:HOH:O	2.09	0.52
1:E:339:PRO:HB3	1:E:354:THR:HG21	1.90	0.52
1:F:218:THR:CG2	1:F:226:ASN:OD1	2.58	0.52
1:E:214:TRP:CZ3	3:F:503:HOH:O	2.54	0.52
1:F:126:ARG:CG	1:F:223:MET:HE1	2.39	0.52
1:B:45:ASN:HB2	3:B:643:HOH:O	2.10	0.52
1:E:223:MET:HE3	3:E:657:HOH:O	2.09	0.52
1:F:223:MET:HG2	3:F:502:HOH:O	2.08	0.52
1:E:43:ASP:O	1:E:45:ASN:O	2.27	0.51
1:E:222:LLP:N1	1:E:257:GLU:OE1	2.44	0.51
1:A:243:GLN:HG2	3:A:569:HOH:O	2.09	0.51
1:A:300:GLN:CD	1:A:379:ARG:HH22	2.19	0.51
1:A:329:PHE:CD2	1:A:337:VAL:HG23	2.46	0.51
1:E:351:HIS:HE1	1:E:356:GLU:OE1	1.93	0.51
1:E:101:PHE:C	3:E:519:HOH:O	2.54	0.51
1:F:222:LLP:O3	1:F:222:LLP:NZ	2.42	0.51
1:A:93:GLU:N	3:A:510:HOH:O	2.44	0.50
1:E:233:ALA:HA	3:E:561:HOH:O	2.10	0.50
1:B:269:ASN:ND2	3:B:506:HOH:O	2.43	0.50
1:E:181:ALA:HB2	3:E:650:HOH:O	2.11	0.50
1:B:267:TRP:HB3	3:B:673:HOH:O	2.11	0.50
1:F:221:CYS:CB	1:F:223:MET:HE3	2.41	0.50
1:E:263:LEU:HD23	1:E:263:LEU:C	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:VAL:N	3:E:503:HOH:O	2.44	0.49
1:A:22:VAL:HG22	1:A:22:VAL:O	2.11	0.49
1:A:309:ARG:HD3	1:A:310:TYR:O	2.13	0.49
1:B:258:VAL:HG21	1:B:263:LEU:HD23	1.94	0.49
1:E:316:LEU:HD21	1:E:328:MET:HE1	1.95	0.49
1:A:231:LEU:HA	3:A:670:HOH:O	2.11	0.49
3:E:682:HOH:O	1:F:126:ARG:CD	2.55	0.49
1:F:263:LEU:HG	3:F:566:HOH:O	2.13	0.49
1:B:122:ARG:NH2	3:B:508:HOH:O	2.46	0.48
1:F:126:ARG:HB3	1:F:223:MET:CE	2.33	0.47
1:E:321:GLU:O	1:E:321:GLU:HG2	2.14	0.47
1:A:146:LYS:CE	3:A:680:HOH:O	2.62	0.47
1:A:305:LYS:HB3	3:A:659:HOH:O	2.14	0.47
1:E:194:PHE:CD2	3:E:582:HOH:O	2.67	0.47
1:E:62:TRP:CD2	1:E:130:PRO:HG3	2.49	0.47
1:A:316:LEU:HD21	1:A:328:MET:HE1	1.95	0.47
1:E:262:ASN:O	1:E:330:GLY:HA2	2.15	0.47
1:F:144:LEU:HG	1:F:187:LEU:HD11	1.97	0.47
1:E:234:GLN:CD	3:E:502:HOH:O	2.54	0.47
1:A:62:TRP:CD2	1:A:130:PRO:HG3	2.50	0.46
1:A:262:ASN:O	1:A:330:GLY:HA2	2.14	0.46
1:B:222:LLP:N1	1:B:257:GLU:OE2	2.48	0.46
1:F:258:VAL:CG2	1:F:263:LEU:HD23	2.45	0.46
1:F:323:ASN:CB	3:F:624:HOH:O	2.52	0.46
