



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:17 PM EDT

PDB ID : 2ZJG / pdb_00002zjg
Title : Crystal structural of mouse kynurenine aminotransferase III
Authors : Han, Q.; Cai, T.; Tagle, D.A.; Robinson, H.; Li, J.
Deposited on : 2008-03-07
Resolution : 3.00 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

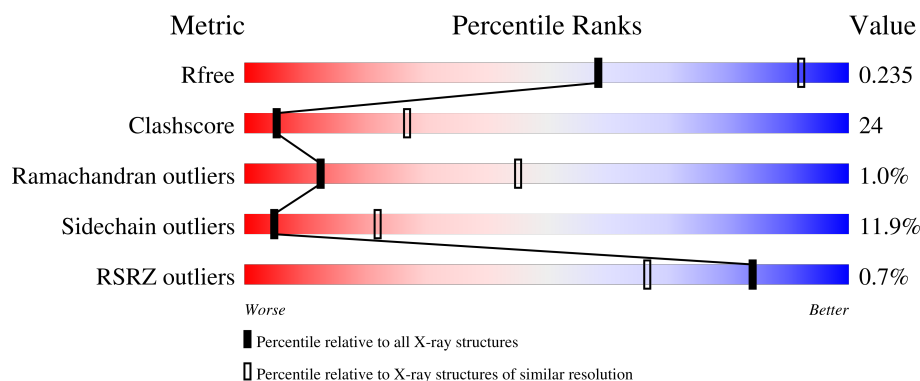
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	410	 55% 36% 8% .
1	B	410	 57% 33% 10%

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
2	GOL	A	500	-	-	X	-
2	GOL	A	501	-	-	X	-
2	GOL	B	503	-	X	-	-

2 Entry composition [i](#)

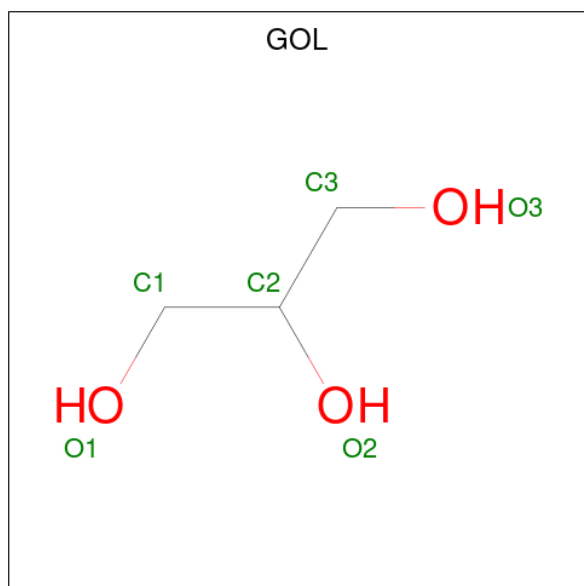
There are 3 unique types of molecules in this entry. The entry contains 6694 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Kynurenine-oxoglutarate transaminase 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	P	S	0	0	0
			3268	2108	537	604	1	18			
1	B	410	Total	C	N	O	P	S	0	0	0
			3268	2108	537	604	1	18			

- 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	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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

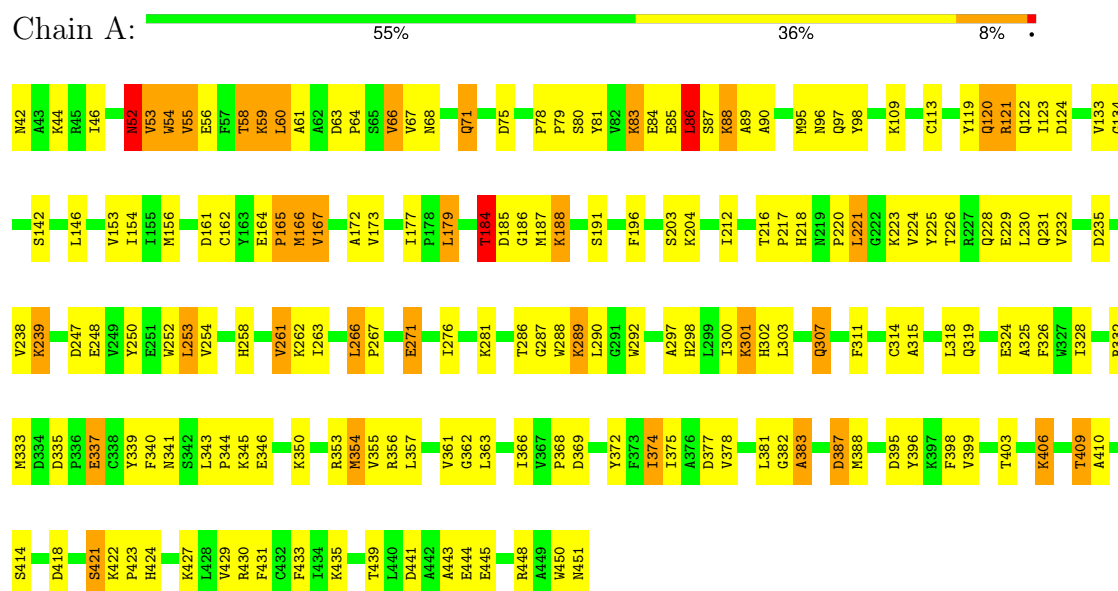
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		
3	B	60	Total	O	0	0
			60	60		

