



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:33 AM UTC

PDB ID : 1D6Y / pdb_00001d6y
Title : CRYSTAL STRUCTURE OF E. COLI COPPER-CONTAINING AMINE
OXIDASE ANAEROBICALLY REDUCED WITH BETA-PHENYLETH
YLAMINE AND COMPLEXED WITH NITRIC OXIDE.
Authors : Wilmot, C.M.; Hajdu, J.; McPherson, M.J.; Knowles, P.F.; Phillips, S.E.V.
Deposited on : 1999-10-16
Resolution : 2.40 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

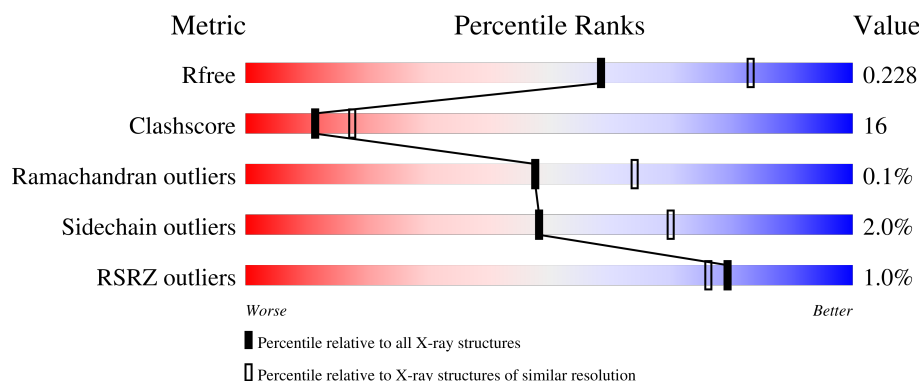
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	727	% 69% 27% ..
1	B	727	% 70% 26% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	HY1	A	2001	-	-	X	-
4	HY1	B	3001	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12823 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 COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	718	Total	C	N	O	S	0	0	0
			5664	3602	965	1075	22			
1	B	720	Total	C	N	O	S	0	0	0
			5683	3614	970	1077	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	466	TYQ	TYR	modified residue	UNP P46883
B	466	TYQ	TYR	modified residue	UNP P46883

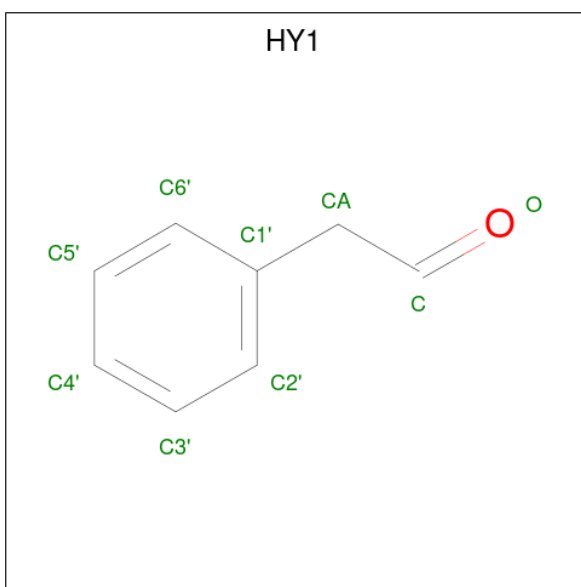
- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

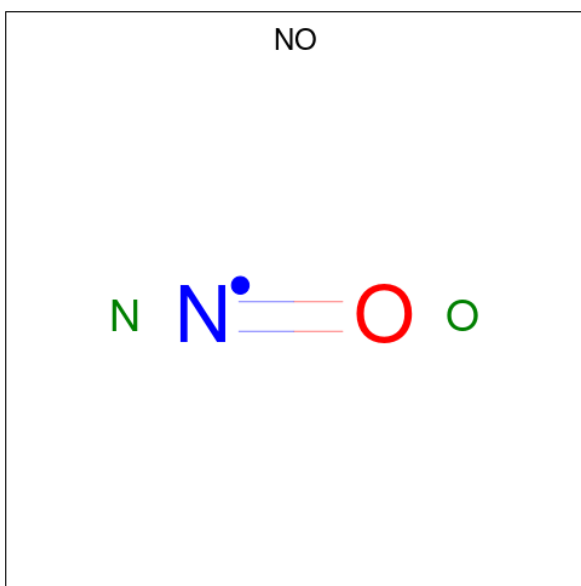
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		

- Molecule 4 is PHENYLACETALDEHYDE (CCD ID: HY1) (formula: C₈H₈O).



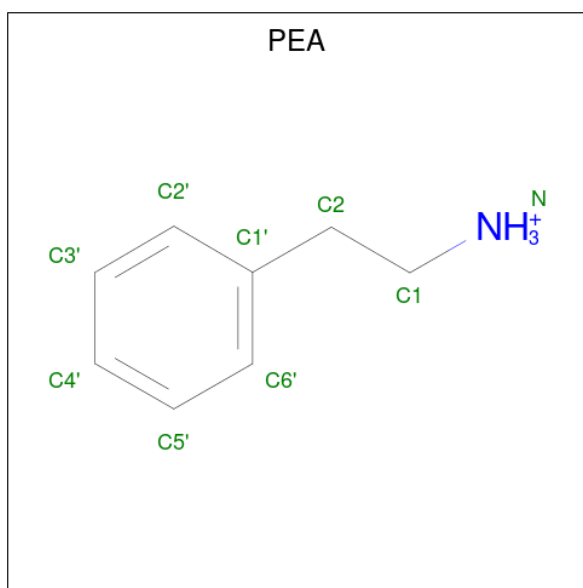
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	8	1		
4	B	1	Total	C	O	0	0
			9	8	1		

- Molecule 5 is NITRIC OXIDE (CCD ID: NO) (formula: NO).



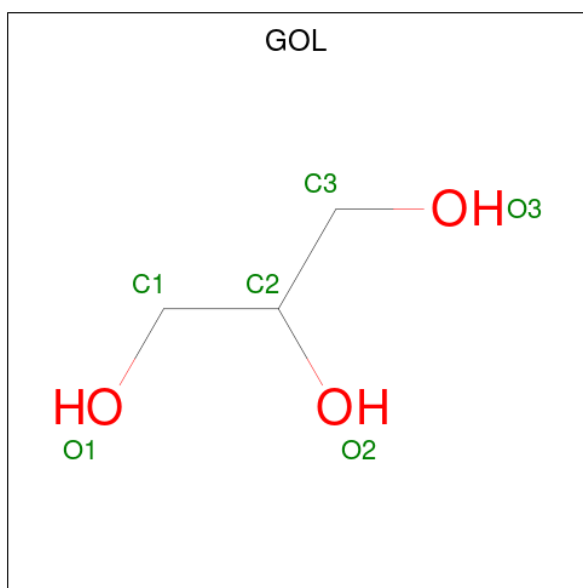
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	N	O	0	0
			2	1	1		
5	B	1	Total	N	O	0	0
			2	1	1		

- Molecule 6 is 2-PHENYLETHYLAMINE (CCD ID: PEA) (formula: $C_8H_{12}N$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			9	8	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

