



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:23 AM UTC

PDB ID : 6OHC / pdb_00006ohc
Title : E. coli Guanine Deaminase
Authors : Shek, R.S.; French, J.B.
Deposited on : 2019-04-05
Resolution : 2.30 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
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

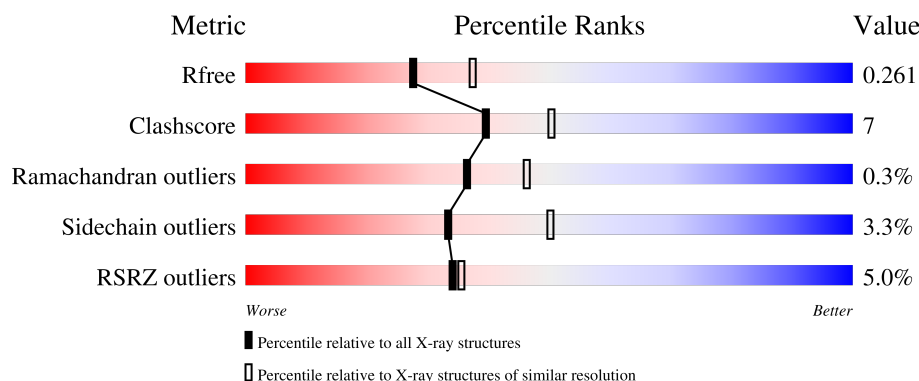
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	439	
1	B	439	
1	C	439	
1	D	439	

2 Entry composition [i](#)

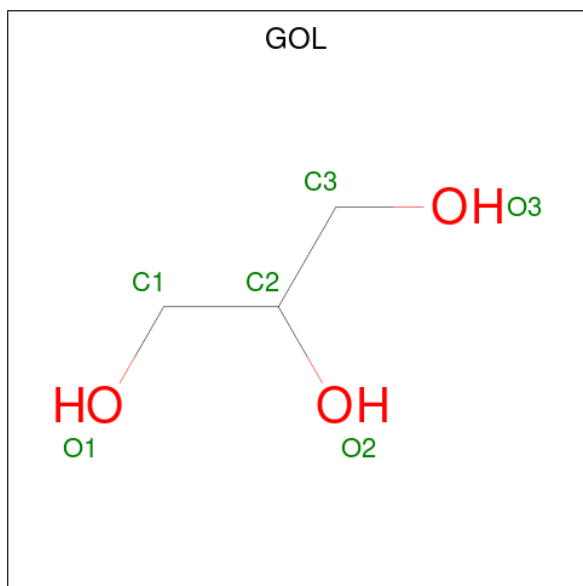
There are 4 unique types of molecules in this entry. The entry contains 13442 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Guanine deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	1	0
			3390	2167	573	633	17			
1	B	430	Total	C	N	O	S	0	0	0
			3428	2191	581	639	17			
1	C	425	Total	C	N	O	S	0	0	0
			3059	1948	532	565	14			
1	D	427	Total	C	N	O	S	0	0	0
			3187	2030	548	595	14			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0

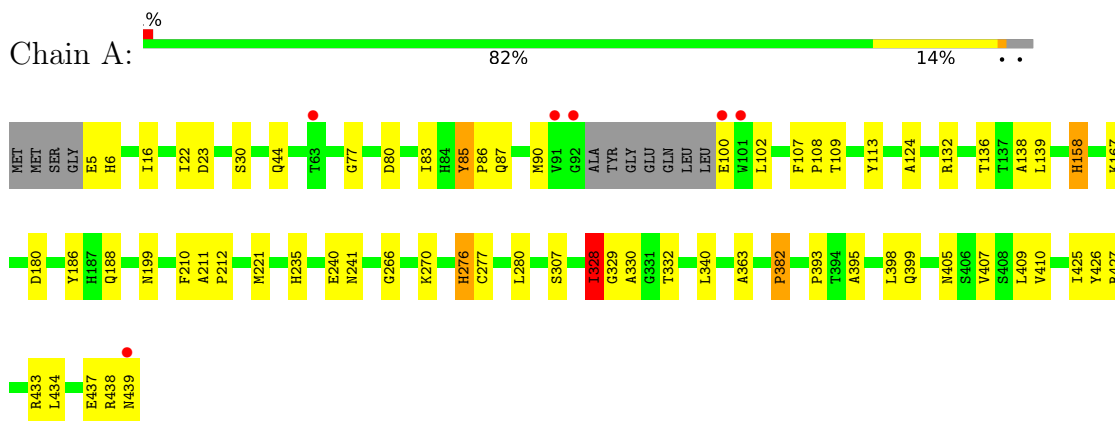
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	134	Total 134	O 134	0	0
4	B	148	Total 148	O 148	0	0
4	C	19	Total 19	O 19	0	0
4	D	61	Total 61	O 61	0	0

