



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:37 AM GMT

PDB ID : 3LPF
Title : Structure of E. coli beta-Glucuronidase bound with a novel, potent inhibitor
1-((6,7-dimethyl-2-oxo-1,2-dihydroquinolin-3-yl)methyl)-1-(2-hydroxyethyl)-3
-(3-methoxyphenyl)thiourea
Authors : Wallace, B.D.; Redinbo, M.R.
Deposited on : 2010-02-05
Resolution : 2.26 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

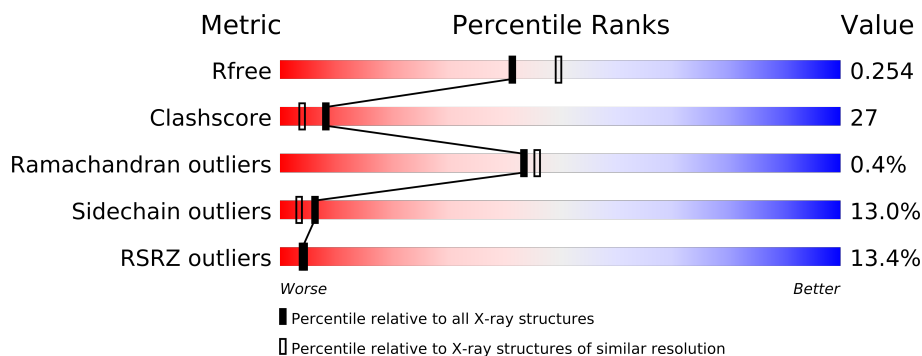
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.26 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}	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	605	
1	B	605	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 10100 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

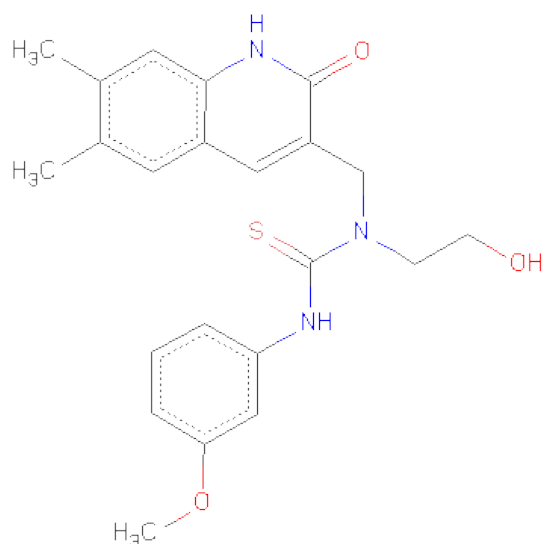
- Molecule 1 is a protein called Beta-glucuronidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	603	Total	C	N	O	S	Se	0	0	0
			4822	3060	833	907	9	13			
1	B	603	Total	C	N	O	S	Se	0	0	0
			4822	3060	833	907	9	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP P05804
A	0	HIS	-	EXPRESSION TAG	UNP P05804
B	-1	SER	-	EXPRESSION TAG	UNP P05804
B	0	HIS	-	EXPRESSION TAG	UNP P05804

- Molecule 2 is 1-[(6,7-DIMETHYL-2-OXO-1,2-DIHYDROQUINOLIN-3-YL)METHYL]-1-(2-HYDROXYETHYL)-3-(3-METHOXYPHENYL)THIOUREA (three-letter code: Z77) (formula: C₂₂H₂₅N₃O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			29	22	3	3	1		
2	B	1	Total	C	N	O	S	0	0
			29	22	3	3	1		

- Molecule 3 is water.

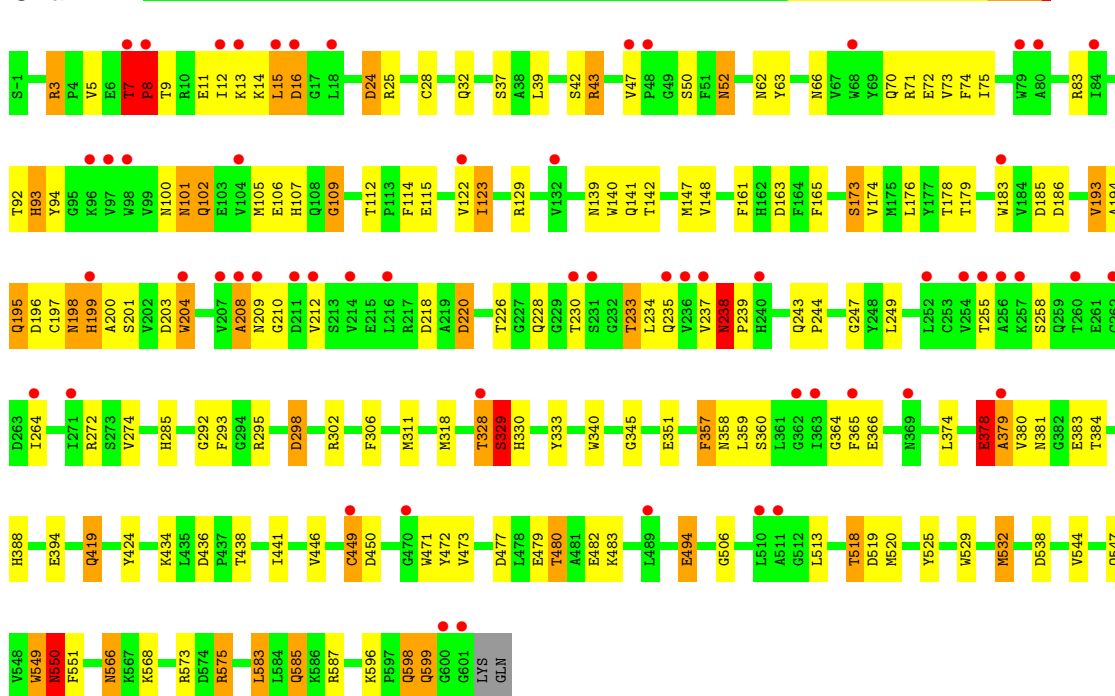
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	269	Total	O	0	0
			269	269		
3	B	129	Total	O	0	0
			129	129		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