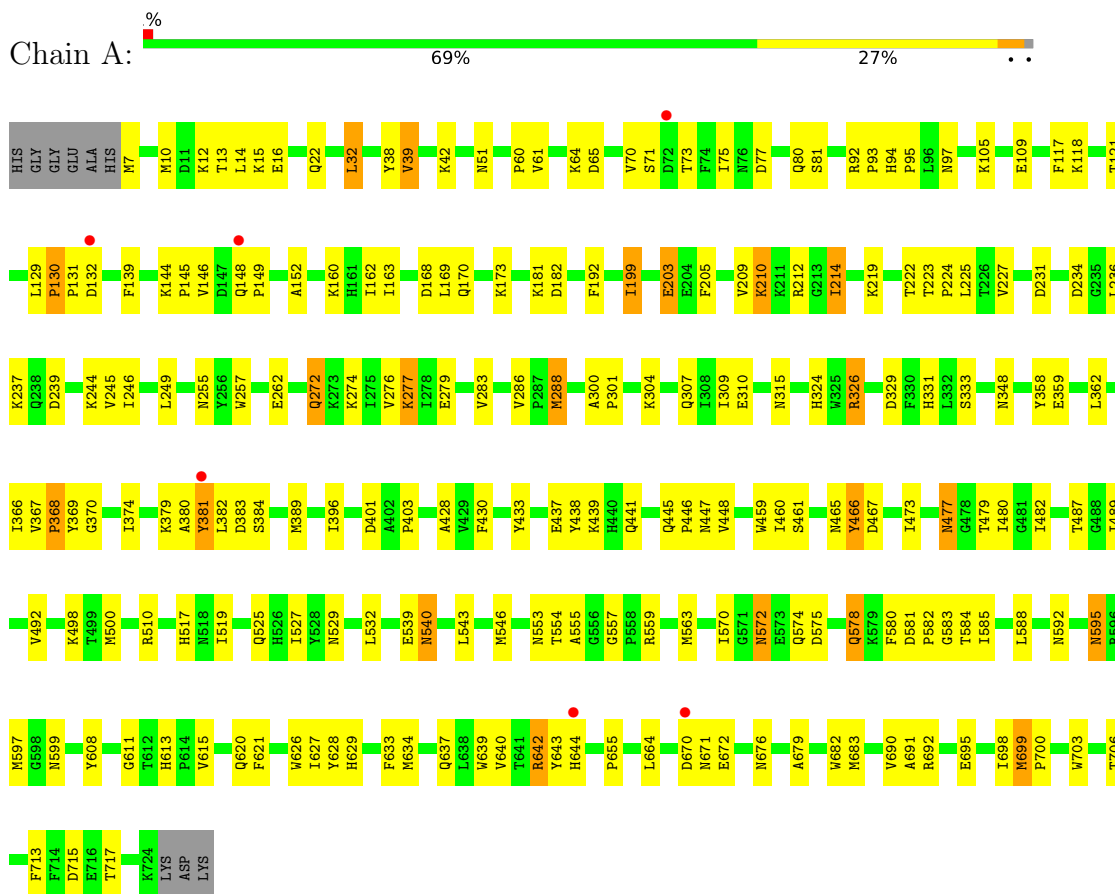
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	746	Total 746	O 746	0	0
8	B	681	Total 681	O 681	0	0

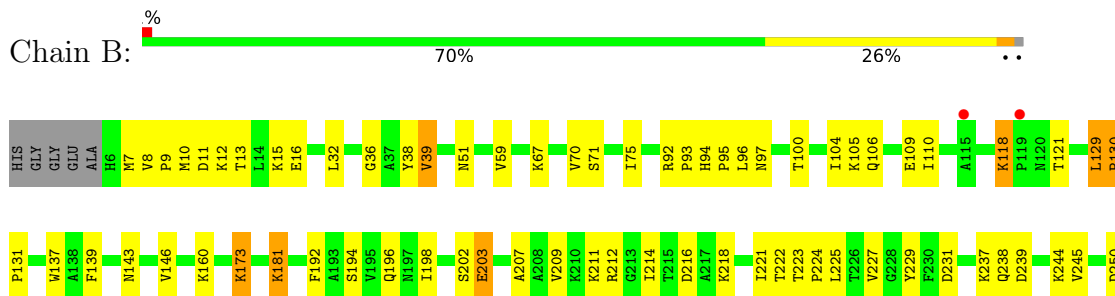
3 Residue-property plots [i](#)

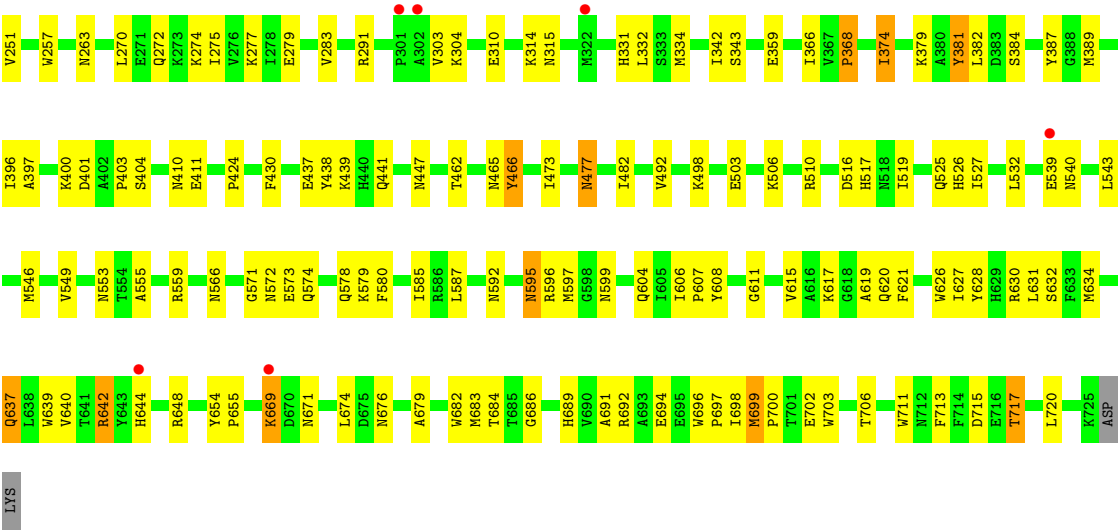
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: COPPER AMINE OXIDASE



• Molecule 1: COPPER AMINE OXIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.24Å 166.48Å 79.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.40) 92.5 (30.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.181 , 0.231 0.183 , 0.228	Depositor DCC
R_{free} test set	2274 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.6	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	0.96	EDS
Total number of atoms	12823	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: NO, CU, CA, GOL, HY1, PEA, TYQ

