Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:13 AM GMT

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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

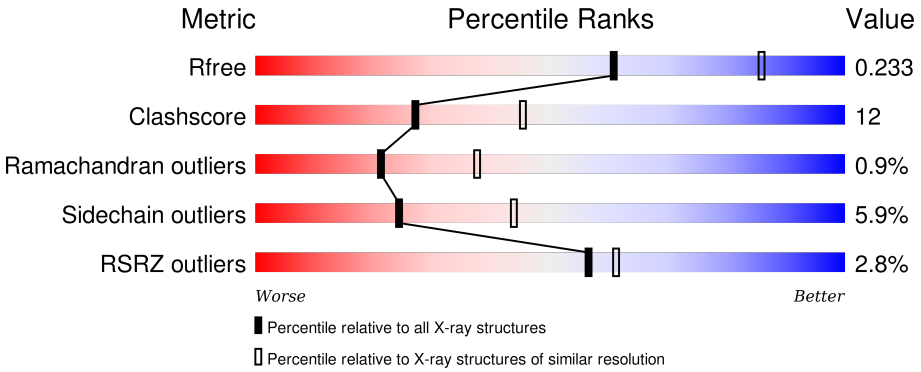
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	83% 16% •
1	B	401	2% 82% 15% •
1	C	401	% 75% 21% •
1	D	401	8% 61% 34% 5%

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	1	-	-	-	X
2	GOL	A	432	-	-	-	X
2	GOL	B	1	-	-	-	X
2	GOL	B	431	-	-	-	X
2	GOL	C	1	-	-	-	X

2 Entry composition

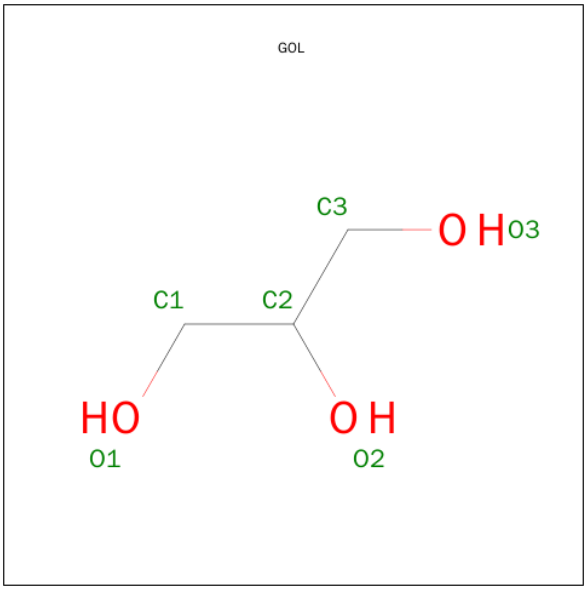
There are 3 unique types of molecules in this entry. The entry contains 13309 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	401	Total	C	N	O	P	S	0	0	0
			3155	2005	551	582	1	16			
1	B	401	Total	C	N	O	P	S	0	0	0
			3155	2005	551	582	1	16			
1	C	401	Total	C	N	O	P	S	0	0	0
			3155	2005	551	582	1	16			
1	D	401	Total	C	N	O	P	S	0	0	0
			3155	2005	551	582	1	16			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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		

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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.

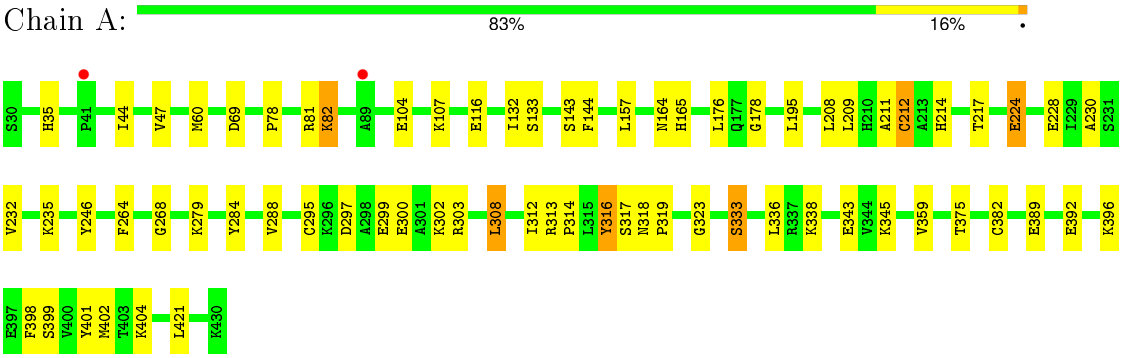
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	201	Total	O	0	0
			201	201		
3	B	168	Total	O	0	0
			168	168		
3	C	161	Total	O	0	0
			161	161		
3	D	123	Total	O	0	0
			123	123		