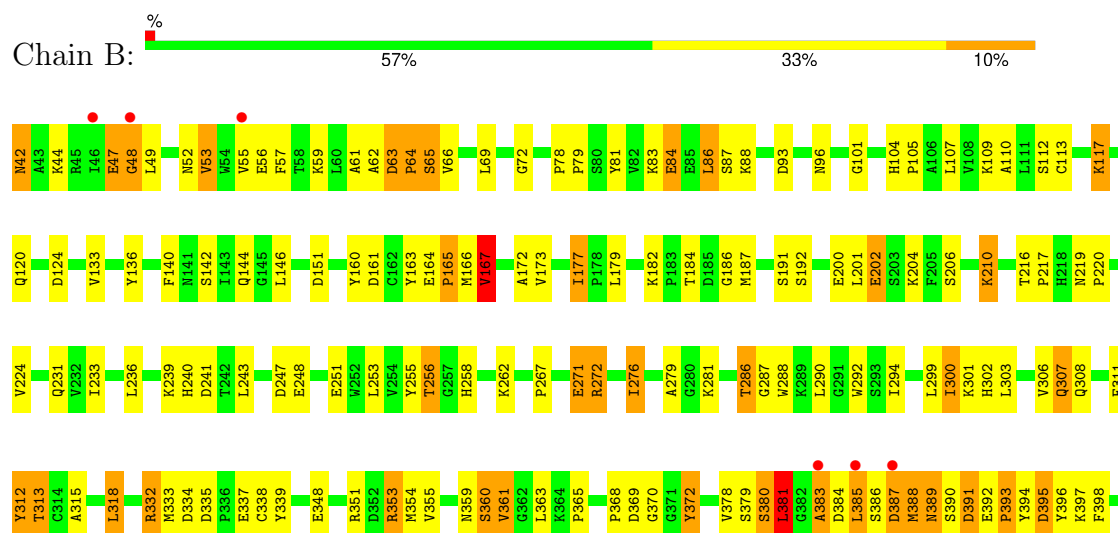
3 Residue-property plots

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: Kynurenine-oxoglutarate transaminase 3



• Molecule 1: Kynurenine-oxoglutarate transaminase 3



W401	W402		H405	K406	K407	L408		I411	P412	V413	S414		K420		E426	K427		F433		S438	T439	L440	D441		E444		R448	A449	W450	W451
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4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.09Å 91.09Å 233.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.58 – 3.00 29.58 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.58-3.00) 97.2 (29.58-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.222 , 0.233 0.223 , 0.235	Depositor DCC
R_{free} test set	999 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6694	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: LLP, 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	1.43	13/3331 (0.4%)	1.29	16/4525 (0.4%)
1	B	1.42	10/3331 (0.3%)	1.29	17/4525 (0.4%)
All	All	1.43	23/6662 (0.3%)	1.29	33/9050 (0.4%)

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	1	5
1	B	1	9
All	All	2	14

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411	ILE	CA-CB	9.55	1.61	1.54
1	B	110	ALA	CA-CB	-7.43	1.41	1.53
1	B	300	ILE	CA-CB	-7.20	1.46	1.54
1	B	200	GLU	CA-C	6.88	1.61	1.52
1	A	154	ILE	CA-CB	-6.40	1.46	1.54
1	A	314	CYS	CA-C	-5.93	1.45	1.53
1	B	113	CYS	CA-C	5.88	1.60	1.52
1	A	225	TYR	C-O	-5.73	1.15	1.23
1	B	173	VAL	CA-CB	5.67	1.59	1.53
1	A	366	ILE	CA-C	-5.61	1.46	1.52
1	A	173	VAL	CA-CB	5.59	1.59	1.53
1	A	377	ASP	CA-C	-5.50	1.45	1.52
1	A	346	GLU	C-O	-5.44	1.17	1.24
1	B	276	ILE	CA-CB	-5.44	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	ILE	CA-CB	5.39	1.60	1.54
1	B	276	ILE	C-O	5.33	1.29	1.24
1	B	306	VAL	CA-CB	-5.30	1.48	1.54
1	A	226	THR	CA-C	-5.29	1.46	1.52
1	B	165	PRO	CA-C	5.23	1.59	1.52
1	A	350	LYS	C-O	-5.14	1.17	1.24
1	A	153	VAL	C-O	5.11	1.29	1.24
1	A	353	ARG	N-CA	-5.11	1.39	1.46
1	A	253	LEU	CA-CB	-5.00	1.46	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	VAL	N-CA-C	9.61	120.42	110.62
1	B	279	ALA	N-CA-C	-7.95	101.92	111.69
1	A	165	PRO	N-CA-C	-7.53	103.71	113.57
1	B	392	GLU	CA-C-N	7.53	127.57	119.89
1	B	392	GLU	C-N-CA	7.53	127.57	119.89
1	A	55	VAL	CB-CA-C	-7.05	102.68	111.92
1	A	443	ALA	N-CA-C	-6.86	103.25	111.69
1	B	167	VAL	N-CA-C	6.83	117.53	110.36
1	A	395	ASP	N-CA-C	6.78	118.67	111.28
1	A	286	THR	N-CA-C	-6.71	104.35	112.54
1	A	439	THR	N-CA-C	-6.48	103.72	111.69
1	B	450	TRP	N-CA-C	-6.38	105.21	112.87
1	B	395	ASP	N-CA-C	6.29	118.94	111.33
1	B	187	MET	N-CA-C	6.09	118.82	111.40
1	B	48	GLY	N-CA-C	-6.07	98.80	113.18
1	B	231	GLN	N-CA-C	5.91	118.48	111.33
1	A	55	VAL	N-CA-C	5.71	116.76	111.45
1	B	355	VAL	N-CA-C	5.70	115.89	110.42
1	B	167	VAL	N-CA-CB	5.62	116.74	110.51
1	A	173	VAL	CA-C-N	-5.45	114.31	119.76
1	A	173	VAL	C-N-CA	-5.45	114.31	119.76
1	B	206	SER	N-CA-C	-5.32	100.89	108.23
1	A	383	ALA	CB-CA-C	5.31	116.33	109.80
1	B	160	TYR	N-CA-C	-5.21	102.68	110.23
1	A	146	LEU	N-CA-C	5.17	121.36	113.61
1	A	409	THR	CB-CA-C	-5.17	99.91	109.37
1	B	233	ILE	N-CA-C	5.16	115.78	110.36
1	B	200	GLU	CA-C-N	5.10	127.43	120.54
1	B	200	GLU	C-N-CA	5.10	127.43	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ALA	N-CA-C	5.06	117.95	110.46
1	B	393	PRO	N-CA-C	5.05	119.14	111.11
1	A	263	ILE	N-CA-C	-5.04	104.79	111.09
1	A	184	THR	N-CA-C	5.00	116.40	110.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	256	THR	CB
1	B	286	THR	CB

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	GLY	Peptide
1	A	289	LYS	Peptide
1	A	362	GLY	Peptide
1	A	388	MET	Peptide
1	A	52	ASN	Peptide
1	B	380	SER	Peptide
1	B	381	LEU	Peptide
1	B	383	ALA	Peptide
1	B	388	MET	Peptide
1	B	389	ASN	Peptide
1	B	391	ASP	Peptide
1	B	47	GLU	Peptide
1	B	61	ALA	Peptide
1	B	63	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3268	0	3235	167	0
1	B	3268	0	3235	183	0
2	A	24	0	32	10	0
2	B	30	0	40	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	44	0	0	0	0
3	B	60	0	0	8	0
All	All	6694	0	6542	318	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 24.