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	0.39	0/5793	1.00	29/7886 (0.4%)
1	B	0.38	0/5813	1.01	27/7912 (0.3%)
All	All	0.39	0/11606	1.00	56/15798 (0.4%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	LYS	CA-C-N	8.08	127.38	118.97
1	B	118	LYS	C-N-CA	8.08	127.38	118.97
1	B	310	GLU	CA-C-N	7.85	127.56	119.56
1	B	310	GLU	C-N-CA	7.85	127.56	119.56
1	B	654	TYR	CA-C-N	7.29	126.92	119.56
1	B	654	TYR	C-N-CA	7.29	126.92	119.56
1	B	699	MET	N-CA-C	7.10	119.11	109.24
1	A	326	ARG	CB-CA-C	-7.04	108.46	116.63
1	B	381	TYR	N-CA-C	6.63	120.30	109.76
1	A	691	ALA	N-CA-C	6.44	118.33	110.41
1	A	713	PHE	N-CA-C	-6.41	104.16	112.23
1	B	39	VAL	N-CA-C	6.32	117.70	108.53
1	B	713	PHE	N-CA-C	-6.18	104.44	112.23
1	B	691	ALA	N-CA-C	6.14	117.96	110.41
1	A	699	MET	N-CA-C	6.04	117.63	109.24
1	A	367	VAL	CA-C-N	6.03	126.51	119.99
1	A	367	VAL	C-N-CA	6.03	126.51	119.99
1	A	310	GLU	CA-C-N	5.96	125.66	119.82
1	A	310	GLU	C-N-CA	5.96	125.66	119.82
1	B	717	THR	CA-C-N	5.95	125.63	119.56
1	B	717	THR	C-N-CA	5.95	125.63	119.56
1	B	270	LEU	N-CA-C	5.93	117.43	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	588	LEU	N-CA-C	-5.86	97.61	107.99
1	B	703	TRP	N-CA-C	5.83	119.07	109.85
1	B	10	MET	N-CA-C	5.72	117.32	111.14
1	B	473	ILE	N-CA-C	5.63	115.70	107.37
1	B	374	ILE	N-CA-C	5.60	117.00	110.62
1	A	309	ILE	N-CA-C	5.54	117.39	108.85
1	A	473	ILE	N-CA-C	5.54	116.07	107.99
1	B	606	ILE	CA-C-N	5.49	125.11	119.56
1	B	606	ILE	C-N-CA	5.49	125.11	119.56
1	A	381	TYR	N-CA-C	5.42	118.46	109.46
1	A	131	PRO	N-CA-C	-5.41	103.64	111.22
1	A	130	PRO	N-CA-C	5.39	117.27	110.70
1	B	129	LEU	N-CA-C	-5.37	101.78	109.24
1	A	262	GLU	N-CA-C	5.36	117.64	110.35
1	A	118	LYS	CA-C-N	5.35	126.53	119.84
1	A	118	LYS	C-N-CA	5.35	126.53	119.84
1	B	689	HIS	N-CA-C	5.33	117.31	108.20
1	A	362	LEU	N-CA-C	-5.30	102.44	110.28
1	A	39	VAL	N-CA-C	5.30	116.94	108.89
1	B	130	PRO	N-CA-C	5.30	117.16	110.70
1	A	578	GLN	N-CA-C	5.23	116.75	108.96
1	A	703	TRP	N-CA-C	5.20	118.06	109.85
1	B	578	GLN	N-CA-C	5.20	116.19	108.60
1	A	717	THR	CA-C-N	5.14	124.80	119.56
1	A	717	THR	C-N-CA	5.14	124.80	119.56
1	A	540	ASN	N-CA-C	5.13	116.63	108.67
1	B	571	GLY	N-CA-C	5.12	122.02	115.32
1	A	272	GLN	N-CA-C	-5.09	107.02	113.18
1	B	503	GLU	N-CA-C	5.06	117.45	111.33
1	B	343	SER	N-CA-C	5.04	117.33	109.52
1	A	690	VAL	N-CA-C	-5.03	100.50	107.80
1	A	383	ASP	N-CA-C	5.01	117.12	111.11
1	A	557	GLY	CA-C-N	5.00	124.78	119.28
1	A	557	GLY	C-N-CA	5.00	124.78	119.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5664	0	5542	201	0
1	B	5683	0	5562	184	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	9	0	8	6	0
4	B	9	0	8	5	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	9	0	12	0	0
7	B	12	0	16	1	0
8	A	746	0	0	14	0
8	B	681	0	0	8	0
All	All	12823	0	11148	363	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 16.