3 Residue-property plots (i)

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.

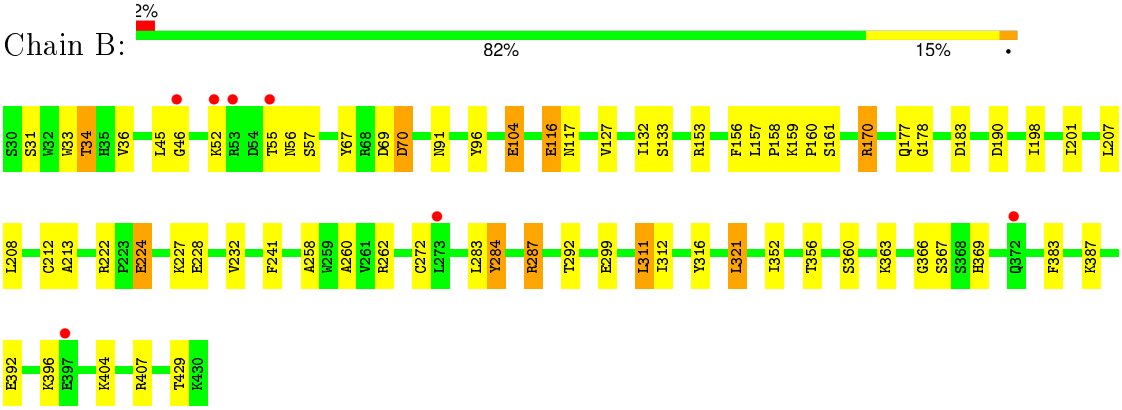
- Molecule 1: Aspartate aminotransferase, mitochondrial

Chain A:



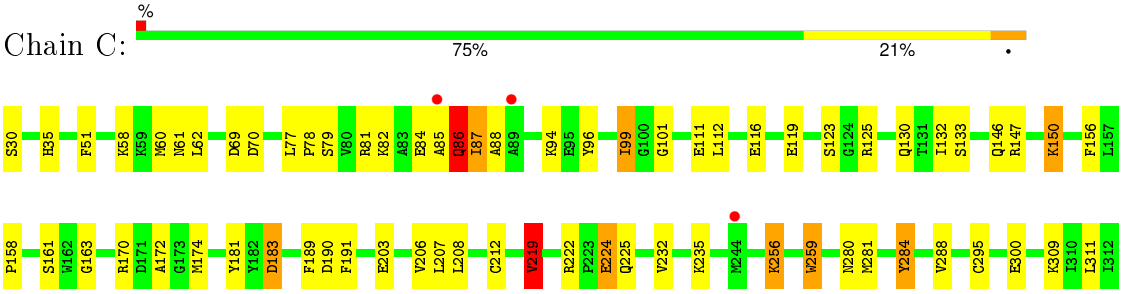
- Molecule 1: Aspartate aminotransferase, mitochondrial

Chain B:



