



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 04:45 PM EDT

PDB ID : 3HLM  
Title : Crystal Structure of Mouse Mitochondrial Aspartate Aminotransferase/Kynurenine Aminotransferase IV  
Authors : Han, Q.; Robinson, H.; Li, J.  
Deposited on : 2009-05-27  
Resolution : 2.50 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

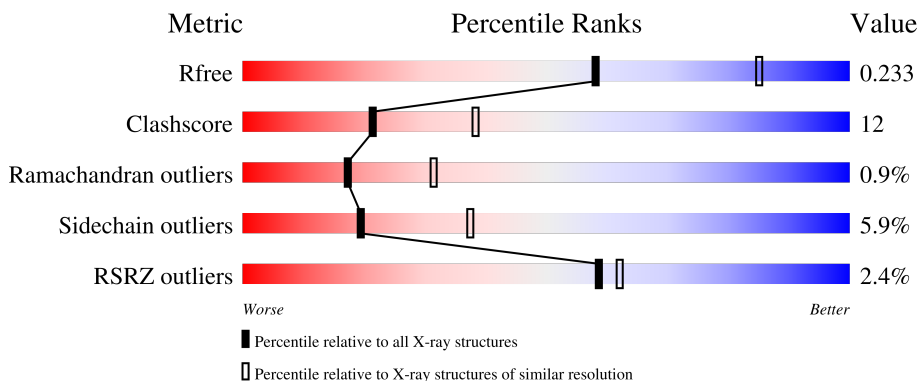
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	401	
1	B	401	
1	C	401	
1	D	401	

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	B	431	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13309 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 Aspartate aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	401	Total 3155	C 2005	N 551	O 582	P 1	S 16	0	0	0
1	B	401	Total 3155	C 2005	N 551	O 582	P 1	S 16	0	0	0
1	C	401	Total 3155	C 2005	N 551	O 582	P 1	S 16	0	0	0
1	D	401	Total 3155	C 2005	N 551	O 582	P 1	S 16	0	0	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

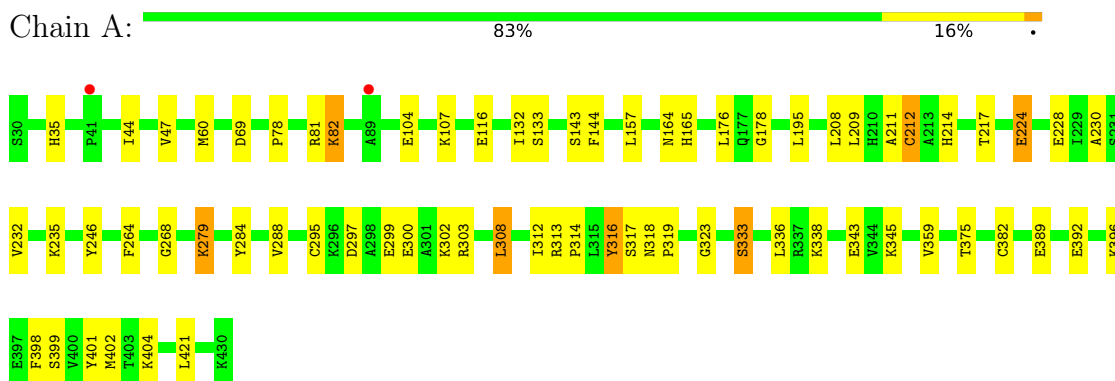
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	201	Total	O	0	0
			201	201		
3	B	168	Total	O	0	0
			168	168		
3	C	161	Total	O	0	0
			161	161		
3	D	123	Total	O	0	0
			123	123		

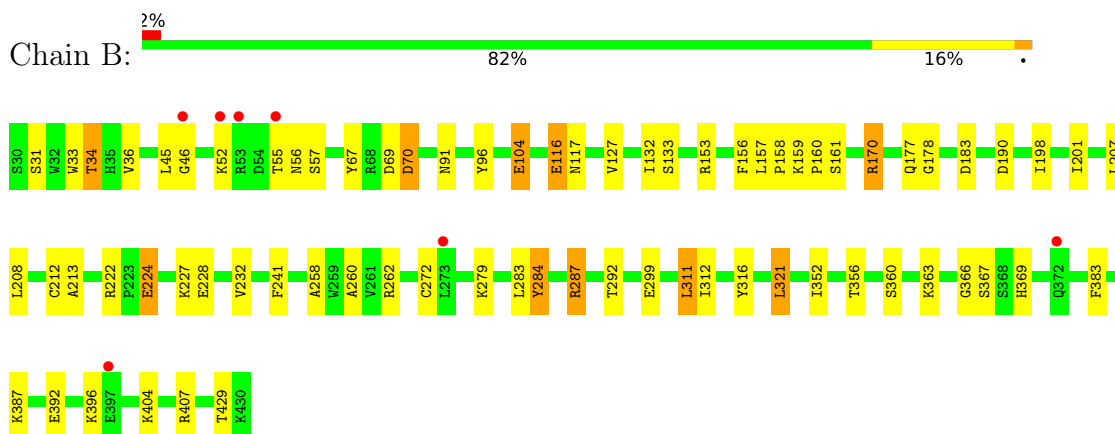
### 3 Residue-property plots

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: Aspartate aminotransferase, mitochondrial