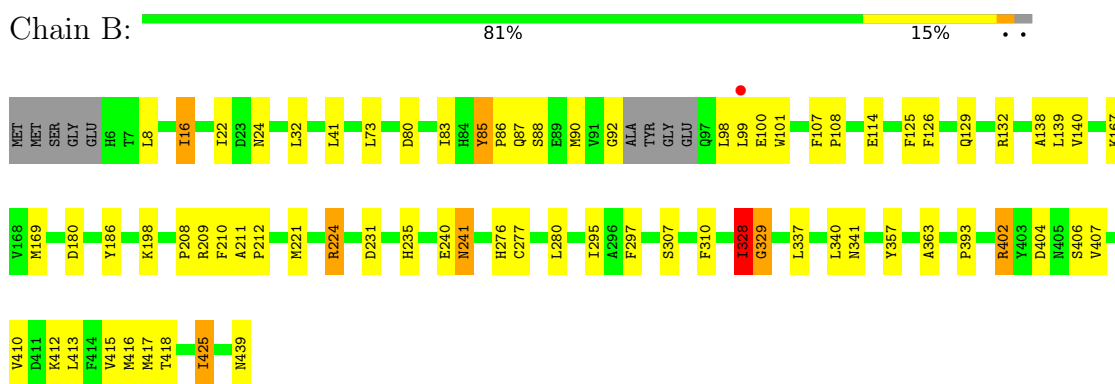
3 Residue-property plots [i](#)

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.