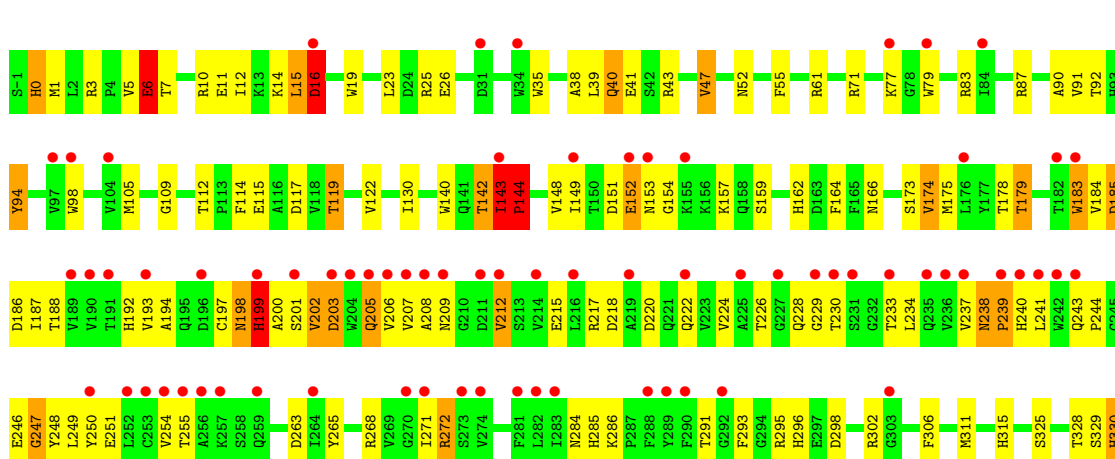
• Molecule 1: Beta-glucuronidase

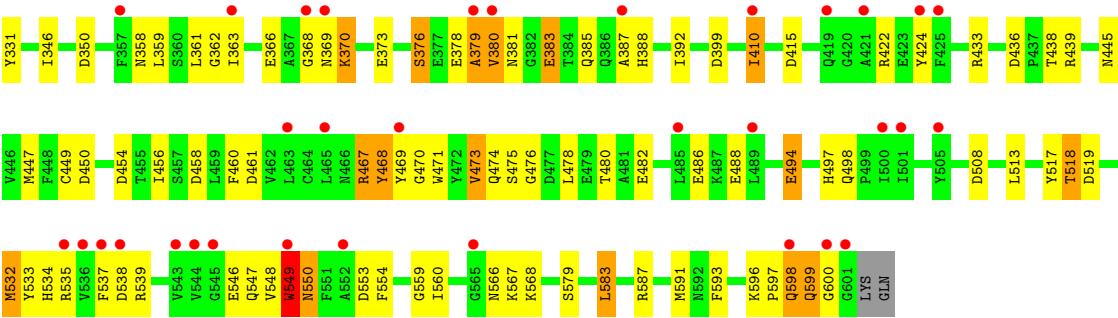
Chain A:



• Molecule 1: Beta-glucuronidase

Chain B:





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.06Å 77.41Å 126.15Å 90.00° 124.66° 90.00°	Depositor
Resolution (Å)	50.00 – 2.26 48.11 – 2.26	Depositor EDS
% Data completeness (in resolution range)	94.6 (50.00-2.26) 94.4 (48.11-2.26)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.88 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.209 , 0.249 0.215 , 0.254	Depositor DCC
R_{free} test set	2976 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 100.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 59263 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Z77

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	0.60	0/4939	1.05	41/6700 (0.6%)
1	B	0.54	2/4939 (0.0%)	0.98	35/6700 (0.5%)
All	All	0.57	2/9878 (0.0%)	1.02	76/13400 (0.6%)

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	6
1	B	0	2
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	239	PRO	N-CD	-7.47	1.37	1.47
1	B	144	PRO	N-CD	6.81	1.57	1.47

