Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 04:31 PM JST

PDB ID	:	6LOX
Title	:	Crystal Structure of human glutaminase with macrocyclic inhibitor
Authors	:	Bian, J.; Li, Z.; Xu, X.; Wang, J.; Li, L.
Deposited on	:	2020-01-07
Resolution	:	3.20 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 (i) 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 (i)) were used in the production of this report:

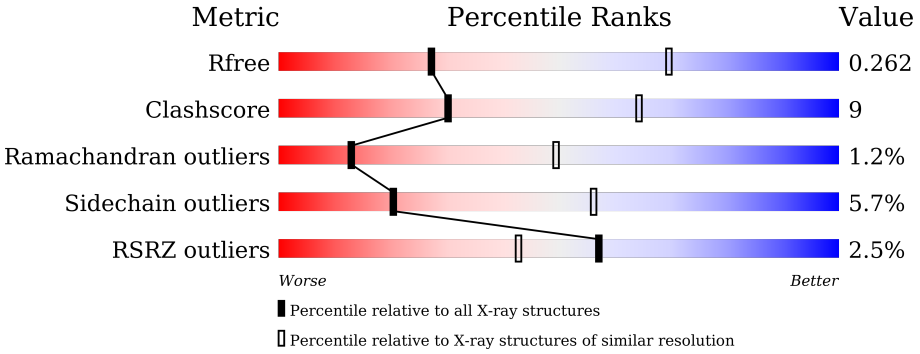
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	534	2% 61% 12% • 24%
1	B	534	2% 62% 13% • 24%
1	C	534	2% 61% 14% • 23%
1	D	534	% 59% 16% • 24%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12089 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 Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	407	3011	1910	506	567	28	0	0	0
1	B	407	2987	1902	495	562	28	0	0	0
1	C	410	3024	1923	511	562	28	0	0	0
1	D	405	2968	1883	494	563	28	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

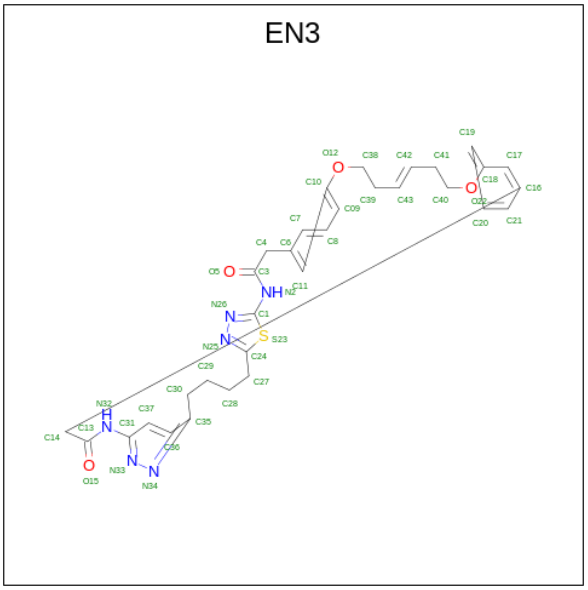
Chain	Residue	Modelled	Actual	Comment	Reference
A	599	HIS	-	expression tag	UNP O94925
A	600	HIS	-	expression tag	UNP O94925
A	601	HIS	-	expression tag	UNP O94925
A	602	HIS	-	expression tag	UNP O94925
A	603	HIS	-	expression tag	UNP O94925
A	604	HIS	-	expression tag	UNP O94925
B	599	HIS	-	expression tag	UNP O94925
B	600	HIS	-	expression tag	UNP O94925
B	601	HIS	-	expression tag	UNP O94925
B	602	HIS	-	expression tag	UNP O94925
B	603	HIS	-	expression tag	UNP O94925
B	604	HIS	-	expression tag	UNP O94925
C	599	HIS	-	expression tag	UNP O94925
C	600	HIS	-	expression tag	UNP O94925
C	601	HIS	-	expression tag	UNP O94925
C	602	HIS	-	expression tag	UNP O94925
C	603	HIS	-	expression tag	UNP O94925
C	604	HIS	-	expression tag	UNP O94925
D	599	HIS	-	expression tag	UNP O94925
D	600	HIS	-	expression tag	UNP O94925
D	601	HIS	-	expression tag	UNP O94925

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	602	HIS	-	expression tag	UNP O94925
D	603	HIS	-	expression tag	UNP O94925
D	604	HIS	-	expression tag	UNP O94925

- Molecule 2 is (E)-15,22-Dioxa-4,11-diaza-5(2,5)-thiadiazola-10(3,6)-pyridazina-1,14(1,3)-dibenzenacyclodocosaphan-18-ene-3,12-dione (three-letter code: EN3) (formula: $C_{32}H_{34}N_6O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			43	32	6	4	1		
2	C	1	Total	C	N	O	S	0	0
			43	32	6	4	1		

- Molecule 3 is water.

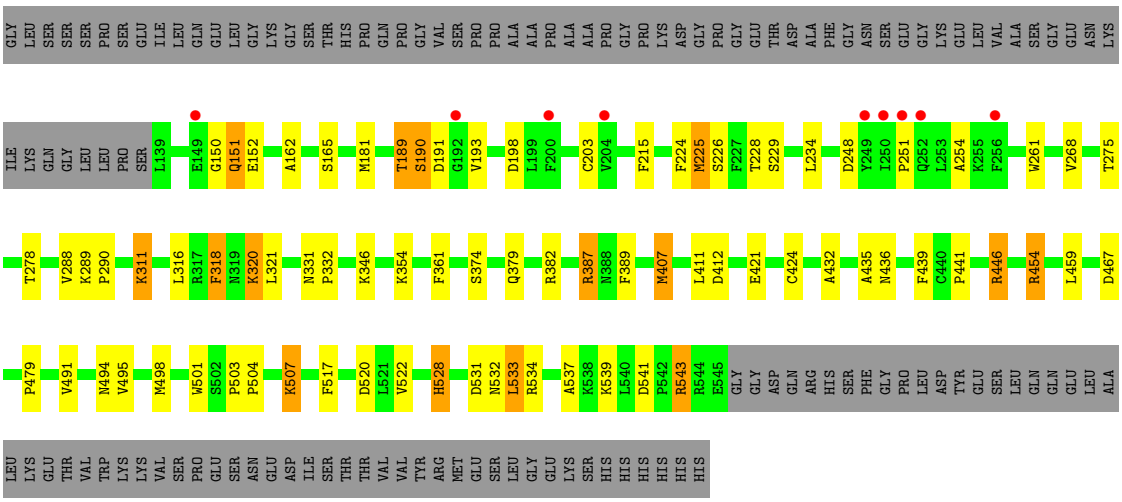
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	4	Total	O	0	0
			4	4		
3	C	3	Total	O	0	0
			3	3		
3	D	3	Total	O	0	0
			3	3		

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.