All (318) 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:387:ASP:OD1	1:B:388:MET:HG3	1.12	1.29
1:B:66:VAL:HG13	1:B:407:LYS:O	1.43	1.19
1:A:88:LYS:HB3	1:A:88:LYS:NZ	1.55	1.12
1:B:334:ASP:HB3	3:B:524:HOH:O	1.48	1.12
1:B:448:ARG:HG3	1:B:448:ARG:HH11	0.97	1.10
1:B:182:LYS:HE3	3:B:535:HOH:O	1.53	1.09
1:A:298:HIS:HA	1:A:301:LYS:HE2	1.33	1.08
1:B:383:ALA:O	1:B:385:LEU:HG	1.51	1.08
1:B:387:ASP:OD1	1:B:388:MET:CG	2.03	1.07
1:A:184:THR:CG2	1:A:186:GLY:H	1.70	1.03
1:A:97:GLN:NE2	1:B:286:THR:HB	1.78	0.98
1:A:42:ASN:HB3	1:B:302:HIS:CE1	1.98	0.98
1:A:430:ARG:HH22	2:A:500:GOL:H11	1.26	0.97
1:A:96:ASN:HD22	1:B:288:TRP:HE1	1.00	0.97
1:A:88:LYS:HB3	1:A:88:LYS:HZ3	1.25	0.93
1:A:288:TRP:HE1	1:B:96:ASN:HD22	1.15	0.93
1:A:184:THR:HG22	1:A:186:GLY:H	1.35	0.91
1:A:88:LYS:HB3	1:A:88:LYS:HZ2	1.29	0.91
1:A:88:LYS:NZ	1:A:88:LYS:CB	2.30	0.91
1:B:448:ARG:HH11	1:B:448:ARG:CG	1.84	0.91
1:B:448:ARG:HG3	1:B:448:ARG:NH1	1.65	0.90
1:B:56:GLU:HA	1:B:59:LYS:HE3	1.52	0.89
1:A:184:THR:HG22	1:A:186:GLY:N	1.89	0.87
1:B:146:LEU:O	1:B:210:LYS:HE2	1.74	0.86
1:A:230:LEU:HD12	1:A:261:VAL:HG22	1.57	0.86
1:A:78:PRO:HG2	1:A:83:LYS:HD2	1.57	0.85
1:A:87:SER:OG	1:B:87:SER:HB2	1.76	0.85
1:B:184:THR:HG23	1:B:186:GLY:H	1.40	0.84
1:B:63:ASP:CG	1:B:65:SER:H	1.85	0.83
1:A:396:TYR:HE1	1:A:414:SER:OG	1.62	0.82
1:B:449:ALA:C	1:B:451:ASN:H	1.86	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASN:ND2	1:B:288:TRP:HE1	1.79	0.80
1:A:88:LYS:HZ2	1:A:88:LYS:CB	1.93	0.77
1:A:60:LEU:HG	1:A:403:THR:HG21	1.66	0.77
1:B:64:PRO:O	1:B:65:SER:HB3	1.84	0.77
1:B:63:ASP:CG	1:B:65:SER:N	2.43	0.76
1:B:63:ASP:C	1:B:65:SER:H	1.93	0.76
1:B:191:SER:OG	1:B:368:PRO:HA	1.85	0.76
1:A:52:ASN:OD1	1:A:55:VAL:HG23	1.85	0.75
1:A:96:ASN:HD22	1:B:288:TRP:NE1	1.82	0.75
1:A:54:TRP:HZ3	1:A:71:GLN:HB3	1.51	0.74
1:B:66:VAL:HG13	1:B:407:LYS:C	2.13	0.73
1:A:230:LEU:CD1	1:A:261:VAL:HG22	2.18	0.72
1:A:430:ARG:HH22	2:A:500:GOL:C1	2.01	0.72
1:B:62:ALA:O	1:B:64:PRO:HD2	1.89	0.72
1:A:162:CYS:O	1:A:166:MET:HB2	1.89	0.72
1:B:380:SER:O	1:B:381:LEU:HD23	1.90	0.71
1:A:184:THR:HG23	1:A:185:ASP:N	2.04	0.71
1:A:97:GLN:HE21	1:B:286:THR:HB	1.54	0.71
1:A:300:ILE:HG22	1:A:300:ILE:O	1.91	0.71
1:B:361:VAL:HG13	1:B:361:VAL:O	1.90	0.70
1:B:361:VAL:O	1:B:361:VAL:CG1	2.38	0.70
1:A:298:HIS:HA	1:A:301:LYS:CE	2.17	0.70
1:B:177:ILE:HG21	1:B:204:LYS:HG3	1.73	0.70
1:B:63:ASP:OD2	1:B:65:SER:HA	1.92	0.70
1:A:399:VAL:HG11	1:A:410:ALA:O	1.92	0.69
1:B:449:ALA:C	1:B:451:ASN:N	2.48	0.69
1:A:184:THR:CG2	1:A:185:ASP:N	2.55	0.69
1:A:343:LEU:N	1:A:344:PRO:HD2	2.08	0.69
1:B:52:ASN:O	1:B:55:VAL:HG12	1.92	0.68
1:A:97:GLN:HE22	1:B:286:THR:HB	1.54	0.68
1:A:324:GLU:HA	1:A:324:GLU:OE2	1.92	0.68
1:B:47:GLU:O	1:B:49:LEU:HG	1.94	0.68
1:A:184:THR:HG23	1:A:186:GLY:H	1.57	0.68
1:A:185:ASP:OD2	1:A:186:GLY:N	2.27	0.68
1:B:389:ASN:HB2	1:B:397:LYS:NZ	2.09	0.67
1:B:177:ILE:CG2	1:B:204:LYS:HG3	2.25	0.67
1:A:184:THR:CG2	1:A:186:GLY:N	2.49	0.67
2:A:500:GOL:H2	2:A:501:GOL:O1	1.95	0.66
1:B:63:ASP:C	1:B:65:SER:N	2.49	0.66
1:B:337:GLU:N	1:B:337:GLU:OE1	2.28	0.66
1:A:98:TYR:CE2	1:B:286:THR:HG22	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:LEU:O	1:B:365:PRO:HD3	1.96	0.65
1:B:177:ILE:O	1:B:177:ILE:HG13	1.96	0.65
1:B:389:ASN:HA	1:B:397:LYS:HE2	1.77	0.65
1:A:341:ASN:O	1:A:344:PRO:HD2	1.97	0.65
1:A:217:PRO:HB2	1:A:250:TYR:HB2	1.78	0.64
1:A:271:GLU:OE1	1:A:271:GLU:N	2.30	0.64
1:A:164:GLU:HB3	1:A:165:PRO:HD3	1.80	0.64
1:A:98:TYR:N	1:B:286:THR:OG1	2.30	0.64
1:B:107:LEU:O	1:B:107:LEU:HD12	1.97	0.64
1:B:62:ALA:O	1:B:64:PRO:CD	2.47	0.63
1:B:420:LYS:HD2	1:B:420:LYS:N	2.12	0.63
1:A:396:TYR:CE1	1:A:414:SER:OG	2.48	0.63
1:A:90:ALA:HB2	1:B:86:LEU:HD13	1.80	0.62
1:A:315:ALA:HA	1:B:287:GLY:O	1.99	0.62
1:B:335:ASP:HB3	1:B:337:GLU:OE1	1.99	0.62
1:A:71:GLN:CD	1:A:71:GLN:H	2.07	0.62
1:A:83:LYS:HE3	1:B:93:ASP:OD2	1.99	0.62
1:A:217:PRO:HG2	1:A:250:TYR:O	2.00	0.62
1:A:161:ASP:OD1	2:A:501:GOL:H31	1.99	0.62
1:B:290:LEU:HD11	1:B:318:LEU:HB3	1.81	0.62
1:B:312:TYR:HD1	1:B:313:THR:HG22	1.65	0.62
1:A:224:VAL:HG23	1:A:369:ASP:HB2	1.80	0.62
1:B:63:ASP:O	1:B:65:SER:N	2.33	0.61
1:B:383:ALA:O	1:B:385:LEU:N	2.33	0.61
1:A:97:GLN:NE2	1:B:286:THR:CB	2.59	0.61
1:A:221:LEU:HD13	1:A:375:ILE:HD12	1.82	0.61
1:A:311:PHE:CD2	1:B:311:PHE:CZ	2.89	0.61
1:A:228:GLN:O	1:A:232:VAL:HG23	2.01	0.60
1:A:71:GLN:H	1:A:71:GLN:NE2	1.98	0.60
1:B:216:THR:HA	1:B:217:PRO:C	2.26	0.60
1:B:332:ARG:O	1:B:338:CYS:HB2	2.01	0.60
1:A:230:LEU:HD12	1:A:261:VAL:CG2	2.29	0.60
1:A:83:LYS:CE	1:B:93:ASP:OD2	2.49	0.60
1:B:56:GLU:O	1:B:59:LYS:HB2	2.02	0.59