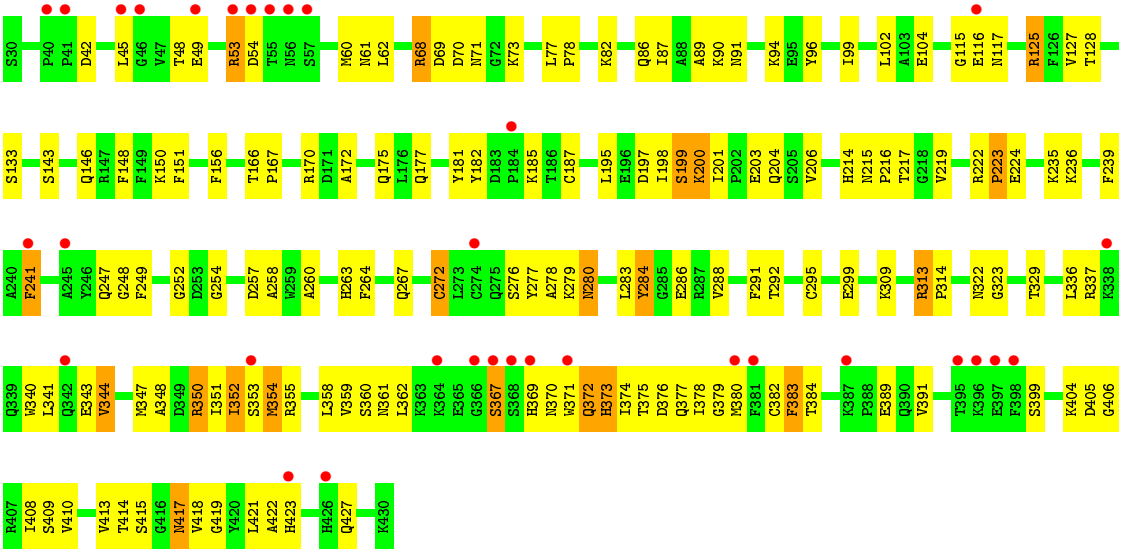
- Molecule 1: Aspartate aminotransferase, mitochondrial

Chain C:



• Molecule 1: Aspartate aminotransferase, mitochondrial

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.83 (at 2.51Å)	Xtriage
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 (5.31%)	DCC
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 61959 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13309	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, LLP