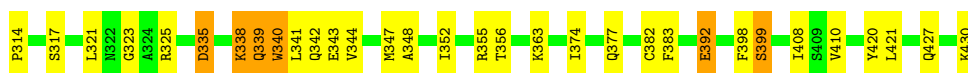


- Molecule 1: Aspartate aminotransferase, mitochondrial

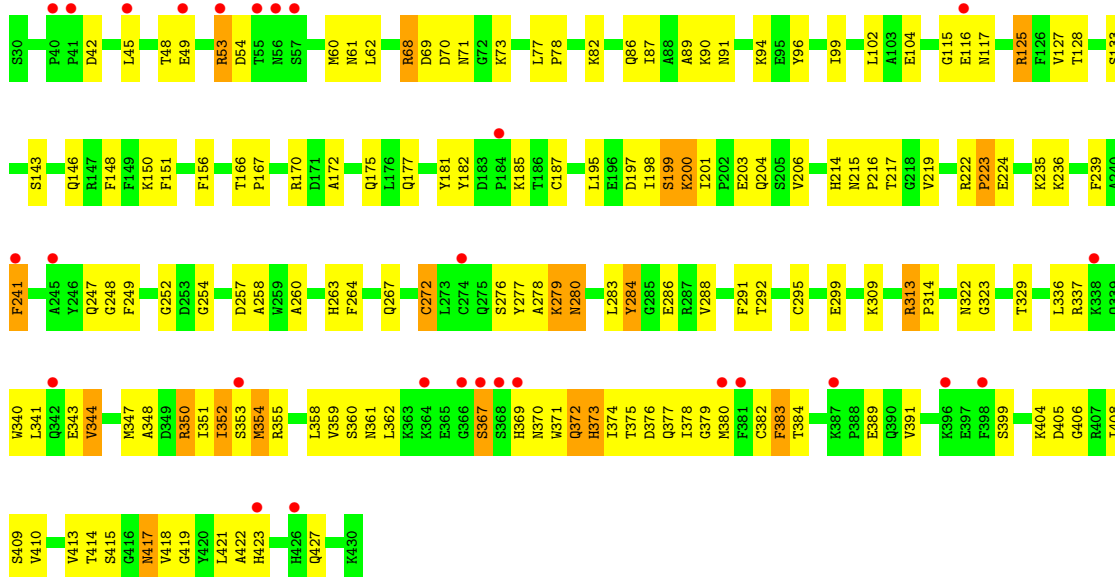


- Molecule 1: Aspartate aminotransferase, mitochondrial





- Molecule 1: Aspartate aminotransferase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	284.32Å 76.79Å 87.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 2.50 29.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.3 (29.90-2.50) 92.3 (29.90-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.5.0044	Depositor
R, $R_{free}$	0.181 , 0.234 0.182 , 0.233	Depositor DCC
$R_{free}$ test set	3126 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.2	Xtrriage
Anisotropy	0.230	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13309	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

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	1.23	4/3203 (0.1%)	0.95	1/4326 (0.0%)
1	B	1.17	1/3203 (0.0%)	0.95	4/4326 (0.1%)
1	C	1.29	6/3203 (0.2%)	1.00	4/4326 (0.1%)
1	D	1.07	4/3203 (0.1%)	0.88	3/4326 (0.1%)
All	All	1.19	15/12812 (0.1%)	0.94	12/17304 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	96	TYR	CE2-CZ	-6.20	1.30	1.38
1	D	96	TYR	CD2-CE2	-5.93	1.30	1.39
1	A	316	TYR	CD1-CE1	-5.71	1.30	1.39
1	C	96	TYR	CD1-CE1	-5.58	1.30	1.39
1	C	181	TYR	CD2-CE2	-5.58	1.30	1.39
1	D	151	PHE	CE2-CZ	5.41	1.47	1.37
1	A	299	GLU	CG-CD	5.28	1.59	1.51
1	B	96	TYR	CD2-CE2	5.22	1.47	1.39
1	A	235	LYS	CD-CE	5.20	1.64	1.51
1	A	302	LYS	CD-CE	5.17	1.64	1.51
1	D	299	GLU	CG-CD	5.16	1.59	1.51
1	C	219	VAL	CB-CG1	-5.07	1.42	1.52
1	C	156	PHE	CD2-CE2	5.07	1.49	1.39
1	C	206	VAL	CB-CG2	-5.03	1.42	1.52
1	C	259	TRP	CB-CG	-5.00	1.41	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	C	183	ASP	CB-CG-OD2	-5.76	113.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ASP	CB-CG-OD1	5.72	123.44	118.30
1	B	311	LEU	CA-CB-CG	5.61	128.20	115.30
1	C	174	MET	CG-SD-CE	5.42	108.88	100.20
1	B	321	LEU	CA-CB-CG	5.34	127.58	115.30
1	C	281	MET	CG-SD-CE	5.33	108.74	100.20
1	D	337	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	D	313	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	C	309	LYS	CD-CE-NZ	-5.18	99.79	111.70
1	D	313	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	366	GLY	N-CA-C	5.14	125.94	113.10

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	3155	0	3128	47	0
1	B	3155	0	3128	44	0
1	C	3155	0	3128	74	0
1	D	3155	0	3128	144	0
2	A	18	0	24	5	0
2	B	12	0	16	3	0
2	C	6	0	8	1	0
3	A	201	0	0	5	0
3	B	168	0	0	7	0
3	C	161	0	0	10	0
3	D	123	0	0	9	0
All	All	13309	0	12560	302	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 12.