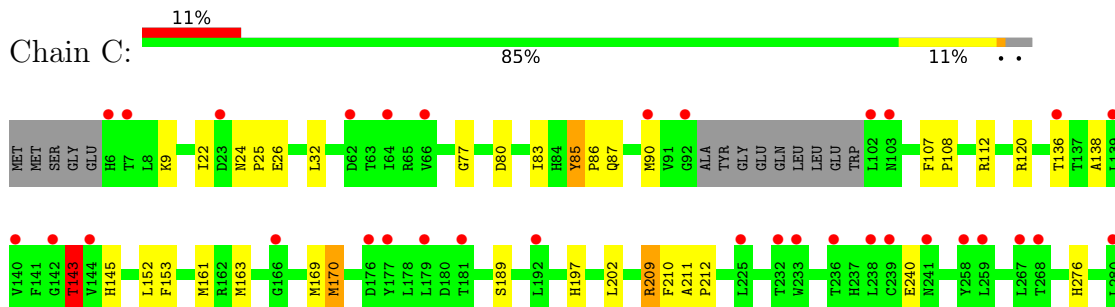
• Molecule 1: Guanine deaminase

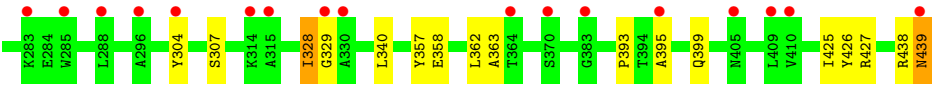


• Molecule 1: Guanine deaminase

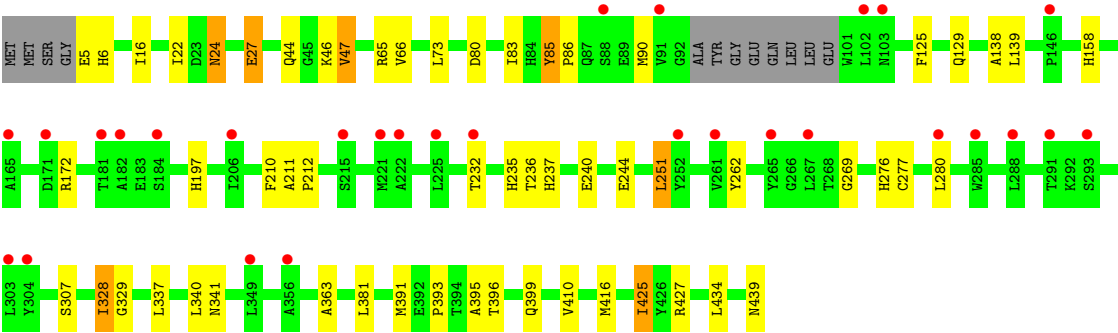
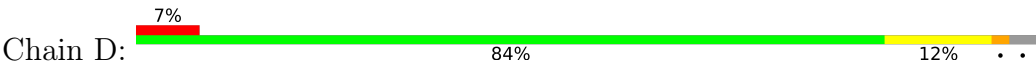


• Molecule 1: Guanine deaminase





● Molecule 1: Guanine deaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.63Å 80.59Å 101.43Å 104.80° 105.72° 105.83°	Depositor
Resolution (Å)	48.91 – 2.30 48.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.91-2.30) 97.8 (48.91-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.209 , 0.258 0.213 , 0.261	Depositor DCC
R_{free} test set	3958 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13442	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	1.13	3/3477 (0.1%)	1.44	6/4722 (0.1%)
1	B	1.15	3/3512 (0.1%)	1.43	5/4761 (0.1%)
1	C	1.09	0/3136	1.43	3/4285 (0.1%)
1	D	1.07	0/3267	1.41	1/4459 (0.0%)
All	All	1.11	6/13392 (0.0%)	1.43	15/18227 (0.1%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	VAL	C-O	7.63	1.32	1.24
1	B	126	PHE	C-O	5.84	1.30	1.24
1	B	415	VAL	C-O	-5.61	1.17	1.24
1	A	382	PRO	C-O	-5.52	1.16	1.24
1	A	276	HIS	CE1-NE2	5.38	1.38	1.32
1	A	158	HIS	CE1-NE2	5.30	1.37	1.32

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	393	PRO	CA-C-O	-6.44	116.55	121.31
1	A	328	ILE	O-C-N	6.31	130.46	122.57
1	A	393	PRO	CA-C-O	-6.26	116.68	121.31
1	A	330	ALA	CA-C-N	5.86	126.52	120.60
1	A	330	ALA	C-N-CA	5.86	126.52	120.60
1	C	439	ASN	CA-C-O	5.67	130.43	120.80
1	A	100	GLU	CA-C-N	5.64	128.16	120.54
1	A	100	GLU	C-N-CA	5.64	128.16	120.54
1	B	132	ARG	CG-CD-NE	-5.59	99.71	112.00
1	B	328	ILE	O-C-N	5.15	129.01	122.57
1	B	114	GLU	CB-CG-CD	5.14	121.34	112.60
1	C	143	THR	CB-CA-C	5.09	119.42	110.36
1	B	329	GLY	CA-C-N	5.09	127.51	120.29
1	B	329	GLY	C-N-CA	5.09	127.51	120.29
1	D	269	GLY	CA-C-O	-5.00	118.06	122.16

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	ILE	Peptide
1	B	328	ILE	Peptide
1	C	328	ILE	Peptide
1	D	328	ILE	Peptide

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	3390	0	3234	46	0
1	B	3428	0	3312	54	0
1	C	3059	0	2604	36	0
1	D	3187	0	2846	44	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	A	134	0	0	5	0
4	B	148	0	0	0	0
4	C	19	0	0	0	0
4	D	61	0	0	1	0
All	All	13442	0	12012	169	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 7.

