



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 12:13 PM UTC

PDB ID : 8Z0G / pdb_00008z0g
Title : Crystal structure of Nelle complexed with isoleucine
Authors : Samygina, V.R.; Subach, O.M.; Vlaskina, A.V.; Gabdukhakov, A.; Subach, F.V.
Deposited on : 2024-04-09
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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

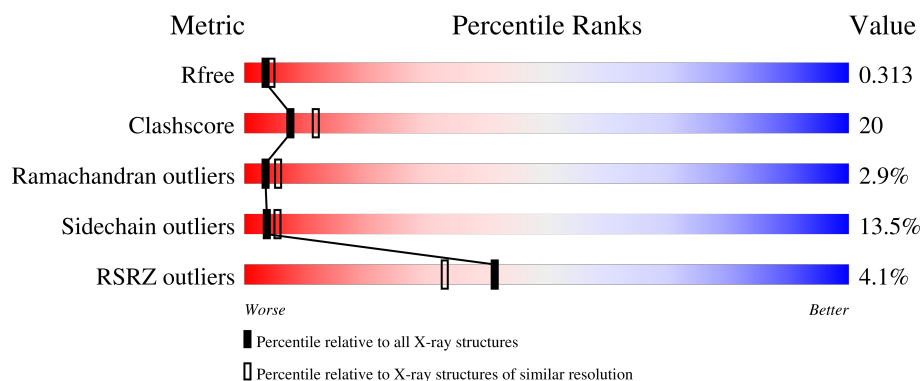
1 Overall quality at a glance

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	593	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4442 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.

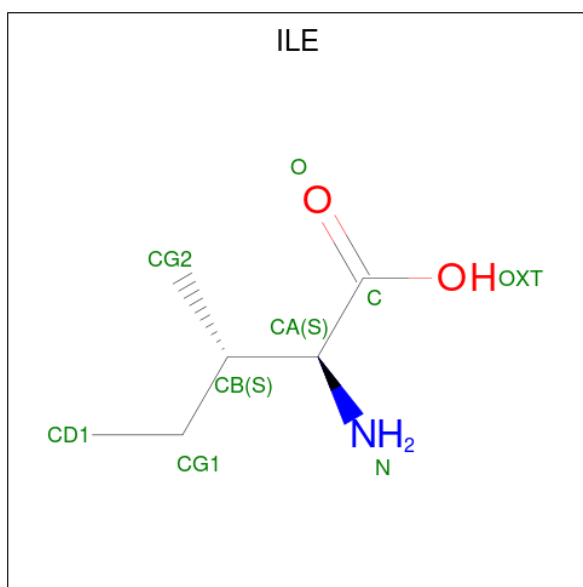
- Molecule 1 is a protein called Leu/Ile/Val-binding protein,Leu/Ile/Val-binding protein,mNeonGreen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	566	Total	C	N	O	S	0	0	0
			4352	2758	746	831	17			

There are 15 discrepancies between the modelled and reference sequences:

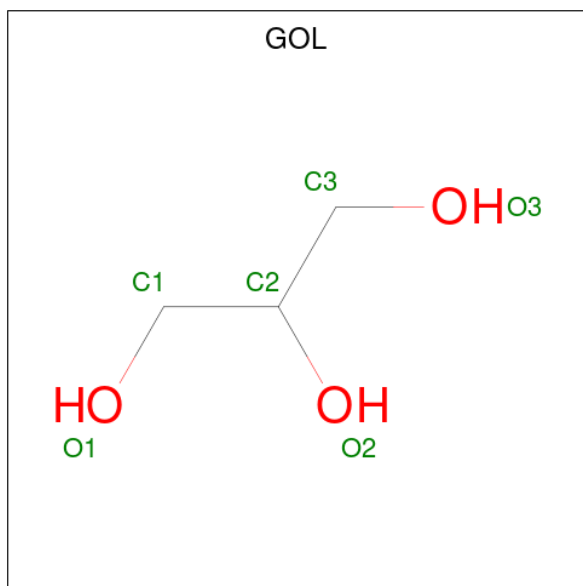
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0AD98
A	14	ALA	-	linker	UNP P0AD98
A	15	GLY	-	linker	UNP P0AD98
A	261	PHE	-	linker	UNP P0AD98
A	262	HIS	-	linker	UNP P0AD98
A	263	ILE	-	linker	UNP P0AD98
A	267	THR	ALA	conflict	UNP P0AD98
A	287	ARG	LYS	conflict	UNP P0AD98
A	315	ARG	LYS	conflict	UNP P0AD98
A	333	ALA	THR	conflict	UNP P0AD98
A	343	ALA	GLU	conflict	UNP P0AD98
A	377	LEU	PRO	conflict	UNP P0AD98
A	411	GLY	ASP	conflict	UNP P0AD98
A	511	HIS	PRO	conflict	UNP P0AD98
A	516	VAL	ILE	conflict	UNP P0AD98

- Molecule 2 is ISOLEUCINE (CCD ID: ILE) (formula: C₆H₁₃NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