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3155	0	3130	47	0
1	B	3155	0	3130	44	0
1	C	3155	0	3130	74	0
1	D	3155	0	3130	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	12568	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:CG	1:D:350:ARG:HH11	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: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:166:THR:HB	1:D:167:PRO:HD3	1.78	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:H	1:B:224:GLU:CD	2.00	0.65
1:B:67:TYR:OH	2:B:1:GOL:H32	1.96	0.64
1:A:359:VAL:HG21	1:A:375:THR:HG23	1.79	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:B:241:PHE:CD1	1:B:272:CYS:SG	2.91	0.63
1:A:246:TYR:HE1	1:A:279:LLP:HD3	1.64	0.63
1:D:125:ARG:HG3	1:D:295:CYS:O	1.99	0.63
1:C:35:HIS:CD2	1:C:35:HIS:H	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: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:104:GLU:HG2	3:B:526:HOH:O	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:D:340:TRP:CE3	1:D:341:LEU:HD13	2.35	0.60
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:A:211:ALA:O	1:A:212:CYS:HB3	2.00	0.60
1:D:373:HIS:CD2	1:D:374:ILE:H	2.20	0.59
1:D:87:ILE:HD11	1:D:329:THR:OG1	2.02	0.59
1:D:283:LEU:O	1:D:284:TYR:C	2.40	0.59
1:D:384:THR:CG2	1:D:408:ILE:HG12	2.33	0.59
1:C:60:MET:HE2	1:C:62:LEU:HD21	1.84	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:CD2	1:A:35:HIS:H	2.20	0.58
1:B:260:ALA:HB3	3:B:522:HOH:O	2.02	0.58
1:A:143:SER:HA	2:A:432:GOL:H12	1.86	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:D:350:ARG:CG	1:D:350:ARG:NH1	2.59	0.56
1:C:35:HIS:HB3	3:D:554:HOH:O	2.03	0.56
1:D:355:ARG:NH1	1:D:377:GLN:HB2	2.20	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:60:MET:SD	1:D:421:LEU:HD13	2.45	0.56
1:B:170:ARG:HD2	3:B:538:HOH:O	2.04	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:D:404:LYS:O	1:D:406:GLY:N	2.39	0.55
1:C:284:TYR:HB2	1:D:94:LYS:O	2.06	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:H	1:A:389:GLU:CD	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:D:373:HIS:O	1:D:375:THR:N	2.41	0.53
1:A:116:GLU:OE2	1:A:116:GLU:HA	2.08	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:370:ASN:C	1:D:371:TRP:CD1	2.83	0.52
1:D:249:PHE:CZ	1:D:380:MET:HE3	2.45	0.52
1:D:150:LYS:HD2	3:D:488:HOH:O	2.10	0.52
1:D:355:ARG:HH12	1:D:377:GLN:CB	2.23	0.51
1:D:146:GLN:HG3	1:D:172:ALA:O	2.09	0.51
1:D:195:LEU:O	1:D:199:SER:OG	2.28	0.51
1:C:99:ILE:HG23	1:C:317:SER:O	2.11	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:D:417:ASN:OD1	1:D:417:ASN:C	2.48	0.51
1:C:222:ARG:NH1	1:C:224:GLU:OE1	2.44	0.51
1:A:288:VAL:CG2	1:A:323:GLY:HA3	2.40	0.51
1:C:94:LYS:O	1:D:284:TYR:HB2	2.11	0.51
1:B:91:ASN:HB2	3:B:560:HOH:O	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:HG3	1:C:125:ARG:O	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:HD23	1:A:208:LEU:C	2.33	0.49
1:D:373:HIS:C	1:D:375:THR:N	2.64	0.49
1:C:256:LYS:HE3	3:C:561:HOH:O	2.13	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:295:CYS:HB3	1:A:300:GLU:HG2	1.95	0.49
1:A:69:ASP:C	1:A:69:ASP:OD1	2.50	0.49
1:D:278:ALA:HB3	1:D:279:LLP:HD3	1.94	0.49
1:D:48:THR:HG23	1:D:61:ASN:HD21	1.78	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:D:413:VAL:O	1:D:413:VAL:HG12	2.12	0.48
1:A:144:PHE:CD1	1:A:308:LEU:HD13	2.48	0.48
1:D:170:ARG:HG3	3:D:450:HOH:O	2.13	0.48
1:D:404:LYS:C	1:D:406:GLY:N	2.66	0.48
1:D:99:ILE:HB	1:D:309:LYS:HG2	1.96	0.48
1:D:358:LEU:HD13	1:D:421:LEU:HD23	1.96	0.48
1:C:355:ARG:NH1	1:C:377:GLN:HB2	2.29	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: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:B:363:LYS:HB2	1:B:363:LYS:HE3	1.74	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:HG12	1:D:219:VAL:O	2.12	0.47