All (169) 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:B:16:ILE:HD11	1:B:32:LEU:HD11	1.33	1.07
1:C:170:MET:HE3	1:C:209:ARG:HD2	1.42	1.01
1:A:186:TYR:CG	1:A:221:MET:HE2	1.99	0.97
1:A:186:TYR:HB2	1:A:221:MET:HE2	1.47	0.96
1:A:186:TYR:CB	1:A:221:MET:HE2	1.99	0.93
1:B:186:TYR:CG	1:B:221:MET:HE2	2.11	0.85
1:B:8:LEU:HD12	1:B:41:LEU:HD22	1.60	0.83
1:B:16:ILE:CD1	1:B:32:LEU:HD11	2.11	0.80
1:C:358:GLU:O	1:C:362:LEU:HD23	1.81	0.80
1:C:143:THR:HG23	1:C:145:HIS:H	1.47	0.79
1:B:73:LEU:HD23	1:B:416:MET:HE1	1.64	0.78
1:D:393:PRO:HB3	1:D:416:MET:SD	2.24	0.78
1:B:186:TYR:CD1	1:B:221:MET:HE2	2.20	0.76
1:D:337:LEU:HD11	1:D:391:MET:HE1	1.67	0.75
1:B:186:TYR:HB2	1:B:221:MET:HE2	1.70	0.74
1:A:186:TYR:CD1	1:A:221:MET:CE	2.73	0.71
1:B:186:TYR:CD1	1:B:221:MET:CE	2.75	0.68
1:B:186:TYR:CB	1:B:221:MET:HE2	2.23	0.68
1:A:186:TYR:CG	1:A:221:MET:CE	2.76	0.68
1:D:197:HIS:CD2	1:D:232:THR:HG22	2.29	0.67
1:C:153:PHE:HD1	1:C:202:LEU:HD23	1.60	0.67
1:A:167:LYS:CE	1:A:188:GLN:HE21	2.09	0.65
1:B:393:PRO:HB3	1:B:416:MET:HG3	1.80	0.64
1:C:87:GLN:HE21	1:C:329:GLY:HA3	1.61	0.63
1:A:439:ASN:H	1:D:439:ASN:HD22	1.46	0.63
1:A:186:TYR:CD1	1:A:221:MET:HE2	2.34	0.62
1:C:152:LEU:HG	1:C:163:MET:HE1	1.81	0.61
1:A:167:LYS:HE2	1:A:188:GLN:NE2	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LYS:NZ	1:A:180:ASP:OD2	2.34	0.60
1:D:197:HIS:HD2	1:D:232:THR:HG22	1.65	0.60
1:D:24:ASN:HD21	1:D:27:GLU:HG3	1.67	0.59
1:A:167:LYS:HE3	1:A:188:GLN:HE21	1.67	0.59
1:B:167:LYS:NZ	1:B:180:ASP:OD2	2.33	0.59
1:B:73:LEU:HD23	1:B:416:MET:CE	2.31	0.58
1:C:152:LEU:CG	1:C:163:MET:HE1	2.33	0.58
1:D:396:THR:H	1:D:399:GLN:HE21	1.51	0.58
1:B:337:LEU:HD22	1:B:417:MET:HA	1.85	0.58
1:D:337:LEU:HD11	1:D:391:MET:CE	2.34	0.58
1:A:167:LYS:CE	1:A:188:GLN:NE2	2.68	0.57
1:D:236:THR:HG22	1:D:237:HIS:N	2.19	0.57
1:B:404:ASP:OD2	1:D:65:ARG:NH1	2.38	0.56
1:D:16:ILE:HD12	1:D:73:LEU:HD21	1.87	0.56
1:D:46:LYS:NZ	4:D:604:HOH:O	2.39	0.55