All (302) 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:D:362:LEU:HD13	1:D:371:TRP:CZ3	1.47	1.45
1:C:78:PRO:HD2	1:C:343:GLU:OE1	1.32	1.26
1:D:362:LEU:CD1	1:D:371:TRP:CZ3	2.33	1.11
1:D:78:PRO:HD2	1:D:343:GLU:OE2	1.56	1.06
1:C:81:ARG:HA	3:C:519:HOH:O	1.56	1.04
1:D:362:LEU:HD13	1:D:371:TRP:CE3	1.96	1.00
1:D:187:CYS:HB2	1:D:373:HIS:ND1	1.76	1.00
1:D:370:ASN:O	1:D:371:TRP:HD1	1.45	0.97
1:D:340:TRP:CE3	1:D:341:LEU:CD1	2.49	0.96
1:C:392:GLU:HG2	3:C:641:HOH:O	1.69	0.92
1:B:222:ARG:HB3	1:B:224:GLU:OE2	1.70	0.91
1:D:362:LEU:HD13	1:D:371:TRP:HZ3	1.29	0.90
1:B:116:GLU:O	1:B:117:ASN:HB2	1.70	0.90
1:D:350:ARG:HG3	1:D:350:ARG:HH11	1.36	0.89
1:D:60:MET:CE	1:D:417:ASN:HD21	1.85	0.88
1:D:340:TRP:CE3	1:D:341:LEU:HD12	2.09	0.88
1:D:60:MET:HE2	1:D:417:ASN:HD21	1.36	0.87
1:D:340:TRP:CZ3	1:D:341:LEU:CD1	2.57	0.86
1:D:362:LEU:CB	1:D:371:TRP:HZ3	1.89	0.85
1:D:187:CYS:CB	1:D:373:HIS:ND1	2.39	0.85
1:D:249:PHE:HZ	1:D:380:MET:HE2	1.41	0.85
1:D:362:LEU:HB3	1:D:371:TRP:CZ3	2.12	0.84
1:C:78:PRO:CD	1:C:343:GLU:OE1	2.22	0.84
1:D:362:LEU:CG	1:D:371:TRP:HZ3	1.90	0.84
1:D:362:LEU:HB3	1:D:371:TRP:HZ3	1.44	0.83
1:D:367:SER:HB3	3:D:440:HOH:O	1.79	0.83
1:D:370:ASN:O	1:D:371:TRP:CD1	2.30	0.83
1:D:340:TRP:CZ3	1:D:341:LEU:HD11	2.15	0.81
1:B:69:ASP:HB2	2:B:1:GOL:O3	1.81	0.80
1:D:362:LEU:CD1	1:D:371:TRP:HZ3	1.83	0.80
1:D:348:ALA:O	1:D:352:ILE:HG13	1.81	0.80
1:B:31:SER:HB3	1:B:34:THR:HG22	1.65	0.79
1:D:350:ARG:HH11	1:D:350:ARG:CG	1.95	0.78
1:D:102:LEU:HG	1:D:104:GLU:HG3	1.65	0.78
1:B:299:GLU:HG2	3:B:541:HOH:O	1.83	0.77
1:A:318:ASN:HB2	1:A:319:PRO:HD2	1.67	0.76
1:D:249:PHE:CZ	1:D:380:MET:HE2	2.20	0.75
1:D:199:SER:O	1:D:236:LYS:HE2	1.86	0.75
1:D:372:GLN:HB2	1:D:376:ASP:OD2	1.88	0.74
1:D:414:THR:OG1	1:D:417:ASN:HB3	1.88	0.74
1:C:340:TRP:CE3	1:C:341:LEU:HD13	2.23	0.73
1:D:125:ARG:CG	1:D:125:ARG:O	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLU:HG3	1:A:404:LYS:HE2	1.70	0.72
1:D:423:HIS:O	1:D:427:GLN:HG2	1.90	0.71
1:D:354:MET:HG2	1:D:413:VAL:HG12	1.72	0.71
1:C:150:LYS:HE2	3:C:531:HOH:O	1.90	0.70
1:C:191:PHE:CE1	1:C:225:GLN:HB3	2.27	0.70
1:D:249:PHE:CZ	1:D:380:MET:CE	2.74	0.69
1:C:170:ARG:HD3	3:C:494:HOH:O	1.93	0.69
1:D:78:PRO:CD	1:D:343:GLU:OE2	2.36	0.68
1:B:70:ASP:HB2	3:B:521:HOH:O	1.92	0.68
1:C:86:GLN:O	1:C:87:ILE:C	2.30	0.68
1:C:398:PHE:O	1:C:399:SER:HB2	1.94	0.67
1:C:256:LYS:HA	1:C:259:TRP:HB2	1.76	0.67
1:D:362:LEU:CB	1:D:371:TRP:CZ3	2.73	0.67
1:D:102:LEU:HG	1:D:104:GLU:CG	2.25	0.67
1:B:352:ILE:O	1:B:356:THR:HG23	1.94	0.67
1:D:166:THR:HB	1:D:167:PRO:HD3	1.78	0.66
1:D:187:CYS:SG	1:D:373:HIS:CE1	2.87	0.66
1:D:373:HIS:HD2	1:D:374:ILE:H	1.44	0.66
1:D:354:MET:HG2	1:D:413:VAL:CG1	2.26	0.66
1:C:355:ARG:HD3	1:C:374:ILE:O	1.94	0.66
1:D:415:SER:HA	1:D:418:VAL:HG12	1.78	0.65
1:D:348:ALA:O	1:D:352:ILE:CG1	2.43	0.65
1:B:224:GLU:CD	1:B:224:GLU:H	2.00	0.65
1:A:359:VAL:HG21	1:A:375:THR:HG23	1.79	0.64
1:B:67:TYR:OH	2:B:1:GOL:H32	1.96	0.64
1:C:86:GLN:O	1:C:88:ALA:N	2.30	0.64
1:D:313:ARG:HB3	1:D:314:PRO:HD3	1.79	0.64
1:A:246:TYR:HE1	1:A:279:LLP:HD3	1.64	0.63
1:B:241:PHE:CD1	1:B:272:CYS:SG	2.91	0.63
1:D:125:ARG:HG3	1:D:295:CYS:O	1.99	0.63
1:C:35:HIS:H	1:C:35:HIS:CD2	2.17	0.63
1:D:78:PRO:HD2	1:D:343:GLU:CD	2.18	0.62
1:A:246:TYR:CE1	1:A:279:LLP:HD3	2.35	0.62
1:D:355:ARG:HH12	1:D:377:GLN:HB2	1.65	0.61
1:C:78:PRO:HD2	1:C:343:GLU:CD	2.17	0.61
1:D:42:ASP:HB3	1:D:45:LEU:HB3	1.82	0.61
1:B:104:GLU:HG2	3:B:526:HOH:O	2.00	0.60
1:D:60:MET:CE	1:D:417:ASN:ND2	2.62	0.60
1:D:125:ARG:O	1:D:125:ARG:HG3	2.00	0.60
1:B:31:SER:HB3	1:B:34:THR:CG2	2.32	0.60
1:D:260:ALA:O	1:D:264:PHE:HD1	1.85	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ASP:CB	2:B:1:GOL:O3	2.50	0.60
1:B:157:LEU:O	1:B:178:GLY:HA2	2.01	0.60
1:D:340:TRP:CE3	1:D:341:LEU:HD13	2.35	0.60
1:A:211:ALA:O	1:A:212:CYS:HB3	2.00	0.60
1:D:87:ILE:HD11	1:D:329:THR:OG1	2.02	0.59
1:D:373:HIS:CD2	1:D:374:ILE:H	2.20	0.59
1:D:283:LEU:O	1:D:284:TYR:C	2.40	0.59
1:C:60:MET:HE2	1:C:62:LEU:HD21	1.84	0.59
1:D:384:THR:CG2	1:D:408:ILE:HG12	2.33	0.59
1:C:77:LEU:HB3	1:C:343:GLU:OE2	2.03	0.59
1:C:340:TRP:CZ3	1:C:341:LEU:HD13	2.37	0.59
1:D:49:GLU:HB3	1:D:53:ARG:NH1	2.16	0.59
1:B:198:ILE:HA	1:B:201:ILE:HD12	1.83	0.59
1:C:222:ARG:O	1:C:225:GLN:N	2.33	0.59
1:D:187:CYS:SG	1:D:373:HIS:ND1	2.76	0.59
1:D:197:ASP:HA	1:D:200:LYS:HD3	1.84	0.58
1:D:358:LEU:O	1:D:362:LEU:HG	2.03	0.58
1:C:60:MET:HE1	1:C:62:LEU:HD11	1.86	0.58
1:A:35:HIS:H	1:A:35:HIS:CD2	2.20	0.58