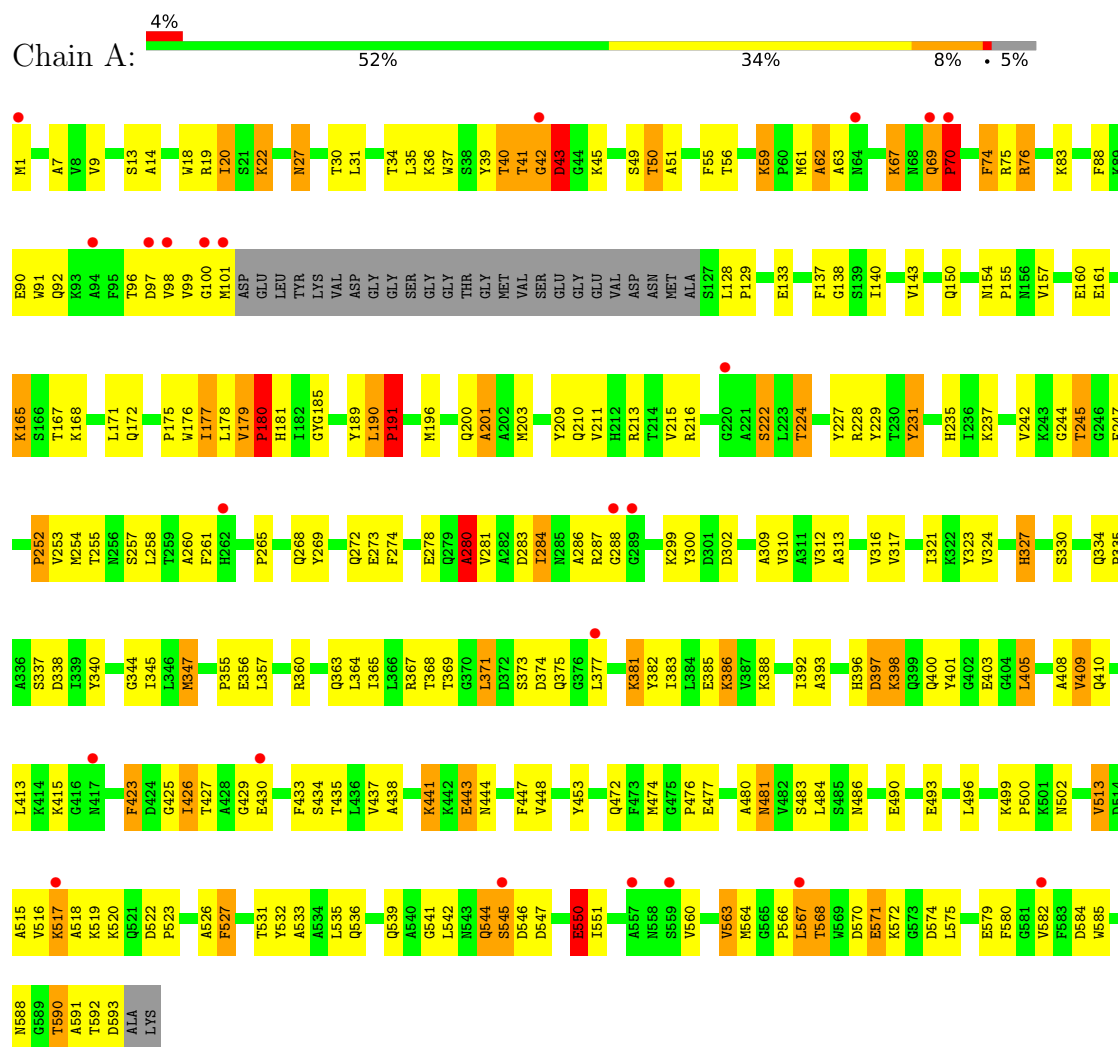
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total	O	0	0
			74	74		

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: Leu/Ile/Val-binding protein,Leu/Ile/Val-binding protein,mNeonGreen



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.13Å 68.15Å 79.48Å 90.00° 112.46° 90.00°	Depositor
Resolution (Å)	22.16 – 2.65 22.16 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.3 (22.16-2.65) 98.3 (22.16-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.63Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.235 , 0.308 0.238 , 0.313	Depositor DCC
R_{free} test set	903 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	11.0	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4442	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CR2, CL, GOL

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	1.28	11/4429 (0.2%)	1.74	61/5997 (1.0%)

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	A	0	4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	ILE	C-O	7.70	1.32	1.24
1	A	215	VAL	C-O	6.77	1.31	1.24
1	A	258	LEU	C-O	6.71	1.32	1.24
1	A	30	THR	C-O	6.17	1.30	1.23
1	A	222	SER	C-O	5.45	1.30	1.23
1	A	280	ALA	C-O	5.40	1.30	1.24
1	A	369	THR	C-O	5.37	1.30	1.23
1	A	486	ASN	C-O	-5.32	1.17	1.24
1	A	401	TYR	C-O	5.30	1.30	1.24
1	A	224	THR	C-O	5.29	1.30	1.24
1	A	443	GLU	C-O	5.02	1.30	1.24

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	TYR	CA-C-O	-9.09	108.28	119.28
1	A	423	PHE	CA-C-O	-7.94	111.59	120.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	PRO	N-CA-C	7.85	128.64	112.47
1	A	570	ASP	CA-CB-CG	7.41	120.00	112.60
1	A	546	ASP	N-CA-C	-7.09	104.20	112.92
1	A	593	ASP	CB-CA-C	-7.08	96.66	110.10
1	A	338	ASP	O-C-N	6.71	129.28	122.03
1	A	435	THR	CA-CB-OG1	-6.63	99.66	109.60
1	A	224	THR	CA-C-O	-6.55	113.77	120.71
1	A	180	PRO	N-CD-CG	-6.37	93.64	103.20
1	A	191	PRO	N-CA-CB	-6.31	96.62	103.25
1	A	571	GLU	CB-CG-CD	6.25	123.23	112.60
1	A	405	LEU	CA-C-N	6.16	128.53	120.28
1	A	405	LEU	C-N-CA	6.16	128.53	120.28
1	A	323	TYR	CA-C-O	-6.14	113.73	120.36
1	A	472	GLN	CB-CA-C	6.12	119.84	109.75
1	A	50	THR	CA-CB-OG1	-6.09	100.47	109.60
1	A	550	GLU	N-CA-CB	6.01	119.15	110.20
1	A	179	VAL	CA-C-N	5.88	127.19	119.84
1	A	179	VAL	C-N-CA	5.88	127.19	119.84
1	A	316	VAL	O-C-N	5.75	127.44	121.87
1	A	400	GLN	CA-C-N	5.74	128.76	120.79
1	A	400	GLN	C-N-CA	5.74	128.76	120.79
1	A	546	ASP	CB-CA-C	5.72	120.22	110.56
1	A	260	ALA	CA-C-O	-5.69	115.27	121.87
1	A	312	VAL	O-C-N	5.65	127.78	121.90
1	A	260	ALA	N-CA-C	-5.59	103.15	110.53
1	A	40	THR	CA-CB-OG1	-5.57	101.25	109.60
1	A	410	GLN	CA-C-N	5.44	126.02	119.98
1	A	410	GLN	C-N-CA	5.44	126.02	119.98
1	A	13	SER	CA-C-O	-5.44	114.67	120.92
1	A	570	ASP	CB-CA-C	5.40	122.74	112.43
1	A	70	PRO	N-CA-CB	-5.39	97.59	103.25
1	A	363	GLN	CB-CA-C	-5.38	100.31	109.03
1	A	201	ALA	CA-C-N	5.38	127.92	120.29
1	A	201	ALA	C-N-CA	5.38	127.92	120.29
1	A	312	VAL	N-CA-C	-5.38	105.48	110.53
1	A	403	GLU	N-CA-C	-5.35	105.45	111.28
1	A	88	PHE	CA-C-O	-5.26	114.29	120.60
1	A	484	LEU	N-CA-C	-5.25	105.46	111.14
1	A	224	THR	CA-CB-OG1	-5.20	101.80	109.60
1	A	527	PHE	CB-CA-C	5.20	120.98	110.38
1	A	441	LYS	CB-CA-C	-5.19	102.97	110.96
1	A	231	TYR	CB-CA-C	5.16	118.67	109.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	PRO	N-CA-CB	-5.13	97.86	103.25
1	A	62	ALA	CA-C-N	5.13	127.11	120.44
1	A	62	ALA	C-N-CA	5.13	127.11	120.44
1	A	245	THR	O-C-N	5.11	129.08	123.25
1	A	13	SER	CA-C-N	5.08	127.34	120.38
1	A	13	SER	C-N-CA	5.08	127.34	120.38
1	A	338	ASP	CA-C-O	-5.08	115.67	120.90
1	A	493	GLU	CA-C-O	-5.06	115.62	121.19
1	A	312	VAL	CA-C-N	5.06	127.06	120.28
1	A	312	VAL	C-N-CA	5.06	127.06	120.28
1	A	550	GLU	CB-CA-C	-5.05	101.45	110.70
1	A	167	THR	CA-CB-OG1	-5.04	102.03	109.60
1	A	189	TYR	O-C-N	5.04	129.33	122.37
1	A	397	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	490	GLU	CA-C-N	5.04	127.03	120.28
1	A	490	GLU	C-N-CA	5.04	127.03	120.28
1	A	27	ASN	CB-CA-C	-5.01	100.37	110.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	179	VAL	Mainchain,Peptide
1	A	190	LEU	Peptide
1	A	429	GLY	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4352	0	4259	175	0
2	A	9	0	10	1	0
3	A	6	0	8	1	0
4	A	1	0	0	0	0
5	A	74	0	0	9	0
All	All	4442	0	4277	175	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 20.