1:A:269:ASN:ND2	1:A:271:ASP:H	2.13	0.46
1:E:88:LEU:HD23	3:E:518:HOH:O	2.15	0.46
1:E:228:GLY:HA2	3:F:510:HOH:O	2.15	0.46
1:F:205:TRP:CH2	1:F:236:GLU:OE2	2.68	0.46
1:A:73:ILE:HG21	1:A:147:LEU:HD12	1.96	0.46
1:B:163:ARG:HG3	3:B:509:HOH:O	2.15	0.46
1:F:134:LYS:HG3	3:F:507:HOH:O	2.16	0.46
1:B:368:LYS:CE	3:B:567:HOH:O	2.62	0.46
1:A:263:LEU:HD23	1:A:263:LEU:C	2.40	0.46
1:B:144:LEU:HG	1:B:187:LEU:HD11	1.98	0.46
1:E:51:THR:HG22	1:E:52:VAL:HG23	1.98	0.46
1:E:183:LEU:HD21	3:E:728:HOH:O	2.16	0.46
1:E:309:ARG:HD2	1:E:311:LEU:HD21	1.98	0.46
1:F:62:TRP:CD2	1:F:130:PRO:HG3	2.51	0.46
1:A:194:PHE:HD1	1:A:200:ASN:H	1.63	0.45
1:F:92:VAL:HG22	3:F:510:HOH:O	2.14	0.45
1:F:132:PHE:CD2	3:F:507:HOH:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:351:HIS:CD2	3:F:637:HOH:O	2.69	0.45
1:A:343:ILE:HG23	3:A:537:HOH:O	2.15	0.45
1:B:362:ALA:CA	3:B:511:HOH:O	2.62	0.45
1:E:53:PHE:C	3:E:524:HOH:O	2.59	0.45
1:E:77:GLN:N	3:E:506:HOH:O	2.42	0.45
1:B:58:LEU:HD13	1:B:59:THR:N	2.32	0.45
1:F:126:ARG:HG2	1:F:223:MET:HE1	1.99	0.45
1:B:258:VAL:HG12	3:B:587:HOH:O	2.16	0.44
1:E:309:ARG:HD2	1:E:311:LEU:CD2	2.47	0.44
1:A:206:ALA:HB2	3:A:537:HOH:O	2.17	0.44
1:A:231:LEU:HD11	3:B:526:HOH:O	2.16	0.44
1:A:255:ILE:HG13	3:A:514:HOH:O	2.17	0.44
1:E:108:ILE:HG23	3:E:519:HOH:O	2.16	0.44
1:A:94:LEU:HD21	3:A:687:HOH:O	2.17	0.44
1:B:362:ALA:N	3:B:511:HOH:O	2.49	0.44
1:E:47:LEU:CD1	1:E:189:PRO:HB2	2.47	0.44
1:F:248:LEU:HA	1:F:254:GLN:O	2.16	0.44
1:B:327:GLU:HB2	3:B:629:HOH:O	2.17	0.44
1:E:269:ASN:ND2	1:E:273:GLU:H	2.16	0.44
1:E:379:ARG:C	1:E:381:TRP:H	2.26	0.44
1:E:35:ALA:C	3:E:526:HOH:O	2.61	0.43
1:B:58:LEU:HD13	1:B:58:LEU:C	2.43	0.43
1:B:244:GLN:HG3	3:B:587:HOH:O	2.17	0.43
1:A:120:MET:HG2	3:A:502:HOH:O	2.18	0.43
1:A:120:MET:O	3:A:502:HOH:O	2.21	0.43
1:E:47:LEU:HD13	1:E:189:PRO:HB2	2.00	0.43
1:F:222:LLP:C4	1:F:286:LEU:HD22	2.48	0.43
1:F:312:THR:CA	3:F:504:HOH:O	2.57	0.43
1:E:83:PRO:HG3	3:F:506:HOH:O	2.18	0.43
1:F:255:ILE:HG13	3:F:504:HOH:O	2.18	0.43