1:A:143:SER:HA	2:A:432:GOL:H12	1.86	0.58
1:B:260:ALA:HB3	3:B:522:HOH:O	2.02	0.58
1:C:84:GLU:HB2	3:C:519:HOH:O	2.04	0.58
1:A:143:SER:HB2	2:A:432:GOL:H2	1.85	0.57
1:D:354:MET:SD	1:D:413:VAL:O	2.63	0.57
1:A:82:LYS:HB3	1:A:336:LEU:HD21	1.84	0.57
1:D:104:GLU:HG2	3:D:473:HOH:O	2.05	0.57
1:C:35:HIS:HB3	3:D:554:HOH:O	2.03	0.56
1:D:350:ARG:CG	1:D:350:ARG:NH1	2.59	0.56
1:B:258:ALA:O	1:B:262:ARG:HG3	2.05	0.56
1:D:82:LYS:HD3	1:D:336:LEU:HD21	1.88	0.56
1:D:355:ARG:NH1	1:D:377:GLN:HB2	2.20	0.56
1:B:170:ARG:HD2	3:B:538:HOH:O	2.04	0.56
1:D:60:MET:SD	1:D:421:LEU:HD13	2.45	0.56
1:C:203:GLU:HB2	3:C:447:HOH:O	2.06	0.56
1:D:73:LYS:NZ	3:D:461:HOH:O	2.38	0.56
1:D:127:VAL:O	1:D:292:THR:HA	2.05	0.56
1:D:404:LYS:C	1:D:406:GLY:H	2.08	0.56
1:B:228:GLU:O	1:B:232:VAL:HG23	2.06	0.55
1:B:158:PRO:HG2	1:B:161:SER:HB2	1.88	0.55
1:C:284:TYR:HB2	1:D:94:LYS:O	2.06	0.55
1:D:404:LYS:O	1:D:406:GLY:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:MET:CG	1:D:413:VAL:HG12	2.36	0.55
1:D:340:TRP:O	1:D:344:VAL:HG13	2.07	0.55
1:A:78:PRO:HD2	1:A:343:GLU:CD	2.28	0.55
1:D:415:SER:C	1:D:417:ASN:H	2.11	0.54
1:D:128:THR:HA	1:D:291:PHE:O	2.07	0.54
1:A:214:HIS:CE1	1:A:217:THR:HG23	2.43	0.54
1:A:389:GLU:CD	1:A:389:GLU:H	2.10	0.54
1:D:288:VAL:HG22	1:D:323:GLY:HA3	1.88	0.54
1:C:340:TRP:CZ3	1:C:341:LEU:CD1	2.91	0.54
1:B:45:LEU:O	1:B:46:GLY:C	2.43	0.53
1:A:116:GLU:OE2	1:A:116:GLU:HA	2.08	0.53
1:D:373:HIS:O	1:D:375:THR:N	2.41	0.53
1:D:362:LEU:CD1	1:D:371:TRP:CE3	2.77	0.53
1:A:318:ASN:HB2	1:A:319:PRO:CD	2.38	0.53
1:D:391:VAL:HG11	1:D:404:LYS:HA	1.91	0.53
1:A:318:ASN:O	1:B:287:ARG:NE	2.41	0.52
1:A:195:LEU:HD11	1:A:232:VAL:HG21	1.91	0.52
1:C:183:ASP:HB2	1:C:190:ASP:HB2	1.90	0.52
1:D:86:GLN:O	1:D:89:ALA:HB3	2.10	0.52
1:D:249:PHE:CZ	1:D:380:MET:HE3	2.45	0.52
1:D:370:ASN:C	1:D:371:TRP:CD1	2.83	0.52
1:D:150:LYS:HD2	3:D:488:HOH:O	2.10	0.52
1:D:146:GLN:HG3	1:D:172:ALA:O	2.09	0.51
1:D:355:ARG:HH12	1:D:377:GLN:CB	2.23	0.51
1:C:99:ILE:HG23	1:C:317:SER:O	2.11	0.51
1:D:195:LEU:O	1:D:199:SER:OG	2.28	0.51
1:D:359:VAL:HA	1:D:362:LEU:HD12	1.92	0.51
1:D:373:HIS:O	1:D:374:ILE:C	2.48	0.51
1:A:288:VAL:CG2	1:A:323:GLY:HA3	2.40	0.51
1:C:222:ARG:NH1	1:C:224:GLU:OE1	2.44	0.51
1:D:417:ASN:OD1	1:D:417:ASN:C	2.48	0.51
1:B:91:ASN:HB2	3:B:560:HOH:O	2.11	0.51
1:C:94:LYS:O	1:D:284:TYR:HB2	2.11	0.51
1:D:182:TYR:CZ	1:D:383:PHE:HD2	2.29	0.51
1:A:396:LYS:HD2	3:A:539:HOH:O	2.11	0.51
1:C:125:ARG:O	1:C:125:ARG:HG3	2.11	0.51
1:C:335:ASP:O	1:C:338:LYS:HB3	2.11	0.50
1:C:339:GLN:O	1:C:340:TRP:C	2.50	0.50
1:A:208:LEU:C	1:A:208:LEU:HD23	2.33	0.49
1:C:256:LYS:HE3	3:C:561:HOH:O	2.13	0.49
1:D:373:HIS:C	1:D:375:THR:N	2.64	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:LEU:O	1:C:112:LEU:HD12	2.12	0.49
1:B:208:LEU:C	1:B:208:LEU:HD23	2.31	0.49
1:D:389:GLU:CD	1:D:389:GLU:H	2.15	0.49
1:A:69:ASP:C	1:A:69:ASP:OD1	2.50	0.49
1:A:295:CYS:HB3	1:A:300:GLU:HG2	1.95	0.49
1:D:48:THR:HG23	1:D:61:ASN:HD21	1.78	0.49
1:D:278:ALA:HB3	1:D:279:LLP:HD3	1.94	0.49
1:C:219:VAL:HG12	1:C:377:GLN:HG2	1.95	0.48
1:C:35:HIS:HE1	1:D:148:PHE:O	1.95	0.48
1:A:60:MET:HE1	1:A:421:LEU:HD13	1.95	0.48
1:D:360:SER:HA	3:D:486:HOH:O	2.13	0.48
1:A:144:PHE:CD1	1:A:308:LEU:HD13	2.48	0.48
1:D:413:VAL:HG12	1:D:413:VAL:O	2.12	0.48
1:D:170:ARG:HG3	3:D:450:HOH:O	2.13	0.48
1:D:99:ILE:HB	1:D:309:LYS:HG2	1.96	0.48
1:D:404:LYS:C	1:D:406:GLY:N	2.66	0.48
1:C:355:ARG:NH1	1:C:377:GLN:HB2	2.29	0.48
1:D:358:LEU:HD13	1:D:421:LEU:HD23	1.96	0.48
1:A:143:SER:O	2:A:432:GOL:O2	2.32	0.48
1:A:398:PHE:O	1:A:399:SER:HB2	2.14	0.47
1:C:232:VAL:HA	1:C:235:LYS:HG2	1.95	0.47
1:A:44:ILE:CD1	2:A:1:GOL:H2	2.45	0.47
1:C:51:PHE:CE1	1:C:61:ASN:HB2	2.49	0.47
1:D:206:VAL:HG22	1:D:239:PHE:HB3	1.97	0.47
3:A:556:HOH:O	1:C:224:GLU:HB2	2.15	0.47
1:B:363:LYS:HB2	1:B:363:LYS:HE3	1.74	0.47
1:C:158:PRO:HG2	1:C:161:SER:HB2	1.96	0.47
1:C:163:GLY:HA3	2:C:1:GOL:H32	1.97	0.47
1:C:170:ARG:CD	3:C:494:HOH:O	2.59	0.47
1:A:228:GLU:O	1:A:232:VAL:HG23	2.15	0.47
1:D:219:VAL:O	1:D:219:VAL:HG12	2.12	0.47
1:D:90:LYS:O	1:D:91:ASN:HB3	2.15	0.46
1:C:410:VAL:O	1:C:410:VAL:HG12	2.15	0.46
1:D:77:LEU:H	1:D:77:LEU:CD1	2.29	0.46
1:D:241:PHE:CD1	1:D:272:CYS:SG	3.08	0.46
1:C:398:PHE:O	1:C:399:SER:CB	2.57	0.46
1:A:157:LEU:O	1:A:178:GLY:HA2	2.14	0.46
1:A:176:LEU:N	1:A:176:LEU:HD22	2.29	0.46
1:D:68:ARG:HH11	1:D:68:ARG:HG2	1.81	0.46
1:D:181:TYR:CE2	1:D:214:HIS:CD2	3.03	0.46