All (175) 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:61:MET:HA	3:A:1202:GOL:H31	1.37	1.01
1:A:171:LEU:HG	5:A:1359:HOH:O	1.63	0.97
1:A:41:THR:HG21	1:A:45:LYS:HB2	1.56	0.85
1:A:253:VAL:HG12	1:A:254:MET:HE2	1.62	0.81
1:A:140:ILE:O	1:A:143:VAL:HG22	1.80	0.81
1:A:513:VAL:O	1:A:517:LYS:NZ	2.14	0.80
1:A:584:ASP:OD1	5:A:1340:HOH:O	2.02	0.77
1:A:383:ILE:HG13	1:A:474:MET:HE1	1.67	0.76
1:A:75:ARG:HD3	1:A:90:GLU:OE2	1.84	0.76
1:A:37:TRP:CH2	1:A:180:PRO:HD3	2.22	0.74
1:A:181:HIS:HE1	5:A:1305:HOH:O	1.69	0.73
1:A:447:PHE:HZ	1:A:474:MET:HE3	1.52	0.72
1:A:513:VAL:HG13	1:A:517:LYS:HZ1	1.55	0.71
1:A:247:PHE:HB2	1:A:254:MET:HE3	1.73	0.71
1:A:280:ALA:O	1:A:284:ILE:HG13	1.91	0.71
1:A:63:ALA:HB1	5:A:1375:HOH:O	1.92	0.69
1:A:545:SER:OG	1:A:550:GLU:HG3	1.93	0.69
1:A:375:GLN:HE22	1:A:477:GLU:H	1.40	0.69
1:A:41:THR:CG2	1:A:45:LYS:HB2	2.24	0.68
1:A:140:ILE:HG22	1:A:254:MET:HE1	1.75	0.68
1:A:41:THR:HG22	1:A:45:LYS:N	2.09	0.67
1:A:41:THR:HG22	1:A:45:LYS:H	1.58	0.67
1:A:191:PRO:O	1:A:191:PRO:HD2	1.93	0.67
1:A:22:LYS:C	1:A:22:LYS:HE3	2.20	0.66
1:A:447:PHE:CZ	1:A:474:MET:HE3	2.29	0.66
1:A:211:VAL:HB	1:A:227:TYR:HB2	1.79	0.65
1:A:37:TRP:CZ3	1:A:180:PRO:HD3	2.31	0.65
1:A:317:VAL:HG22	1:A:345:ILE:HD12	1.80	0.64
1:A:41:THR:CG2	1:A:45:LYS:H	2.10	0.64
1:A:140:ILE:CG2	1:A:254:MET:HE1	2.27	0.64
1:A:317:VAL:HG22	1:A:345:ILE:CD1	2.27	0.64
1:A:405:LEU:O	1:A:408:ALA:O	2.15	0.63
1:A:383:ILE:CG1	1:A:474:MET:HE1	2.27	0.63
1:A:381:LYS:O	1:A:385:GLU:HG3	1.99	0.63
1:A:280:ALA:HB3	1:A:535:LEU:HD12	1.80	0.63
1:A:533:ALA:CB	1:A:564:MET:HE2	2.29	0.61
1:A:280:ALA:CB	1:A:535:LEU:HD12	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ARG:HE	1:A:92:GLN:HE21	1.50	0.60
1:A:334:GLN:HB3	1:A:335:PRO:HD3	1.84	0.60
1:A:41:THR:HG21	1:A:45:LYS:CB	2.31	0.60
1:A:190:LEU:O	1:A:200:GLN:NE2	2.35	0.60
1:A:35:LEU:HB3	1:A:51:ALA:HB3	1.83	0.59
1:A:500:PRO:HG2	1:A:526:ALA:HB1	1.85	0.59
1:A:253:VAL:CG1	1:A:254:MET:HE2	2.32	0.59
1:A:518:ALA:HB3	5:A:1333:HOH:O	2.02	0.59
1:A:90:GLU:HB3	1:A:160:GLU:HG3	1.85	0.59
1:A:367:ARG:HD2	1:A:574:ASP:OD1	2.02	0.59
1:A:513:VAL:HG13	1:A:517:LYS:NZ	2.17	0.59
1:A:517:LYS:HE3	1:A:523:PRO:HG3	1.85	0.58
1:A:75:ARG:HE	1:A:92:GLN:NE2	2.02	0.58
1:A:499:LYS:NZ	1:A:502:ASN:OD1	2.34	0.58
1:A:41:THR:HG23	1:A:43:ASP:CB	2.33	0.58
1:A:408:ALA:O	1:A:409:VAL:HB	2.05	0.57
1:A:517:LYS:NZ	1:A:523:PRO:HG3	2.20	0.57
1:A:368:THR:HA	1:A:575:LEU:HD11	1.87	0.56
1:A:397:ASP:O	1:A:398:LYS:HB2	2.06	0.56
1:A:69:GLN:HB2	1:A:70:PRO:HD2	1.88	0.56
1:A:324:VAL:HG21	1:A:340:TYR:CZ	2.41	0.56
1:A:499:LYS:HE2	1:A:500:PRO:O	2.06	0.56
1:A:517:LYS:O	1:A:518:ALA:C	2.49	0.55
1:A:191:PRO:O	1:A:191:PRO:CD	2.55	0.55
1:A:513:VAL:C	1:A:517:LYS:HZ3	2.12	0.54
1:A:138:GLY:HA3	1:A:242:VAL:O	2.06	0.54
1:A:273:GLU:O	1:A:531:THR:HG21	2.08	0.54
1:A:137:PHE:O	1:A:242:VAL:HG23	2.08	0.54
1:A:415:LYS:O	1:A:415:LYS:HD3	2.08	0.54
1:A:453:TYR:CE1	2:A:1201:ILE:HG22	2.43	0.54
1:A:517:LYS:CE	1:A:523:PRO:HG3	2.37	0.54
1:A:22:LYS:HE2	1:A:34:THR:OG1	2.08	0.54
1:A:541:GLY:O	1:A:544:GLN:O	2.26	0.53
1:A:567:LEU:O	1:A:568:THR:C	2.51	0.53
1:A:327:HIS:HE1	1:A:340:TYR:OH	1.91	0.53
1:A:588:ASN:HD21	1:A:590:THR:HG22	1.73	0.53
1:A:443:GLU:O	1:A:444:ASN:C	2.51	0.53
1:A:405:LEU:HD13	1:A:476:PRO:HG3	1.91	0.53
1:A:313:ALA:O	1:A:317:VAL:HG23	2.09	0.52
1:A:281:VAL:HG23	1:A:535:LEU:HD11	1.91	0.52
1:A:286:ALA:C	1:A:288:GLY:H	2.17	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:NH1	1:A:91:TRP:CD2	2.78	0.52
1:A:41:THR:HA	1:A:257:SER:O	2.09	0.51
1:A:425:GLY:O	1:A:426:ILE:HD13	2.10	0.51
1:A:564:MET:HE3	1:A:567:LEU:HD21	1.94	0.50
1:A:128:LEU:HB3	1:A:129:PRO:HD2	1.93	0.50
1:A:18:TRP:CE3	1:A:76:ARG:HG3	2.46	0.50
1:A:499:LYS:O	1:A:580:PHE:O	2.30	0.50
1:A:585:TRP:CE3	1:A:591:ALA:HB2	2.47	0.50
1:A:447:PHE:C	1:A:447:PHE:CD2	2.90	0.50
1:A:545:SER:CB	1:A:550:GLU:HG3	2.42	0.49