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	549	TRP	CB-CA-C	17.72	145.84	110.40
1	A	329	SER	CB-CA-C	14.82	138.26	110.10
1	A	379	ALA	N-CA-C	11.13	141.06	111.00
1	A	208	ALA	CB-CA-C	-10.96	93.66	110.10
1	B	549	TRP	N-CA-C	-10.54	82.55	111.00
1	A	449	CYS	N-CA-C	-9.89	84.29	111.00
1	A	358	ASN	N-CA-CB	-9.33	93.80	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	PRO	CB-CA-C	8.72	133.80	112.00
1	B	363	ILE	CB-CA-C	-8.69	94.23	111.60
1	A	209	ASN	N-CA-CB	8.67	126.21	110.60
1	A	24	ASP	N-CA-C	-8.56	87.89	111.00
1	A	329	SER	N-CA-C	-8.31	88.57	111.00
1	B	554	PHE	N-CA-CB	-8.30	95.67	110.60
1	A	549	TRP	C-N-CA	-8.12	101.40	121.70
1	B	379	ALA	N-CA-C	8.01	132.62	111.00
1	B	239	PRO	N-CA-CB	-7.95	93.77	103.30
1	A	8	PRO	N-CA-C	-7.86	91.67	112.10
1	B	583	LEU	CA-CB-CG	7.75	133.12	115.30
1	B	90	ALA	CB-CA-C	7.67	121.60	110.10
1	A	93	HIS	CB-CA-C	7.64	125.67	110.40
1	A	583	LEU	CA-CB-CG	7.41	132.34	115.30
1	A	378	GLU	CB-CA-C	7.39	125.18	110.40
1	A	598	GLN	CB-CA-C	-7.32	95.76	110.40
1	B	143	ILE	N-CA-C	7.22	130.49	111.00
1	B	468	TYR	N-CA-C	-7.18	91.61	111.00
1	B	471	TRP	N-CA-C	7.17	130.37	111.00
1	A	7	THR	N-CA-C	7.17	130.37	111.00
1	A	450	ASP	N-CA-CB	7.12	123.42	110.60
1	A	328	THR	N-CA-C	-7.02	92.06	111.00
1	B	16	ASP	N-CA-C	-6.96	92.22	111.00
1	A	379	ALA	CB-CA-C	-6.85	99.83	110.10
1	B	379	ALA	N-CA-CB	-6.80	100.58	110.10
1	A	209	ASN	N-CA-C	6.76	129.26	111.00
1	B	380	VAL	N-CA-C	-6.74	92.80	111.00
1	B	154	GLY	N-CA-C	6.34	128.94	113.10
1	B	109	GLY	N-CA-C	-6.20	97.60	113.10
1	A	101	ASN	CB-CA-C	-6.20	98.01	110.40
1	A	199	HIS	N-CA-C	6.13	127.55	111.00
1	B	379	ALA	CB-CA-C	-6.10	100.94	110.10
1	B	449	CYS	N-CA-C	-6.09	94.55	111.00
1	A	94	TYR	N-CA-CB	-6.06	99.69	110.60
1	A	16	ASP	N-CA-C	-6.05	94.66	111.00
1	A	109	GLY	N-CA-C	-6.05	97.97	113.10
1	A	520	MSE	N-CA-C	6.03	127.29	111.00
1	B	6	GLU	N-CA-C	5.99	127.17	111.00
1	A	575	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	471	TRP	N-CA-C	5.91	126.95	111.00
1	A	472	TYR	N-CA-CB	5.80	121.04	110.60
1	A	102	GLN	N-CA-CB	5.80	121.03	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	554	PHE	N-CA-C	5.79	126.64	111.00
1	B	246	GLU	N-CA-C	5.74	126.49	111.00
1	B	247	GLY	N-CA-C	5.67	127.28	113.10
1	A	379	ALA	N-CA-CB	-5.67	102.16	110.10
1	B	239	PRO	N-CD-CG	-5.65	94.73	103.20
1	A	209	ASN	CB-CA-C	-5.62	99.16	110.40
1	A	550	ASN	N-CA-C	5.62	126.16	111.00
1	A	293	PHE	N-CA-CB	-5.60	100.51	110.60
1	B	358	ASN	N-CA-CB	-5.57	100.57	110.60
1	B	239	PRO	N-CA-C	5.55	126.54	112.10
1	A	380	VAL	N-CA-C	-5.53	96.08	111.00
1	A	365	PHE	N-CA-C	5.50	125.85	111.00
1	A	50	SER	N-CA-C	-5.43	96.35	111.00
1	B	376	SER	CB-CA-C	5.41	120.37	110.10
1	B	549	TRP	N-CA-CB	5.36	120.24	110.60
1	A	210	GLY	N-CA-C	5.26	126.25	113.10
1	A	357	PHE	CB-CA-C	5.24	120.88	110.40
1	B	560	ILE	CB-CA-C	-5.24	101.12	111.60
1	A	380	VAL	N-CA-CB	5.22	123.00	111.50
1	B	144	PRO	N-CD-CG	-5.20	95.40	103.20
1	A	25	ARG	N-CA-CB	5.17	119.90	110.60
1	B	550	ASN	N-CA-CB	5.17	119.90	110.60
1	B	246	GLU	CB-CA-C	-5.12	100.16	110.40
1	B	91	VAL	N-CA-CB	5.10	122.72	111.50
1	B	549	TRP	CA-C-N	-5.09	105.99	117.20
1	B	199	HIS	N-CA-C	5.06	124.67	111.00
1	B	92	THR	CA-C-N	-5.02	106.15	117.20