All (363) 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:181:LYS:H	1:B:181:LYS:HE2	0.99	1.11
1:A:304:LYS:H	1:B:315:ASN:HD21	0.97	0.97
1:A:642:ARG:HB2	1:A:642:ARG:HH11	1.28	0.96
1:B:181:LYS:H	1:B:181:LYS:CE	1.81	0.91
1:B:181:LYS:HE2	1:B:181:LYS:N	1.84	0.91
1:A:288:MET:HE2	1:A:288:MET:HA	1.53	0.89
1:B:572:ASN:HB2	1:B:671:ASN:HD21	1.38	0.87
1:B:642:ARG:HH11	1:B:642:ARG:HB2	1.41	0.86
1:B:572:ASN:HB2	1:B:671:ASN:ND2	1.92	0.82
1:B:669:LYS:NZ	1:B:669:LYS:HA	1.96	0.81
1:A:38:TYR:H	1:A:51:ASN:HD21	1.29	0.80
1:A:272:GLN:HE21	1:A:274:LYS:HZ3	1.28	0.80
1:A:580:PHE:H	1:A:637:GLN:HE21	1.29	0.79
1:B:525:GLN:HE22	1:B:620:GLN:H	1.30	0.79
1:A:304:LYS:H	1:B:315:ASN:ND2	1.79	0.79
1:A:553:ASN:ND2	1:A:555:ALA:H	1.81	0.78
1:A:227:VAL:HG12	1:A:244:LYS:HG3	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:MET:HE2	1:A:7:MET:HA	1.66	0.77
1:A:210:LYS:HE2	1:A:210:LYS:HA	1.66	0.77
1:A:642:ARG:HH11	1:A:642:ARG:CB	1.98	0.77
1:B:221:ILE:HD11	1:B:250:ASP:HB2	1.66	0.77
1:A:249:LEU:HD23	1:A:288:MET:HE1	1.66	0.76
1:A:71:SER:OG	1:A:73:THR:HG22	1.86	0.76
8:A:2268:HOH:O	1:B:400:LYS:HD2	1.83	0.76
1:B:525:GLN:NE2	1:B:620:GLN:H	1.84	0.76
1:A:38:TYR:H	1:A:51:ASN:ND2	1.84	0.76
1:B:227:VAL:HG12	1:B:244:LYS:HG3	1.68	0.75
1:B:669:LYS:HA	1:B:669:LYS:HZ1	1.52	0.75
1:A:203:GLU:CD	1:A:203:GLU:H	1.96	0.74
1:A:22:GLN:NE2	1:A:307:GLN:HE22	1.86	0.73
1:B:237:LYS:HE2	1:B:239:ASP:HB3	1.70	0.73
1:B:644:HIS:HB3	8:B:3315:HOH:O	1.87	0.73
1:A:358:TYR:CD2	1:A:359:GLU:HG3	2.24	0.72
1:A:279:GLU:OE1	1:A:374:ILE:HD11	1.89	0.72
1:A:379:LYS:HG3	1:A:381:TYR:CZ	2.25	0.72
1:B:12:LYS:O	1:B:16:GLU:HG2	1.90	0.72
1:A:315:ASN:HD21	1:B:304:LYS:H	1.36	0.71
1:B:334:MET:HE2	1:B:411:GLU:HG3	1.71	0.70
1:B:221:ILE:CD1	1:B:250:ASP:HB2	2.21	0.70
1:B:580:PHE:H	1:B:637:GLN:NE2	1.89	0.69
1:B:8:VAL:HG23	1:B:9:PRO:HD2	1.73	0.69
1:B:94:HIS:HD2	1:B:96:LEU:H	1.39	0.69
1:A:525:GLN:NE2	1:A:620:GLN:H	1.90	0.69
1:A:304:LYS:N	1:B:315:ASN:HD21	1.81	0.69
1:B:540:ASN:HB3	1:B:676:ASN:ND2	2.08	0.68
1:B:699:MET:HE3	1:B:702:GLU:HG3	1.75	0.68
1:A:525:GLN:HE22	1:A:620:GLN:H	1.42	0.68
1:B:94:HIS:CD2	1:B:96:LEU:H	2.12	0.68
1:A:225:LEU:HD22	1:A:381:TYR:CE1	2.29	0.67
1:A:272:GLN:NE2	1:A:274:LYS:HZ3	1.91	0.67
1:A:540:ASN:HB3	1:A:676:ASN:ND2	2.10	0.67
1:A:209:VAL:HG12	1:A:214:ILE:HB	1.77	0.67
1:B:532:LEU:HD11	1:B:683:MET:HE2	1.75	0.66
1:B:699:MET:HE3	1:B:702:GLU:CG	2.26	0.66
1:A:563:MET:HE2	1:B:620:GLN:HB2	1.78	0.65
1:B:366:ILE:HD11	1:B:627:ILE:HD11	1.78	0.65
1:A:286:VAL:HG12	1:A:288:MET:HE3	1.76	0.65
1:B:8:VAL:CG2	1:B:9:PRO:HD2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:LYS:O	1:B:517:HIS:HD2	1.78	0.65
1:A:670:ASP:OD2	1:A:672:GLU:HG3	1.96	0.65
1:A:237:LYS:NZ	1:A:239:ASP:HB3	2.12	0.65
1:A:592:ASN:HD21	1:A:676:ASN:HD21	1.45	0.64
1:B:572:ASN:HD22	1:B:671:ASN:HD21	1.45	0.64
1:B:642:ARG:HH11	1:B:642:ARG:CB	2.11	0.64
1:B:231:ASP:HB2	1:B:626:TRP:CZ2	2.33	0.64
1:A:94:HIS:HB3	1:A:97:ASN:ND2	2.14	0.63
1:A:227:VAL:CG1	1:A:244:LYS:HG3	2.29	0.62
1:A:22:GLN:HE22	1:A:307:GLN:HE22	1.44	0.62
1:A:272:GLN:NE2	1:A:274:LYS:NZ	2.48	0.62
1:A:500:MET:HG3	1:B:599:ASN:ND2	2.15	0.61
1:B:381:TYR:CD2	1:B:466:TYQ:N5	2.66	0.61
1:B:574:GLN:H	1:B:671:ASN:ND2	1.98	0.61
1:A:441:GLN:OE1	1:A:447:ASN:HB2	2.00	0.61
1:B:13:THR:HG22	1:B:75:ILE:HD11	1.83	0.61
1:A:149:PRO:HA	1:A:170:GLN:HE21	1.65	0.60
1:B:387:TYR:CZ	4:B:3001:HY1:HA1	2.35	0.60
1:B:580:PHE:H	1:B:637:GLN:HE21	1.49	0.60
1:A:572:ASN:HD21	1:A:575:ASP:CG	2.09	0.60
1:B:553:ASN:ND2	1:B:555:ALA:H	2.00	0.60
1:A:214:ILE:N	1:A:214:ILE:HD12	2.17	0.59
1:B:382:LEU:N	1:B:382:LEU:HD12	2.18	0.59
1:A:570:ILE:HD13	1:A:578:GLN:HE22	1.67	0.59
1:B:257:TRP:HH2	4:B:3001:HY1:H3	1.67	0.59
1:B:441:GLN:OE1	1:B:447:ASN:HB2	2.02	0.59
1:B:692:ARG:NH1	1:B:694:GLU:HB2	2.16	0.59
1:A:580:PHE:H	1:A:637:GLN:NE2	1.97	0.59
1:B:717:THR:HB	1:B:720:LEU:HG	1.83	0.59
1:B:225:LEU:HD22	1:B:381:TYR:CE1	2.38	0.58
1:B:291:ARG:NH1	1:B:516:ASP:OD2	2.36	0.58
1:B:679:ALA:HB2	8:B:3366:HOH:O	2.03	0.58
1:A:629:HIS:HB2	8:A:2378:HOH:O	2.02	0.58
1:A:326:ARG:HH12	1:B:303:VAL:HG22	1.68	0.58
1:A:73:THR:HG23	1:A:77:ASP:OD2	2.03	0.58
1:A:77:ASP:O	1:A:81:SER:HB3	2.03	0.58
1:A:381:TYR:HD2	1:A:466:TYQ:HN52	1.40	0.58
1:A:12:LYS:O	1:A:16:GLU:HG3	2.04	0.58
1:B:216:ASP:OD1	1:B:218:LYS:HB2	2.03	0.58
1:B:209:VAL:HG12	1:B:214:ILE:HB	1.86	0.58
1:B:173:LYS:NZ	1:B:173:LYS:HB3	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:HD3	8:A:2377:HOH:O	2.04	0.57
1:A:572:ASN:C	1:A:572:ASN:HD22	2.11	0.57
1:A:203:GLU:CD	1:A:203:GLU:N	2.63	0.57
1:A:477:ASN:C	1:A:477:ASN:HD22	2.12	0.56
1:B:173:LYS:HB3	1:B:173:LYS:HZ3	1.71	0.56
1:B:368:PRO:HB2	1:B:621:PHE:CZ	2.41	0.56
1:B:595:ASN:C	1:B:595:ASN:HD22	2.12	0.56
1:A:13:THR:HG22	1:A:75:ILE:HD11	1.88	0.56
1:A:38:TYR:N	1:A:51:ASN:HD21	2.02	0.56
1:A:643:TYR:O	1:A:644:HIS:CD2	2.59	0.56
1:A:276:VAL:O	1:A:277:LYS:HB2	2.05	0.56
1:A:381:TYR:CD2	1:A:466:TYQ:N5	2.67	0.56
1:B:574:GLN:HB2	1:B:671:ASN:CG	2.31	0.56
1:B:203:GLU:CD	1:B:203:GLU:H	2.14	0.56
1:B:366:ILE:HD12	1:B:631:LEU:CD1	2.36	0.56
1:A:532:LEU:HD11	1:A:683:MET:HE2	1.88	0.55
1:A:492:VAL:HB	1:A:519:ILE:HG23	1.88	0.55
1:B:639:TRP:HB2	1:B:682:TRP:HB2	1.87	0.55
1:A:129:LEU:HD12	1:A:130:PRO:HD2	1.87	0.55
1:B:251:VAL:HG12	1:B:251:VAL:O	2.07	0.55
1:A:237:LYS:HZ3	1:A:239:ASP:HB3	1.69	0.55
1:B:379:LYS:HG3	1:B:381:TYR:CZ	2.41	0.54
1:A:288:MET:HA	1:A:288:MET:CE	2.32	0.54