1:A:165:LYS:NZ	1:A:165:LYS:HB2	2.26	0.49
1:A:481:ASN:HD22	1:A:483:SER:H	1.59	0.49
1:A:9:VAL:HG22	1:A:300:TYR:HB2	1.95	0.49
1:A:133:GLU:HG2	1:A:150:GLN:OE1	2.13	0.48
1:A:268:GLN:O	1:A:272:GLN:HG3	2.13	0.48
1:A:392:ILE:HD13	1:A:413:LEU:HD13	1.95	0.48
1:A:129:PRO:O	1:A:155:PRO:HG3	2.12	0.48
1:A:344:GLY:HA2	1:A:364:LEU:CD1	2.43	0.48
1:A:42:GLY:N	1:A:257:SER:O	2.35	0.48
1:A:513:VAL:HG13	1:A:517:LYS:CE	2.44	0.48
1:A:547:ASP:O	1:A:551:ILE:HG13	2.14	0.48
1:A:43:ASP:OD2	1:A:45:LYS:HE2	2.14	0.47
1:A:500:PRO:HG2	1:A:526:ALA:CB	2.45	0.47
1:A:560:VAL:O	1:A:566:PRO:HA	2.13	0.47
1:A:67:LYS:HD3	5:A:1375:HOH:O	2.14	0.47
1:A:76:ARG:NH1	1:A:91:TRP:CE3	2.83	0.47
1:A:447:PHE:CD2	1:A:448:VAL:N	2.82	0.47
1:A:481:ASN:HD21	1:A:483:SER:HB2	1.80	0.46
1:A:171:LEU:HD22	1:A:175:PRO:HG3	1.98	0.46
1:A:74:PHE:N	1:A:74:PHE:CD2	2.84	0.46
1:A:20:ILE:HD13	1:A:20:ILE:N	2.31	0.46
1:A:244:GLY:O	1:A:245:THR:HG23	2.15	0.46
1:A:382:TYR:CE1	1:A:386:LYS:HD3	2.50	0.46
1:A:177:ILE:HD12	1:A:177:ILE:HA	1.71	0.46
1:A:181:HIS:CD2	1:A:213:ARG:HD2	2.50	0.46
1:A:181:HIS:HD2	1:A:213:ARG:HE	1.64	0.46
1:A:31:LEU:O	1:A:55:PHE:HD2	1.98	0.45
1:A:533:ALA:HB1	1:A:564:MET:HE2	1.97	0.45
1:A:133:GLU:HG3	1:A:235:HIS:CE1	2.50	0.45
1:A:357:LEU:HA	1:A:360:ARG:HH21	1.81	0.45
1:A:274:PHE:O	1:A:278:GLU:HG3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ASP:OD2	1:A:532:TYR:OH	2.30	0.45
1:A:388:LYS:HD2	5:A:1343:HOH:O	2.16	0.45
1:A:536:GLN:O	1:A:539:GLN:HB3	2.17	0.45
1:A:14:ALA:HA	1:A:261:PHE:CD2	2.52	0.45
1:A:154:ASN:HB3	1:A:157:VAL:HG22	1.99	0.45
1:A:388:LYS:CD	5:A:1343:HOH:O	2.65	0.45
1:A:133:GLU:OE2	1:A:235:HIS:HE1	2.00	0.44
1:A:588:ASN:OD1	1:A:590:THR:N	2.50	0.44
1:A:396:HIS:O	1:A:425:GLY:HA2	2.16	0.44
1:A:515:ALA:O	1:A:516:VAL:C	2.60	0.44
1:A:36:LYS:HD3	1:A:36:LYS:HA	1.72	0.44
1:A:317:VAL:HG22	1:A:345:ILE:HD11	2.00	0.44
1:A:337:SER:CB	1:A:347:MET:HE1	2.47	0.44
1:A:344:GLY:HA2	1:A:364:LEU:HD11	2.00	0.44
1:A:36:LYS:HD3	1:A:50:THR:HG22	2.00	0.43
1:A:59:LYS:HB3	1:A:59:LYS:HE2	1.80	0.43
1:A:229:TYR:HA	1:A:237:LYS:O	2.18	0.43
1:A:269:TYR:HD1	1:A:527:PHE:HE2	1.66	0.43
1:A:393:ALA:O	1:A:448:VAL:HA	2.18	0.43
1:A:408:ALA:O	1:A:409:VAL:CB	2.65	0.43
1:A:584:ASP:N	1:A:592:THR:O	2.47	0.43
1:A:269:TYR:CD1	1:A:527:PHE:HE2	2.37	0.43
1:A:588:ASN:OD1	1:A:588:ASN:C	2.61	0.43
1:A:474:MET:HA	1:A:496:LEU:O	2.19	0.43
1:A:203:MET:HE3	1:A:231:TYR:CD1	2.54	0.42
1:A:253:VAL:HG12	1:A:254:MET:CE	2.41	0.42
1:A:55:PHE:CD1	1:A:211:VAL:HG22	2.54	0.42
1:A:100:GLY:O	1:A:101:MET:C	2.61	0.42
1:A:564:MET:CE	1:A:567:LEU:HD11	2.48	0.42
1:A:522:ASP:C	1:A:522:ASP:OD1	2.62	0.42
1:A:56:THR:O	1:A:209:TYR:HA	2.19	0.42
1:A:541:GLY:HA3	1:A:551:ILE:HG23	2.01	0.42
1:A:39:TYR:CE1	1:A:176:TRP:O	2.73	0.42
1:A:438:ALA:O	1:A:441:LYS:HB2	2.19	0.42
1:A:49:SER:HA	1:A:216:ARG:O	2.20	0.42
1:A:433:PHE:O	1:A:437:VAL:HG23	2.19	0.42
1:A:302:ASP:HB2	1:A:309:ALA:HA	2.02	0.41
1:A:481:ASN:HD22	1:A:481:ASN:C	2.27	0.41
1:A:481:ASN:HD22	1:A:483:SER:N	2.18	0.41
1:A:536:GLN:HE22	1:A:563:VAL:H	1.66	0.41
1:A:355:PRO:HG3	1:A:371:LEU:HB3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:HIS:CE1	1:A:423:PHE:CE2	3.09	0.41
1:A:397:ASP:HA	1:A:426:ILE:O	2.19	0.41
1:A:481:ASN:ND2	1:A:483:SER:HB2	2.35	0.41
1:A:517:LYS:C	1:A:519:LYS:N	2.79	0.41
1:A:474:MET:HG3	1:A:496:LEU:CB	2.51	0.41
1:A:337:SER:HB3	1:A:347:MET:HE1	2.01	0.41
1:A:55:PHE:CD2	1:A:55:PHE:N	2.89	0.41
1:A:143:VAL:O	1:A:143:VAL:HG23	2.21	0.40
1:A:7:ALA:HB2	1:A:321:ILE:HG21	2.04	0.40
1:A:36:LYS:CD	1:A:50:THR:HG22	2.52	0.40
1:A:517:LYS:O	1:A:519:LYS:N	2.54	0.40
1:A:41:THR:HG23	1:A:43:ASP:HB2	2.02	0.40
1:A:255:THR:HG23	5:A:1353:HOH:O	2.20	0.40
1:A:274:PHE:CE2	1:A:299:LYS:HD3	2.57	0.40
1:A:405:LEU:HD13	1:A:476:PRO:CG	2.52	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	559/593 (94%)	504 (90%)	39 (7%)	16 (3%)	3 5