1:F:223:MET:HE2	3:F:502:HOH:O	2.18	0.43
1:F:325:VAL:HG11	3:F:705:HOH:O	2.18	0.43
1:F:337:VAL:HG22	3:F:581:HOH:O	2.18	0.43
1:A:379:ARG:O	1:A:379:ARG:CG	2.66	0.42
1:B:123:SER:O	1:B:223:MET:HE2	2.19	0.42
1:A:286:LEU:HG	1:A:287:PRO:HD2	2.01	0.42
1:E:231:LEU:HD11	3:F:510:HOH:O	2.19	0.42
1:B:329:PHE:CZ	3:B:511:HOH:O	2.73	0.42
1:E:73:ILE:HG21	1:E:147:LEU:HD12	2.01	0.42
1:F:300:GLN:NE2	1:F:379:ARG:HH22	2.18	0.42
1:F:23:GLY:N	3:F:518:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LEU:HA	1:A:254:GLN:O	2.20	0.41
1:B:62:TRP:CD2	1:B:130:PRO:HG3	2.55	0.41
1:B:246:LEU:HA	3:B:533:HOH:O	2.19	0.41
1:E:102:ARG:HA	3:E:519:HOH:O	2.20	0.41
1:F:295:LEU:CD1	3:F:634:HOH:O	2.59	0.41
1:A:112:GLN:N	1:A:113:PRO:CD	2.83	0.41
1:F:328:MET:C	3:F:529:HOH:O	2.63	0.41
1:F:52:VAL:O	1:F:189:PRO:HD2	2.21	0.41
1:A:144:LEU:HD13	1:A:187:LEU:HD11	2.01	0.41
1:A:305:LYS:CB	3:A:659:HOH:O	2.67	0.41
1:E:195:SER:CB	3:E:647:HOH:O	2.61	0.41
1:E:284:ILE:HG13	1:E:285:ILE:HD12	2.03	0.41
1:A:380:ASP:C	1:A:380:ASP:OD1	2.63	0.41
1:B:205:TRP:HH2	1:B:236:GLU:OE2	2.04	0.41
1:E:37:ILE:C	3:E:526:HOH:O	2.63	0.41
1:E:61:GLU:CD	3:E:509:HOH:O	2.64	0.41
1:F:265:LEU:HD13	1:F:328:MET:HE2	2.03	0.41
1:A:54:THR:HG22	1:A:151:TRP:CD2	2.56	0.41
1:B:186:LEU:HG	3:B:509:HOH:O	2.20	0.41
1:A:380:ASP:OD1	1:A:380:ASP:O	2.39	0.40
1:A:228:GLY:HA2	3:B:526:HOH:O	2.21	0.40
1:B:23:GLY:N	3:B:514:HOH:O	2.54	0.40
1:E:337:VAL:C	3:E:505:HOH:O	2.65	0.40
1:F:312:THR:C	3:F:504:HOH:O	2.63	0.40
1:F:242:CYS:SG	1:F:344:LEU:HD13	2.61	0.40
1:E:268:ILE:HD11	1:E:326:ARG:NH2	2.36	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	362/364 (100%)	350 (97%)	12 (3%)	0	100	100
1	B	360/364 (99%)	350 (97%)	10 (3%)	0	100	100
1	E	361/364 (99%)	348 (96%)	13 (4%)	0	100	100
1	F	360/364 (99%)	351 (98%)	9 (2%)	0	100	100
All	All	1443/1456 (99%)	1399 (97%)	44 (3%)	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	314/316 (99%)	294 (94%)	20 (6%)	16	3
1	B	314/316 (99%)	300 (96%)	14 (4%)	24	6