1:A:692:ARG:HG3	1:A:695:GLU:HG3	1.90	0.54
1:B:404:SER:HB2	7:B:3003:GOL:H12	1.88	0.54
1:A:149:PRO:HA	1:A:170:GLN:NE2	2.22	0.54
1:A:664:LEU:HD21	1:A:682:TRP:CD2	2.43	0.54
1:B:59:VAL:HB	1:B:71:SER:HB2	1.89	0.54
1:B:546:MET:HB2	1:B:585:ILE:HB	1.90	0.54
1:B:579:LYS:HA	1:B:637:GLN:NE2	2.22	0.54
1:B:221:ILE:N	1:B:221:ILE:HD12	2.22	0.53
1:A:160:LYS:HB2	8:A:2542:HOH:O	2.09	0.53
1:A:574:GLN:H	1:A:671:ASN:ND2	2.05	0.53
1:B:214:ILE:HD12	1:B:214:ILE:N	2.23	0.53
1:B:617:LYS:HA	8:B:3241:HOH:O	2.08	0.53
1:A:105:LYS:O	1:A:109:GLU:HG3	2.09	0.52
1:B:477:ASN:HD22	1:B:477:ASN:C	2.16	0.52
1:A:94:HIS:HB3	1:A:97:ASN:HD21	1.73	0.52
1:A:498:LYS:NZ	1:A:498:LYS:HB3	2.25	0.52
1:A:382:LEU:HD13	1:A:655:PRO:HB2	1.91	0.52
1:A:482:ILE:HB	1:A:706:THR:OG1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:MET:HG3	1:A:14:LEU:HD23	1.92	0.52
1:A:574:GLN:HG2	1:A:671:ASN:CG	2.34	0.52
1:B:181:LYS:HE3	8:B:3672:HOH:O	2.09	0.52
1:A:326:ARG:HH12	1:B:303:VAL:CG2	2.23	0.52
1:B:543:LEU:HD22	1:B:640:VAL:HG21	1.91	0.52
1:A:163:ILE:N	1:A:163:ILE:HD12	2.25	0.51
1:A:633:PHE:HA	1:A:639:TRP:CZ2	2.45	0.51
1:A:117:PHE:CZ	1:A:121:THR:HB	2.45	0.51
1:A:368:PRO:HB2	1:A:621:PHE:CZ	2.45	0.51
1:B:384:SER:HA	1:B:389:MET:HG3	1.92	0.51
1:B:94:HIS:HB3	1:B:97:ASN:ND2	2.26	0.51
1:A:396:ILE:CD1	1:A:428:ALA:HB2	2.40	0.51
1:A:595:ASN:C	1:A:595:ASN:ND2	2.68	0.51
1:A:162:ILE:C	1:A:163:ILE:HD12	2.36	0.51
1:A:543:LEU:HD22	1:A:640:VAL:HG21	1.92	0.51
1:B:94:HIS:CD2	1:B:96:LEU:HB2	2.46	0.51
1:A:595:ASN:ND2	1:A:599:ASN:H	2.09	0.51
1:B:527:ILE:HD12	1:B:634:MET:HE3	1.93	0.51
8:A:2268:HOH:O	1:B:397:ALA:HB1	2.10	0.50
1:B:129:LEU:HD12	1:B:130:PRO:HD2	1.92	0.50
1:A:366:ILE:HD11	1:A:627:ILE:HD11	1.93	0.50
1:A:595:ASN:C	1:A:595:ASN:HD22	2.19	0.50
1:A:595:ASN:HB2	1:A:715:ASP:OD1	2.12	0.50
1:A:368:PRO:HB2	1:A:621:PHE:HZ	1.75	0.50
1:A:597:MET:SD	1:B:516:ASP:HA	2.52	0.50
1:B:194:SER:O	1:B:198:ILE:HG13	2.11	0.50
1:A:366:ILE:HA	1:A:381:TYR:O	2.11	0.50
1:B:516:ASP:HB3	1:B:519:ILE:HB	1.94	0.50
1:A:639:TRP:HB2	1:A:682:TRP:HB2	1.93	0.50
1:A:231:ASP:HB2	1:A:626:TRP:CZ2	2.46	0.49
1:B:368:PRO:HB2	1:B:621:PHE:HZ	1.77	0.49
1:A:527:ILE:HD12	1:A:634:MET:CE	2.42	0.49
1:A:210:LYS:HE2	1:A:214:ILE:O	2.11	0.49
1:B:100:THR:O	1:B:104:ILE:HG13	2.13	0.49
1:A:326:ARG:NH1	1:B:303:VAL:HG22	2.26	0.49
1:A:366:ILE:HG12	1:A:368:PRO:HD3	1.94	0.49
1:A:403:PRO:HG3	1:A:430:PHE:CD2	2.47	0.49
1:A:439:LYS:NZ	1:A:447:ASN:HD21	2.11	0.49
1:A:42:LYS:HD2	8:A:2468:HOH:O	2.12	0.49
1:A:381:TYR:CD2	4:A:2001:HY1:H	2.48	0.48
1:B:218:LYS:HD2	1:B:218:LYS:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LYS:HE2	8:A:2448:HOH:O	2.12	0.48
1:A:348:ASN:HD22	1:A:348:ASN:C	2.21	0.48
1:B:203:GLU:CD	1:B:203:GLU:N	2.71	0.48
1:A:60:PRO:HD2	8:A:2673:HOH:O	2.13	0.48
1:B:272:GLN:HE21	1:B:274:LYS:HD3	1.77	0.48
1:B:580:PHE:N	1:B:637:GLN:HE21	2.12	0.48
1:A:553:ASN:HD22	1:A:554:THR:N	2.12	0.48
1:A:517:HIS:CE1	1:B:596:ARG:HH11	2.31	0.48
1:A:553:ASN:HD21	1:A:555:ALA:H	1.57	0.48
1:B:36:GLY:HA2	1:B:314:LYS:HE2	1.95	0.48
1:B:492:VAL:HB	1:B:519:ILE:HG23	1.96	0.48
1:A:370:GLY:HA2	1:B:559:ARG:HH22	1.79	0.47
1:B:227:VAL:CG1	1:B:244:LYS:HG3	2.40	0.47
1:B:587:LEU:HD23	1:B:604:GLN:HA	1.96	0.47
1:B:595:ASN:C	1:B:595:ASN:ND2	2.66	0.47
1:B:209:VAL:CG1	1:B:214:ILE:HB	2.44	0.47
1:B:572:ASN:CB	1:B:671:ASN:HD21	2.19	0.47
1:A:160:LYS:NZ	1:A:239:ASP:OD1	2.45	0.47
1:B:105:LYS:O	1:B:109:GLU:HG3	2.14	0.47
1:B:118:LYS:HB2	1:B:121:THR:OG1	2.15	0.47
1:A:64:LYS:O	1:A:65:ASP:HB3	2.14	0.47
1:A:32:LEU:HB2	1:A:39:VAL:HB	1.96	0.47
1:B:196:GLN:HE22	1:B:222:THR:H	1.61	0.47
1:B:466:TYQ:HN51	4:B:3001:HY1:C	2.27	0.47
1:A:7:MET:CE	1:A:71:SER:HA	2.44	0.47
1:A:467:ASP:HB2	1:A:487:THR:HG23	1.97	0.47
1:B:7:MET:HE3	1:B:70:VAL:C	2.40	0.47
1:B:439:LYS:NZ	1:B:447:ASN:HD21	2.13	0.47
1:A:439:LYS:HZ1	1:A:447:ASN:ND2	2.13	0.46
1:A:192:PHE:CE2	4:A:2001:HY1:H5	2.51	0.46
1:B:332:LEU:HD13	1:B:342:ILE:HD13	1.96	0.46
1:B:595:ASN:ND2	1:B:597:MET:H	2.14	0.46
1:A:438:TYR:CD1	1:B:698:ILE:HD13	2.50	0.46
1:A:546:MET:HE3	8:A:2534:HOH:O	2.15	0.46
1:B:277:LYS:HE2	1:B:279:GLU:HG2	1.97	0.46
1:A:529:ASN:HD21	1:A:682:TRP:HE3	1.61	0.46
1:A:510:ARG:HG3	1:A:510:ARG:HH11	1.80	0.46
1:B:382:LEU:HD22	1:B:655:PRO:HB2	1.97	0.46
1:A:396:ILE:HG23	1:A:401:ASP:HB2	1.98	0.46
1:B:572:ASN:ND2	1:B:671:ASN:HD21	2.13	0.46
1:B:579:LYS:HA	1:B:637:GLN:HE22	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:LYS:NZ	1:A:447:ASN:ND2	2.64	0.45
1:B:160:LYS:HE3	1:B:239:ASP:OD1	2.16	0.45
1:A:581:ASP:HB3	1:A:584:THR:HG23	1.97	0.45
1:A:572:ASN:HB2	1:A:671:ASN:ND2	2.32	0.45
1:A:466:TYQ:N5	4:A:2001:HY1:H	2.32	0.45
1:A:572:ASN:CG	1:A:671:ASN:HD21	2.24	0.45
1:B:291:ARG:HG3	1:B:291:ARG:HH11	1.82	0.45
1:A:382:LEU:CD1	1:A:655:PRO:HB2	2.47	0.45
1:B:359:GLU:CD	1:B:648:ARG:HH22	2.24	0.45
1:B:549:VAL:HG11	1:B:566:ASN:ND2	2.32	0.45
1:B:580:PHE:CD2	1:B:607:PRO:HD2	2.52	0.45
1:A:433:TYR:CE2	1:B:403:PRO:HD3	2.52	0.45
1:B:573:GLU:HA	1:B:674:LEU:HD11	1.99	0.45
1:A:608:TYR:HE2	1:B:608:TYR:HE2	1.64	0.45
1:B:207:ALA:O	1:B:211:LYS:HG2	2.16	0.45
1:B:632:SER:HB3	8:B:3243:HOH:O	2.16	0.45
1:A:192:PHE:HE2	4:A:2001:HY1:H5	1.81	0.45
1:B:196:GLN:NE2	1:B:222:THR:H	2.15	0.45
1:A:222:THR:HB	1:A:245:VAL:CG1	2.46	0.44
1:A:331:HIS:HE1	1:A:333:SER:HB3	1.82	0.44
1:B:251:VAL:O	1:B:251:VAL:CG1	2.64	0.44
1:B:410:ASN:OD1	1:B:424:PRO:HA	2.17	0.44
1:A:642:ARG:HH11	1:A:642:ARG:CG	2.31	0.44