1:B:388:MET:O	1:B:390:SER:N	2.34	0.59
1:B:380:SER:O	1:B:380:SER:OG	2.20	0.59
1:A:97:GLN:NE2	1:B:286:THR:H	2.00	0.59
1:A:248:GLU:OE1	1:A:262:LYS:HG2	2.01	0.59
1:A:300:ILE:O	1:A:300:ILE:CG2	2.51	0.59
1:B:140:PHE:CZ	1:B:144:GLN:HG3	2.38	0.59
1:A:84:GLU:O	1:A:88:LYS:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:HIS:CE1	1:B:42:ASN:HB2	2.38	0.59
1:B:391:ASP:CG	1:B:391:ASP:O	2.44	0.59
1:B:312:TYR:CD1	1:B:313:THR:HG22	2.38	0.59
1:B:449:ALA:O	1:B:451:ASN:N	2.36	0.58
1:A:63:ASP:O	1:A:66:VAL:HG13	2.03	0.58
1:A:185:ASP:OD2	1:A:187:MET:N	2.36	0.58
1:A:98:TYR:CZ	1:B:286:THR:HG22	2.38	0.58
1:B:182:LYS:CE	3:B:535:HOH:O	2.30	0.58
1:B:272:ARG:NH1	3:B:545:HOH:O	2.35	0.58
1:A:55:VAL:HG12	1:A:56:GLU:N	2.20	0.57
1:A:315:ALA:O	1:A:319:GLN:HG3	2.04	0.57
1:A:287:GLY:O	1:B:315:ALA:HA	2.05	0.57
1:A:368:PRO:HD3	1:A:374:ILE:HD12	1.86	0.57
1:A:341:ASN:C	1:A:344:PRO:HD2	2.30	0.57
1:B:63:ASP:OD2	1:B:65:SER:N	2.37	0.57
1:B:81:TYR:HA	1:B:84:GLU:HB2	1.85	0.57
1:A:97:GLN:HE21	1:B:286:THR:CB	2.18	0.56
1:B:389:ASN:HB2	1:B:397:LYS:HZ3	1.70	0.56
1:B:88:LYS:HD3	3:B:548:HOH:O	2.06	0.56
1:B:63:ASP:OD2	1:B:65:SER:CA	2.54	0.56
1:B:224:VAL:HG23	1:B:369:ASP:HB2	1.88	0.56
1:A:343:LEU:N	1:A:344:PRO:CD	2.69	0.56
1:A:311:PHE:HD2	1:B:311:PHE:CZ	2.24	0.55
1:B:253:LEU:O	1:B:370:GLY:HA2	2.06	0.55
1:A:56:GLU:C	1:A:58:THR:H	2.14	0.55
1:A:42:ASN:HB3	1:B:302:HIS:ND1	2.20	0.55
1:A:288:TRP:HE1	1:B:96:ASN:ND2	1.97	0.55
1:B:48:GLY:O	1:B:49:LEU:HD23	2.06	0.55
1:A:161:ASP:OD1	2:A:501:GOL:C3	2.55	0.55
1:B:241:ASP:HA	1:B:272:ARG:NH2	2.22	0.55
1:B:47:GLU:O	1:B:48:GLY:C	2.51	0.54
1:A:164:GLU:HB3	1:A:165:PRO:CD	2.36	0.54
1:B:42:ASN:N	3:B:520:HOH:O	2.41	0.54
1:B:79:PRO:HG3	1:B:339:TYR:CE1	2.42	0.54
1:B:385:LEU:CD1	1:B:394:TYR:CE1	2.90	0.54
1:B:427:LYS:NZ	3:B:527:HOH:O	2.40	0.54
1:B:146:LEU:O	1:B:210:LYS:CE	2.49	0.54
1:B:380:SER:C	1:B:381:LEU:HD23	2.33	0.54
1:A:179:LEU:N	1:A:179:LEU:HD23	2.22	0.54
1:B:164:GLU:HB3	1:B:165:PRO:HD3	1.90	0.54
1:B:117:LYS:HE2	1:B:333:MET:HE3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASP:OD2	1:A:124:ASP:C	2.51	0.53
1:A:184:THR:HG23	1:A:185:ASP:H	1.71	0.53
1:A:98:TYR:CE2	1:B:286:THR:CG2	2.91	0.53
1:A:59:LYS:O	1:A:60:LEU:C	2.50	0.53
1:A:63:ASP:OD2	1:A:63:ASP:C	2.51	0.53
1:B:151:ASP:O	1:B:172:ALA:HB1	2.07	0.53
1:A:430:ARG:NH2	2:A:500:GOL:H11	2.08	0.53
2:A:500:GOL:C2	2:A:501:GOL:O1	2.57	0.53
1:B:248:GLU:OE1	1:B:262:LYS:HG2	2.09	0.53
1:B:448:ARG:CG	1:B:448:ARG:NH1	2.48	0.52
1:A:119:TYR:HB3	1:A:121:ARG:HG3	1.92	0.52
1:B:383:ALA:O	1:B:385:LEU:CG	2.41	0.52
1:A:66:VAL:HG23	1:A:67:VAL:N	2.24	0.52
1:B:256:THR:OG1	1:B:348:GLU:OE1	2.28	0.52
1:B:385:LEU:HD12	1:B:394:TYR:CE1	2.44	0.52
1:B:290:LEU:CD1	1:B:318:LEU:HB3	2.39	0.52
1:B:351:ARG:HD2	1:B:368:PRO:HD2	1.91	0.52
1:A:361:VAL:HG23	1:A:363:LEU:HG	1.93	0.51
1:B:177:ILE:O	1:B:177:ILE:CG1	2.58	0.51
1:A:97:GLN:NE2	1:A:97:GLN:HA	2.24	0.51
1:A:297:ALA:O	1:A:301:LYS:HB2	2.10	0.51
1:B:241:ASP:OD1	1:B:272:ARG:NH2	2.43	0.51
1:B:391:ASP:O	1:B:391:ASP:OD1	2.29	0.51
1:A:79:PRO:O	1:A:80:SER:C	2.54	0.51
1:A:85:GLU:O	1:A:86:LEU:C	2.52	0.51
1:B:101:GLY:HA2	1:B:313:THR:HB	1.92	0.51
1:A:253:LEU:HD21	1:A:343:LEU:HD23	1.93	0.51
1:B:276:ILE:HA	1:B:292:TRP:O	2.11	0.50
1:B:161:ASP:OD1	2:B:502:GOL:H31	2.11	0.50
1:B:258:HIS:CD2	1:B:369:ASP:HB3	2.46	0.50
1:B:117:LYS:HE2	1:B:333:MET:CE	2.41	0.50
1:B:294:ILE:HD12	3:B:533:HOH:O	2.11	0.50
1:B:389:ASN:O	1:B:389:ASN:OD1	2.29	0.50
1:A:56:GLU:C	1:A:58:THR:N	2.70	0.50
1:A:120:GLN:O	1:A:121:ARG:HB3	2.12	0.50
1:A:387:ASP:OD1	1:A:387:ASP:N	2.28	0.50
1:B:450:TRP:O	1:B:451:ASN:OD1	2.30	0.50
1:A:97:GLN:HE22	1:B:286:THR:H	1.59	0.50
1:A:142:SER:HA	1:A:303:LEU:HD11	1.94	0.49
1:A:382:GLY:O	1:A:383:ALA:C	2.56	0.49
1:B:53:VAL:HG13	1:B:57:PHE:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:HIS:HB3	2:A:502:GOL:H2	1.94	0.49
1:B:389:ASN:HB2	1:B:397:LYS:HZ1	1.78	0.49
1:A:374:ILE:HG13	1:A:375:ILE:N	2.27	0.49
1:B:62:ALA:O	1:B:63:ASP:C	2.55	0.49
1:B:398:PHE:C	1:B:398:PHE:CD2	2.90	0.49
1:B:379:SER:HB3	1:B:427:LYS:HG3	1.95	0.48
1:A:161:ASP:OD1	2:A:501:GOL:H2	2.14	0.48
1:A:398:PHE:CD2	1:A:398:PHE:C	2.91	0.48
1:B:66:VAL:HG22	1:B:407:LYS:HB3	1.96	0.48
1:A:410:ALA:HB1	1:A:430:ARG:O	2.14	0.48
1:B:64:PRO:O	1:B:65:SER:CB	2.58	0.48
1:A:223:LYS:NZ	1:A:229:GLU:OE1	2.48	0.47
1:A:307:GLN:HE21	1:A:307:GLN:HB2	1.40	0.47
1:B:124:ASP:C	1:B:124:ASP:OD2	2.57	0.47
1:B:444:GLU:O	1:B:448:ARG:HB2	2.15	0.47
1:A:61:ALA:HB1	1:A:68:ASN:ND2	2.30	0.47
1:A:133:VAL:HG21	1:B:133:VAL:HG21	1.96	0.47
1:B:161:ASP:OD2	2:B:502:GOL:H11	2.15	0.47
1:A:187:MET:HB3	1:A:188:LYS:HG3	1.96	0.47