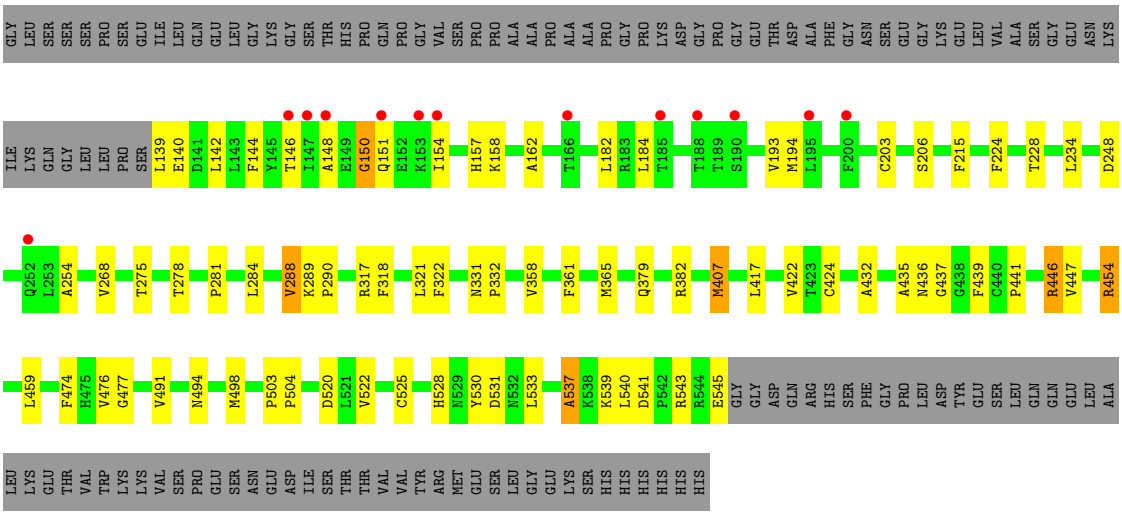
• Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain A:



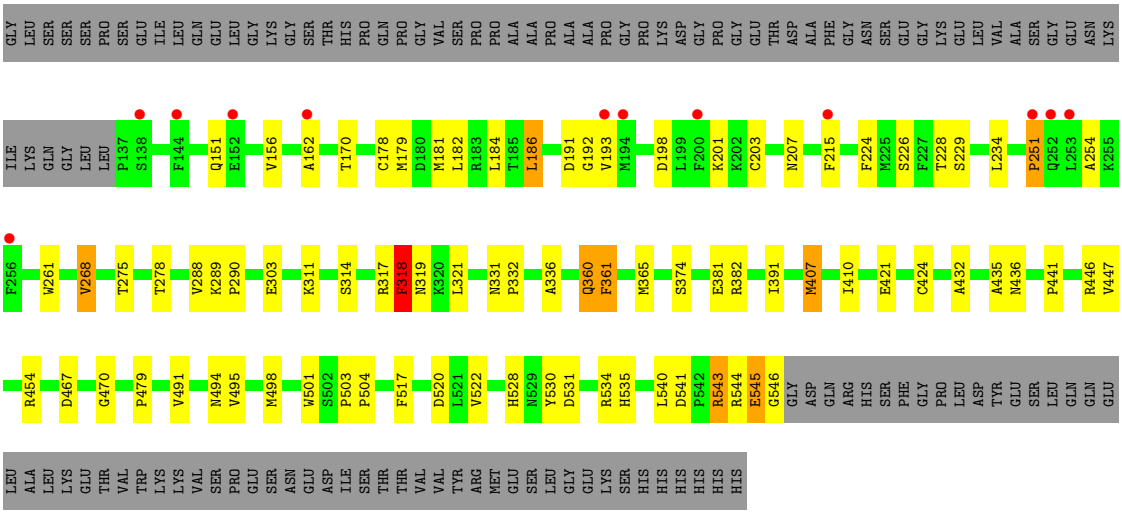
• Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain B:



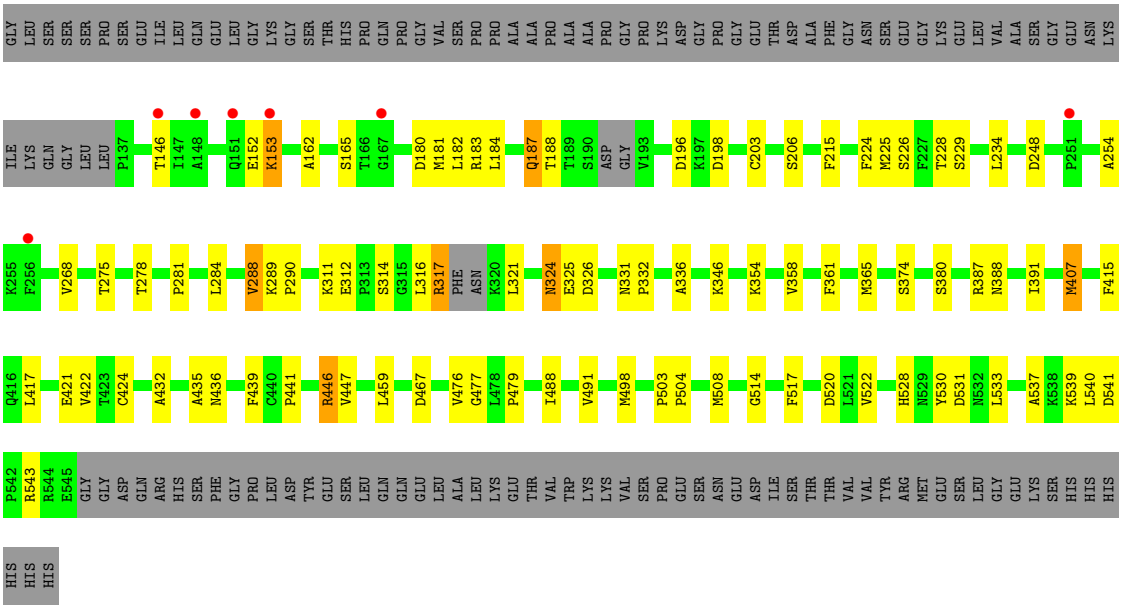
• Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain C:



- Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.97Å 138.67Å 177.67Å 90.00° 94.16° 90.00°	Depositor
Resolution (Å)	47.14 – 3.20 47.10 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.14-3.20) 98.7 (47.10-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.222 , 0.260 0.224 , 0.262	Depositor DCC
R_{free} test set	1936 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	55.3	Xtriage
Anisotropy	1.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 75.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12089	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: EN3

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	0.42	0/3080	0.81	1/4183 (0.0%)
1	B	0.41	0/3058	0.81	0/4161
1	C	0.42	0/3095	0.80	0/4205
1	D	0.41	0/3035	0.79	0/4128
All	All	0.41	0/12268	0.80	1/16677 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	534	ARG	CG-CD-NE	5.54	123.44	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3011	0	2794	57	0
1	B	2987	0	2733	61	0
1	C	3024	0	2814	51	0
1	D	2968	0	2718	63	0
2	A	43	0	0	4	0
2	C	43	0	0	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	0	0
3	B	4	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
All	All	12089	0	11059	215	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 9.