1:A:459:TRP:CZ2	1:A:461:SER:HB2	2.52	0.44
1:A:225:LEU:HD22	1:A:381:TYR:CZ	2.52	0.44
1:B:143:ASN:OD1	1:B:143:ASN:O	2.36	0.44
1:B:212:ARG:NH1	1:B:283:VAL:HA	2.33	0.44
1:B:439:LYS:HZ1	1:B:447:ASN:ND2	2.16	0.44
1:B:549:VAL:HG11	1:B:566:ASN:HD22	1.82	0.44
1:B:592:ASN:HD21	1:B:676:ASN:HD21	1.65	0.44
1:A:437:GLU:OE2	1:B:700:PRO:HB3	2.17	0.44
1:B:8:VAL:CG2	1:B:9:PRO:CD	2.96	0.44
1:B:580:PHE:N	1:B:637:GLN:NE2	2.64	0.44
1:A:209:VAL:CG1	1:A:214:ILE:HB	2.46	0.44
1:A:227:VAL:HG12	1:A:244:LYS:CG	2.42	0.44
1:B:595:ASN:HB2	1:B:715:ASP:OD1	2.18	0.44
1:A:181:LYS:HG3	1:A:182:ASP:OD2	2.18	0.43
1:A:611:GLY:HA3	8:A:2221:HOH:O	2.18	0.43
1:A:698:ILE:HD13	1:B:438:TYR:CD1	2.53	0.43
1:A:539:GLU:HB2	8:A:2438:HOH:O	2.18	0.43
1:A:132:ASP:OD2	1:A:148:GLN:OE1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ASN:HA	8:A:2358:HOH:O	2.18	0.43
1:B:506:LYS:HE2	1:B:510:ARG:HH12	1.83	0.43
1:A:324:HIS:HD2	1:A:329:ASP:OD1	2.01	0.43
1:A:396:ILE:HD12	1:A:428:ALA:HB2	2.01	0.43
1:B:139:PHE:O	1:B:143:ASN:HA	2.19	0.43
1:A:10:MET:HG3	1:A:14:LEU:CD2	2.49	0.43
1:A:559:ARG:NH2	1:B:621:PHE:HE1	2.16	0.43
1:B:238:GLN:HE21	1:B:238:GLN:HA	1.83	0.43
1:B:482:ILE:HB	1:B:706:THR:OG1	2.19	0.43
1:B:585:ILE:HD13	1:B:711:TRP:CH2	2.52	0.43
1:A:234:ASP:OD2	1:A:236:LEU:HD12	2.19	0.43
1:B:396:ILE:HG23	1:B:401:ASP:HB2	1.99	0.43
1:A:205:PHE:O	1:A:209:VAL:HG23	2.19	0.43
1:B:637:GLN:HA	1:B:684:THR:HB	2.01	0.43
1:A:225:LEU:HD12	1:A:246:ILE:HG12	2.01	0.43
1:A:695:GLU:HB3	1:A:699:MET:HG3	2.01	0.43
1:B:229:TYR:HB3	1:B:630:ARG:HD2	2.00	0.43
1:B:465:ASN:HD21	1:B:466:TYQ:CE1	2.32	0.43
1:A:628:TYR:CD1	1:A:628:TYR:C	2.97	0.43
1:B:139:PHE:CD1	1:B:139:PHE:C	2.97	0.43
1:B:642:ARG:HH11	1:B:642:ARG:CG	2.32	0.43
1:A:445:GLN:HE21	1:A:446:PRO:HD3	1.84	0.42
1:A:574:GLN:HG2	1:A:671:ASN:CB	2.49	0.42
1:B:516:ASP:OD1	1:B:517:HIS:N	2.52	0.42
1:B:619:ALA:CB	1:B:634:MET:HE2	2.49	0.42
1:B:696:TRP:CD2	1:B:697:PRO:HA	2.55	0.42
1:A:498:LYS:HB3	1:A:498:LYS:HZ2	1.84	0.42
1:B:366:ILE:HA	1:B:381:TYR:O	2.20	0.42
1:A:381:TYR:CG	4:A:2001:HY1:H	2.54	0.42
1:A:527:ILE:HD12	1:A:634:MET:HE2	2.00	0.42
1:B:332:LEU:HD13	1:B:342:ILE:CD1	2.50	0.42
1:B:611:GLY:HA3	8:B:3246:HOH:O	2.20	0.42
1:A:61:VAL:HG22	1:A:70:VAL:HG12	2.01	0.42
1:A:130:PRO:HB3	8:A:2298:HOH:O	2.18	0.42
1:A:152:ALA:HB2	1:A:169:LEU:HD11	2.01	0.42
1:A:439:LYS:HZ2	1:A:447:ASN:HD21	1.67	0.42
1:A:572:ASN:C	1:A:572:ASN:ND2	2.75	0.42
1:B:202:SER:OG	1:B:275:ILE:HD12	2.20	0.42
1:A:139:PHE:CD1	1:A:139:PHE:C	2.97	0.42
1:A:214:ILE:N	1:A:214:ILE:CD1	2.82	0.42
1:A:92:ARG:HA	1:A:93:PRO:HD2	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:THR:HB	1:A:245:VAL:HG13	2.02	0.42
1:A:437:GLU:O	1:B:700:PRO:HA	2.20	0.42
1:B:106:GLN:O	1:B:110:ILE:HG13	2.20	0.42
1:A:144:LYS:HA	1:A:145:PRO:HD3	1.92	0.42
1:A:447:ASN:CG	1:A:448:VAL:N	2.78	0.42
1:A:300:ALA:HA	1:A:301:PRO:HD3	1.88	0.42
1:A:366:ILE:CD1	1:A:627:ILE:HD11	2.50	0.42
1:B:403:PRO:HG3	1:B:430:PHE:CD2	2.54	0.42
1:B:381:TYR:CG	4:B:3001:HY1:H	2.55	0.41
1:B:506:LYS:HD3	1:B:506:LYS:C	2.44	0.41
1:A:212:ARG:NH1	1:A:283:VAL:HA	2.35	0.41
1:B:94:HIS:HD2	1:B:96:LEU:HB2	1.85	0.41
1:B:222:THR:HB	1:B:245:VAL:HG13	2.01	0.41
1:A:7:MET:HE1	1:A:71:SER:HA	2.02	0.41
1:A:553:ASN:ND2	1:A:553:ASN:C	2.78	0.41
1:A:582:PRO:C	1:B:615:VAL:HG12	2.45	0.41
1:B:130:PRO:HA	1:B:131:PRO:HD3	1.81	0.41
1:B:238:GLN:HA	1:B:238:GLN:NE2	2.35	0.41
1:B:462:THR:HG23	1:B:466:TYQ:O	2.20	0.41
1:A:379:LYS:HE2	1:A:381:TYR:OH	2.21	0.41
1:A:384:SER:HA	1:A:389:MET:HG3	2.03	0.41
1:A:608:TYR:CZ	1:A:615:VAL:HG21	2.55	0.41
1:A:465:ASN:HB2	1:A:489:ILE:O	2.21	0.41
1:B:637:GLN:HE21	1:B:637:GLN:HB2	1.68	0.41
1:A:546:MET:HB2	1:A:585:ILE:HB	2.02	0.41
1:A:700:PRO:HB3	1:B:437:GLU:OE2	2.21	0.41
1:B:15:LYS:HE2	8:B:3496:HOH:O	2.21	0.41
1:A:51:ASN:N	1:A:51:ASN:HD22	2.17	0.41
1:A:257:TRP:HH2	4:A:2001:HY1:H3	1.86	0.41
1:A:366:ILE:HD11	1:A:380:ALA:HB1	2.02	0.41
1:A:460:ILE:HG21	1:B:439:LYS:HE2	2.03	0.41
1:A:595:ASN:HD21	1:A:599:ASN:H	1.69	0.41
1:A:664:LEU:HD21	1:A:682:TRP:CE2	2.55	0.41
1:B:223:THR:HA	1:B:224:PRO:HD3	1.83	0.41
1:B:627:ILE:HG23	1:B:628:TYR:N	2.36	0.41
1:A:396:ILE:HD13	1:A:428:ALA:HB2	2.02	0.41
1:A:477:ASN:HD22	1:A:479:THR:H	1.69	0.41
1:A:581:ASP:C	1:A:583:GLY:H	2.28	0.41
1:A:22:GLN:NE2	1:A:307:GLN:NE2	2.62	0.40
1:A:369:TYR:CD1	1:A:379:LYS:HG2	2.56	0.40
1:A:679:ALA:HB2	8:A:2694:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:TYR:H	1:B:51:ASN:ND2	2.19	0.40
1:B:97:ASN:ND2	1:B:331:HIS:NE2	2.70	0.40
1:A:168:ASP:HB3	1:A:173:LYS:HG2	2.03	0.40
1:B:67:LYS:HE2	1:B:67:LYS:HB3	1.86	0.40
1:B:95:PRO:HB3	1:B:146:VAL:HG21	2.03	0.40
1:A:129:LEU:HD12	1:A:130:PRO:CD	2.51	0.40
1:A:237:LYS:HZ2	1:A:239:ASP:HB3	1.85	0.40
1:A:223:THR:HA	1:A:224:PRO:HD3	1.95	0.40
1:A:479:THR:HG22	1:A:480:ILE:N	2.35	0.40
1:B:32:LEU:HB2	1:B:39:VAL:HB	2.04	0.40
1:B:192:PHE:HE2	4:B:3001:HY1:H5	1.87	0.40
1:B:263:ASN:HA	1:B:374:ILE:HD11	2.03	0.40
1:A:95:PRO:HB3	1:A:146:VAL:HG21	2.03	0.40
1:A:199:ILE:HG23	1:A:205:PHE:CD2	2.57	0.40
1:B:9:PRO:HB2	8:B:3583:HOH:O	2.20	0.40
1:B:92:ARG:HA	1:B:93:PRO:HD2	1.85	0.40
1:B:221:ILE:HD13	1:B:250:ASP:HB2	2.03	0.40
1:B:526:HIS:O	1:B:686:GLY:HA2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	715/727 (98%)	689 (96%)	25 (4%)	1 (0%)	48	64
1	B	717/727 (99%)	692 (96%)	25 (4%)	0	100	100
All	All	1432/1454 (98%)	1381 (96%)	50 (4%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	LYS