1:B:221:MET:HE3	1:B:221:MET:HA	1.87	0.55
1:C:90:MET:HE2	1:C:329:GLY:HA2	1.88	0.55
1:C:340:LEU:HD11	1:C:363:ALA:HB2	1.89	0.55
1:B:92:GLY:O	1:B:101:TRP:HZ3	1.90	0.55
1:A:80:ASP:O	1:A:138:ALA:HA	2.08	0.54
1:A:132:ARG:HH22	1:D:439:ASN:HA	1.72	0.54
1:C:83:ILE:HG13	1:C:328:ILE:HB	1.90	0.54
1:A:83:ILE:HG13	1:A:328:ILE:HB	1.90	0.53
1:B:90:MET:HE3	1:B:329:GLY:CA	2.39	0.53
1:C:153:PHE:CD1	1:C:202:LEU:HD23	2.43	0.53
1:A:438:ARG:O	1:A:439:ASN:CB	2.57	0.52
1:A:199:ASN:C	1:A:199:ASN:HD22	2.18	0.52
1:C:90:MET:HE2	1:C:329:GLY:CA	2.40	0.52
1:B:413:LEU:HD12	1:B:417:MET:HG2	1.92	0.52
1:B:80:ASP:O	1:B:138:ALA:HA	2.11	0.51
1:A:5:GLU:HA	1:A:44:GLN:HG2	1.92	0.50
1:B:404:ASP:HB3	1:D:65:ARG:HD2	1.92	0.50
1:C:438:ARG:O	1:C:439:ASN:HB3	2.11	0.50
1:D:24:ASN:N	1:D:24:ASN:OD1	2.43	0.50
1:C:80:ASP:O	1:C:138:ALA:HA	2.11	0.50
1:D:83:ILE:HG13	1:D:328:ILE:HB	1.93	0.50
1:C:87:GLN:NE2	1:C:90:MET:HE1	2.27	0.50
1:A:107:PHE:HB2	1:A:108:PRO:HD3	1.94	0.50
1:D:172:ARG:NH1	1:D:251:LEU:HG	2.27	0.50
1:D:80:ASP:O	1:D:138:ALA:HA	2.12	0.50
1:A:22:ILE:HD12	1:A:22:ILE:C	2.36	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ILE:C	1:D:22:ILE:HD12	2.37	0.50
1:C:107:PHE:HB2	1:C:108:PRO:HD3	1.95	0.49
1:B:98:LEU:O	1:B:100:GLU:N	2.45	0.49
1:C:24:ASN:ND2	1:C:26:GLU:CB	2.76	0.49
1:A:340:LEU:HD11	1:A:363:ALA:HB2	1.94	0.48
1:B:169:MET:HE2	1:B:208:PRO:N	2.28	0.48
1:C:169:MET:HE3	1:C:189:SER:OG	2.14	0.48
1:C:24:ASN:OD1	1:C:25:PRO:HD2	2.13	0.48
1:C:438:ARG:O	1:C:439:ASN:CB	2.62	0.48
1:B:8:LEU:HD12	1:B:41:LEU:CD2	2.38	0.48
1:C:161:MET:HE3	1:C:163:MET:HG3	1.96	0.48
1:D:236:THR:CG2	1:D:237:HIS:N	2.77	0.48
1:B:22:ILE:C	1:B:22:ILE:HD12	2.39	0.47
1:A:124:ALA:HA	4:A:729:HOH:O	2.14	0.47
1:C:211:ALA:HB3	1:C:212:PRO:HD3	1.97	0.47
1:D:5:GLU:HA	1:D:44:GLN:CG	2.45	0.47
1:C:426:TYR:CD2	1:C:427:ARG:HG3	2.49	0.47
1:B:85:TYR:N	1:B:86:PRO:CD	2.77	0.47
1:C:22:ILE:C	1:C:22:ILE:HD12	2.39	0.47