All (215) 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:C:407:MET:O	1:C:407:MET:SD	2.04	1.15
1:D:182:LEU:HD23	1:D:203:CYS:SG	2.08	0.94
1:C:541:ASP:OD1	1:C:543:ARG:HG2	1.69	0.92
1:B:157:HIS:HD2	1:B:158:LYS:N	1.72	0.88
1:A:234:LEU:HD22	1:A:520:ASP:HB3	1.57	0.87
1:D:234:LEU:HD22	1:D:520:ASP:HB3	1.57	0.87
1:B:234:LEU:HD22	1:B:520:ASP:HB3	1.57	0.85
1:A:507:LYS:H	1:A:507:LYS:HD3	1.42	0.84
1:A:387:ARG:CG	1:A:387:ARG:HH11	1.91	0.84
1:B:157:HIS:CD2	1:B:158:LYS:N	2.46	0.83
1:D:498:MET:HE1	1:D:517:PHE:CE2	2.14	0.82
1:B:321:LEU:HD23	2:C:701:EN3:C31	2.10	0.81
1:C:234:LEU:HD22	1:C:520:ASP:HB3	1.59	0.81
1:D:182:LEU:CD2	1:D:203:CYS:SG	2.69	0.81
1:B:144:PHE:CE1	1:B:154:ILE:HD13	2.17	0.79
1:D:187:GLN:HA	1:D:187:GLN:HE21	1.50	0.77
1:C:318:PHE:HB3	1:C:467:ASP:OD2	1.86	0.75
1:B:144:PHE:CD1	1:B:154:ILE:HD13	2.21	0.75
1:D:324:ASN:C	1:D:324:ASN:HD22	1.88	0.75
1:A:479:PRO:HG3	1:B:530:TYR:CE1	2.23	0.73
2:A:701:EN3:C1	1:D:321:LEU:HD13	2.19	0.73
1:A:387:ARG:HH11	1:A:387:ARG:HG2	1.53	0.73
1:A:268:VAL:HG13	1:A:436:ASN:OD1	1.90	0.71
1:A:268:VAL:CG1	1:A:436:ASN:OD1	2.38	0.71
1:C:268:VAL:HG12	1:C:436:ASN:OD1	1.93	0.69
1:D:498:MET:HE1	1:D:517:PHE:HE2	1.55	0.69
1:B:541:ASP:OD1	1:B:543:ARG:HD2	1.93	0.69
1:C:479:PRO:HG3	1:D:530:TYR:CE1	2.28	0.67
1:C:268:VAL:CG2	1:C:495:VAL:O	2.43	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:VAL:HG13	1:A:436:ASN:CG	2.15	0.66
1:C:407:MET:SD	1:C:407:MET:C	2.74	0.65
1:D:324:ASN:C	1:D:324:ASN:ND2	2.51	0.64
1:C:268:VAL:HG23	1:C:495:VAL:O	1.97	0.64
1:C:318:PHE:HA	1:C:467:ASP:OD1	1.97	0.64
1:A:150:GLY:O	1:A:151:GLN:O	2.16	0.63
1:C:268:VAL:HG12	1:C:436:ASN:CG	2.19	0.63
1:A:162:ALA:HB1	1:A:215:PHE:HE1	1.63	0.62
1:D:162:ALA:HB1	1:D:215:PHE:HE1	1.64	0.62
1:B:477:GLY:HA3	1:B:528:HIS:CD2	2.34	0.62
1:B:162:ALA:HB1	1:B:215:PHE:HE1	1.64	0.62
1:C:162:ALA:HB1	1:C:215:PHE:HE1	1.63	0.62
1:A:522:VAL:CG1	1:A:528:HIS:HB2	2.30	0.61
1:B:182:LEU:HD23	1:B:203:CYS:SG	2.40	0.61
1:A:528:HIS:CD2	1:B:454:ARG:CD	2.85	0.60
1:C:454:ARG:NH1	1:D:531:ASP:OD1	2.36	0.59
1:C:544:ARG:O	1:C:545:GLU:CB	2.50	0.59
1:B:157:HIS:CD2	1:B:158:LYS:H	2.20	0.59
1:B:224:PHE:O	1:B:228:THR:HG23	2.03	0.59
1:A:224:PHE:O	1:A:228:THR:HG23	2.03	0.59
1:B:522:VAL:CG1	1:B:528:HIS:HB2	2.32	0.59
1:D:224:PHE:O	1:D:228:THR:HG23	2.02	0.59
1:A:251:PRO:HA	1:A:254:ALA:HB3	1.85	0.58
1:B:144:PHE:CD1	1:B:154:ILE:CD1	2.86	0.58
1:D:522:VAL:CG1	1:D:528:HIS:HB2	2.33	0.58
1:C:224:PHE:O	1:C:228:THR:HG23	2.04	0.58
1:D:477:GLY:HA3	1:D:528:HIS:CD2	2.38	0.58
1:C:522:VAL:CG1	1:C:528:HIS:HB2	2.34	0.57
1:C:179:MET:HA	1:C:179:MET:HE2	1.85	0.57
1:A:528:HIS:CD2	1:B:454:ARG:HD2	2.40	0.57
1:B:268:VAL:HG12	1:B:436:ASN:HB2	1.85	0.56
1:D:467:ASP:HB3	1:D:508:MET:HE1	1.86	0.56
1:C:479:PRO:HD3	1:D:530:TYR:OH	2.05	0.56
1:A:321:LEU:HD23	2:A:701:EN3:N32	2.20	0.56
1:B:321:LEU:HD22	2:C:701:EN3:N32	2.20	0.56
1:C:179:MET:HA	1:C:179:MET:CE	2.36	0.55
1:B:139:LEU:HG	1:B:142:LEU:H	1.71	0.55
1:B:331:ASN:HB2	1:B:332:PRO:HD2	1.89	0.55
1:B:476:VAL:C	1:B:528:HIS:HD2	2.10	0.55
1:D:182:LEU:HD21	1:D:203:CYS:CB	2.37	0.55
1:B:321:LEU:CD2	2:C:701:EN3:C31	2.82	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:GLY:HA3	1:D:312:GLU:OE1	2.08	0.54
1:D:182:LEU:HD21	1:D:203:CYS:HB3	1.89	0.54