1	E	313/316 (99%)	292 (93%)	21 (7%)	15	2
1	F	314/316 (99%)	303 (96%)	11 (4%)	32	11
All	All	1255/1264 (99%)	1189 (95%)	66 (5%)	20	4

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	60	VAL
1	A	107	LYS
1	A	137	LEU
1	A	144	LEU
1	A	146	LYS
1	A	147	LEU
1	A	182	LEU
1	A	183	LEU
1	A	229	SER
1	A	238	VAL
1	A	269	ASN
1	A	276	LEU

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Mol	Chain	Res	Type
1	A	286	LEU
1	A	309	ARG
1	A	361	LEU
1	A	370	THR
1	A	378	GLU
1	A	380	ASP
1	A	385	LEU
1	B	42	PRO
1	B	46	ASN
1	B	60	VAL
1	B	65	GLU
1	B	112	GLN
1	B	137	LEU
1	B	176	LYS
1	B	183	LEU
1	B	218	THR
1	B	251	GLU
1	B	276	LEU
1	B	286	LEU
1	B	344	LEU
1	B	356	GLU
1	E	46	ASN
1	E	51	THR
1	E	60	VAL
1	E	112	GLN
1	E	137	LEU
1	E	144	LEU
1	E	147	LEU
1	E	182	LEU
1	E	183	LEU
1	E	196	SER
1	E	229	SER
1	E	238	VAL
1	E	243	GLN
1	E	269	ASN
1	E	276	LEU
1	E	285	ILE
1	E	286	LEU
1	E	309	ARG
1	E	337	VAL
1	E	361	LEU
1	E	385	LEU

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Mol	Chain	Res	Type
1	F	46	ASN
1	F	60	VAL
1	F	112	GLN
1	F	137	LEU
1	F	171	PRO
1	F	176	LYS
1	F	180	LYS
1	F	183	LEU
1	F	276	LEU
1	F	286	LEU
1	F	356	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	142	GLN
1	A	254	GLN
1	A	269	ASN
1	A	351	HIS
1	B	45	ASN
1	B	56	HIS
1	B	143	GLN
1	B	200	ASN
1	B	254	GLN
1	E	106	ASN
1	E	112	GLN
1	E	143	GLN
1	E	149	GLN
1	E	226	ASN
1	E	269	ASN
1	E	300	GLN
1	E	351	HIS
1	F	45	ASN
1	F	56	HIS
1	F	143	GLN
1	F	200	ASN
1	F	254	GLN
1	F	300	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LLP	E	222	1	23,24,25	0.60	0	25,32,34	1.55	5 (20%)
1	LLP	B	222	1	23,24,25	0.62	0	25,32,34	1.47	6 (24%)
1	LLP	A	222	1	23,24,25	0.61	0	25,32,34	1.36	4 (16%)
1	LLP	F	222	1	23,24,25	0.55	0	25,32,34	1.47	5 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	E	222	1	-	4/16/17/19	0/1/1/1
1	LLP	B	222	1	-	3/16/17/19	0/1/1/1
1	LLP	A	222	1	-	4/16/17/19	0/1/1/1
1	LLP	F	222	1	-	4/16/17/19	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	LLP	OP4-C5'-C5	3.77	116.42	109.36