1:B:389:ASN:HA	1:B:397:LYS:CE	2.43	0.47
1:A:231:GLN:HG3	1:A:231:GLN:O	2.15	0.46
1:A:318:LEU:HD11	1:B:318:LEU:HD22	1.97	0.46
1:B:267:PRO:O	2:B:501:GOL:O3	2.32	0.46
1:B:63:ASP:OD1	1:B:65:SER:N	2.49	0.46
1:B:408:LEU:HD12	1:B:408:LEU:HA	1.76	0.46
1:A:81:TYR:HA	1:A:84:GLU:HG3	1.97	0.46
1:B:78:PRO:HD2	1:B:83:LYS:HD2	1.98	0.46
1:A:212:ILE:O	1:A:212:ILE:HG23	2.14	0.46
1:B:300:ILE:O	1:B:301:LYS:C	2.58	0.46
1:A:53:VAL:O	1:A:56:GLU:HB2	2.15	0.46
1:A:86:LEU:O	1:A:89:ALA:N	2.48	0.46
1:A:258:HIS:CE1	1:A:369:ASP:OD1	2.69	0.46
1:A:75:ASP:OD1	1:A:435:LYS:HA	2.16	0.46
1:B:191:SER:HB2	1:B:369:ASP:OD2	2.15	0.46
1:A:90:ALA:O	1:B:83:LYS:HG2	2.16	0.46
1:A:95:MET:HE2	1:A:95:MET:HA	1.97	0.46
1:B:107:LEU:HD12	1:B:107:LEU:C	2.39	0.46
1:A:235:ASP:O	1:A:239:LYS:HB3	2.16	0.46
1:A:363:LEU:HD22	1:A:378:VAL:HG12	1.97	0.45
1:B:359:ASN:C	1:B:361:VAL:H	2.23	0.45
1:A:53:VAL:C	1:A:55:VAL:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LYS:O	1:B:62:ALA:HB3	2.15	0.45
1:A:247:ASP:C	1:A:247:ASP:OD1	2.59	0.45
1:B:59:LYS:O	1:B:62:ALA:CB	2.64	0.45
1:B:69:LEU:HD13	1:B:354:MET:HE1	1.99	0.45
1:B:179:LEU:HD23	1:B:179:LEU:HA	1.76	0.45
1:A:121:ARG:NH2	1:A:122:GLN:O	2.50	0.45
1:B:142:SER:HA	1:B:303:LEU:HD11	1.99	0.45
1:A:302:HIS:CE1	1:B:42:ASN:CB	3.00	0.44
1:A:381:LEU:HD12	1:A:381:LEU:HA	1.83	0.44
1:B:401:TRP:CD1	1:B:405:HIS:HD2	2.35	0.44
1:A:42:ASN:CB	1:B:302:HIS:ND1	2.80	0.44
1:A:42:ASN:CB	1:B:302:HIS:CE1	2.87	0.44
1:A:354:MET:HE1	1:A:431:PHE:HB3	1.98	0.44
1:A:441:ASP:O	1:A:444:GLU:HB3	2.17	0.44
1:B:104:HIS:HA	1:B:105:PRO:HD3	1.69	0.44
1:A:276:ILE:HA	1:A:292:TRP:O	2.18	0.44
1:B:62:ALA:C	1:B:64:PRO:CD	2.90	0.44
1:B:253:LEU:O	1:B:370:GLY:CA	2.65	0.44
1:A:164:GLU:N	1:A:165:PRO:HD2	2.33	0.44
1:B:219:ASN:HA	1:B:220:PRO:HA	1.79	0.44
1:A:403:THR:OG1	1:A:409:THR:HG22	2.18	0.43
1:B:201:LEU:O	1:B:202:GLU:C	2.60	0.43
1:B:385:LEU:HD11	1:B:394:TYR:CE1	2.53	0.43
1:B:359:ASN:C	1:B:361:VAL:N	2.72	0.43
1:A:177:ILE:HB	1:A:204:LYS:HE3	1.99	0.43
1:A:341:ASN:O	1:A:344:PRO:HG2	2.18	0.43
1:B:307:GLN:HE21	1:B:307:GLN:HB2	1.42	0.43
1:B:69:LEU:HD12	1:B:408:LEU:HD21	2.01	0.43
1:B:120:GLN:OE1	1:B:120:GLN:HA	2.19	0.43
1:A:63:ASP:OD2	1:A:64:PRO:N	2.51	0.43
1:A:79:PRO:HG3	1:A:339:TYR:CE1	2.53	0.43
1:A:288:TRP:O	1:A:289:LYS:C	2.61	0.43
1:B:389:ASN:O	1:B:389:ASN:CG	2.61	0.43
1:A:63:ASP:HA	1:A:64:PRO:HD3	1.70	0.43
1:B:353:ARG:HH11	1:B:444:GLU:HG3	1.84	0.43
1:A:363:LEU:HD21	1:A:381:LEU:HD22	2.00	0.43
1:A:332:ARG:O	1:A:333:MET:C	2.60	0.42
1:B:395:ASP:HB3	1:B:426:GLU:O	2.19	0.42
1:A:216:THR:HA	1:A:217:PRO:C	2.43	0.42
1:A:406:LYS:HD2	1:A:450:TRP:CD2	2.54	0.42
1:B:381:LEU:HD23	1:B:381:LEU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TRP:CE3	1:A:340:PHE:HB3	2.55	0.42
1:A:335:ASP:HB3	1:A:337:GLU:HG2	2.01	0.42
1:B:413:VAL:O	1:B:414:SER:C	2.60	0.42
1:B:450:TRP:O	1:B:450:TRP:CD1	2.72	0.42
1:A:356:ARG:O	1:A:357:LEU:C	2.59	0.42
1:B:255:TYR:HB3	1:B:348:GLU:OE2	2.20	0.42
1:A:422:LYS:N	1:A:423:PRO:CD	2.82	0.42
1:A:161:ASP:CG	2:A:501:GOL:H2	2.45	0.42
1:B:359:ASN:O	1:B:360:SER:C	2.63	0.42
1:A:325:ALA:O	1:A:326:PHE:C	2.59	0.42
1:A:343:LEU:HB3	1:A:344:PRO:HD3	2.01	0.42
1:A:418:ASP:CG	1:A:421:SER:HB2	2.45	0.42
1:A:196:PHE:CE1	1:A:229:GLU:HG2	2.55	0.42
1:B:163:TYR:O	1:B:167:VAL:HG13	2.20	0.42
1:A:433:PHE:C	1:A:435:LYS:H	2.28	0.41
1:B:66:VAL:HG22	1:B:407:LYS:HA	2.02	0.41
1:B:393:PRO:HB2	1:B:396:TYR:HD2	1.85	0.41
1:A:335:ASP:CB	1:A:337:GLU:HG2	2.50	0.41
1:B:56:GLU:HG3	1:B:59:LYS:CE	2.49	0.41
1:B:299:LEU:HA	1:B:299:LEU:HD23	1.87	0.41
1:A:83:LYS:HE2	1:B:93:ASP:OD2	2.19	0.41
1:A:221:LEU:HD13	1:A:221:LEU:HA	1.87	0.41
1:A:86:LEU:O	1:A:87:SER:C	2.62	0.41
1:A:266:LEU:O	1:A:267:PRO:C	2.60	0.41
1:B:87:SER:O	1:B:88:LYS:C	2.61	0.41
1:A:341:ASN:O	1:A:344:PRO:CD	2.68	0.41
1:B:163:TYR:OH	1:B:247:ASP:OD2	2.35	0.41
1:A:79:PRO:HG3	1:A:339:TYR:CZ	2.56	0.41
1:A:307:GLN:NE2	1:A:311:PHE:CZ	2.89	0.41
1:A:433:PHE:C	1:A:435:LYS:N	2.78	0.41
1:B:402:MET:HG2	1:B:408:LEU:O	2.20	0.41
1:A:337:GLU:HG2	1:A:337:GLU:H	1.55	0.41
1:A:218:HIS:HE1	1:A:220:PRO:HD2	1.85	0.41
1:B:271:GLU:CD	1:B:271:GLU:N	2.79	0.40
1:B:440:LEU:O	1:B:441:ASP:C	2.64	0.40
1:B:136:TYR:CE1	1:B:166:MET:HE3	2.57	0.40
1:B:372:TYR:HA	1:B:433:PHE:CZ	2.56	0.40
1:B:248:GLU:O	1:B:251:GLU:HB3	2.21	0.40
1:B:271:GLU:CD	1:B:271:GLU:H	2.22	0.40
1:A:86:LEU:HA	1:A:86:LEU:HD23	1.73	0.40
1:B:236:LEU:O	1:B:240:HIS:HB2	2.22	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	407/410 (99%)	371 (91%)	32 (8%)	4 (1%)	12	45
1	B	407/410 (99%)	369 (91%)	34 (8%)	4 (1%)	12	45
All	All	814/820 (99%)	740 (91%)	66 (8%)	8 (1%)	12	45