1:A:498:MET:HE3	1:A:517:PHE:CE2	2.43	0.53
1:B:322:PHE:H	2:C:701:EN3:C36	2.21	0.53
1:A:189:THR:O	1:A:190:SER:C	2.47	0.53
1:D:316:LEU:O	1:D:317:ARG:C	2.46	0.52
1:B:148:ALA:C	1:B:150:GLY:H	2.12	0.52
1:B:144:PHE:CE1	1:B:154:ILE:CD1	2.92	0.52
1:C:268:VAL:HG22	1:C:495:VAL:C	2.30	0.52
1:A:268:VAL:HG23	1:A:495:VAL:C	2.30	0.51
1:C:318:PHE:N	1:C:318:PHE:CD1	2.78	0.51
1:D:331:ASN:HB2	1:D:332:PRO:HD2	1.92	0.51
1:D:182:LEU:CD2	1:D:203:CYS:CB	2.89	0.51
1:C:498:MET:HE3	1:C:517:PHE:CE2	2.46	0.51
1:D:182:LEU:CD2	1:D:203:CYS:HB3	2.41	0.50
1:A:522:VAL:HG11	1:A:528:HIS:HB2	1.92	0.50
1:D:365:MET:HG3	1:D:447:VAL:HG11	1.93	0.50
1:B:144:PHE:HD1	1:B:154:ILE:CD1	2.25	0.50
1:C:331:ASN:HB2	1:C:332:PRO:HD2	1.93	0.50
1:C:178:CYS:HB2	1:C:207:ASN:OD1	2.12	0.49
1:C:530:TYR:CE1	1:D:479:PRO:HG3	2.47	0.49
1:A:528:HIS:CD2	1:B:454:ARG:HD3	2.46	0.49
1:D:180:ASP:OD1	1:D:183:ARG:NH2	2.45	0.49
1:A:387:ARG:HG2	1:A:387:ARG:NH1	2.20	0.49
1:D:346:LYS:HB3	1:D:354:LYS:HG2	1.94	0.49
1:C:365:MET:HG3	1:C:447:VAL:HG11	1.94	0.49
1:C:268:VAL:CG2	1:C:495:VAL:C	2.80	0.49
1:A:454:ARG:NH1	1:B:531:ASP:OD1	2.46	0.49
1:C:181:MET:HG2	1:C:203:CYS:HA	1.95	0.49
1:A:379:GLN:O	1:A:382:ARG:HG2	2.13	0.48
1:A:432:ALA:HB1	1:A:441:PRO:HG3	1.95	0.48
1:C:182:LEU:HD23	1:C:203:CYS:SG	2.53	0.48
1:D:432:ALA:HB1	1:D:441:PRO:HG3	1.95	0.48
1:D:467:ASP:HB3	1:D:508:MET:CE	2.43	0.48
1:A:318:PHE:HB3	1:A:467:ASP:OD2	2.13	0.48
1:A:331:ASN:HB2	1:A:332:PRO:HD2	1.94	0.48
1:C:360:GLN:HG3	1:C:361:PHE:N	2.28	0.48
1:B:365:MET:HG3	1:B:447:VAL:HG11	1.95	0.48
1:A:181:MET:HG2	1:A:203:CYS:HA	1.96	0.48
1:A:387:ARG:HH11	1:A:387:ARG:HG3	1.75	0.48
1:B:321:LEU:HD23	2:C:701:EN3:C37	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:VAL:HG22	1:C:495:VAL:O	2.14	0.48
1:A:346:LYS:HB3	1:A:354:LYS:HG2	1.96	0.47
1:A:531:ASP:OD1	1:B:454:ARG:NH1	2.47	0.47
1:B:379:GLN:O	1:B:382:ARG:HG2	2.15	0.47
1:B:321:LEU:CD2	2:C:701:EN3:N32	2.78	0.47
1:B:432:ALA:HB1	1:B:441:PRO:HG3	1.96	0.47
1:D:476:VAL:C	1:D:528:HIS:HD2	2.18	0.47
1:B:498:MET:HB3	1:B:498:MET:HE2	1.52	0.47
1:C:545:GLU:O	1:C:546:GLY:C	2.53	0.47
1:B:321:LEU:HB3	2:C:701:EN3:C37	2.45	0.47
1:A:165:SER:HA	1:A:225:MET:SD	2.55	0.47
1:D:321:LEU:N	1:D:321:LEU:HD23	2.29	0.47
1:D:407:MET:SD	1:D:407:MET:C	2.94	0.47
1:C:251:PRO:HA	1:C:254:ALA:HB3	1.98	0.46
1:B:476:VAL:O	1:B:528:HIS:HD2	1.99	0.46
1:C:156:VAL:HG21	1:C:186:LEU:HD21	1.98	0.46
1:A:503:PRO:N	1:A:504:PRO:CD	2.79	0.46
1:C:226:SER:O	1:C:229:SER:HB3	2.16	0.46
1:C:503:PRO:N	1:C:504:PRO:CD	2.79	0.46
1:A:407:MET:SD	1:A:407:MET:C	2.94	0.46
1:D:541:ASP:OD1	1:D:543:ARG:HD2	2.14	0.46
1:B:278:THR:HA	1:B:424:CYS:HB2	1.98	0.46
1:A:268:VAL:HG13	1:A:436:ASN:CB	2.46	0.46
1:C:494:ASN:OD1	1:D:533:LEU:HB2	2.16	0.46
1:A:537:ALA:C	1:A:539:LYS:H	2.20	0.45
1:B:522:VAL:HG13	1:B:528:HIS:HB2	1.97	0.45
1:B:537:ALA:C	1:B:539:LYS:H	2.18	0.45
1:D:317:ARG:H	1:D:317:ARG:NE	2.14	0.45
1:B:407:MET:SD	1:B:407:MET:C	2.95	0.45
1:A:541:ASP:OD1	1:A:543:ARG:HD3	2.16	0.45
1:B:358:VAL:HG11	1:B:417:LEU:HD22	1.98	0.45
1:C:541:ASP:OD1	1:C:543:ARG:NH1	2.46	0.45
1:B:503:PRO:N	1:B:504:PRO:CD	2.79	0.45
1:C:278:THR:HA	1:C:424:CYS:HB2	1.99	0.45
1:D:152:GLU:O	1:D:153:LYS:CB	2.65	0.45
1:D:289:LYS:N	1:D:290:PRO:HD2	2.32	0.45
1:D:165:SER:HA	1:D:225:MET:CE	2.47	0.45