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	GLN	Peptide
1	A	238	ASN	Peptide
1	A	329	SER	Peptide
1	A	364	GLY	Peptide
1	A	519	ASP	Peptide
1	A	92	THR	Peptide
1	B	143	ILE	Peptide
1	B	549	TRP	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4822	0	0	101	1
1	B	4822	0	0	156	1
2	A	29	0	0	1	0
2	B	29	0	0	3	0
3	A	269	0	0	35	0
3	B	129	0	0	30	0
All	All	10100	0	0	258	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (258) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:598:GLN:CG	1:A:598:GLN:O	1.82	1.18
1:B:151:ASP:OD1	1:B:153:ASN:O	1.71	1.06
1:B:534:HIS:ND1	3:B:619:HOH:O	1.90	1.02
1:A:7:THR:O	3:A:853:HOH:O	1.80	0.99
1:A:247:GLY:O	1:A:249:LEU:CD1	2.13	0.97
1:B:186:ASP:N	3:B:728:HOH:O	1.97	0.97
1:A:3:ARG:NH2	3:A:872:HOH:O	1.96	0.96
1:A:9:THR:OG1	3:A:852:HOH:O	1.84	0.94
1:A:596:LYS:N	3:A:771:HOH:O	1.99	0.94
1:A:318:MSE:SE	3:A:791:HOH:O	2.34	0.94
1:B:548:VAL:CG1	1:B:549:TRP:O	2.17	0.92
1:B:207:VAL:CG1	1:B:208:ALA:O	2.19	0.90
1:B:238:ASN:CG	1:B:238:ASN:O	2.10	0.89
1:A:199:HIS:ND1	1:A:200:ALA:N	2.21	0.88
1:B:598:GLN:CG	1:B:598:GLN:O	2.22	0.87
1:B:23:LEU:N	3:B:633:HOH:O	2.05	0.87
1:A:306:PHE:O	3:A:868:HOH:O	1.91	0.87
1:B:298:ASP:OD2	3:B:717:HOH:O	1.94	0.86
1:B:415:ASP:OD2	3:B:729:HOH:O	1.94	0.82
1:B:25:ARG:N	3:B:720:HOH:O	2.11	0.82
1:A:24:ASP:O	1:A:63:TYR:OH	1.98	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:72:GLU:OE1	3:A:857:HOH:O	1.98	0.81
1:A:550:ASN:N	3:A:832:HOH:O	2.11	0.81
1:B:203:ASP:OD1	1:B:233:THR:OG1	1.99	0.81
1:A:7:THR:O	3:A:834:HOH:O	1.98	0.81
1:A:479:GLU:OE1	3:A:784:HOH:O	1.97	0.80
1:B:184:VAL:CG1	3:B:728:HOH:O	2.30	0.80
1:A:228:GLN:N	3:A:811:HOH:O	2.14	0.79
1:B:579:SER:O	3:B:724:HOH:O	2.00	0.79
1:B:366:GLU:OE1	3:B:626:HOH:O	1.99	0.79
1:A:62:ASN:ND2	3:A:701:HOH:O	2.17	0.78
1:A:203:ASP:OD2	1:A:233:THR:OG1	2.00	0.78
1:B:212:VAL:CG2	1:B:229:GLY:O	2.31	0.78
1:B:140:TRP:CE3	1:B:379:ALA:O	2.38	0.76
1:A:83:ARG:N	3:A:808:HOH:O	2.19	0.75
1:B:205:GLN:NE2	1:B:206:VAL:O	2.20	0.75
1:B:378:GLU:O	3:B:709:HOH:O	2.06	0.74
1:B:185:ASP:N	3:B:728:HOH:O	2.20	0.73
1:A:243:GLN:OE1	3:A:819:HOH:O	2.06	0.73
1:B:7:THR:OG1	3:B:707:HOH:O	2.06	0.73
1:B:83:ARG:NH1	1:B:183:TRP:CZ3	2.57	0.72
1:A:15:LEU:CD2	1:A:15:LEU:O	2.37	0.72
1:B:517:TYR:OH	3:B:651:HOH:O	2.07	0.72
1:A:165:PHE:O	3:A:666:HOH:O	2.07	0.72
1:B:362:GLY:CA	3:B:733:HOH:O	2.39	0.71
1:A:208:ALA:C	3:A:839:HOH:O	2.30	0.70
1:B:306:PHE:CZ	1:B:311:MSE:CE	2.75	0.70
1:A:105:MSE:CE	1:A:115:GLU:CA	2.69	0.70
1:B:1:MSE:CE	1:B:87:ARG:NH1	2.54	0.70
1:A:198:ASN:OD1	1:A:237:VAL:O	2.10	0.70
1:B:205:GLN:OE1	1:B:207:VAL:CG2	2.39	0.70
1:A:37:SER:O	3:A:795:HOH:O	2.09	0.70
1:B:166:ASN:O	3:B:608:HOH:O	2.09	0.69
2:A:604:Z77:SAF	2:A:604:Z77:CAJ	2.80	0.68
1:A:8:PRO:CA	3:A:853:HOH:O	2.41	0.68
1:A:195:GLN:OE1	1:A:195:GLN:N	2.27	0.68
1:B:205:GLN:CD	1:B:207:VAL:CG2	2.62	0.68
1:A:482:GLU:OE2	3:A:724:HOH:O	2.12	0.68
1:A:140:TRP:CE3	1:A:379:ALA:O	2.47	0.67
1:B:368:GLY:O	1:B:370:LYS:CB	2.41	0.67
1:B:10:ARG:NH2	1:B:79:TRP:NE1	2.42	0.67
1:B:447:MSE:CE	1:B:468:TYR:O	2.43	0.66
1:B:547:GLN:CB	3:B:606:HOH:O	2.44	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:238:ASN:O	3:B:701:HOH:O	2.13	0.66
1:B:143:ILE:CG2	1:B:143:ILE:O	2.43	0.66
1:A:419:GLN:O	3:A:810:HOH:O	2.13	0.66
1:A:436:ASP:O	3:A:688:HOH:O	2.14	0.66
1:A:585:GLN:CG	3:A:636:HOH:O	2.43	0.66
1:A:112:THR:O	3:A:628:HOH:O	2.14	0.65
1:B:105:MSE:CE	1:B:115:GLU:CA	2.74	0.65
1:A:15:LEU:CD1	1:A:173:SER:CB	2.75	0.65
1:A:203:ASP:CG	1:A:233:THR:OG1	2.35	0.64
1:B:548:VAL:C	1:B:549:TRP:O	2.25	0.63
1:B:192:HIS:O	1:B:199:HIS:CG	2.51	0.63
1:B:244:PRO:CB	1:B:593:PHE:CE1	2.81	0.63
1:A:147:MSE:CE	1:A:161:PHE:CZ	2.82	0.63
1:B:183:TRP:CD1	1:B:208:ALA:CB	2.81	0.63
1:A:7:THR:CB	1:A:8:PRO:CD	2.78	0.62
1:B:467:ARG:NH1	1:B:467:ARG:CG	2.63	0.62