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	609/615 (99%)	596 (98%)	13 (2%)	47	69
1	B	611/615 (99%)	599 (98%)	12 (2%)	48	70
All	All	1220/1230 (99%)	1195 (98%)	25 (2%)	48	70

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	80	GLN
1	A	199	ILE
1	A	203	GLU
1	A	210	LYS
1	A	214	ILE
1	A	288	MET
1	A	368	PRO
1	A	477	ASN
1	A	572	ASN
1	A	595	ASN
1	A	613	HIS
1	A	642	ARG
1	B	11	ASP
1	B	137	TRP
1	B	173	LYS
1	B	181	LYS
1	B	203	GLU
1	B	368	PRO
1	B	477	ASN
1	B	539	GLU
1	B	595	ASN
1	B	637	GLN

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Mol	Chain	Res	Type
1	B	642	ARG
1	B	669	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	51	ASN
1	A	53	GLN
1	A	97	ASN
1	A	120	ASN
1	A	143	ASN
1	A	148	GLN
1	A	170	GLN
1	A	178	GLN
1	A	196	GLN
1	A	200	ASN
1	A	201	ASN
1	A	263	ASN
1	A	272	GLN
1	A	307	GLN
1	A	315	ASN
1	A	324	HIS
1	A	327	ASN
1	A	348	ASN
1	A	445	GLN
1	A	447	ASN
1	A	477	ASN
1	A	517	HIS
1	A	525	GLN
1	A	529	ASN
1	A	540	ASN
1	A	541	ASN
1	A	553	ASN
1	A	564	GLN
1	A	567	GLN
1	A	572	ASN
1	A	595	ASN
1	A	599	ASN
1	A	637	GLN
1	A	660	HIS
1	A	666	GLN