1:C:432:ALA:HB1	1:C:441:PRO:HG3	1.98	0.45
1:B:284:LEU:HD13	1:B:288:VAL:HG23	1.99	0.45
1:C:498:MET:HB3	1:C:498:MET:HE2	1.55	0.45
1:A:494:ASN:OD1	1:B:533:LEU:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LEU:HA	1:A:533:LEU:HD22	1.77	0.44
1:A:533:LEU:HB2	1:B:494:ASN:OD1	2.17	0.44
1:B:322:PHE:H	2:C:701:EN3:C37	2.30	0.44
1:A:226:SER:O	1:A:229:SER:HB3	2.17	0.44
1:D:181:MET:HA	1:D:184:LEU:HD12	1.99	0.44
1:D:324:ASN:ND2	1:D:326:ASP:H	2.16	0.44
2:A:701:EN3:N2	1:D:321:LEU:HD13	2.33	0.44
1:C:289:LYS:N	1:C:290:PRO:HD2	2.33	0.44
1:D:439:PHE:CZ	1:D:446:ARG:HG3	2.53	0.44
1:D:226:SER:O	1:D:229:SER:HB3	2.17	0.44
1:D:388:ASN:HD22	1:D:415:PHE:HE1	1.64	0.44
1:D:537:ALA:C	1:D:539:LYS:H	2.22	0.44
1:A:435:ALA:HB2	1:A:491:VAL:HG13	1.99	0.43
1:D:435:ALA:HB2	1:D:491:VAL:HG13	2.00	0.43
1:A:248:ASP:HA	1:A:254:ALA:HB2	2.00	0.43
1:B:193:VAL:O	1:B:194:MET:HG2	2.18	0.43
1:A:289:LYS:N	1:A:290:PRO:HD2	2.32	0.43
1:D:503:PRO:N	1:D:504:PRO:CD	2.81	0.43
1:D:522:VAL:HG11	1:D:528:HIS:HB2	2.00	0.43
1:C:522:VAL:HG13	1:C:528:HIS:HB2	2.01	0.43
1:D:268:VAL:HG12	1:D:436:ASN:HB2	2.01	0.43
1:A:268:VAL:HG23	1:A:495:VAL:O	2.19	0.43
1:B:289:LYS:N	1:B:290:PRO:HD2	2.33	0.43
1:B:144:PHE:HE1	1:B:154:ILE:HD13	1.76	0.43
1:B:332:PRO:CG	1:B:459:LEU:HD13	2.48	0.43
1:A:498:MET:HE2	1:A:498:MET:HB3	1.54	0.42
1:C:534:ARG:HG2	1:C:535:HIS:CE1	2.54	0.42
1:B:439:PHE:CZ	1:B:446:ARG:HG3	2.53	0.42
1:C:435:ALA:HB2	1:C:491:VAL:HG13	2.00	0.42
1:D:278:THR:HA	1:D:424:CYS:HB2	2.01	0.42
1:D:488:ILE:HD12	1:D:514:GLY:HA3	2.01	0.42
1:A:507:LYS:H	1:A:507:LYS:CD	2.18	0.42
1:B:281:PRO:HA	1:B:422:VAL:O	2.19	0.42
1:B:435:ALA:HB2	1:B:491:VAL:HG13	2.00	0.42
1:D:196:ASP:C	1:D:198:ASP:H	2.23	0.42
1:D:324:ASN:HD22	1:D:324:ASN:N	2.17	0.42
1:D:248:ASP:HA	1:D:254:ALA:HB2	2.02	0.42
1:A:311:LYS:HD3	1:B:474:PHE:CD2	2.54	0.42
1:A:320:LYS:HE2	2:A:701:EN3:C7	2.50	0.41
1:D:196:ASP:C	1:D:198:ASP:N	2.72	0.41
1:A:439:PHE:CZ	1:A:446:ARG:HG3	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ASN:ND2	1:B:437:GLY:N	2.68	0.41
1:D:281:PRO:HA	1:D:422:VAL:O	2.19	0.41
1:D:284:LEU:HD13	1:D:288:VAL:HG23	2.02	0.41
1:B:157:HIS:CD2	1:B:157:HIS:C	2.94	0.41
1:D:336:ALA:HA	1:D:391:ILE:HG21	2.02	0.41
1:A:261:TRP:HA	1:A:501:TRP:O	2.21	0.41
1:C:261:TRP:HA	1:C:501:TRP:O	2.20	0.41
1:C:410:ILE:HD13	1:C:410:ILE:HA	1.94	0.41
1:D:332:PRO:CG	1:D:459:LEU:HD13	2.51	0.41
1:B:248:ASP:HA	1:B:254:ALA:HB2	2.01	0.41
1:A:278:THR:HA	1:A:424:CYS:HB2	2.02	0.41
1:C:336:ALA:HA	1:C:391:ILE:HG21	2.02	0.41
1:D:374:SER:HB2	1:D:421:GLU:OE2	2.21	0.41
1:B:139:LEU:HD12	1:B:140:GLU:H	1.86	0.41
1:C:374:SER:HB2	1:C:421:GLU:OE2	2.21	0.41
1:C:530:TYR:OH	1:D:479:PRO:HD3	2.21	0.41
1:A:389:PHE:CD1	1:A:411:LEU:HD13	2.57	0.40
1:A:374:SER:HB2	1:A:421:GLU:OE2	2.21	0.40
1:A:332:PRO:CG	1:A:459:LEU:HD13	2.51	0.40
1:A:522:VAL:HG13	1:A:528:HIS:HB2	2.03	0.40
1:D:358:VAL:HG11	1:D:417:LEU:HD22	2.03	0.40
1:B:525:CYS:HA	1:B:540:LEU:O	2.21	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	405/534 (76%)	387 (96%)	11 (3%)	7 (2%)	9 42
1	B	405/534 (76%)	383 (95%)	18 (4%)	4 (1%)	15 54
1	C	408/534 (76%)	388 (95%)	13 (3%)	7 (2%)	9 42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	399/534 (75%)	386 (97%)	12 (3%)	1 (0%)	41	74
All	All	1617/2136 (76%)	1544 (96%)	54 (3%)	19 (1%)	13	49