1:D:62:LEU:HD13	1:D:408:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:HIS:HE1	1:B:429:THR:O	1.97	0.46
1:C:208:LEU:HD23	1:C:208:LEU:C	2.36	0.46
1:D:185:LYS:O	3:D:465:HOH:O	2.21	0.46
1:A:303:ARG:HD2	1:B:36:VAL:O	2.16	0.46
1:D:60:MET:HG2	1:D:417:ASN:ND2	2.31	0.46
1:B:156:PHE:CD2	1:B:177:GLN:HB2	2.50	0.45
1:C:82:LYS:O	1:C:85:ALA:HB3	2.16	0.45
1:A:313:ARG:HB3	1:A:314:PRO:HD3	1.98	0.45
1:D:355:ARG:HG3	1:D:410:VAL:HG11	1.98	0.45
1:A:214:HIS:HE1	1:A:217:THR:HG23	1.82	0.45
1:C:288:VAL:CG2	1:C:323:GLY:HA3	2.47	0.45
1:D:277:TYR:HA	1:D:280:ASN:OD1	2.16	0.45
1:B:392:GLU:HG3	1:B:404:LYS:NZ	2.32	0.45
1:B:321:LEU:HD21	3:B:628:HOH:O	2.17	0.45
1:D:286:GLU:CD	1:D:322:ASN:HD22	2.19	0.45
1:C:382:CYS:HB3	1:C:408:ILE:HG12	1.99	0.45
1:D:175:GLN:HG3	3:D:508:HOH:O	2.16	0.45
1:B:283:LEU:O	1:B:284:TYR:C	2.54	0.45
1:C:146:GLN:HG3	1:C:172:ALA:O	2.17	0.45
1:B:56:ASN:OD1	1:B:57:SER:N	2.51	0.44
1:D:69:ASP:OD2	1:D:73:LYS:HB2	2.18	0.44
1:D:156:PHE:CD2	1:D:177:GLN:HB2	2.52	0.44
1:A:312:ILE:HG23	1:A:316:TYR:CZ	2.53	0.44
1:A:333:SER:O	1:A:333:SER:OG	2.34	0.44
1:B:45:LEU:HA	1:B:45:LEU:HD23	1.54	0.44
1:D:60:MET:HE3	1:D:417:ASN:HD21	1.79	0.44
1:C:101:GLY:HA3	1:C:130:GLN:HB3	2.00	0.44
1:C:420:TYR:O	1:C:421:LEU:C	2.53	0.43
1:C:341:LEU:HD12	1:C:341:LEU:HA	1.27	0.43
1:D:115:GLY:O	1:D:117:ASN:N	2.52	0.43
1:D:54:ASP:OD2	1:D:399:SER:OG	2.33	0.43
1:C:147:ARG:HB2	3:C:497:HOH:O	2.18	0.43
1:B:127:VAL:O	1:B:292:THR:HA	2.18	0.43
1:C:116:GLU:N	3:C:457:HOH:O	2.51	0.43
1:D:260:ALA:O	1:D:264:PHE:CD1	2.70	0.43
1:C:348:ALA:O	1:C:352:ILE:HG13	2.19	0.43
1:C:78:PRO:O	1:C:81:ARG:N	2.52	0.43
1:C:51:PHE:CD1	1:C:61:ASN:HB2	2.53	0.43
1:C:340:TRP:CE3	1:C:341:LEU:CD1	2.97	0.43
1:A:44:ILE:HD12	2:A:1:GOL:H2	2.00	0.43
1:A:338:LYS:HE2	1:A:338:LYS:HB3	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:GLN:NE2	1:C:430:LYS:HE2	2.34	0.42
1:D:350:ARG:HG3	1:D:350:ARG:O	2.18	0.42
1:A:268:GLY:HA2	3:A:594:HOH:O	2.19	0.42
1:A:230:ALA:HB2	1:A:264:PHE:CE1	2.54	0.42
1:D:77:LEU:H	1:D:77:LEU:HD12	1.84	0.42
1:D:355:ARG:NH2	1:D:379:GLY:O	2.51	0.42
1:C:295:CYS:HB3	1:C:300:GLU:OE1	2.19	0.42
1:B:117:ASN:HD22	1:B:117:ASN:HA	1.59	0.42
1:C:58:LYS:HE3	1:C:420:TYR:CD1	2.55	0.42
1:C:344:VAL:HA	1:C:347:MET:HE2	2.01	0.42
1:A:81:ARG:HG3	3:A:610:HOH:O	2.19	0.42
1:B:241:PHE:CE1	1:B:272:CYS:SG	3.13	0.42
1:D:198:ILE:HA	1:D:201:ILE:CD1	2.49	0.42
1:B:407:ARG:HE	1:B:407:ARG:HB3	1.57	0.42
1:C:79:SER:HB3	1:C:339:GLN:HG2	2.02	0.42
1:D:86:GLN:HE21	1:D:86:GLN:HB3	1.54	0.42
1:D:222:ARG:O	1:D:223:PRO:C	2.57	0.42
1:A:132:ILE:HD12	1:B:132:ILE:HD12	2.01	0.42
1:C:313:ARG:HB3	1:C:314:PRO:HD3	2.02	0.42
1:D:362:LEU:CD2	1:D:422:ALA:HB1	2.50	0.42
1:C:280:ASN:OD1	1:C:280:ASN:C	2.57	0.41
1:D:77:LEU:HD12	1:D:77:LEU:N	2.34	0.41
1:B:33:TRP:O	1:B:34:THR:C	2.57	0.41
1:D:214:HIS:CE1	1:D:217:THR:HG23	2.56	0.41
1:B:153:ARG:HA	1:B:153:ARG:NE	2.35	0.41
1:B:183:ASP:HB2	1:B:190:ASP:HB2	2.01	0.41
1:C:58:LYS:HE3	1:C:420:TYR:CE1	2.55	0.41
1:D:215:ASN:HA	1:D:216:PRO:HA	1.72	0.41
1:C:35:HIS:H	1:C:35:HIS:HD2	1.65	0.41
1:D:286:GLU:OE2	1:D:322:ASN:ND2	2.53	0.41
1:D:288:VAL:CG2	1:D:323:GLY:HA3	2.49	0.41
1:D:361:ASN:HD22	1:D:419:GLY:HA2	1.85	0.41
1:A:47:VAL:HG13	1:A:401:TYR:HB3	2.02	0.41
1:A:224:GLU:HB3	1:C:224:GLU:OE2	2.21	0.41
1:B:212:CYS:O	1:B:213:ALA:HB3	2.20	0.41
1:C:189:PHE:HE2	1:C:191:PHE:HD1	1.69	0.41
1:D:69:ASP:C	1:D:69:ASP:OD1	2.60	0.41
1:D:203:GLU:O	1:D:204:GLN:HB2	2.20	0.41
1:D:247:GLN:NE2	1:D:258:ALA:HB2	2.36	0.41
1:D:276:SER:OG	1:D:279:LLP:OP2	2.26	0.41
1:D:373:HIS:CD2	1:D:374:ILE:N	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ASN:O	1:A:165:HIS:C	2.59	0.41
1:C:112:LEU:HD12	1:C:112:LEU:C	2.41	0.41
1:C:321:LEU:HD22	1:C:325:ARG:NE	2.36	0.41
1:B:312:ILE:HG23	1:B:316:TYR:CZ	2.56	0.40
1:D:248:GLY:N	1:D:257:ASP:OD2	2.54	0.40
1:D:347:MET:O	1:D:351:ILE:HG12	2.20	0.40
1:B:159:LYS:HA	1:B:160:PRO:HA	1.93	0.40
1:C:132:ILE:H	1:C:132:ILE:HG12	1.73	0.40
1:A:402:MET:HE2	1:A:402:MET:HB3	1.92	0.40
1:D:263:HIS:O	1:D:267:GLN:HG2	2.21	0.40
1:A:209:LEU:HA	3:A:509:HOH:O	2.21	0.40
1:A:308:LEU:HD12	1:A:308:LEU:HA	1.75	0.40
1:C:69:ASP:OD1	1:C:69:ASP:C	2.58	0.40
1:D:198:ILE:HA	1:D:201:ILE:HD12	2.03	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	398/401 (99%)	380 (96%)	16 (4%)	2 (0%)	29	48
1	B	398/401 (99%)	379 (95%)	18 (4%)	1 (0%)	41	61
1	C	398/401 (99%)	369 (93%)	24 (6%)	5 (1%)	12	21
1	D	398/401 (99%)	351 (88%)	41 (10%)	6 (2%)	10	18
All	All	1592/1604 (99%)	1479 (93%)	99 (6%)	14 (1%)	17	31