1:D:90:LYS:O	1:D:91:ASN:HB3	2.15	0.46
1:D:77:LEU:H	1:D:77:LEU:CD1	2.29	0.46
1:C:410:VAL:HG12	1:C:410:VAL:O	2.15	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:D:68:ARG:HH11	1:D:68:ARG:HG2	1.81	0.46
1:A:176:LEU:HD22	1:A:176:LEU:N	2.29	0.46
1:D:181:TYR:CE2	1:D:214:HIS:CD2	3.03	0.46
1:A:157:LEU:O	1:A:178:GLY:HA2	2.14	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: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:B:369:HIS:HE1	1:B:429:THR:O	1.97	0.46
1:D:60:MET:HG2	1:D:417:ASN:ND2	2.31	0.46
1:A:303:ARG:HD2	1:B:36:VAL:O	2.16	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:D:355:ARG:HG3	1:D:410:VAL:HG11	1.98	0.45
1:A:313:ARG:HB3	1:A:314:PRO:HD3	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:D:286:GLU:CD	1:D:322:ASN:HD22	2.19	0.45
1:B:321:LEU:HD21	3:B:628:HOH:O	2.17	0.45
1:D:175:GLN:HG3	3:D:508:HOH:O	2.16	0.45
1:C:382:CYS:HB3	1:C:408:ILE:HG12	1.99	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: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:B:56:ASN:OD1	1:B:57:SER:N	2.51	0.44
1:A:333:SER:O	1:A:333:SER:OG	2.34	0.44
1:A:312:ILE:HG23	1:A:316:TYR:CZ	2.53	0.44
1:D:60:MET:HE3	1:D:417:ASN:HD21	1.79	0.44
1:B:45:LEU:HA	1:B:45:LEU:HD23	1.54	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:D:260:ALA:O	1:D:264:PHE:CD1	2.70	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: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:340:TRP:CE3	1:C:341:LEU:CD1	2.97	0.43
1:C:51:PHE:CD1	1:C:61:ASN:HB2	2.53	0.43
1:A:44:ILE:HD12	2:A:1:GOL:H2	2.00	0.43
1:A:338:LYS:HB3	1:A:338:LYS:HE2	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:ARG:HG3	1:D:350:ARG:O	2.18	0.42
1:C:427:GLN:NE2	1:C:430:LYS:HE2	2.34	0.42
1:A:268:GLY:HA2	3:A:594:HOH:O	2.19	0.42
1:D:355:ARG:NH2	1:D:379:GLY:O	2.51	0.42
1:D:77:LEU:HD12	1:D:77:LEU:H	1.84	0.42
1:A:230:ALA:HB2	1:A:264:PHE:CE1	2.54	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:B:241:PHE:CE1	1:B:272:CYS:SG	3.13	0.42
1:A:81:ARG:HG3	3:A:610:HOH:O	2.19	0.42
1:D:198:ILE:HA	1:D:201:ILE:CD1	2.49	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:B:407:ARG:HE	1:B:407:ARG:HB3	1.57	0.42
1:D:362:LEU:CD2	1:D:422:ALA:HB1	2.50	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:77:LEU:N	1:D:77:LEU:HD12	2.34	0.41
1:C:280:ASN:C	1:C:280:ASN:OD1	2.57	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:183:ASP:HB2	1:B:190:ASP:HB2	2.01	0.41
1:B:153:ARG:HA	1:B:153:ARG:NE	2.35	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:D:373:HIS:CD2	1:D:374:ILE:N	2.87	0.41
1:A:224:GLU:HB3	1:C:224:GLU:OE2	2.21	0.41
1:C:189:PHE:HE2	1:C:191:PHE:HD1	1.69	0.41
1:D:69:ASP:OD1	1:D:69:ASP:C	2.60	0.41
1:D:276:SER:OG	1:D:279:LLP:OP2	2.26	0.41
1:B:212:CYS:O	1:B:213:ALA:HB3	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:LEU:C	1:C:112:LEU:HD12	2.41	0.41
1:A:164:ASN:O	1:A:165:HIS:C	2.59	0.41
1:C:321:LEU:HD22	1:C:325:ARG:NE	2.36	0.41
1:D:347:MET:O	1:D:351:ILE:HG12	2.20	0.40
1:D:248:GLY:N	1:D:257:ASP:OD2	2.54	0.40
1:B:312:ILE:HG23	1:B:316:TYR:CZ	2.56	0.40
1:C:132:ILE:H	1:C:132:ILE:HG12	1.73	0.40
1:B:159:LYS:HA	1:B:160:PRO:HA	1.93	0.40
1:A:402:MET:HB3	1:A:402:MET:HE2	1.92	0.40
1:D:263:HIS:O	1:D:267:GLN:HG2	2.21	0.40
1:A:308:LEU:HA	1:A:308:LEU:HD12	1.75	0.40
1:D:198:ILE:HA	1:D:201:ILE:HD12	2.03	0.40
1:A:209:LEU:HA	3:A:509:HOH:O	2.21	0.40
1:C:69:ASP:C	1:C:69:ASP:OD1	2.58	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%)	34	55
1	B	398/401 (99%)	379 (95%)	18 (4%)	1 (0%)	46	68
1	C	398/401 (99%)	369 (93%)	24 (6%)	5 (1%)	15	26
1	D	398/401 (99%)	351 (88%)	41 (10%)	6 (2%)	13	22
All	All	1592/1604 (99%)	1479 (93%)	99 (6%)	14 (1%)	21	37