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	152	GLU
1	C	191	ASP
1	C	192	GLY
1	C	545	GLU
1	D	153	LYS
1	A	190	SER
1	B	317	ARG
1	C	318	PHE
1	A	191	ASP
1	A	316	LEU
1	A	318	PHE
1	A	193	VAL
1	B	151	GLN
1	B	537	ALA
1	C	151	GLN
1	C	193	VAL
1	C	317	ARG
1	B	150	GLY

5.3.2 Protein sidechains (i)

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	308/458 (67%)	291 (94%)	17 (6%)	21	57
1	B	300/458 (66%)	289 (96%)	11 (4%)	34	68
1	C	308/458 (67%)	284 (92%)	24 (8%)	12	43
1	D	301/458 (66%)	284 (94%)	17 (6%)	21	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1217/1832 (66%)	1148 (94%)	69 (6%)	20 56

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	THR
1	A	198	ASP
1	A	225	MET
1	A	275	THR
1	A	288	VAL
1	A	311	LYS
1	A	320	LYS
1	A	361	PHE
1	A	387	ARG
1	A	407	MET
1	A	412	ASP
1	A	446	ARG
1	A	454	ARG
1	A	507	LYS
1	A	528	HIS
1	A	533	LEU
1	A	543	ARG
1	B	146	THR
1	B	184	LEU
1	B	206	SER
1	B	275	THR
1	B	288	VAL
1	B	318	PHE
1	B	361	PHE
1	B	407	MET
1	B	446	ARG
1	B	454	ARG
1	B	545	GLU
1	C	170	THR
1	C	184	LEU
1	C	186	LEU
1	C	198	ASP
1	C	201	LYS
1	C	251	PRO
1	C	268	VAL
1	C	275	THR
1	C	288	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	303	GLU
1	C	311	LYS
1	C	314	SER
1	C	318	PHE
1	C	319	ASN
1	C	321	LEU
1	C	360	GLN
1	C	361	PHE
1	C	381	GLU
1	C	382	ARG
1	C	407	MET
1	C	446	ARG
1	C	531	ASP
1	C	540	LEU
1	C	543	ARG
1	D	146	THR
1	D	187	GLN
1	D	188	THR
1	D	206	SER
1	D	275	THR
1	D	288	VAL
1	D	311	LYS
1	D	314	SER
1	D	317	ARG
1	D	324	ASN
1	D	325	GLU
1	D	361	PHE
1	D	380	SER
1	D	387	ARG
1	D	407	MET
1	D	446	ARG
1	D	540	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	A	285	GLN
1	A	388	ASN
1	B	157	HIS
1	B	205	GLN
1	B	528	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	360	GLN
1	C	455	ASN
1	D	187	GLN
1	D	324	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\| > 2$
2	EN3	A	701	-	44,47,47	2.71	10 (22%)	49,61,61	1.78	12 (24%)
2	EN3	C	701	-	44,47,47	2.57	9 (20%)	49,61,61	1.82	13 (26%)

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	EN3	A	701	-	-	12/31/34/34	0/4/5/5
2	EN3	C	701	-	-	11/31/34/34	0/4/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	EN3	N26-N25	11.65	1.60	1.37
2	A	701	EN3	N26-N25	11.39	1.59	1.37
2	A	701	EN3	C24-S23	-6.66	1.53	1.73
2	C	701	EN3	C24-S23	-6.01	1.55	1.73
2	A	701	EN3	C1-N2	5.38	1.46	1.36
2	C	701	EN3	C1-N2	5.04	1.45	1.36
2	A	701	EN3	C13-N32	4.86	1.46	1.35
2	A	701	EN3	C27-C24	4.83	1.52	1.49
2	A	701	EN3	C3-N2	4.82	1.46	1.35
2	C	701	EN3	C13-N32	4.53	1.45	1.35
2	C	701	EN3	C3-N2	4.29	1.45	1.35
2	C	701	EN3	C27-C24	3.13	1.51	1.49
2	C	701	EN3	O5-C3	-3.07	1.17	1.23
2	A	701	EN3	C31-N32	2.44	1.45	1.40
2	C	701	EN3	C35-N34	-2.37	1.31	1.33
2	A	701	EN3	C14-C16	2.34	1.55	1.51
2	A	701	EN3	O22-C18	2.24	1.42	1.37
2	C	701	EN3	C31-N32	2.13	1.45	1.40
2	A	701	EN3	O15-C13	-2.11	1.19	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	EN3	C35-N34-N33	5.67	122.60	119.77
2	C	701	EN3	C1-N2-C3	-4.26	118.03	129.54
2	A	701	EN3	C4-C6-C11	-4.21	113.72	120.38
2	C	701	EN3	C4-C3-N2	4.04	123.11	114.77
2	C	701	EN3	C4-C6-C11	-3.62	114.65	120.38
2	C	701	EN3	C4-C6-C7	3.33	125.66	120.89
2	C	701	EN3	C31-N32-C13	-3.31	122.33	128.25
2	A	701	EN3	C31-N32-C13	-3.27	122.40	128.25
2	A	701	EN3	C29-C30-C35	-3.20	103.06	113.11
2	C	701	EN3	C21-C16-C17	3.08	122.86	118.54
2	A	701	EN3	C1-N2-C3	-2.86	121.82	129.54
2	C	701	EN3	C31-N33-N34	2.78	121.34	119.37
2	A	701	EN3	C14-C13-N32	2.72	120.38	114.77
2	C	701	EN3	C14-C16-C17	-2.70	116.10	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	701	EN3	O5-C3-N2	-2.44	119.17	123.63
2	A	701	EN3	C7-C6-C11	2.43	121.95	118.54
2	C	701	EN3	C16-C14-C13	-2.39	105.48	112.57
2	A	701	EN3	C4-C6-C7	2.39	124.31	120.89
2	A	701	EN3	C8-C09-C10	2.14	122.39	118.96
2	C	701	EN3	C29-C30-C35	-2.13	106.41	113.11
2	C	701	EN3	C37-C31-N32	-2.09	116.81	123.06
2	A	701	EN3	C38-O12-C10	-2.08	112.49	117.93
2	C	701	EN3	C38-O12-C10	-2.07	112.50	117.93
2	A	701	EN3	C6-C4-C3	2.04	118.61	112.57
2	A	701	EN3	C37-C31-N33	-2.00	118.73	122.56

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	EN3	C24-C27-C28-C29
2	A	701	EN3	C28-C29-C30-C35
2	A	701	EN3	O12-C38-C39-C43
2	A	701	EN3	O22-C40-C41-C42
2	C	701	EN3	C40-C41-C42-C43
2	A	701	EN3	N33-C31-N32-C13
2	A	701	EN3	C37-C31-N32-C13
2	C	701	EN3	C19-C18-O22-C40
2	C	701	EN3	C17-C18-O22-C40
2	C	701	EN3	C09-C10-O12-C38
2	C	701	EN3	C11-C10-O12-C38
2	A	701	EN3	C19-C18-O22-C40
2	A	701	EN3	C17-C18-O22-C40
2	C	701	EN3	C28-C29-C30-C35
2	C	701	EN3	C37-C31-N32-C13
2	C	701	EN3	N33-C31-N32-C13
2	A	701	EN3	C27-C28-C29-C30
2	C	701	EN3	C27-C28-C29-C30
2	A	701	EN3	C39-C38-O12-C10
2	C	701	EN3	C41-C40-O22-C18
2	A	701	EN3	C41-C40-O22-C18
2	A	701	EN3	C38-C39-C43-C42
2	C	701	EN3	C24-C27-C28-C29