1:B:26:GLU:OE1	1:B:26:GLU:CA	2.47	0.62
1:B:19:TRP:CD1	1:B:47:VAL:CG1	2.83	0.61
1:B:470:GLY:O	1:B:475:SER:CA	2.49	0.61
1:A:311:MSE:CE	1:A:340:TRP:CB	2.79	0.61
1:A:8:PRO:O	1:B:77:LYS:NZ	2.33	0.61
1:B:205:GLN:NE2	1:B:207:VAL:CG2	2.64	0.61
1:B:410:ILE:N	1:B:410:ILE:CD1	2.65	0.60
1:A:107:HIS:CE1	1:A:394:GLU:OE1	2.55	0.60
1:B:10:ARG:CB	1:B:10:ARG:NH1	2.65	0.60
1:B:284:ASN:O	1:B:286:LYS:NZ	2.35	0.60
1:B:15:LEU:O	1:B:16:ASP:C	2.39	0.60
1:A:378:GLU:O	3:A:610:HOH:O	2.16	0.60
1:A:203:ASP:OD1	1:A:233:THR:OG1	2.22	0.58
1:B:330:HIS:O	1:B:331:TYR:CD2	2.57	0.58
1:B:183:TRP:O	1:B:208:ALA:CB	2.52	0.58
1:B:537:PHE:O	1:B:596:LYS:NZ	2.37	0.58
1:A:244:PRO:O	1:A:345:GLY:O	2.22	0.57
1:B:215:GLU:CD	1:B:217:ARG:NH2	2.58	0.57
1:B:350:ASP:OD2	1:B:399:ASP:OD2	2.23	0.56
1:B:238:ASN:C	3:B:701:HOH:O	2.42	0.56
1:B:142:THR:CG2	1:B:144:PRO:O	2.53	0.56
1:B:162:HIS:CD2	1:B:164:PHE:CZ	2.94	0.56
1:A:292:GLY:O	1:A:547:GLN:CA	2.54	0.56
1:B:140:TRP:CD2	1:B:379:ALA:O	2.58	0.56
1:A:11:GLU:OE2	1:A:11:GLU:N	2.39	0.56
1:B:152:GLU:CG	1:B:153:ASN:N	2.67	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:15:LEU:CD1	1:B:173:SER:OG	2.54	0.55
1:A:434:LYS:NZ	3:A:704:HOH:O	2.39	0.55
1:B:193:VAL:C	1:B:199:HIS:CD2	2.79	0.55
1:A:357:PHE:O	1:A:374:LEU:CD2	2.54	0.55
1:B:553:ASP:OD2	3:B:710:HOH:O	2.18	0.55
1:B:183:TRP:CD1	1:B:183:TRP:N	2.75	0.54
1:A:43:ARG:NH2	3:A:703:HOH:O	2.40	0.54
1:A:139:ASN:N	1:A:142:THR:CG2	2.70	0.54
1:B:183:TRP:CA	1:B:263:ASP:OD2	2.56	0.54
1:B:469:TYR:N	1:B:533:TYR:OH	2.40	0.54
1:A:140:TRP:CD2	1:A:379:ALA:O	2.61	0.54
1:B:381:ASN:ND2	3:B:680:HOH:O	2.40	0.54
1:B:508:ASP:OD1	1:B:568:LYS:NZ	2.41	0.53
1:B:83:ARG:CD	1:B:179:THR:CG2	2.86	0.53
1:B:239:PRO:O	3:B:701:HOH:O	2.19	0.53
1:B:330:HIS:C	1:B:331:TYR:CD2	2.82	0.53
1:B:15:LEU:CD1	1:B:173:SER:CB	2.87	0.53
1:B:198:ASN:O	1:B:199:HIS:CB	2.56	0.53
1:A:106:GLU:N	3:A:763:HOH:O	2.41	0.53
1:B:117:ASP:OD1	1:B:119:THR:OG1	2.27	0.53
1:A:598:GLN:O	1:A:599:GLN:CB	2.57	0.52
1:A:100:ASN:ND2	1:A:129:ARG:NH1	2.58	0.52
1:A:39:LEU:N	1:A:70:GLN:OE1	2.41	0.52
1:B:10:ARG:CB	1:B:10:ARG:CZ	2.87	0.52
1:B:361:LEU:CD1	2:B:604:Z77:CAZ	2.87	0.52
1:B:519:ASP:OD2	1:B:519:ASP:N	2.42	0.52
1:B:35:TRP:NE1	1:B:98:TRP:CD1	2.77	0.52
1:A:24:ASP:OD1	3:A:826:HOH:O	2.19	0.52
1:B:112:THR:N	3:B:655:HOH:O	2.42	0.51
1:B:194:ALA:CB	1:B:199:HIS:CD2	2.94	0.51
1:B:388:HIS:CD2	1:B:424:TYR:OH	2.64	0.51
1:A:212:VAL:CG2	1:A:230:THR:CA	2.89	0.51
1:B:83:ARG:NH1	1:B:183:TRP:CH2	2.78	0.51
1:B:240:HIS:ND1	1:B:250:TYR:OH	2.44	0.51
1:B:199:HIS:ND1	1:B:200:ALA:N	2.59	0.50
1:B:15:LEU:CD1	1:B:173:SER:CA	2.88	0.50
1:A:208:ALA:CB	3:A:839:HOH:O	2.59	0.50
1:B:248:TYR:CD2	1:B:249:LEU:N	2.79	0.50
1:B:433:ARG:NH1	1:B:461:ASP:OD1	2.44	0.50
1:B:597:PRO:CB	1:B:600:GLY:O	2.59	0.50
1:B:11:GLU:OE2	1:B:11:GLU:N	2.45	0.50
1:A:203:ASP:OD1	1:A:233:THR:CB	2.60	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:193:VAL:CG1	1:B:285:HIS:NE2	2.75	0.50
1:B:250:TYR:CD2	1:B:271:ILE:CD1	2.95	0.49
1:A:436:ASP:OD1	1:A:438:THR:CG2	2.61	0.49
1:B:14:LYS:CB	1:B:174:VAL:CG2	2.91	0.49
1:A:518:THR:O	1:A:525:TYR:CD1	2.65	0.49
1:B:202:VAL:CG1	1:B:234:LEU:CD2	2.90	0.49
1:A:506:GLY:N	1:A:529:TRP:CZ3	2.80	0.49
1:A:13:LYS:O	1:A:174:VAL:O	2.31	0.49
1:B:315:HIS:CE1	3:B:668:HOH:O	2.65	0.49
1:B:330:HIS:N	1:B:330:HIS:CD2	2.81	0.49
1:B:194:ALA:N	1:B:199:HIS:CD2	2.80	0.48
1:B:295:ARG:O	1:B:329:SER:CB	2.61	0.48
1:B:361:LEU:CD1	2:B:604:Z77:N3	2.76	0.48
1:A:52:ASN:ND2	1:A:52:ASN:N	2.61	0.48
1:B:40:GLN:CG	3:B:682:HOH:O	2.62	0.48
1:B:291:THR:O	1:B:325:SER:OG	2.31	0.48
1:A:494:GLU:OE1	3:A:717:HOH:O	2.20	0.48
1:B:10:ARG:NH2	1:B:79:TRP:CD1	2.82	0.47
1:A:477:ASP:OD1	1:A:480:THR:CG2	2.61	0.47
1:A:566:ASN:ND2	1:A:568:LYS:N	2.62	0.47
1:A:549:TRP:CA	3:A:832:HOH:O	2.62	0.47
1:B:293:PHE:N	1:B:293:PHE:CD2	2.81	0.47