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	TYR

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Mol	Chain	Res	Type
1	C	284	TYR
1	D	284	TYR
1	B	284	TYR
1	C	86	GLN
1	D	116	GLU
1	D	280	ASN
1	C	87	ILE
1	D	252	GLY
1	D	405	ASP
1	A	212	CYS
1	C	339	GLN
1	C	340	TRP
1	D	254	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	333/333 (100%)	323 (97%)	10 (3%)	41	68
1	B	333/333 (100%)	316 (95%)	17 (5%)	24	45
1	C	333/333 (100%)	309 (93%)	24 (7%)	14	28
1	D	333/333 (100%)	305 (92%)	28 (8%)	11	21
All	All	1332/1332 (100%)	1253 (94%)	79 (6%)	19	37

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LYS
1	A	104	GLU
1	A	107	LYS
1	A	133	SER
1	A	224	GLU
1	A	308	LEU
1	A	317	SER
1	A	333	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	345	LYS
1	A	382	CYS
1	B	34	THR
1	B	52	LYS
1	B	55	THR
1	B	70	ASP
1	B	104	GLU
1	B	116	GLU
1	B	133	SER
1	B	170	ARG
1	B	207	LEU
1	B	224	GLU
1	B	227	LYS
1	B	311	LEU
1	B	360	SER
1	B	367	SER
1	B	383	PHE
1	B	387	LYS
1	B	396	LYS
1	C	30	SER
1	C	70	ASP
1	C	86	GLN
1	C	99	ILE
1	C	111	GLU
1	C	119	GLU
1	C	123	SER
1	C	133	SER
1	C	150	LYS
1	C	207	LEU
1	C	212	CYS
1	C	219	VAL
1	C	224	GLU
1	C	256	LYS
1	C	311	LEU
1	C	313	ARG
1	C	335	ASP
1	C	338	LYS
1	C	342	GLN
1	C	356	THR
1	C	363	LYS
1	C	383	PHE
1	C	392	GLU

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Mol	Chain	Res	Type
1	C	399	SER
1	D	53	ARG
1	D	68	ARG
1	D	70	ASP
1	D	71	ASN
1	D	125	ARG
1	D	133	SER
1	D	143	SER
1	D	199	SER
1	D	200	LYS
1	D	223	PRO
1	D	224	GLU
1	D	235	LYS
1	D	241	PHE
1	D	272	CYS
1	D	344	VAL
1	D	350	ARG
1	D	352	ILE
1	D	353	SER
1	D	354	MET
1	D	367	SER
1	D	369	HIS
1	D	372	GLN
1	D	373	HIS
1	D	378	ILE
1	D	382	CYS
1	D	383	PHE
1	D	409	SER
1	D	417	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	146	GLN
1	B	86	GLN
1	B	91	ASN
1	B	117	ASN
1	B	322	ASN
1	B	342	GLN
1	B	361	ASN
1	B	369	HIS