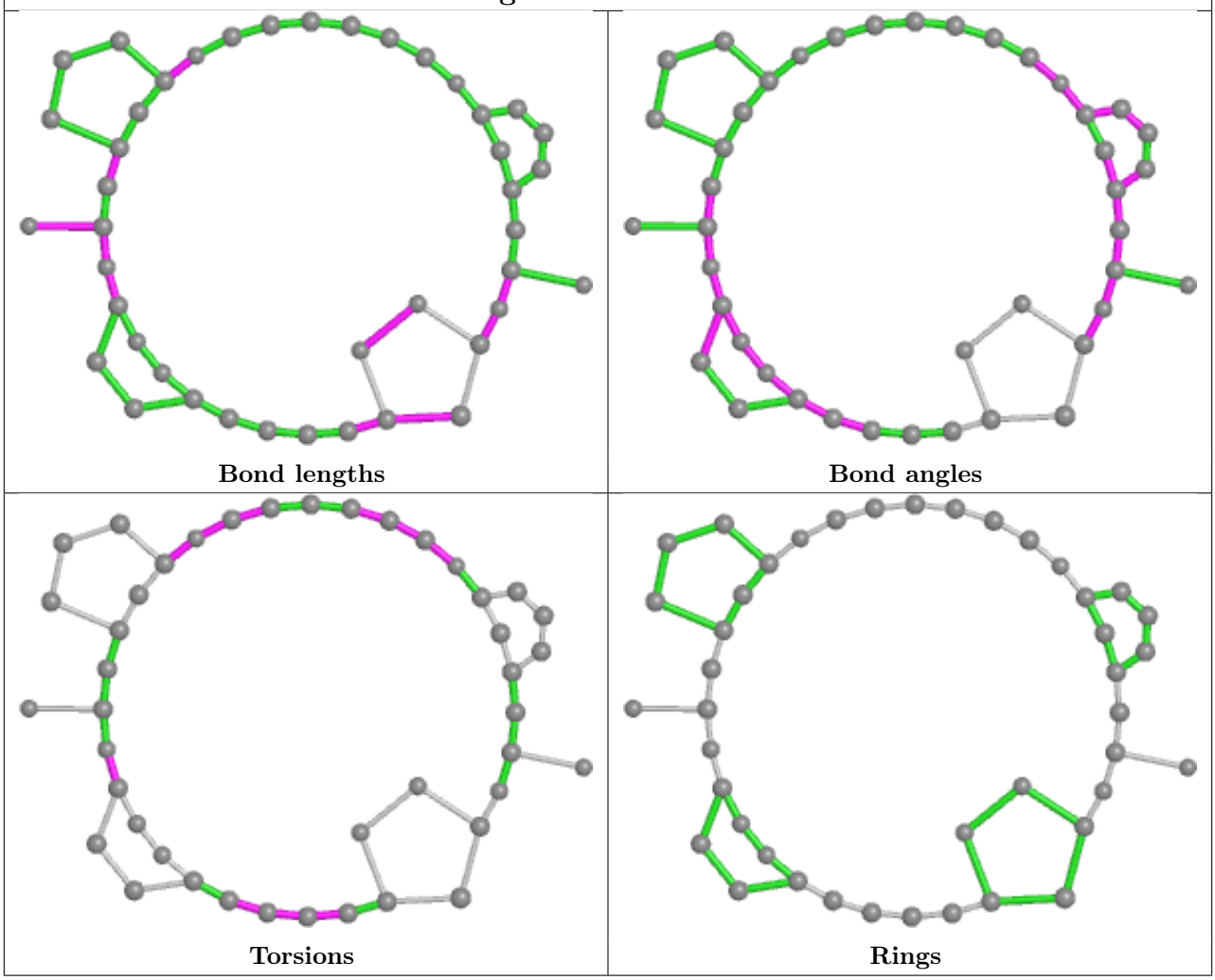
There are no ring outliers.

2 monomers are involved in 12 short contacts:

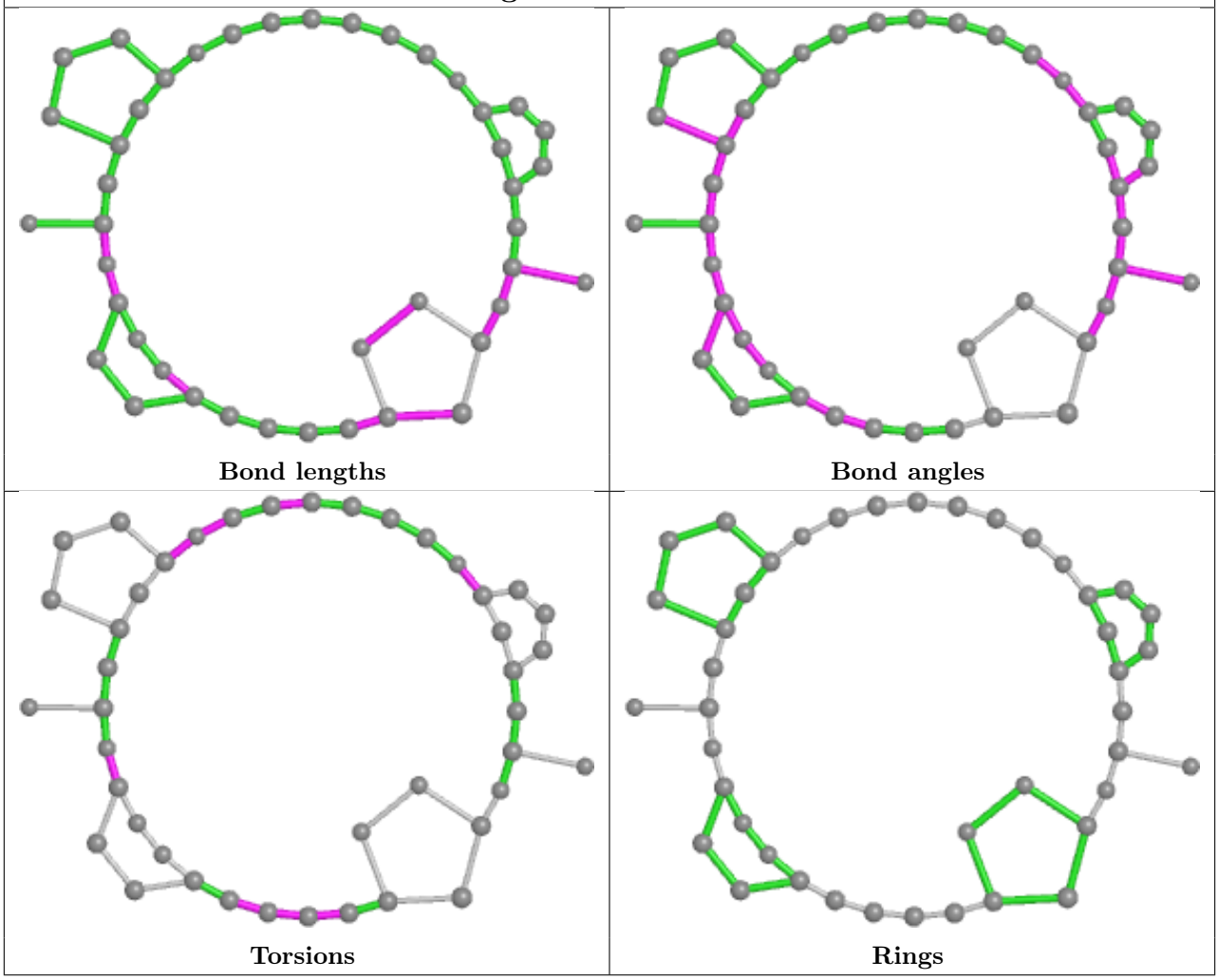
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	EN3	4	0
2	C	701	EN3	8	0

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 then 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.