1:A:73:VAL:CG2	1:A:74:PHE:N	2.77	0.47
1:A:446:VAL:O	1:A:449:CYS:O	2.32	0.47
1:A:483:LYS:NZ	3:A:757:HOH:O	2.48	0.47
1:A:193:VAL:O	1:A:285:HIS:NE2	2.48	0.47
1:A:328:THR:C	1:A:329:SER:O	2.46	0.47
2:B:604:Z77:SAF	2:B:604:Z77:CAJ	3.03	0.46
1:B:532:MSE:CG	1:B:533:TYR:N	2.77	0.46
1:B:35:TRP:CD1	1:B:98:TRP:CD1	3.04	0.46
1:B:203:ASP:CG	1:B:233:THR:OG1	2.54	0.46
1:B:238:ASN:OD1	1:B:238:ASN:O	2.30	0.46
1:B:144:PRO:O	1:B:144:PRO:CD	2.63	0.46
1:B:35:TRP:CD1	1:B:98:TRP:CG	3.03	0.46
1:A:194:ALA:C	1:A:196:ASP:N	2.67	0.46
1:B:43:ARG:NH1	1:B:55:PHE:CD1	2.84	0.46
1:A:100:ASN:O	1:A:101:ASN:CB	2.62	0.46
1:B:460:PHE:O	1:B:498:GLN:NE2	2.49	0.46
1:B:254:VAL:N	1:B:265:TYR:O	2.49	0.46
1:A:238:ASN:N	3:A:789:HOH:O	2.48	0.46
1:B:469:TYR:O	1:B:473:VAL:O	2.35	0.45
1:A:114:PHE:N	1:A:114:PHE:CD2	2.84	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:14:LYS:C	1:A:16:ASP:N	2.69	0.45
1:B:470:GLY:O	1:B:476:GLY:N	2.49	0.45
1:A:381:ASN:C	1:A:381:ASN:OD1	2.54	0.45
1:B:373:GLU:CA	3:B:702:HOH:O	2.64	0.45
1:A:198:ASN:OD1	1:A:237:VAL:C	2.55	0.45
1:B:383:GLU:O	1:B:387:ALA:N	2.50	0.45
1:B:212:VAL:CG1	1:B:230:THR:CG2	2.95	0.45
1:B:212:VAL:CA	1:B:255:THR:O	2.64	0.45
1:A:220:ASP:OD2	1:A:220:ASP:N	2.50	0.45
1:B:538:ASP:O	1:B:599:GLN:CG	2.65	0.45
1:B:215:GLU:OE1	1:B:217:ARG:NH2	2.49	0.45
1:B:385:GLN:NE2	1:B:424:TYR:O	2.50	0.45
1:B:94:TYR:C	1:B:94:TYR:CD2	2.90	0.45
1:B:247:GLY:O	1:B:249:LEU:CD1	2.64	0.44
1:B:559:GLY:N	3:B:611:HOH:O	2.50	0.44
1:A:123:ILE:O	1:A:123:ILE:CG2	2.63	0.44
1:A:183:TRP:CD1	1:A:183:TRP:N	2.85	0.44
1:B:546:GLU:OE2	1:B:587:ARG:NH1	2.49	0.44
1:B:250:TYR:CE2	1:B:271:ILE:CD1	3.00	0.44
1:A:249:LEU:CD1	1:A:249:LEU:N	2.80	0.44
1:B:467:ARG:CD	1:B:469:TYR:CE1	3.00	0.44
1:B:193:VAL:CA	1:B:199:HIS:CD2	3.01	0.44
1:A:366:GLU:CG	3:A:710:HOH:O	2.64	0.44
1:B:445:ASN:ND2	1:B:467:ARG:NH2	2.66	0.44
1:A:183:TRP:CZ3	1:A:185:ASP:CB	3.02	0.43
1:B:486:GLU:OE1	1:B:539:ARG:NH1	2.51	0.43
1:B:187:ILE:CG2	1:B:188:THR:N	2.81	0.43
1:B:162:HIS:CD2	1:B:164:PHE:CE2	3.06	0.43
1:B:369:ASN:CA	1:B:370:LYS:CB	2.96	0.43
1:B:482:GLU:CB	1:B:532:MSE:CE	2.96	0.43
1:A:330:HIS:CD2	1:A:351:GLU:OE1	2.72	0.43
1:A:482:GLU:CB	1:A:532:MSE:CE	2.97	0.43
1:B:376:SER:N	1:B:380:VAL:O	2.51	0.43
1:A:298:ASP:OD1	1:A:573:ARG:NH2	2.52	0.43
1:B:243:GLN:O	1:B:247:GLY:N	2.52	0.43
1:A:550:ASN:ND2	1:A:551:PHE:N	2.66	0.43
1:B:244:PRO:CG	1:B:593:PHE:CE1	3.01	0.43
1:B:422:ARG:NH2	1:B:458:ASP:OD2	2.52	0.43
1:A:238:ASN:C	1:A:238:ASN:ND2	2.72	0.42
1:B:217:ARG:N	1:B:251:GLU:O	2.52	0.42
1:B:239:PRO:N	3:B:701:HOH:O	2.52	0.42
1:B:296:HIS:ND1	1:B:331:TYR:OH	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:14:LYS:C	1:B:16:ASP:N	2.73	0.42
1:B:494:GLU:O	1:B:497:HIS:CD2	2.73	0.42
1:B:518:THR:OG1	1:B:518:THR:O	2.37	0.42
1:A:139:ASN:OD1	1:A:141:GLN:N	2.53	0.41
1:A:28:CYS:CB	1:A:32:GLN:NE2	2.83	0.41
1:B:239:PRO:CA	3:B:701:HOH:O	2.68	0.41
1:A:381:ASN:O	1:A:384:THR:N	2.54	0.41
1:A:295:ARG:O	1:A:333:TYR:OH	2.37	0.41
1:B:52:ASN:O	3:B:627:HOH:O	2.21	0.41
1:B:436:ASP:OD1	1:B:438:THR:OG1	2.39	0.41
1:B:328:THR:O	1:B:329:SER:C	2.59	0.41
1:A:186:ASP:OD2	1:A:204:TRP:CH2	2.73	0.41
1:A:15:LEU:O	1:A:16:ASP:C	2.57	0.41
1:A:238:ASN:CB	3:A:789:HOH:O	2.68	0.41
1:A:538:ASP:OD2	1:A:587:ARG:NH2	2.53	0.41
1:B:238:ASN:ND2	1:B:238:ASN:O	2.53	0.41
1:B:0:HIS:N	1:B:0:HIS:CD2	2.88	0.41
1:B:38:ALA:O	1:B:39:LEU:C	2.56	0.41
1:B:224:VAL:CG2	1:B:224:VAL:O	2.69	0.40
1:A:93:HIS:O	1:A:109:GLY:O	2.38	0.40
1:B:272:ARG:NH2	1:B:439:ARG:NE	2.69	0.40
1:A:197:CYS:O	1:A:238:ASN:ND2	2.55	0.40
1:B:5:VAL:CG1	1:B:6:GLU:N	2.84	0.40
1:B:447:MSE:CE	1:B:469:TYR:CE2	3.05	0.40
1:A:388:HIS:CD2	1:A:424:TYR:OH	2.74	0.40
1:B:239:PRO:C	3:B:701:HOH:O	2.59	0.40
1:B:105:MSE:CE	1:B:114:PHE:O	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:366:GLU:OE2	1:B:474:GLN:N[2_555]	2.05	0.15