1	E	222	LLP	OP4-C5'-C5	3.59	116.08	109.36
1	F	222	LLP	CD-CE-NZ	3.50	120.11	110.83
1	E	222	LLP	C5-C4-C4'	3.44	126.78	121.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	LLP	C5-C4-C4'	3.28	126.53	121.47
1	A	222	LLP	OP4-C5'-C5	3.03	115.03	109.36
1	F	222	LLP	OP2-P-OP4	-2.97	98.92	106.67
1	B	222	LLP	OP2-P-OP4	-2.85	99.23	106.67
1	A	222	LLP	C3-C4-C4'	-2.83	115.28	120.40
1	E	222	LLP	O3-C3-C2	2.74	123.27	117.58
1	B	222	LLP	C5-C4-C4'	2.73	125.69	121.47
1	E	222	LLP	C3-C4-C4'	-2.63	115.66	120.40
1	F	222	LLP	OP4-C5'-C5	2.60	114.22	109.36
1	F	222	LLP	O3-C3-C2	2.52	122.80	117.58
1	F	222	LLP	OP3-P-OP2	2.39	116.76	107.80
1	A	222	LLP	O3-C3-C2	2.35	122.45	117.58
1	B	222	LLP	CD-CE-NZ	2.32	116.97	110.83
1	E	222	LLP	OP2-P-OP4	-2.19	100.96	106.67
1	B	222	LLP	C3-C4-C4'	-2.08	116.64	120.40
1	B	222	LLP	O3-C3-C2	2.00	121.73	117.58

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	222	LLP	N-CA-CB-CG
1	A	222	LLP	C-CA-CB-CG
1	B	222	LLP	N-CA-CB-CG
1	B	222	LLP	C-CA-CB-CG
1	E	222	LLP	N-CA-CB-CG
1	E	222	LLP	C-CA-CB-CG
1	F	222	LLP	N-CA-CB-CG
1	F	222	LLP	C-CA-CB-CG
1	F	222	LLP	C4-C4'-NZ-CE
1	B	222	LLP	C4-C4'-NZ-CE
1	E	222	LLP	C4-C4'-NZ-CE
1	A	222	LLP	C4-C4'-NZ-CE
1	A	222	LLP	CG-CD-CE-NZ
1	E	222	LLP	CG-CD-CE-NZ
1	F	222	LLP	CE-CD-CG-CB

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	222	LLP	2	0
1	B	222	LLP	2	0
1	A	222	LLP	2	0
1	F	222	LLP	4	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	363/364 (99%)	0.44	20 (5%)	30 36	14, 30, 50, 88	1 (0%)
1	B	362/364 (99%)	0.44	19 (5%)	33 39	20, 31, 50, 62	0
1	E	363/364 (99%)	0.46	29 (7%)	18 21	21, 30, 51, 87	0
1	F	362/364 (99%)	0.64	28 (7%)	19 23	20, 33, 52, 69	0
All	All	1450/1456 (99%)	0.49	96 (6%)	24 29	14, 31, 51, 88	1 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	PHE	9.1
1	A	22	VAL	9.1
1	E	194	PHE	7.8
1	E	22	VAL	7.2
1	F	385	LEU	5.0
1	B	385	LEU	4.7
1	A	37	ILE	3.9
1	F	344	LEU	3.8
1	E	46	ASN	3.7
1	E	47	LEU	3.6
1	A	385	LEU	3.5
1	E	37	ILE	3.4
1	F	40	GLU	3.4
1	E	385	LEU	3.3