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%)	48 76
1	B	333/333 (100%)	316 (95%)	17 (5%)	29 52
1	C	333/333 (100%)	309 (93%)	24 (7%)	18 33
1	D	333/333 (100%)	305 (92%)	28 (8%)	14 25
All	All	1332/1332 (100%)	1253 (94%)	79 (6%)	24 44

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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Mol	Chain	Res	Type
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

Some 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

There are no RNA molecules in this entry.

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

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	A	279	1	23,24,25	3.56	13 (56%)	28,32,34	2.88	7 (25%)
1	LLP	B	279	1	23,24,25	2.97	11 (47%)	28,32,34	2.32	8 (28%)
1	LLP	C	279	1	23,24,25	3.24	12 (52%)	28,32,34	2.34	6 (21%)
1	LLP	D	279	1	23,24,25	2.47	7 (30%)	28,32,34	2.58	9 (32%)

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	279	1	-	0/15/17/19	0/1/1/1
1	LLP	B	279	1	-	0/15/17/19	0/1/1/1
1	LLP	C	279	1	-	0/15/17/19	0/1/1/1
1	LLP	D	279	1	-	0/15/17/19	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	LLP	C3-C2	-8.01	1.35	1.40
1	C	279	LLP	O3-C3	-7.82	1.18	1.37
1	A	279	LLP	O3-C3	-7.62	1.19	1.37
1	B	279	LLP	O3-C3	-7.24	1.20	1.37
1	C	279	LLP	C3-C2	-6.94	1.36	1.40
1	D	279	LLP	O3-C3	-6.85	1.21	1.37
1	B	279	LLP	C3-C2	-5.76	1.36	1.40
1	C	279	LLP	P-OP3	-5.30	1.35	1.54
1	A	279	LLP	P-OP3	-5.26	1.35	1.54
1	A	279	LLP	P-OP2	-4.79	1.37	1.54
1	A	279	LLP	P-OP1	-4.65	1.35	1.51
1	B	279	LLP	P-OP3	-4.56	1.38	1.54
1	B	279	LLP	P-OP2	-4.47	1.38	1.54
1	C	279	LLP	P-OP2	-4.09	1.40	1.54
1	C	279	LLP	P-OP1	-4.03	1.37	1.51
1	B	279	LLP	P-OP1	-3.64	1.39	1.51
1	A	279	LLP	P-OP4	-3.28	1.49	1.60
1	C	279	LLP	C4-C3	-3.23	1.36	1.40
1	B	279	LLP	C4-C3	-3.03	1.36	1.40
1	B	279	LLP	C4-C5	-3.01	1.37	1.42
1	C	279	LLP	C4-C5	-2.79	1.38	1.42
1	B	279	LLP	P-OP4	-2.58	1.51	1.60
1	C	279	LLP	P-OP4	-2.52	1.51	1.60
1	A	279	LLP	C4-C3	-2.50	1.37	1.40
1	A	279	LLP	C4-C5	-2.29	1.38	1.42
1	A	279	LLP	CA-N	-2.20	1.40	1.47
1	D	279	LLP	C6-N1	2.01	1.38	1.34
1	C	279	LLP	CD-CE	2.23	1.58	1.51
1	D	279	LLP	CD-CE	2.28	1.58	1.51
1	B	279	LLP	C4'-NZ	2.40	1.34	1.27
1	B	279	LLP	C4-C4'	2.46	1.51	1.46
1	D	279	LLP	C2-N1	2.64	1.39	1.34
1	C	279	LLP	C4'-NZ	2.95	1.36	1.27
1	A	279	LLP	C4'-NZ	3.04	1.36	1.27
1	A	279	LLP	C4-C4'	3.16	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	279	LLP	C4'-NZ	3.31	1.37	1.27
1	C	279	LLP	C4-C4'	3.39	1.52	1.46
1	B	279	LLP	CE-NZ	3.78	1.54	1.46
1	A	279	LLP	CD-CE	3.84	1.63	1.51
1	C	279	LLP	CE-NZ	3.92	1.55	1.46
1	D	279	LLP	C4-C4'	4.13	1.53	1.46
1	A	279	LLP	CE-NZ	5.21	1.57	1.46
1	D	279	LLP	CE-NZ	5.79	1.58	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	279	LLP	OP2-P-OP4	-3.71	95.89	106.56
1	B	279	LLP	C5'-C5-C6	-3.26	113.12	119.28
1	A	279	LLP	C3-C4-C5	-3.00	115.86	118.11