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	601/605 (99%)	579 (96%)	20 (3%)	2 (0%)	50	54
1	B	601/605 (99%)	556 (92%)	42 (7%)	3 (0%)	38	38
All	All	1202/1210 (99%)	1135 (94%)	62 (5%)	5 (0%)	43	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	PRO
1	A	239	PRO
1	B	143	ILE
1	B	370	LYS
1	B	144	PRO

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	509/500 (102%)	450 (88%)	59 (12%)	8	5
1	B	509/500 (102%)	436 (86%)	73 (14%)	5	2
All	All	1018/1000 (102%)	886 (87%)	132 (13%)	6	3

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	5	VAL
1	A	7	THR
1	A	12	ILE
1	A	15	LEU
1	A	42	SER
1	A	43	ARG
1	A	47	VAL
1	A	52	ASN
1	A	66	ASN
1	A	71	ARG
1	A	75	ILE

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Mol	Chain	Res	Type
1	A	102	GLN
1	A	122	VAL
1	A	123	ILE
1	A	148	VAL
1	A	163	ASP
1	A	173	SER
1	A	176	LEU
1	A	178	THR
1	A	179	THR
1	A	193	VAL
1	A	198	ASN
1	A	201	SER
1	A	204	TRP
1	A	218	ASP
1	A	220	ASP
1	A	226	THR
1	A	233	THR
1	A	234	LEU
1	A	235	GLN
1	A	238	ASN
1	A	255	THR
1	A	258	SER
1	A	264	ILE
1	A	272	ARG
1	A	274	VAL
1	A	298	ASP
1	A	302	ARG
1	A	329	SER
1	A	359	LEU
1	A	360	SER
1	A	378	GLU
1	A	383	GLU
1	A	419	GLN
1	A	441	ILE
1	A	473	VAL
1	A	480	THR
1	A	494	GLU
1	A	513	LEU
1	A	518	THR
1	A	532	MSE
1	A	544	VAL
1	A	550	ASN

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Mol	Chain	Res	Type
1	A	566	ASN
1	A	575	ARG
1	A	583	LEU
1	A	585	GLN
1	A	599	GLN
1	B	0	HIS
1	B	3	ARG
1	B	6	GLU
1	B	12	ILE
1	B	15	LEU
1	B	16	ASP
1	B	40	GLN
1	B	41	GLU
1	B	47	VAL
1	B	61	ARG
1	B	71	ARG
1	B	94	TYR
1	B	119	THR
1	B	122	VAL
1	B	130	ILE
1	B	142	THR
1	B	148	VAL
1	B	149	ILE
1	B	152	GLU
1	B	157	LYS
1	B	159	SER
1	B	174	VAL
1	B	175	MSE
1	B	178	THR
1	B	179	THR
1	B	183	TRP
1	B	185	ASP
1	B	197	CYS
1	B	198	ASN
1	B	199	HIS
1	B	201	SER
1	B	202	VAL
1	B	203	ASP
1	B	205	GLN
1	B	209	ASN
1	B	212	VAL
1	B	218	ASP

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Mol	Chain	Res	Type
1	B	220	ASP
1	B	222	GLN
1	B	226	THR
1	B	228	GLN
1	B	237	VAL
1	B	238	ASN
1	B	241	LEU
1	B	268	ARG
1	B	272	ARG
1	B	302	ARG
1	B	330	HIS
1	B	346	ILE
1	B	359	LEU
1	B	383	GLU
1	B	392	ILE
1	B	410	ILE
1	B	450	ASP
1	B	454	ASP
1	B	456	ILE
1	B	467	ARG
1	B	473	VAL
1	B	478	LEU
1	B	480	THR
1	B	488	GLU
1	B	494	GLU
1	B	513	LEU
1	B	518	THR
1	B	532	MSE
1	B	535	ARG
1	B	550	ASN
1	B	566	ASN
1	B	567	LYS
1	B	583	LEU
1	B	591	MSE
1	B	598	GLN
1	B	599	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	Z77	A	604	-	31,31,31	1.42	4 (12%)	41,43,43	1.85	6 (14%)
2	Z77	B	604	-	31,31,31	1.47	3 (9%)	41,43,43	1.38	6 (14%)