1	A	195	SER	3.3
1	E	36	THR	3.2
1	E	198	THR	3.0
1	B	205	TRP	3.0
1	E	210	TYR	3.0
1	F	193	TYR	3.0
1	E	156	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	255	ILE	2.9
1	F	194	PHE	2.8
1	B	209	LYS	2.8
1	F	23	GLY	2.8
1	E	196	SER	2.8
1	E	38	LEU	2.8
1	E	174	GLY	2.8
1	B	23	GLY	2.7
1	B	239	ASP	2.7
1	A	28	LYS	2.6
1	B	45	ASN	2.6
1	B	255	ILE	2.6
1	B	40	GLU	2.6
1	F	196	SER	2.6
1	E	238	VAL	2.6
1	F	350	ILE	2.6
1	A	198	THR	2.5
1	E	378	GLU	2.5
1	F	323	ASN	2.5
1	F	47	LEU	2.5
1	E	32	VAL	2.5
1	B	210	TYR	2.5
1	F	383	ILE	2.5
1	A	205	TRP	2.4
1	F	122	ARG	2.4
1	F	174	GLY	2.4
1	B	47	LEU	2.4
1	B	344	LEU	2.4
1	E	205	TRP	2.4
1	F	45	ASN	2.4
1	A	156	THR	2.4
1	A	238	VAL	2.4
1	E	258	VAL	2.4
1	E	380	ASP	2.4
1	E	383	ILE	2.4
1	A	107	LYS	2.3
1	F	180	LYS	2.3
1	F	205	TRP	2.3
1	E	45	ASN	2.3
1	F	321	GLU	2.3
1	F	345	TYR	2.3
1	E	241	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	196	SER	2.3
1	F	66	PHE	2.3
1	E	190	VAL	2.3
1	F	238	VAL	2.3
1	F	58	LEU	2.2
1	B	252	ASP	2.2
1	E	104	VAL	2.2
1	A	214	TRP	2.2
1	E	114	ASN	2.2
1	E	28	LYS	2.2
1	A	46	ASN	2.2
1	E	346	LYS	2.2
1	A	47	LEU	2.2
1	F	46	ASN	2.2
1	B	350	ILE	2.2
1	A	190	VAL	2.1
1	B	300	GLN	2.1
1	F	268	ILE	2.1
1	F	175	VAL	2.1
1	B	46	ASN	2.1
1	A	196	SER	2.1
1	B	195	SER	2.1
1	B	194	PHE	2.1
1	E	193	TYR	2.1
1	A	380	ASP	2.0
1	E	195	SER	2.0
1	F	44	PRO	2.0
1	A	321	GLU	2.0
1	F	356	GLU	2.0
1	B	268	ILE	2.0
1	F	126	ARG	2.0
1	A	239	ASP	2.0
1	A	384	VAL	2.0

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

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
1	LLP	F	222	24/25	0.97	0.08	24,32,36,38	0
1	LLP	B	222	24/25	0.98	0.08	22,27,30,33	0
1	LLP	E	222	24/25	0.98	0.06	22,26,29,30	0
1	LLP	A	222	24/25	0.98	0.06	21,26,28,30	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

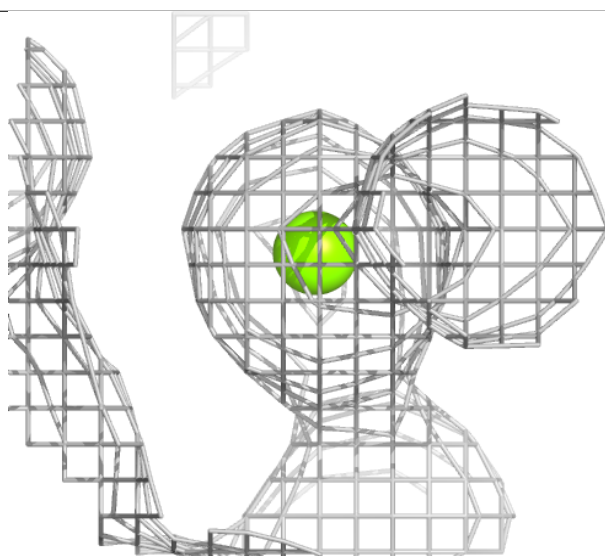
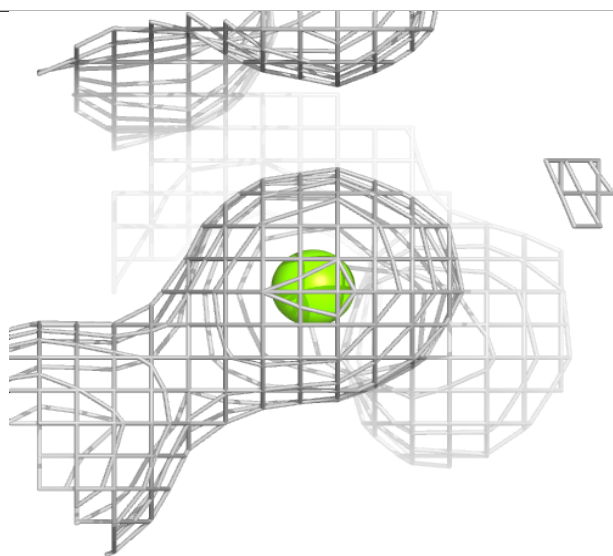
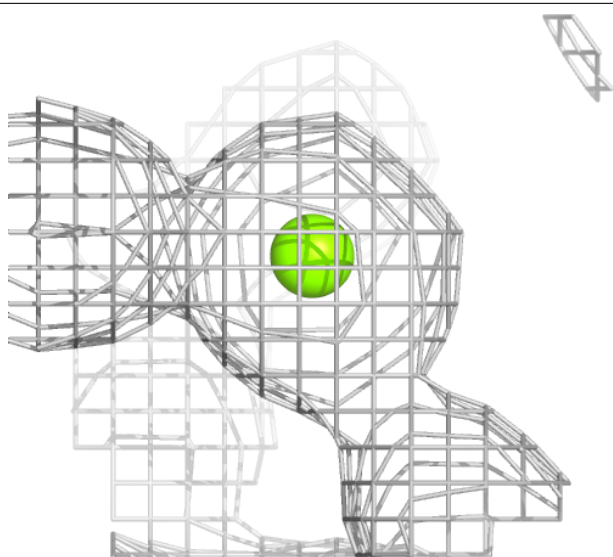
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	B	402	1/1	0.97	0.09	43,43,43,43	0