1:B:32:LEU:HD22	1:B:357:TYR:CE1	2.49	0.47
1:B:169:MET:CE	1:B:208:PRO:N	2.77	0.47
1:A:22:ILE:HD12	1:A:22:ILE:O	2.15	0.46
1:A:158:HIS:CG	1:D:158:HIS:CE1	3.02	0.46
1:B:340:LEU:HD11	1:B:363:ALA:HB2	1.97	0.46
1:B:98:LEU:C	1:B:100:GLU:H	2.23	0.46
1:D:139:LEU:HG	1:D:235:HIS:CE1	2.50	0.46
1:A:277:CYS:HB3	1:A:280:LEU:HD11	1.98	0.46
1:D:85:TYR:N	1:D:86:PRO:CD	2.79	0.46
1:B:83:ILE:HG13	1:B:328:ILE:HB	1.98	0.46
1:A:426:TYR:CD2	1:A:427:ARG:HG2	2.51	0.46
1:B:90:MET:HE3	1:B:329:GLY:HA2	1.97	0.46
1:D:236:THR:HG21	1:D:262:TYR:CZ	2.51	0.46
1:D:22:ILE:HD12	1:D:22:ILE:O	2.16	0.46
1:A:139:LEU:HG	1:A:235:HIS:CE1	2.51	0.45
1:B:198:LYS:CE	1:B:231:ASP:OD2	2.65	0.45
1:B:439:ASN:HD22	1:C:439:ASN:H	1.64	0.45
1:B:22:ILE:HD12	1:B:22:ILE:O	2.16	0.45
1:D:340:LEU:HD11	1:D:363:ALA:HB2	1.97	0.45
1:A:85:TYR:N	1:A:86:PRO:CD	2.80	0.45
1:A:186:TYR:HB2	1:A:221:MET:CE	2.33	0.45
1:A:398:LEU:HD11	1:B:88:SER:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:GLN:NE2	1:C:329:GLY:HA3	2.31	0.45
1:D:125:PHE:O	1:D:129:GLN:HG2	2.16	0.45
1:D:90:MET:HE2	1:D:329:GLY:CA	2.46	0.45
1:B:169:MET:CE	1:B:208:PRO:CD	2.95	0.44
1:B:277:CYS:HB3	1:B:280:LEU:HD11	1.99	0.44
1:B:107:PHE:HB2	1:B:108:PRO:HD3	1.98	0.44
1:D:47:VAL:HG11	1:D:381:LEU:O	2.18	0.44
1:B:240:GLU:O	1:B:307:SER:HB3	2.17	0.44
1:A:240:GLU:O	1:A:307:SER:HB3	2.18	0.44
1:A:332:THR:O	1:B:402:ARG:NH2	2.51	0.43
1:C:22:ILE:HD12	1:C:22:ILE:O	2.18	0.43
1:B:341:ASN:HB2	1:B:418:THR:O	2.18	0.43
1:D:47:VAL:CG1	1:D:381:LEU:O	2.66	0.43
1:A:211:ALA:HB3	1:A:212:PRO:HD3	2.00	0.43
1:A:439:ASN:C	4:A:644:HOH:O	2.60	0.43
1:C:85:TYR:N	1:C:86:PRO:CD	2.81	0.43
1:A:427:ARG:HD2	1:A:434:LEU:HD11	2.00	0.43
1:D:240:GLU:O	1:D:307:SER:HB3	2.19	0.43
1:B:241:ASN:OD1	1:B:241:ASN:C	2.61	0.43
1:D:211:ALA:HB3	1:D:212:PRO:HD3	2.01	0.43
1:A:16:ILE:HD13	1:A:409:LEU:HD21	2.01	0.43
1:A:395:ALA:H	1:A:399:GLN:HE21	1.67	0.42
1:D:5:GLU:HA	1:D:44:GLN:CD	2.43	0.42
1:B:125:PHE:O	1:B:129:GLN:HG2	2.18	0.42