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	Z77	A	604	-	-	0/17/17/17	0/1/3/3
2	Z77	B	604	-	-	0/17/17/17	0/1/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	604	Z77	CAW-N1	-4.12	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	604	Z77	CAM-CAY	4.03	1.41	1.35
2	B	604	Z77	CAT-SAF	4.03	1.74	1.67
2	B	604	Z77	CAM-CAY	3.48	1.40	1.35
2	A	604	Z77	CAT-SAF	3.20	1.72	1.67
2	A	604	Z77	CAW-N1	-3.03	1.35	1.41
2	A	604	Z77	CAZ-N3	2.50	1.41	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	604	Z77	N1-CAT-N2	6.23	122.98	115.81
2	A	604	Z77	SAF-CAT-N2	-6.01	116.20	124.49
2	B	604	Z77	CAM-CAY-CAZ	4.70	119.21	115.58
2	A	604	Z77	CAM-CAY-CAZ	4.60	119.13	115.58
2	A	604	Z77	CAY-CAP-N2	3.14	118.60	113.35
2	A	604	Z77	CAA-OAS-CAX	-2.91	110.47	117.54
2	B	604	Z77	CBA-CBB-N3	2.77	120.47	118.23
2	B	604	Z77	CAP-CAY-CAZ	2.66	125.61	120.11
2	B	604	Z77	CAP-N2-CAT	-2.64	117.64	122.30
2	A	604	Z77	CAO-N2-CAT	-2.57	117.27	121.79
2	B	604	Z77	CAP-CAY-CAM	-2.49	115.18	121.97
2	B	604	Z77	SAF-CAT-N2	-2.40	121.18	124.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	603/605 (99%)	0.71	57 (9%) 8 10	21, 47, 105, 138	0
1	B	603/605 (99%)	1.12	105 (17%) 2 2	29, 84, 165, 230	0
All	All	1206/1210 (99%)	0.91	162 (13%) 4 4	21, 66, 140, 230	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	545	GLY	8.4
1	B	212	VAL	8.0
1	B	214	VAL	8.0
1	B	231	SER	7.7
1	A	208	ALA	7.5
1	B	204	TRP	7.4
1	A	199	HIS	7.2
1	B	208	ALA	7.2
1	B	207	VAL	5.9
1	B	240	HIS	5.9
1	B	463	LEU	5.9
1	B	209	ASN	5.8
1	B	239	PRO	5.8
1	A	264	ILE	5.6
1	B	357	PHE	5.5
1	B	152	GLU	5.5
1	B	225	ALA	5.4
1	B	206	VAL	5.2
1	B	230	THR	5.1
1	A	230	THR	5.1
1	B	271	ILE	5.0
1	A	207	VAL	5.0
1	A	252	LEU	4.9
1	B	601	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	489	LEU	4.9
1	A	8	PRO	4.8
1	B	600	GLY	4.8
1	B	270	GLY	4.7
1	B	501	ILE	4.7
1	A	209	ASN	4.7
1	B	250	TYR	4.6
1	A	256	ALA	4.6
1	B	252	LEU	4.5
1	B	425	PHE	4.5
1	B	199	HIS	4.5
1	A	363	ILE	4.4
1	B	500	ILE	4.4
1	B	254	VAL	4.4
1	B	274	VAL	4.4
1	B	379	ALA	4.3
1	B	289	TYR	4.3
1	A	98	TRP	4.3
1	B	191	THR	4.2
1	B	216	LEU	4.2
1	B	241	LEU	4.0
1	B	283	ILE	3.9
1	B	290	PHE	3.9
1	B	424	TYR	3.8
1	B	16	ASP	3.8
1	B	203	ASP	3.8
1	B	149	ILE	3.8
1	A	254	VAL	3.7
1	B	79	TRP	3.7
1	B	380	VAL	3.7
1	B	253	CYS	3.7
1	B	469	TYR	3.7
1	B	255	THR	3.6
1	B	282	LEU	3.6
1	B	537	PHE	3.6
1	B	236	VAL	3.6
1	B	229	GLY	3.6
1	A	216	LEU	3.5
1	A	379	ALA	3.4
1	A	214	VAL	3.4
1	B	598	GLN	3.4
1	A	231	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	259	GLN	3.3
1	A	7	THR	3.3
1	B	235	GLN	3.3
1	B	227	GLY	3.3
1	B	153	ASN	3.3
1	B	98	TRP	3.2
1	A	79	TRP	3.2
1	B	189	VAL	3.2
1	A	84	ILE	3.2
1	B	242	TRP	3.2
1	B	281	PHE	3.1
1	B	256	ALA	3.1
1	B	292	GLY	3.1
1	B	549	TRP	3.1
1	B	104	VAL	3.1
1	A	601	GLY	3.1
1	B	196	ASP	3.0
1	B	84	ILE	3.0
1	A	257	LYS	2.9
1	B	536	VAL	2.9
1	B	369	ASN	2.9
1	B	190	VAL	2.9
1	A	15	LEU	2.8
1	A	68	TRP	2.8
1	A	47	VAL	2.8
1	A	260	THR	2.8
1	A	16	ASP	2.8
1	A	13	LYS	2.8
1	A	211	ASP	2.8
1	B	543	VAL	2.8
1	A	240	HIS	2.7
1	B	205	GLN	2.7
1	A	104	VAL	2.7
1	A	183	TRP	2.7
1	B	273	SER	2.7
1	B	264	ILE	2.7
1	A	365	PHE	2.7
1	A	97	VAL	2.6
1	A	122	VAL	2.6
1	B	182	THR	2.6
1	B	544	VAL	2.6
1	B	34	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	288	PHE	2.6
1	B	368	GLY	2.6
1	A	132	VAL	2.6
1	A	212	VAL	2.6
1	A	470	GLY	2.5
1	B	222	GLN	2.5
1	B	211	ASP	2.5
1	A	237	VAL	2.5
1	A	255	THR	2.5
1	A	18	LEU	2.5
1	A	236	VAL	2.4
1	A	449	CYS	2.4
1	A	235	GLN	2.4
1	B	183	TRP	2.4
1	A	362	GLY	2.3
1	B	465	LEU	2.3
1	B	535	ARG	2.3
1	B	143	ILE	2.3
1	B	419	GLN	2.3
1	A	328	THR	2.3
1	A	48	PRO	2.3
1	A	262	CYS	2.3
1	B	565	GLY	2.2
1	B	363	ILE	2.2
1	B	155	LYS	2.2
1	B	421	ALA	2.2
1	B	193	VAL	2.2
1	A	600	GLY	2.2
1	B	233	THR	2.2
1	A	96	LYS	2.2
1	B	505	TYR	2.2
1	B	538	ASP	2.2
1	A	511	ALA	2.2
1	B	552	ALA	2.2
1	A	489	LEU	2.2
1	A	510	LEU	2.2
1	B	303	GLY	2.1
1	B	77	LYS	2.1
1	A	12	ILE	2.1
1	B	410	ILE	2.1
1	B	176	LEU	2.1
1	B	257	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	201	SER	2.1
1	B	97	VAL	2.1
1	B	219	ALA	2.1
1	A	204	TRP	2.0
1	A	271	ILE	2.0
1	B	237	VAL	2.0
1	A	80	ALA	2.0
1	B	387	ALA	2.0
1	A	369	ASN	2.0
1	B	31	ASP	2.0
1	B	485	LEU	2.0
1	B	243	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	Z77	B	604	29/29	0.26	1.84	63,75,94,123	5
2	Z77	A	604	29/29	0.18	0.18	48,65,106,111	2

6.5 Other polymers ⓘ

There are no such residues in this entry.