2	MG	B	401	1/1	0.98	0.13	39,39,39,39	0
2	MG	B	403	1/1	0.98	0.19	36,36,36,36	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.

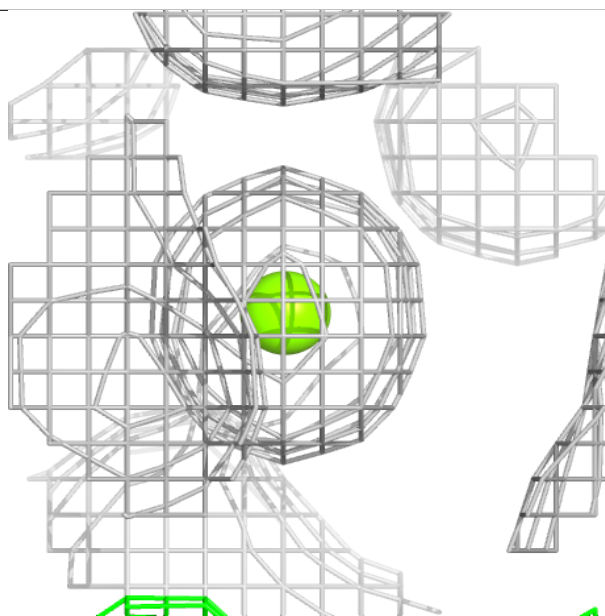
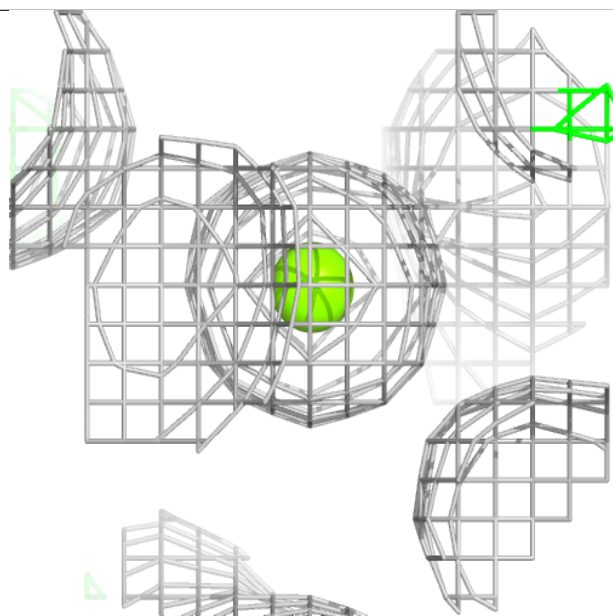
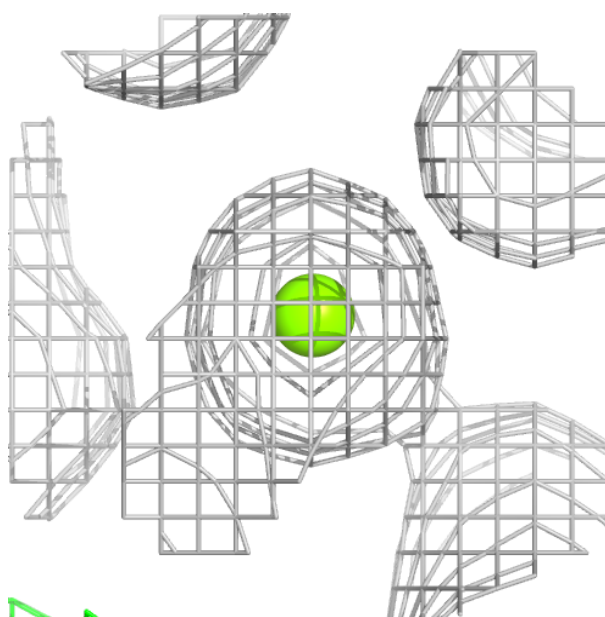
**Electron density around MG B 402:**

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