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Mol	Chain	Res	Type
1	C	35	HIS
1	C	86	GLN
1	C	322	ASN
1	C	361	ASN
1	C	423	HIS
1	C	427	GLN
1	D	61	ASN
1	D	71	ASN
1	D	86	GLN
1	D	91	ASN
1	D	322	ASN
1	D	373	HIS
1	D	417	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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	D	279	1	23,24,25	2.44	7 (30%)	25,32,34	2.54	8 (32%)
1	LLP	B	279	1	23,24,25	2.80	12 (52%)	25,32,34	2.20	6 (24%)
1	LLP	C	279	1	23,24,25	3.00	12 (52%)	25,32,34	2.34	6 (24%)
1	LLP	A	279	1	23,24,25	3.28	13 (56%)	25,32,34	2.54	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	D	279	1	-	7/16/17/19	0/1/1/1
1	LLP	B	279	1	-	7/16/17/19	0/1/1/1
1	LLP	C	279	1	-	9/16/17/19	0/1/1/1
1	LLP	A	279	1	-	9/16/17/19	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	279	LLP	O3-C3	-7.87	1.18	1.37
1	A	279	LLP	O3-C3	-7.67	1.19	1.37
1	B	279	LLP	O3-C3	-7.28	1.20	1.37
1	D	279	LLP	O3-C3	-6.89	1.21	1.37
1	A	279	LLP	C3-C2	-5.67	1.35	1.40
1	D	279	LLP	CE-NZ	5.50	1.58	1.46
1	C	279	LLP	P-OP3	-4.97	1.35	1.54
1	A	279	LLP	CE-NZ	4.95	1.57	1.46
1	A	279	LLP	P-OP3	-4.94	1.35	1.54
1	C	279	LLP	C3-C2	-4.93	1.36	1.40
1	A	279	LLP	P-OP1	-4.54	1.35	1.50
1	A	279	LLP	P-OP2	-4.50	1.37	1.54
1	B	279	LLP	P-OP3	-4.29	1.38	1.54
1	B	279	LLP	P-OP2	-4.20	1.38	1.54
1	B	279	LLP	C3-C2	-4.11	1.36	1.40
1	C	279	LLP	P-OP1	-3.91	1.37	1.50
1	C	279	LLP	P-OP2	-3.85	1.40	1.54
1	D	279	LLP	C4-C4'	3.81	1.53	1.46
1	C	279	LLP	CE-NZ	3.73	1.55	1.46
1	B	279	LLP	CE-NZ	3.59	1.54	1.46
1	B	279	LLP	P-OP1	-3.52	1.39	1.50
1	A	279	LLP	CD-CE	3.47	1.63	1.51
1	A	279	LLP	P-OP4	-3.40	1.49	1.60
1	B	279	LLP	C4-C5	-3.25	1.37	1.42
1	C	279	LLP	C4-C4'	3.13	1.52	1.46
1	D	279	LLP	C2-N1	3.08	1.39	1.33
1	D	279	LLP	C4'-NZ	3.03	1.37	1.27
1	C	279	LLP	C4-C5	-3.01	1.38	1.42
1	A	279	LLP	C4-C4'	2.92	1.52	1.46
1	A	279	LLP	C4'-NZ	2.79	1.36	1.27
1	C	279	LLP	C4-C3	-2.77	1.36	1.40
1	C	279	LLP	C4'-NZ	2.71	1.36	1.27
1	B	279	LLP	P-OP4	-2.68	1.51	1.60
1	C	279	LLP	P-OP4	-2.61	1.51	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	279	LLP	C4-C3	-2.60	1.36	1.40
1	A	279	LLP	C4-C5	-2.48	1.38	1.42
1	A	279	LLP	CA-N	-2.44	1.40	1.48
1	B	279	LLP	C4-C4'	2.28	1.51	1.46
1	B	279	LLP	C4'-NZ	2.23	1.34	1.27
1	A	279	LLP	C4-C3	-2.16	1.37	1.40
1	D	279	LLP	CD-CE	2.08	1.58	1.51
1	D	279	LLP	C6-N1	2.05	1.38	1.34
1	C	279	LLP	CD-CE	2.04	1.58	1.51
1	B	279	LLP	CA-N	-2.03	1.42	1.48

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	279	LLP	OP4-C5'-C5	9.54	127.53	109.35
1	C	279	LLP	OP4-C5'-C5	8.79	126.10	109.35
1	B	279	LLP	OP4-C5'-C5	8.16	124.91	109.35
1	A	279	LLP	CD-CE-NZ	7.02	128.13	110.93
1	A	279	LLP	OP4-C5'-C5	6.63	121.98	109.35
1	D	279	LLP	C4-C3-C2	4.49	122.97	120.19
1	C	279	LLP	C4-C3-C2	4.34	122.87	120.19
1	A	279	LLP	OP2-P-OP4	-4.07	95.89	106.73
1	B	279	LLP	C5'-C5-C6	-3.80	113.12	119.37
1	D	279	LLP	C4-C4'-NZ	-3.46	108.42	124.31
1	B	279	LLP	C4-C4'-NZ	-3.35	108.93	124.31
1	A	279	LLP	C3-C4-C5	-3.12	115.86	118.26
1	C	279	LLP	C3-C4-C5	-3.12	115.87	118.26
1	C	279	LLP	C4-C4'-NZ	-2.99	110.56	124.31
1	A	279	LLP	C5'-C5-C6	-2.97	114.49	119.37
1	A	279	LLP	C4-C3-C2	2.83	121.94	120.19
1	D	279	LLP	OP2-P-OP1	2.70	121.26	110.68
1	C	279	LLP	C5'-C5-C6	-2.63	115.05	119.37
1	B	279	LLP	OP2-P-OP4	-2.62	99.76	106.73
1	D	279	LLP	C5'-C5-C6	-2.58	115.14	119.37
1	A	279	LLP	C4-C4'-NZ	-2.56	112.54	124.31
1	D	279	LLP	C3-C4-C5	-2.39	116.43	118.26
1	D	279	LLP	OP3-P-OP4	-2.34	100.50	106.73
1	B	279	LLP	OP3-P-OP2	2.24	116.19	107.64
1	B	279	LLP	C3-C4-C5	-2.22	116.56	118.26
1	D	279	LLP	C5-C4-C4'	2.22	125.21	121.56
1	C	279	LLP	OP2-P-OP1	2.05	118.72	110.68