Ligand EN3 A 701



Ligand EN3 C 701



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	407/534 (76%)	-0.01	9 (2%)	62	48	33, 61, 98, 145	0
1	B	407/534 (76%)	0.03	13 (3%)	47	31	38, 62, 103, 144	0
1	C	410/534 (76%)	-0.01	12 (2%)	51	36	38, 62, 102, 130	0
1	D	405/534 (75%)	0.01	7 (1%)	70	57	35, 63, 97, 136	0
All	All	1629/2136 (76%)	0.01	41 (2%)	57	43	33, 62, 100, 145	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	GLN	4.4
1	D	251	PRO	3.7
1	A	249	TYR	3.7
1	B	147	ILE	3.7
1	C	252	GLN	3.6
1	C	253	LEU	3.3
1	B	151	GLN	3.3
1	A	251	PRO	3.1
1	C	193	VAL	3.0
1	A	256	PHE	3.0
1	B	146	THR	3.0
1	D	153	LYS	2.9
1	B	200	PHE	2.7
1	D	151	GLN	2.7
1	B	188	THR	2.7
1	C	144	PHE	2.6
1	B	252	GLN	2.6
1	B	148	ALA	2.6
1	B	195	LEU	2.6
1	C	251	PRO	2.6
1	A	200	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	153	LYS	2.6
1	C	200	PHE	2.5
1	A	192	GLY	2.5
1	C	194	MET	2.5
1	C	256	PHE	2.4
1	D	148	ALA	2.4
1	A	149	GLU	2.3
1	D	146	THR	2.3
1	C	215	PHE	2.3
1	B	154	ILE	2.3
1	C	162	ALA	2.2
1	B	166	THR	2.2
1	C	138	SER	2.1
1	B	190	SER	2.1
1	A	250	ILE	2.1
1	D	167	GLY	2.1
1	D	256	PHE	2.0
1	C	152	GLU	2.0
1	B	185	THR	2.0
1	A	204	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

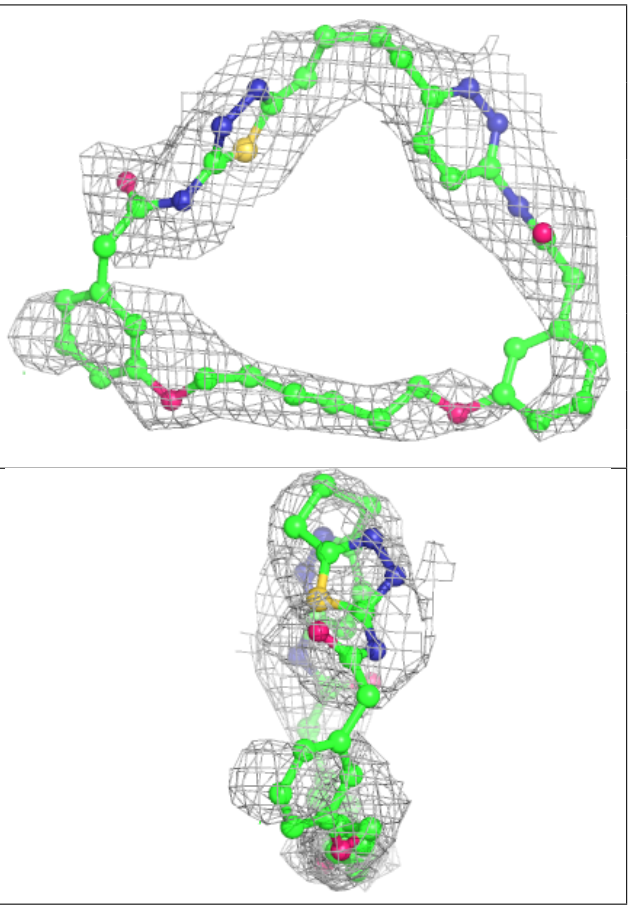
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EN3	A	701	43/43	0.87	0.33	53,91,115,124	0
2	EN3	C	701	43/43	0.90	0.32	53,79,105,109	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.

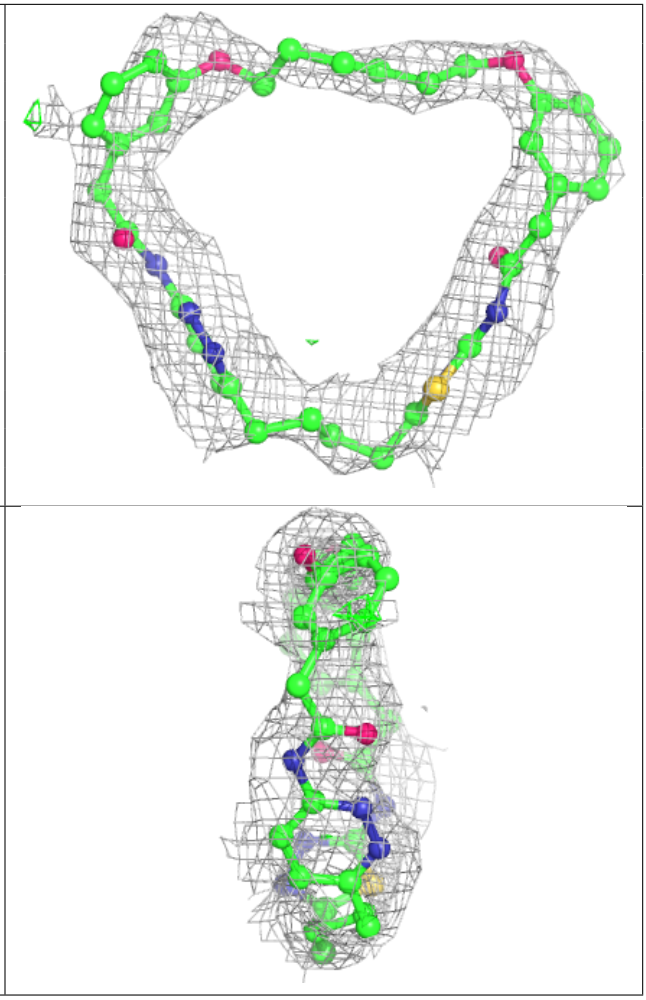
Electron density around EN3 A 701:

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



Electron density around EN3 C 701:

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



6.5 Other polymers (i)

There are no such residues in this entry.