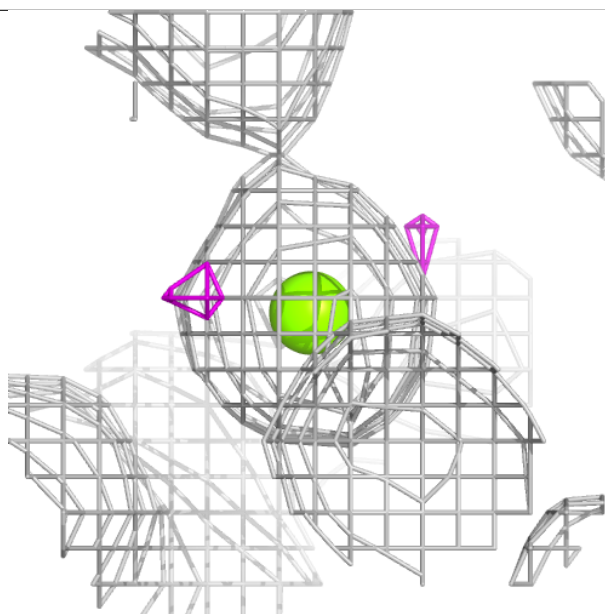
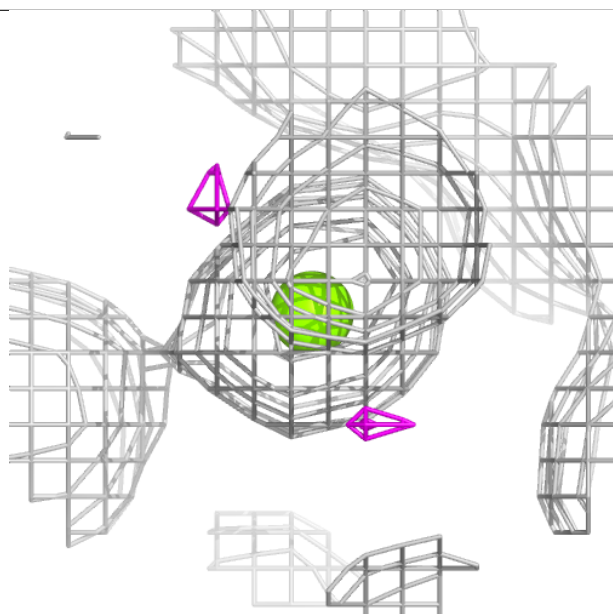
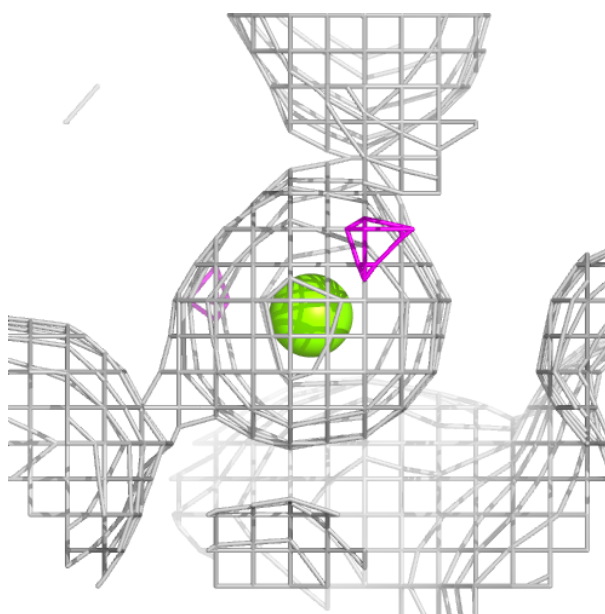
**Electron density around MG B 401:**

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



**Electron density around MG B 403:**

$2mF_o-DF_c$  (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.