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	64	PRO
1	B	65	SER
1	B	312	TYR
1	A	86	LEU
1	A	203	SER
1	A	60	LEU
1	A	54	TRP
1	B	72	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	357/357 (100%)	310 (87%)	47 (13%)	4	18
1	B	357/357 (100%)	319 (89%)	38 (11%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	714/714 (100%)	629 (88%)	85 (12%)	5 22

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LYS
1	A	52	ASN
1	A	53	VAL
1	A	58	THR
1	A	59	LYS
1	A	66	VAL
1	A	71	GLN
1	A	83	LYS
1	A	86	LEU
1	A	88	LYS
1	A	109	LYS
1	A	113	CYS
1	A	120	GLN
1	A	121	ARG
1	A	123	ILE
1	A	156	MET
1	A	166	MET
1	A	167	VAL
1	A	179	LEU
1	A	184	THR
1	A	188	LYS
1	A	191	SER
1	A	221	LEU
1	A	238	VAL
1	A	239	LYS
1	A	254	VAL
1	A	261	VAL
1	A	266	LEU
1	A	271	GLU
1	A	290	LEU
1	A	301	LYS
1	A	307	GLN
1	A	328	ILE
1	A	337	GLU
1	A	345	LYS
1	A	354	MET
1	A	355	VAL