1:C:77:GLY:HA3	1:C:136:THR:OG1	2.20	0.42
1:B:211:ALA:HB3	1:B:212:PRO:HD3	2.01	0.42
1:C:161:MET:CE	1:C:163:MET:SD	3.07	0.42
1:C:439:ASN:C	1:C:439:ASN:OD1	2.63	0.42
1:D:427:ARG:HD2	1:D:434:LEU:HD11	2.01	0.42
1:A:158:HIS:CE1	1:D:158:HIS:CG	3.07	0.42
1:D:277:CYS:HB3	1:D:280:LEU:HD11	2.01	0.42
1:B:425:ILE:N	1:B:425:ILE:HD12	2.35	0.42
1:A:87:GLN:OE1	1:A:329:GLY:HA3	2.20	0.42
1:B:406:SER:O	1:B:412:LYS:NZ	2.53	0.41
1:A:30:SER:HB3	4:A:629:HOH:O	2.20	0.41
1:B:139:LEU:HG	1:B:235:HIS:CE1	2.55	0.41
1:C:395:ALA:H	1:C:399:GLN:NE2	2.19	0.41
1:A:266:GLY:HA2	4:A:671:HOH:O	2.20	0.41
1:B:208:PRO:O	1:B:209:ARG:C	2.64	0.41
1:C:240:GLU:O	1:C:307:SER:HB3	2.20	0.41
1:D:395:ALA:HB3	1:D:399:GLN:HE22	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:425:ILE:HD12	1:D:425:ILE:N	2.35	0.41
1:A:77:GLY:HA3	1:A:136:THR:OG1	2.19	0.41
1:A:86:PRO:HA	1:A:113:TYR:CZ	2.56	0.41
1:A:102:LEU:HB3	1:A:107:PHE:CE2	2.55	0.41
1:A:405:ASN:HB2	4:A:692:HOH:O	2.21	0.41
1:B:297:PHE:CE1	1:B:310:PHE:HB3	2.56	0.41
1:C:32:LEU:HD22	1:C:357:TYR:CE1	2.55	0.41
1:D:197:HIS:ND1	1:D:197:HIS:C	2.79	0.41
1:B:295:ILE:HG21	1:B:310:PHE:CE1	2.56	0.41
1:D:5:GLU:HA	1:D:44:GLN:NE2	2.36	0.40
1:A:90:MET:HG3	1:A:109:THR:OG1	2.21	0.40
1:C:304:TYR:OH	1:D:341:ASN:ND2	2.50	0.40
1:B:224:ARG:HH11	1:B:224:ARG:HG3	1.85	0.40
1:B:404:ASP:CB	1:D:65:ARG:HD2	2.51	0.40
1:B:22:ILE:C	1:B:22:ILE:CD1	2.95	0.40
1:B:87:GLN:OE1	1:B:329:GLY:HA3	2.21	0.40
1:C:197:HIS:ND1	1:C:197:HIS:C	2.80	0.40
1:D:24:ASN:ND2	1:D:27:GLU:HG3	2.33	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	425/439 (97%)	411 (97%)	13 (3%)	1 (0%)	43	55
1	B	426/439 (97%)	411 (96%)	13 (3%)	2 (0%)	24	31
1	C	421/439 (96%)	408 (97%)	12 (3%)	1 (0%)	43	55
1	D	423/439 (96%)	409 (97%)	13 (3%)	1 (0%)	43	55
All	All	1695/1756 (96%)	1639 (97%)	51 (3%)	5 (0%)	36	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	99	LEU
1	A	276	HIS
1	B	276	HIS
1	C	276	HIS
1	D	276	HIS