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	A	70	PRO
1	A	180	PRO
1	A	191	PRO
1	A	409	VAL
1	A	480	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	542	LEU
1	A	196	MET
1	A	280	ALA
1	A	327	HIS
1	A	568	THR
1	A	42	GLY
1	A	398	LYS
1	A	62	ALA
1	A	201	ALA
1	A	563	VAL

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	450/469 (96%)	390 (87%)	60 (13%)	4 6

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	19	ARG
1	A	20	ILE
1	A	22	LYS
1	A	27	ASN
1	A	40	THR
1	A	41	THR
1	A	43	ASP
1	A	59	LYS
1	A	67	LYS
1	A	69	GLN
1	A	70	PRO
1	A	74	PHE
1	A	76	ARG
1	A	83	LYS
1	A	96	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	97	ASP
1	A	98	VAL
1	A	99	VAL
1	A	161	GLU
1	A	165	LYS
1	A	168	LYS
1	A	172	GLN
1	A	177	ILE
1	A	178	LEU
1	A	210	GLN
1	A	222	SER
1	A	224	THR
1	A	228	ARG
1	A	252	PRO
1	A	265	PRO
1	A	287	ARG
1	A	310	VAL
1	A	330	SER
1	A	347	MET
1	A	356	GLU
1	A	365	ILE
1	A	371	LEU
1	A	373	SER
1	A	374	ASP
1	A	377	LEU
1	A	381	LYS
1	A	386	LYS
1	A	426	ILE
1	A	427	THR
1	A	430	GLU
1	A	434	SER
1	A	481	ASN
1	A	513	VAL
1	A	517	LYS
1	A	520	LYS
1	A	544	GLN
1	A	545	SER
1	A	550	GLU
1	A	567	LEU
1	A	571	GLU
1	A	572	LYS
1	A	579	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	582	VAL
1	A	590	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	132	HIS
1	A	181	HIS
1	A	212	HIS
1	A	235	HIS
1	A	256	ASN
1	A	296	GLN
1	A	314	ASN
1	A	327	HIS
1	A	375	GLN
1	A	396	HIS
1	A	399	GLN
1	A	481	ASN
1	A	509	ASN
1	A	536	GLN
1	A	543	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CR2	A	185	1	20,20,21	3.87	6 (30%)	25,27,29	5.21	15 (60%)