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Mol	Chain	Res	Type
1	A	372	TYR
1	A	374	ILE
1	A	387	ASP
1	A	406	LYS
1	A	421	SER
1	A	427	LYS
1	A	429	VAL
1	A	445	GLU
1	A	448	ARG
1	A	451	ASN
1	B	42	ASN
1	B	44	LYS
1	B	53	VAL
1	B	84	GLU
1	B	86	LEU
1	B	109	LYS
1	B	112	SER
1	B	117	LYS
1	B	167	VAL
1	B	177	ILE
1	B	192	SER
1	B	202	GLU
1	B	210	LYS
1	B	239	LYS
1	B	243	LEU
1	B	256	THR
1	B	271	GLU
1	B	272	ARG
1	B	286	THR
1	B	307	GLN
1	B	308	GLN
1	B	313	THR
1	B	318	LEU
1	B	332	ARG
1	B	353	ARG
1	B	360	SER
1	B	361	VAL
1	B	372	TYR
1	B	378	VAL
1	B	381	LEU
1	B	384	ASP
1	B	385	LEU

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Mol	Chain	Res	Type
1	B	386	SER
1	B	387	ASP
1	B	420	LYS
1	B	438	SER
1	B	439	THR
1	B	448	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	71	GLN
1	A	96	ASN
1	A	97	GLN
1	A	231	GLN
1	A	307	GLN
1	A	341	ASN
1	A	451	ASN
1	B	94	ASN
1	B	96	ASN
1	B	97	GLN
1	B	144	GLN
1	B	240	HIS
1	B	302	HIS
1	B	307	GLN
1	B	359	ASN
1	B	405	HIS

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	LLP	A	281	1	23,24,25	1.97	6 (26%)	25,32,34	1.83	7 (28%)
1	LLP	B	281	1	23,24,25	2.08	8 (34%)	25,32,34	2.17	7 (28%)

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	LLP	A	281	1	-	8/16/17/19	0/1/1/1
1	LLP	B	281	1	-	8/16/17/19	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281	LLP	O3-C3	-5.79	1.23	1.36
1	B	281	LLP	O3-C3	-4.16	1.27	1.36
1	B	281	LLP	C2-N1	3.37	1.39	1.33
1	B	281	LLP	P-OP3	-3.31	1.42	1.54
1	A	281	LLP	C2-N1	3.22	1.39	1.33
1	A	281	LLP	C3-C2	-3.21	1.37	1.41
1	B	281	LLP	CE-NZ	3.11	1.53	1.46
1	B	281	LLP	P-OP2	-2.87	1.44	1.54
1	B	281	LLP	C4'-NZ	2.82	1.36	1.27
1	B	281	LLP	CG-CB	2.48	1.62	1.52
1	B	281	LLP	C4-C4'	2.12	1.51	1.46
1	A	281	LLP	P-OP3	-2.10	1.47	1.54
1	A	281	LLP	P-OP2	-2.01	1.47	1.54
1	A	281	LLP	CD-CE	2.01	1.58	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	LLP	C4-C3-C2	-5.17	117.23	120.14
1	B	281	LLP	OP4-C5'-C5	5.01	118.75	109.36
1	B	281	LLP	C4-C4'-NZ	-4.78	101.99	124.04
1	A	281	LLP	OP4-C5'-C5	4.15	117.13	109.36
1	A	281	LLP	C3-C4-C5	3.37	120.98	118.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	LLP	C4-C3-C2	-3.22	118.33	120.14
1	B	281	LLP	C3-C4-C5	3.02	120.70	118.28
1	A	281	LLP	C4-C4'-NZ	-3.00	110.22	124.04
1	A	281	LLP	C5-C4-C4'	-2.70	117.31	121.47
1	B	281	LLP	OP3-P-OP2	2.59	117.53	107.80
1	A	281	LLP	C5-C6-N1	-2.58	119.63	123.83
1	B	281	LLP	O3-C3-C2	2.54	122.85	117.58
1	A	281	LLP	O3-C3-C4	2.25	125.51	119.44
1	B	281	LLP	C5-C6-N1	-2.01	120.56	123.83