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	351/379 (93%)	339 (97%)	12 (3%)	32	49
1	B	361/379 (95%)	351 (97%)	10 (3%)	38	56
1	C	256/379 (68%)	247 (96%)	9 (4%)	32	48
1	D	294/379 (78%)	283 (96%)	11 (4%)	30	45
All	All	1262/1516 (83%)	1220 (97%)	42 (3%)	33	50

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	23	ASP
1	A	85	TYR
1	A	210	PHE
1	A	241	ASN
1	A	270	LYS
1	A	382	PRO
1	A	407	VAL
1	A	410	VAL
1	A	425	ILE
1	A	433	ARG
1	A	437	GLU
1	B	16	ILE
1	B	24	ASN
1	B	85	TYR
1	B	210	PHE
1	B	224	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	241	ASN
1	B	402	ARG
1	B	407	VAL
1	B	410	VAL
1	B	425	ILE
1	C	9	LYS
1	C	85	TYR
1	C	112	ARG
1	C	120	ARG
1	C	143	THR
1	C	170	MET
1	C	209	ARG
1	C	210	PHE
1	C	425	ILE
1	D	6	HIS
1	D	24	ASN
1	D	27	GLU
1	D	47	VAL
1	D	66	VAL
1	D	85	TYR
1	D	210	PHE
1	D	244	GLU
1	D	251	LEU
1	D	410	VAL
1	D	425	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	145	HIS
1	A	188	GLN
1	A	199	ASN
1	A	255	HIS
1	A	341	ASN
1	A	399	GLN
1	B	59	GLN
1	B	103	ASN
1	B	145	HIS
1	B	317	GLN
1	B	348	GLN
1	B	399	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	44	GLN
1	C	87	GLN
1	C	105	HIS
1	C	218	GLN
1	C	341	ASN
1	C	399	GLN
1	D	44	GLN
1	D	105	HIS
1	D	129	GLN
1	D	158	HIS
1	D	188	GLN
1	D	341	ASN
1	D	399	GLN
1	D	405	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are 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	GOL	A	501	-	5,5,5	0.09	0	5,5,5	0.36	0
2	GOL	B	501	-	5,5,5	0.30	0	5,5,5	0.48	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	GOL	A	501	-	-	1/4/4/4	-
2	GOL	B	501	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	O1-C1-C2-O2
2	B	501	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	428/439 (97%)	-0.04	6 (1%) 73 75	30, 47, 65, 104	1 (0%)
1	B	430/439 (97%)	-0.07	1 (0%) 91 91	34, 46, 62, 88	0
1	C	425/439 (96%)	0.94	50 (11%) 9 10	54, 86, 116, 131	0
1	D	427/439 (97%)	0.71	29 (6%) 23 25	39, 76, 122, 136	0
All	All	1710/1756 (97%)	0.39	86 (5%) 34 35	30, 57, 113, 136	1 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	GLY	5.8
1	D	222	ALA	4.7
1	D	356	ALA	4.7
1	D	206	ILE	4.5
1	A	91	VAL	4.1
1	A	101	TRP	3.6
1	A	439	ASN	3.3
1	D	171	ASP	3.1
1	D	304	TYR	3.1
1	C	225	LEU	3.1
1	D	267	LEU	3.0
1	C	64	ILE	3.0
1	D	103	ASN	2.8
1	C	330	ALA	2.8
1	C	66	VAL	2.8
1	D	181	THR	2.7
1	C	102	LEU	2.7
1	B	99	LEU	2.7
1	C	285	TRP	2.7
1	C	364	THR	2.6
1	C	103	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	293	SER	2.6
1	C	92	GLY	2.6
1	C	410	VAL	2.6
1	D	182	ALA	2.6
1	C	23	ASP	2.6
1	C	405	ASN	2.6
1	C	176	ASP	2.5
1	D	221	MET	2.5
1	C	268	THR	2.5
1	C	304	TYR	2.5
1	A	100	GLU	2.5
1	C	142	GLY	2.5
1	D	102	LEU	2.5
1	C	90	MET	2.5
1	C	241	ASN	2.5
1	C	296	ALA	2.5
1	C	439	ASN	2.4
1	C	239	CYS	2.4
1	C	179	LEU	2.4
1	C	166	GLY	2.3
1	C	7	THR	2.3
1	D	88	SER	2.3
1	C	288	LEU	2.3
1	C	283	LYS	2.3
1	D	91	VAL	2.3
1	C	314	LYS	2.3
1	C	181	THR	2.3
1	C	232	THR	2.3
1	C	140	VAL	2.3
1	D	303	LEU	2.2
1	C	395	ALA	2.2
1	D	252	TYR	2.2
1	C	233	TRP	2.2
1	D	184	SER	2.2
1	D	215	SER	2.2
1	D	280	LEU	2.2
1	A	63	THR	2.2
1	C	62	ASP	2.2
1	C	329	GLY	2.2
1	C	177	TYR	2.2
1	C	259	LEU	2.2
1	D	232	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	192	LEU	2.1
1	D	261	VAL	2.1
1	D	146	PRO	2.1
1	C	370	SER	2.1
1	D	165	ALA	2.1
1	D	265	TYR	2.1
1	C	383	GLY	2.1
1	D	291	THR	2.1
1	C	238	LEU	2.1
1	C	267	LEU	2.1
1	C	409	LEU	2.1
1	D	349	LEU	2.1
1	C	136	THR	2.0
1	C	236	THR	2.0
1	C	139	LEU	2.0
1	C	258	TYR	2.0
1	C	144	VAL	2.0
1	D	285	TRP	2.0
1	C	315	ALA	2.0
1	C	6	HIS	2.0
1	C	280	LEU	2.0
1	D	225	LEU	2.0
1	D	288	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
-----	------	-------	-----	-------	------	-----	-----------------------------	-------

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	501	6/6	0.84	0.13	59,63,64,65	0
2	GOL	A	501	6/6	0.91	0.13	59,59,60,60	0
3	ZN	C	501	1/1	0.98	0.05	73,73,73,73	0
3	ZN	D	501	1/1	0.98	0.06	67,67,67,67	0
3	ZN	A	502	1/1	1.00	0.02	37,37,37,37	0
3	ZN	B	502	1/1	1.00	0.02	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.