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	CR2	A	185	1	-	0/6/25/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	CR2	CB2-CA2	14.92	1.49	1.35
1	A	185	CR2	CA2-C2	-4.75	1.43	1.48
1	A	185	CR2	CA1-C1	-3.83	1.45	1.49
1	A	185	CR2	C2-N3	-3.02	1.33	1.40
1	A	185	CR2	CE1-CD1	2.60	1.43	1.38
1	A	185	CR2	CD1-CG2	-2.09	1.35	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	CR2	O2-C2-CA2	-15.10	121.38	131.02
1	A	185	CR2	C2-N3-C1	-13.01	102.23	108.08
1	A	185	CR2	CA2-C2-N3	9.32	111.32	103.50
1	A	185	CR2	C1-CA1-N1	-7.76	95.69	112.85
1	A	185	CR2	CD1-CE1-CZ	4.94	125.10	119.88
1	A	185	CR2	C2-CA2-N2	-3.90	106.16	108.95
1	A	185	CR2	N3-C1-N2	3.76	116.10	111.75
1	A	185	CR2	CA3-N3-C2	3.61	131.60	123.67
1	A	185	CR2	CD2-CE2-CZ	-3.26	116.43	119.88
1	A	185	CR2	CE2-CD2-CG2	3.25	125.42	121.22
1	A	185	CR2	CE1-CD1-CG2	-3.13	117.17	121.22
1	A	185	CR2	C3-CA3-N3	3.01	119.28	112.43
1	A	185	CR2	CA1-C1-N3	-2.87	118.67	122.52
1	A	185	CR2	CB2-CA2-C2	2.82	125.77	122.36
1	A	185	CR2	O3-C3-CA3	-2.22	115.47	125.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
2	ILE	A	1201	-	8,8,8	0.89	1 (12%)	9,10,10	0.56	0
3	GOL	A	1202	-	5,5,5	0.41	0	5,5,5	0.84	0

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
2	ILE	A	1201	-	-	4/10/10/10	-
3	GOL	A	1202	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	ILE	OXT-C	-2.02	1.24	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

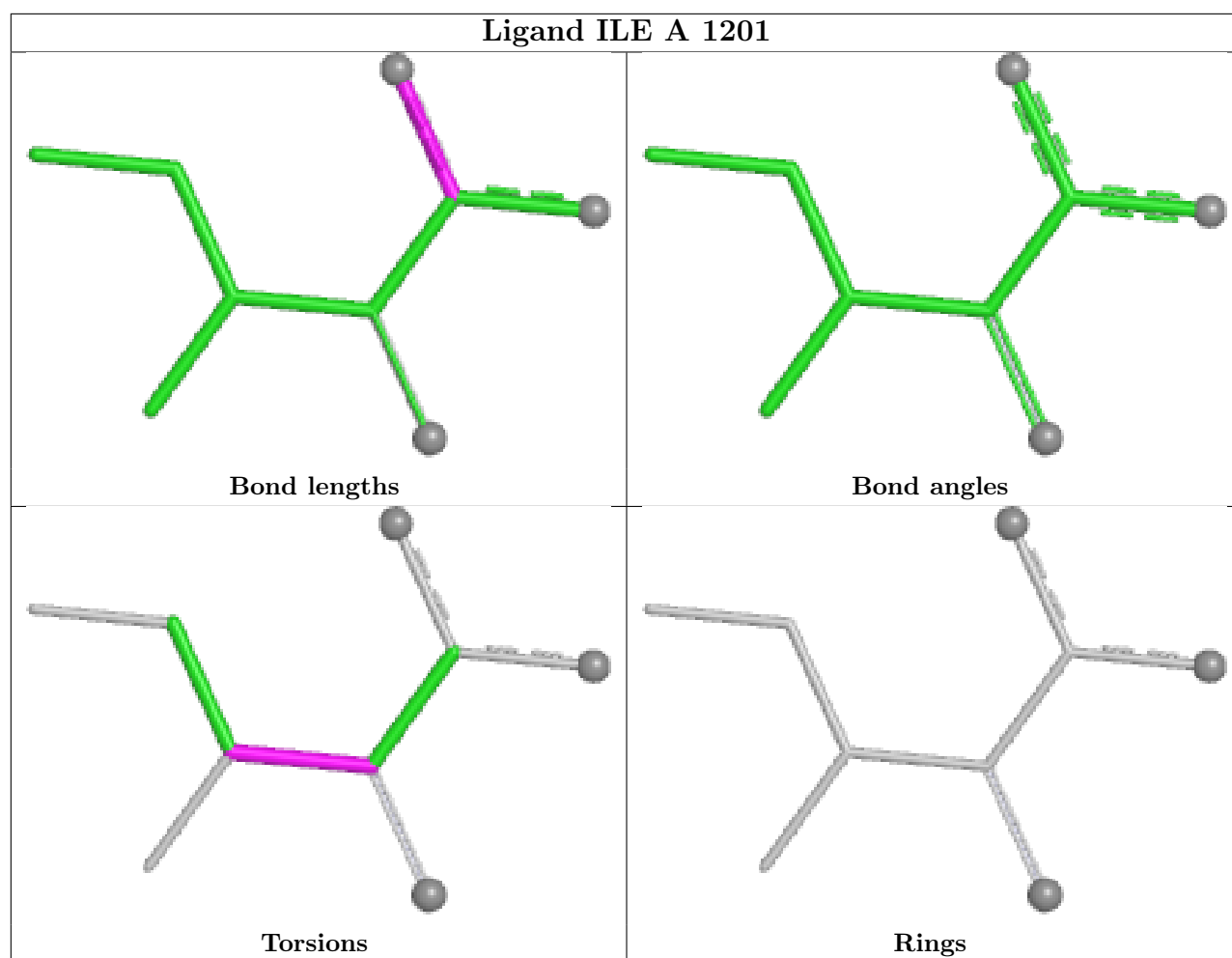
Mol	Chain	Res	Type	Atoms
2	A	1201	ILE	C-CA-CB-CG2
3	A	1202	GOL	O1-C1-C2-C3
3	A	1202	GOL	C1-C2-C3-O3
3	A	1202	GOL	O1-C1-C2-O2
3	A	1202	GOL	O2-C2-C3-O3
2	A	1201	ILE	N-CA-CB-CG1
2	A	1201	ILE	C-CA-CB-CG1
2	A	1201	ILE	N-CA-CB-CG2