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	281	LLP	C5'-OP4-P-OP2
1	A	281	LLP	C5'-OP4-P-OP3
1	A	281	LLP	O-C-CA-CB
1	B	281	LLP	C5'-OP4-P-OP1
1	B	281	LLP	C5'-OP4-P-OP2
1	B	281	LLP	C5'-OP4-P-OP3
1	A	281	LLP	C4-C4'-NZ-CE
1	B	281	LLP	C3-C4-C4'-NZ
1	A	281	LLP	C5'-OP4-P-OP1
1	B	281	LLP	C5-C4-C4'-NZ
1	B	281	LLP	C4-C4'-NZ-CE
1	A	281	LLP	C3-C4-C4'-NZ
1	B	281	LLP	CD-CE-NZ-C4'
1	A	281	LLP	CD-CE-NZ-C4'
1	A	281	LLP	N-CA-CB-CG
1	B	281	LLP	CA-CB-CG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

9 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	GOL	A	503	-	5,5,5	0.49	0	5,5,5	0.72	0
2	GOL	B	503	-	5,5,5	0.72	0	5,5,5	2.22	4 (80%)
2	GOL	B	501	-	5,5,5	0.60	0	5,5,5	0.56	0
2	GOL	B	504	-	5,5,5	0.40	0	5,5,5	0.33	0
2	GOL	A	502	-	5,5,5	0.53	0	5,5,5	0.28	0
2	GOL	B	500	-	5,5,5	0.57	0	5,5,5	0.88	0
2	GOL	B	502	-	5,5,5	0.47	0	5,5,5	0.53	0
2	GOL	A	500	-	5,5,5	0.91	0	5,5,5	2.64	4 (80%)
2	GOL	A	501	-	5,5,5	0.37	0	5,5,5	1.11	1 (20%)

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	503	-	-	1/4/4/4	-
2	GOL	B	503	-	-	2/4/4/4	-
2	GOL	B	501	-	-	2/4/4/4	-
2	GOL	B	504	-	-	2/4/4/4	-
2	GOL	A	502	-	-	2/4/4/4	-
2	GOL	B	500	-	-	2/4/4/4	-
2	GOL	B	502	-	-	2/4/4/4	-
2	GOL	A	500	-	-	0/4/4/4	-
2	GOL	A	501	-	-	1/4/4/4	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	GOL	C3-C2-C1	-3.53	98.87	111.80
2	A	500	GOL	O3-C3-C2	-3.02	96.78	110.38
2	A	500	GOL	O2-C2-C1	-2.89	97.21	109.18
2	B	503	GOL	C3-C2-C1	-2.60	102.26	111.80
2	B	503	GOL	O2-C2-C3	2.42	119.18	109.18
2	B	503	GOL	O3-C3-C2	2.39	121.12	110.38
2	B	503	GOL	O1-C1-C2	-2.27	100.18	110.38
2	A	500	GOL	O1-C1-C2	-2.23	100.35	110.38
2	A	501	GOL	O2-C2-C1	2.08	117.77	109.18

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	GOL	O1-C1-C2-O2
2	A	502	GOL	O1-C1-C2-C3
2	B	500	GOL	O1-C1-C2-C3
2	B	502	GOL	O1-C1-C2-C3
2	B	503	GOL	C1-C2-C3-O3
2	B	504	GOL	O1-C1-C2-C3
2	B	500	GOL	O1-C1-C2-O2
2	B	502	GOL	O1-C1-C2-O2
2	B	503	GOL	O2-C2-C3-O3
2	B	504	GOL	O1-C1-C2-O2
2	B	501	GOL	O1-C1-C2-O2
2	A	501	GOL	O2-C2-C3-O3
2	A	503	GOL	O1-C1-C2-O2
2	B	501	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	GOL	1	0
2	A	502	GOL	1	0
2	B	502	GOL	2	0
2	A	500	GOL	5	0
2	A	501	GOL	6	0

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 [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	409/410 (99%)	-0.19	0	100 100	12, 25, 56, 76	0
1	B	409/410 (99%)	-0.13	6 (1%)	72 49	13, 28, 66, 80	0
All	All	818/820 (99%)	-0.16	6 (0%)	84 66	12, 26, 58, 80	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	387	ASP	2.4
1	B	46	ILE	2.3
1	B	385	LEU	2.2
1	B	48	GLY	2.2
1	B	383	ALA	2.1
1	B	55	VAL	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(Å ²)	Q < 0.9
1	LLP	A	281	24/25	0.94	0.10	17,24,31,32	0
1	LLP	B	281	24/25	0.96	0.07	19,23,29,31	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
2	GOL	B	504	6/6	0.32	0.35	88,90,90,91	0
2	GOL	A	503	6/6	0.55	0.28	75,75,77,77	0
2	GOL	B	500	6/6	0.61	0.25	57,66,67,69	0
2	GOL	A	502	6/6	0.78	0.16	37,48,53,54	0
2	GOL	A	501	6/6	0.78	0.15	43,48,49,51	0
2	GOL	B	502	6/6	0.80	0.22	49,55,57,58	0
2	GOL	B	501	6/6	0.83	0.20	55,57,58,59	0
2	GOL	A	500	6/6	0.91	0.10	17,20,23,31	0
2	GOL	B	503	6/6	0.93	0.14	38,40,46,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.