There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	279	LLP	C3-C4-C4'-NZ
1	A	279	LLP	C4-C5-C5'-OP4
1	A	279	LLP	C6-C5-C5'-OP4
1	A	279	LLP	C5'-OP4-P-OP1
1	A	279	LLP	C5'-OP4-P-OP2
1	A	279	LLP	C5'-OP4-P-OP3
1	A	279	LLP	N-CA-CB-CG
1	A	279	LLP	C-CA-CB-CG
1	B	279	LLP	C4-C5-C5'-OP4
1	B	279	LLP	C6-C5-C5'-OP4
1	C	279	LLP	C3-C4-C4'-NZ
1	C	279	LLP	C5'-OP4-P-OP1
1	C	279	LLP	C5'-OP4-P-OP2
1	C	279	LLP	C5'-OP4-P-OP3
1	D	279	LLP	C4-C5-C5'-OP4
1	D	279	LLP	C6-C5-C5'-OP4
1	B	279	LLP	C4-C4'-NZ-CE
1	B	279	LLP	C3-C4-C4'-NZ
1	B	279	LLP	CA-CB-CG-CD
1	D	279	LLP	C3-C4-C4'-NZ
1	C	279	LLP	CA-CB-CG-CD
1	D	279	LLP	CA-CB-CG-CD
1	D	279	LLP	C5-C4-C4'-NZ
1	D	279	LLP	C4-C4'-NZ-CE
1	A	279	LLP	CA-CB-CG-CD
1	D	279	LLP	CD-CE-NZ-C4'
1	C	279	LLP	CD-CE-NZ-C4'
1	C	279	LLP	C4-C4'-NZ-CE
1	B	279	LLP	CD-CE-NZ-C4'
1	B	279	LLP	C5-C4-C4'-NZ
1	C	279	LLP	C5-C4-C4'-NZ
1	C	279	LLP	CE-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	279	LLP	2	0
1	A	279	LLP	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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	B	431	-	5,5,5	0.95	0	5,5,5	1.11	1 (20%)
2	GOL	B	1	-	5,5,5	0.35	0	5,5,5	0.73	0
2	GOL	A	1	-	5,5,5	0.59	0	5,5,5	1.65	2 (40%)
2	GOL	A	432	-	5,5,5	0.73	0	5,5,5	1.01	0
2	GOL	A	431	-	5,5,5	0.49	0	5,5,5	0.63	0
2	GOL	C	1	-	5,5,5	0.30	0	5,5,5	0.73	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	431	-	-	2/4/4/4	-
2	GOL	B	1	-	-	4/4/4/4	-
2	GOL	A	1	-	-	2/4/4/4	-
2	GOL	A	432	-	-	3/4/4/4	-
2	GOL	A	431	-	-	4/4/4/4	-
2	GOL	C	1	-	-	2/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	GOL	O2-C2-C1	-2.24	99.26	109.12
2	B	431	GOL	O2-C2-C3	2.05	118.15	109.12
2	A	1	GOL	C3-C2-C1	2.02	119.56	111.70

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	GOL	O1-C1-C2-C3
2	A	431	GOL	O1-C1-C2-O2
2	A	431	GOL	O1-C1-C2-C3
2	B	1	GOL	O1-C1-C2-C3
2	B	1	GOL	C1-C2-C3-O3
2	B	431	GOL	C1-C2-C3-O3
2	A	431	GOL	C1-C2-C3-O3
2	A	432	GOL	C1-C2-C3-O3
2	C	1	GOL	O1-C1-C2-C3
2	A	432	GOL	O2-C2-C3-O3
2	B	1	GOL	O1-C1-C2-O2
2	C	1	GOL	O1-C1-C2-O2
2	A	1	GOL	O1-C1-C2-O2
2	B	431	GOL	O2-C2-C3-O3
2	B	1	GOL	O2-C2-C3-O3
2	A	432	GOL	O1-C1-C2-C3
2	A	431	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	GOL	3	0
2	A	1	GOL	2	0
2	A	432	GOL	3	0
2	C	1	GOL	1	0

## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	400/401 (99%)	-0.42	2 (0%) 91 91	17, 31, 44, 53	0
1	B	400/401 (99%)	-0.29	7 (1%) 68 71	20, 34, 63, 84	0
1	C	400/401 (99%)	-0.28	2 (0%) 91 91	18, 33, 50, 61	0
1	D	400/401 (99%)	0.28	28 (7%) 16 16	20, 53, 85, 91	0
All	All	1600/1604 (99%)	-0.18	39 (2%) 59 62	17, 35, 73, 91	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	398	PHE	4.5
1	D	353	SER	4.0
1	D	45	LEU	3.9
1	B	55	THR	3.8
1	D	55	THR	3.6
1	D	342	GLN	3.1
1	D	396	LYS	3.1
1	B	46	GLY	3.0
1	C	89	ALA	2.9
1	D	426	HIS	2.9
1	A	41	PRO	2.8
1	D	53	ARG	2.8
1	D	366	GLY	2.6
1	D	369	HIS	2.6
1	D	274	CYS	2.5
1	B	372	GLN	2.4
1	C	85	ALA	2.4
1	D	368	SER	2.4
1	D	338	LYS	2.3
1	D	57	SER	2.3
1	D	241	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	381	PHE	2.3
1	D	41	PRO	2.2
1	D	387	LYS	2.2
1	D	56	ASN	2.2
1	B	53	ARG	2.2
1	D	423	HIS	2.2
1	D	49	GLU	2.2
1	D	245	ALA	2.1
1	B	52	LYS	2.1
1	D	40	PRO	2.1
1	D	367	SER	2.1
1	B	273	LEU	2.1
1	B	397	GLU	2.1
1	D	184	PRO	2.1
1	D	380	MET	2.0
1	D	116	GLU	2.0
1	D	364	LYS	2.0
1	A	89	ALA	2.0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	LLP	D	279	24/25	0.95	0.19	33,51,57,59	0
1	LLP	C	279	24/25	0.96	0.17	18,27,41,43	0
1	LLP	A	279	24/25	0.96	0.19	18,28,35,38	0
1	LLP	B	279	24/25	0.97	0.18	29,36,43,47	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	GOL	B	431	6/6	0.65	0.44	49,57,60,61	0
2	GOL	A	1	6/6	0.83	0.26	36,47,51,54	0
2	GOL	C	1	6/6	0.90	0.22	61,62,62,63	0
2	GOL	A	432	6/6	0.95	0.22	33,36,37,40	0
2	GOL	A	431	6/6	0.96	0.19	40,41,43,47	0
2	GOL	B	1	6/6	0.96	0.15	39,43,44,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.