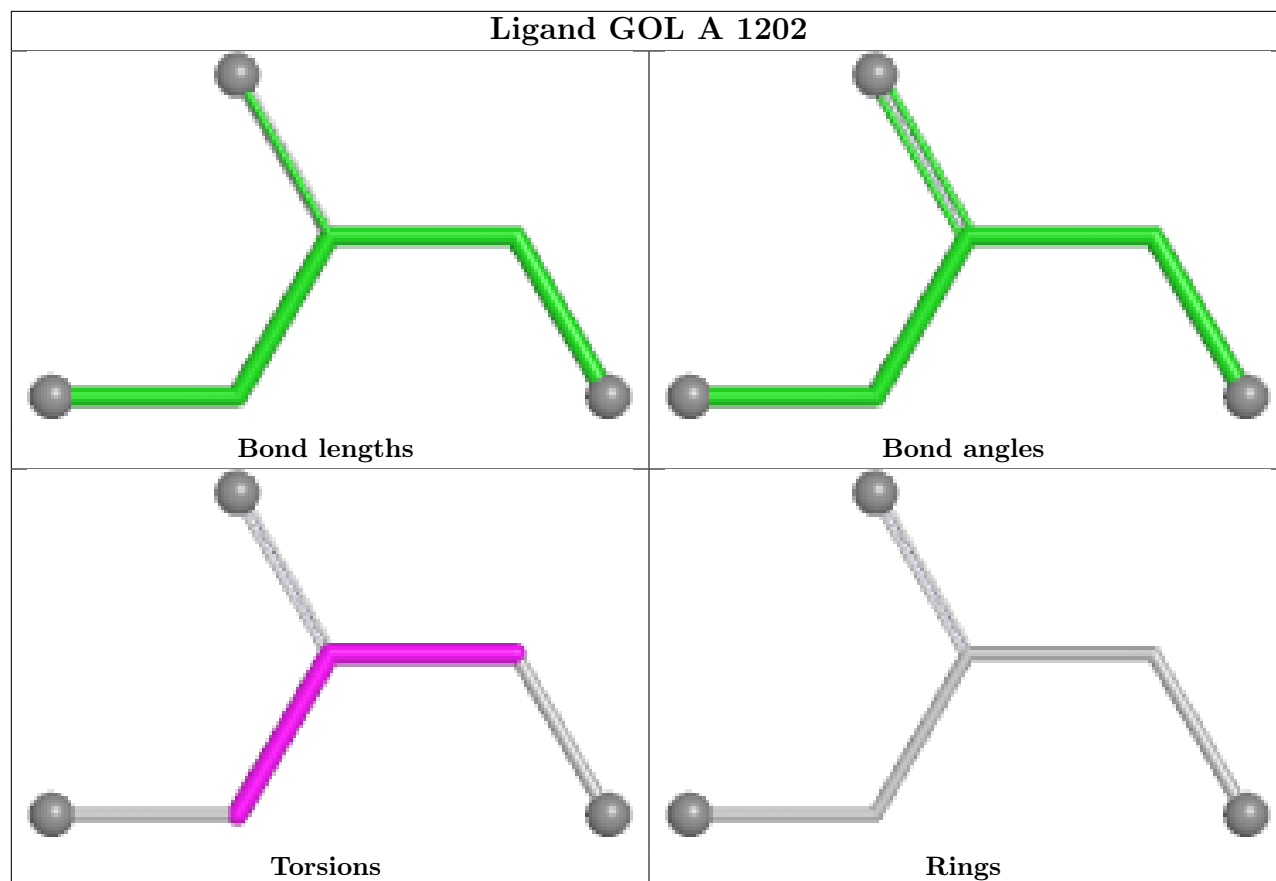
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	ILE	1	0
3	A	1202	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	565/593 (95%)	0.49	23 (4%) 41 33	16, 29, 46, 93	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	MET	6.6
1	A	220	GLY	3.7
1	A	100	GLY	3.7
1	A	69	GLN	3.3
1	A	70	PRO	3.2
1	A	42	GLY	2.8
1	A	289	GLY	2.8
1	A	377	LEU	2.8
1	A	262	HIS	2.7
1	A	582	VAL	2.5
1	A	97	ASP	2.4
1	A	545	SER	2.4
1	A	430	GLU	2.3
1	A	517	LYS	2.3
1	A	288	GLY	2.2
1	A	417	ASN	2.2
1	A	1	MET	2.1
1	A	64	ASN	2.1
1	A	557	ALA	2.1
1	A	98	VAL	2.1
1	A	94	ALA	2.0
1	A	567	LEU	2.0
1	A	559	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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($\text{\AA}^2$)	Q<0.9
1	CR2	A	185	19/20	0.92	0.11	18,22,26,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

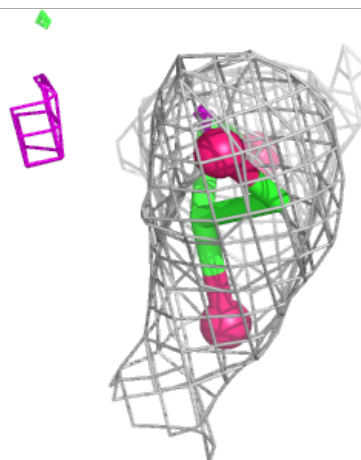
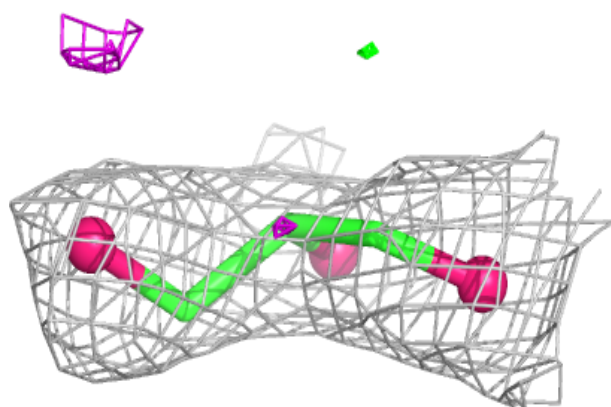
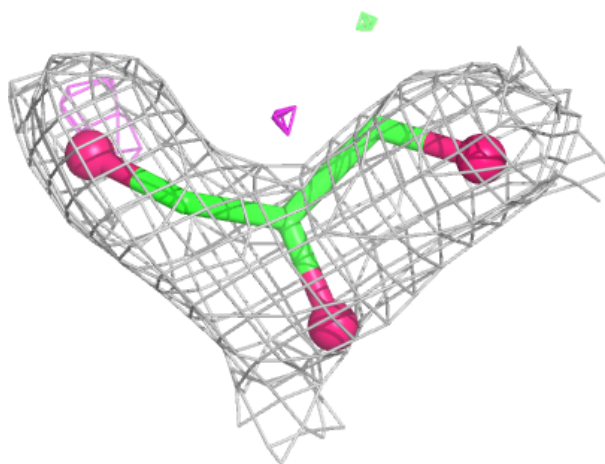
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	1202	6/6	0.91	0.17	35,36,41,45	0
2	ILE	A	1201	9/9	0.96	0.08	23,29,30,33	0
4	CL	A	1320	1/1	0.99	0.04	33,33,33,33	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.