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Mol	Chain	Res	Type
1	A	671	ASN
1	A	676	ASN
1	B	51	ASN
1	B	94	HIS
1	B	97	ASN
1	B	143	ASN
1	B	148	GLN
1	B	172	ASN
1	B	196	GLN
1	B	200	ASN
1	B	201	ASN
1	B	238	GLN
1	B	272	GLN
1	B	315	ASN
1	B	327	ASN
1	B	350	ASN
1	B	447	ASN
1	B	477	ASN
1	B	517	HIS
1	B	525	GLN
1	B	529	ASN
1	B	540	ASN
1	B	541	ASN
1	B	553	ASN
1	B	566	ASN
1	B	567	GLN
1	B	572	ASN
1	B	595	ASN
1	B	599	ASN
1	B	637	GLN
1	B	671	ASN
1	B	676	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	TYQ	A	466	1	13,14,15	1.21	2 (15%)	13,19,21	0.70	0
1	TYQ	B	466	1	13,14,15	1.03	1 (7%)	13,19,21	0.77	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
1	TYQ	A	466	1	-	0/5/6/8	0/1/1/1
1	TYQ	B	466	1	-	2/5/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	TYQ	CE2-N5	2.55	1.46	1.38
1	A	466	TYQ	CE2-CZ	-2.48	1.38	1.40
1	B	466	TYQ	CE2-N5	2.39	1.45	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	466	TYQ	O-C-CA-CB
1	B	466	TYQ	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	466	TYQ	3	0
1	B	466	TYQ	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	$\# Z > 2$
7	GOL	B	2004	-	5,5,5	0.48	0	5,5,5	0.60	0
4	HY1	A	2001	-	8,9,9	1.79	2 (25%)	10,10,10	0.72	0
5	NO	B	3002	2	0,1,1	-	-	-	-	-
4	HY1	B	3001	-	8,9,9	1.43	2 (25%)	10,10,10	0.80	1 (10%)
6	PEA	A	2003	-	9,9,9	1.35	1 (11%)	10,10,10	0.65	0
7	GOL	B	3003	-	5,5,5	0.40	0	5,5,5	0.44	0
5	NO	A	2002	-	0,1,1	-	-	-	-	-

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
7	GOL	B	2004	-	-	2/4/4/4	-
4	HY1	A	2001	-	-	0/3/3/3	0/1/1/1
4	HY1	B	3001	-	-	0/3/3/3	0/1/1/1
6	PEA	A	2003	-	-	1/3/3/3	0/1/1/1
7	GOL	B	3003	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2001	HY1	C3'-C2'	3.37	1.44	1.38
4	A	2001	HY1	C5'-C6'	2.61	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3001	HY1	C3'-C2'	2.51	1.43	1.38
6	A	2003	PEA	C3'-C2'	2.33	1.42	1.38
4	B	3001	HY1	C5'-C6'	2.14	1.42	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3001	HY1	C1'-CA-C	-2.13	109.24	113.92

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2003	PEA	N-C1-C2-C1'
7	B	2004	GOL	C1-C2-C3-O3
7	B	2004	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	HY1	6	0
4	B	3001	HY1	5	0
7	B	3003	GOL	1	0

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	717/727 (98%)	-0.35	6 (0%) 82 80	22, 37, 59, 82	0
1	B	719/727 (98%)	-0.24	8 (1%) 78 74	26, 41, 63, 74	0
All	All	1436/1454 (98%)	-0.29	14 (0%) 79 76	22, 39, 62, 82	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	644	HIS	3.4
1	B	644	HIS	3.0
1	B	119	PRO	2.9
1	B	301	PRO	2.9
1	B	302	ALA	2.9
1	B	539	GLU	2.7
1	A	72	ASP	2.6
1	A	670	ASP	2.5
1	B	669	LYS	2.4
1	B	322	MET	2.3
1	A	381	TYR	2.3
1	A	132	ASP	2.2
1	A	148	GLN	2.1
1	B	115	ALA	2.1

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	TYQ	A	466	14/15	0.86	0.17	39,53,58,61	0
1	TYQ	B	466	14/15	0.87	0.15	36,55,61,63	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
4	HY1	A	2001	9/9	0.76	0.16	54,55,57,60	0
4	HY1	B	3001	9/9	0.77	0.15	52,54,62,67	0
7	GOL	B	2004	6/6	0.80	0.15	58,60,61,61	0
7	GOL	B	3003	6/6	0.84	0.16	56,57,57,58	0
3	CA	A	803	1/1	0.89	0.12	72,72,72,72	0
6	PEA	A	2003	9/9	0.89	0.10	35,37,38,39	0
5	NO	A	2002	2/2	0.90	0.21	60,60,60,60	0
5	NO	B	3002	2/2	0.93	0.11	48,48,48,49	0
3	CA	B	803	1/1	0.95	0.11	74,74,74,74	0
2	CU	A	801	1/1	0.99	0.02	43,43,43,43	0
3	CA	B	802	1/1	1.00	0.02	39,39,39,39	0
3	CA	A	802	1/1	1.00	0.04	33,33,33,33	0
2	CU	B	801	1/1	1.00	0.03	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.