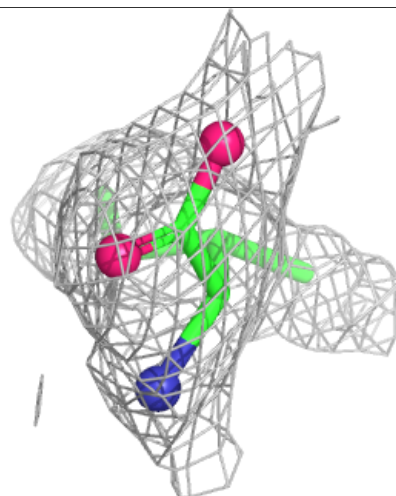
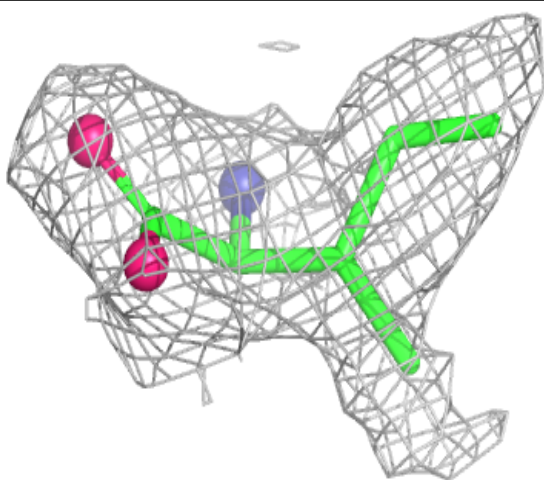
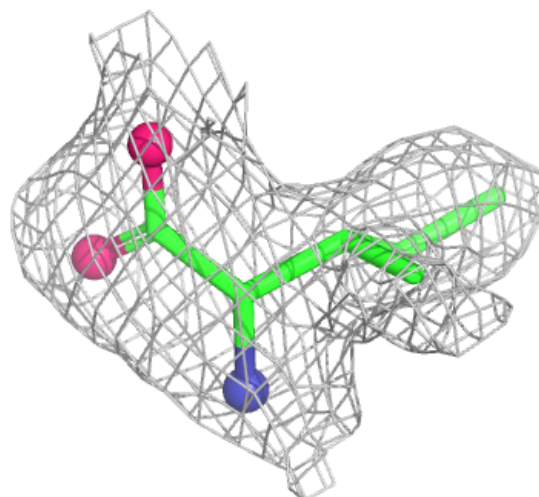
Electron density around GOL A 1202:

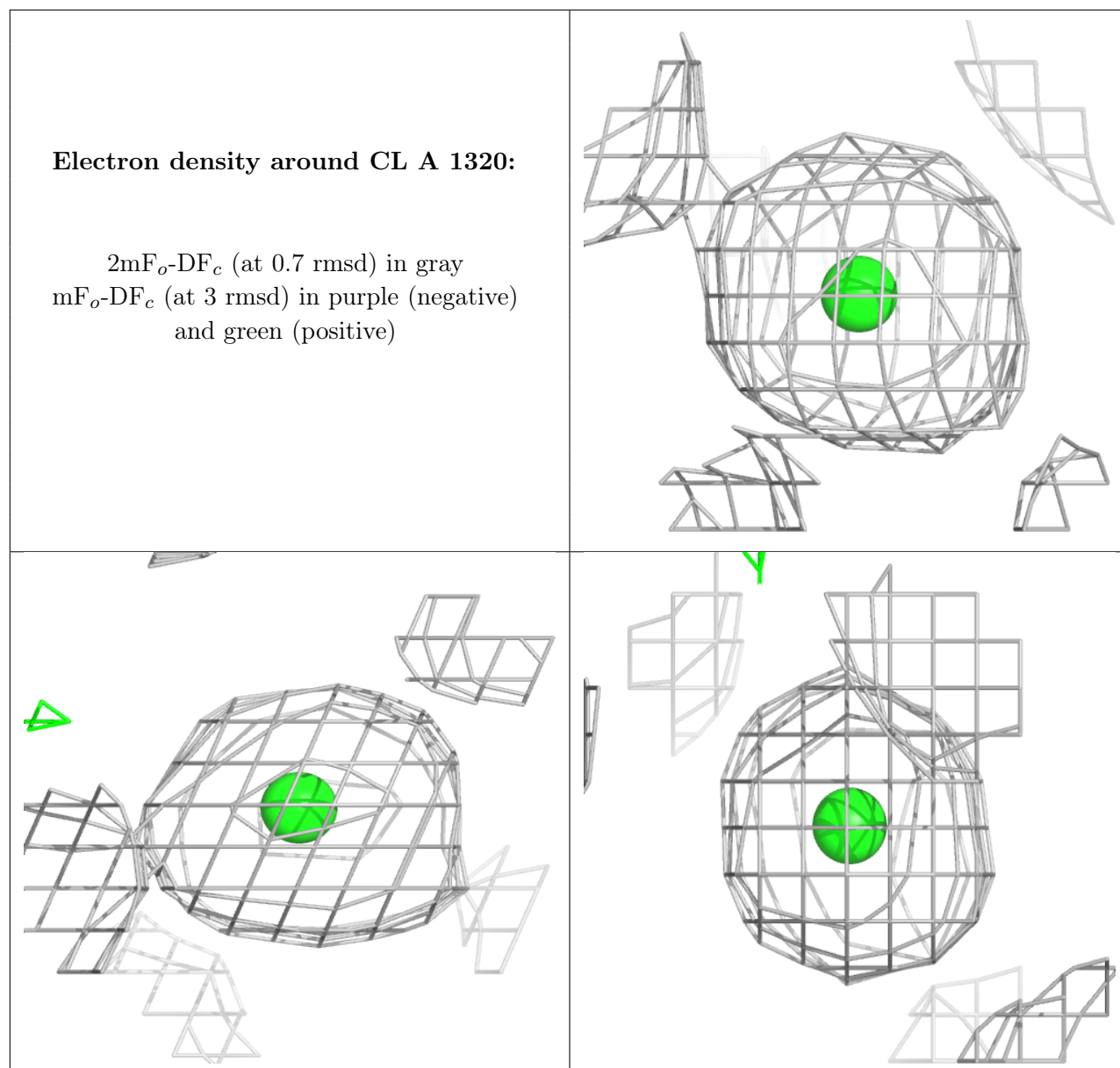
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ILE A 1201:

$2mF_o-DF_c$ (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.