1	D	279	LLP	C4-C4'-NZ	-2.99	108.42	125.06
1	C	279	LLP	C3-C4-C5	-2.99	115.87	118.11
1	B	279	LLP	C4-C4'-NZ	-2.90	108.93	125.06
1	C	279	LLP	C4-C4'-NZ	-2.61	110.56	125.06
1	A	279	LLP	C5'-C5-C6	-2.53	114.49	119.28
1	B	279	LLP	O-C-CA	-2.44	119.13	125.49
1	B	279	LLP	OP2-P-OP4	-2.36	99.76	106.56
1	A	279	LLP	C4-C4'-NZ	-2.25	112.54	125.06
1	D	279	LLP	C3-C4-C5	-2.24	116.43	118.11
1	C	279	LLP	C5'-C5-C6	-2.23	115.05	119.28
1	D	279	LLP	O-C-CA	-2.20	119.76	125.49
1	D	279	LLP	C5'-C5-C6	-2.19	115.14	119.28
1	A	279	LLP	O-C-CA	-2.18	119.81	125.49
1	D	279	LLP	OP3-P-OP4	-2.10	100.50	106.56
1	B	279	LLP	C3-C4-C5	-2.07	116.56	118.11
1	D	279	LLP	C5'-C5-C4	2.08	124.96	121.47
1	C	279	LLP	C5'-C5-C4	2.11	125.02	121.47
1	B	279	LLP	OP3-P-OP2	2.31	116.19	107.38
1	B	279	LLP	C5'-C5-C4	2.50	125.67	121.47
1	C	279	LLP	OP2-P-OP1	2.53	118.72	110.58
1	D	279	LLP	C5-C4-C4'	2.57	125.21	121.52
1	D	279	LLP	OP2-P-OP1	3.32	121.26	110.58
1	A	279	LLP	OP4-C5'-C5	7.86	121.98	108.99
1	B	279	LLP	OP4-C5'-C5	9.63	124.91	108.99
1	C	279	LLP	OP4-C5'-C5	10.35	126.10	108.99
1	A	279	LLP	CD-CE-NZ	10.48	128.13	110.98
1	D	279	LLP	OP4-C5'-C5	11.21	127.53	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates 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	A	1	-	5,5,5	0.58	0	5,5,5	1.63	2 (40%)
2	GOL	A	431	-	5,5,5	0.51	0	5,5,5	0.54	0
2	GOL	A	432	-	5,5,5	0.70	0	5,5,5	1.02	0
2	GOL	B	1	-	5,5,5	0.41	0	5,5,5	0.67	0
2	GOL	B	431	-	5,5,5	0.93	0	5,5,5	1.15	1 (20%)
2	GOL	C	1	-	5,5,5	0.25	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	A	1	-	-	0/4/4/4	0/0/0/0
2	GOL	A	431	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	432	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1	-	-	0/4/4/4	0/0/0/0
2	GOL	B	431	-	-	0/4/4/4	0/0/0/0
2	GOL	C	1	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	GOL	O2-C2-C1	-2.05	99.26	108.65
2	B	431	GOL	O2-C2-C3	2.07	118.15	108.65
2	A	1	GOL	C3-C2-C1	2.15	119.56	111.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	GOL	2	0
2	A	432	GOL	3	0
2	B	1	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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	400/401 (99%)	-0.38	2 (0%) 91 92	17, 31, 44, 53	0
1	B	400/401 (99%)	-0.25	7 (1%) 71 75	20, 34, 63, 84	0
1	C	400/401 (99%)	-0.24	3 (0%) 87 89	18, 33, 50, 61	0
1	D	400/401 (99%)	0.33	33 (8%) 14 15	20, 53, 85, 91	0
All	All	1600/1604 (99%)	-0.13	45 (2%) 56 61	17, 35, 73, 91	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	398	PHE	4.6
1	D	353	SER	4.1
1	B	55	THR	4.0
1	D	45	LEU	4.0
1	D	55	THR	3.8
1	D	396	LYS	3.3
1	D	342	GLN	3.3
1	B	46	GLY	3.2
1	D	426	HIS	3.1
1	C	89	ALA	3.1
1	A	41	PRO	3.0
1	D	366	GLY	2.9
1	D	53	ARG	2.9
1	D	369	HIS	2.7
1	D	274	CYS	2.6
1	C	85	ALA	2.6
1	B	372	GLN	2.5
1	D	368	SER	2.5
1	D	41	PRO	2.4
1	D	57	SER	2.4
1	D	241	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	381	PHE	2.4
1	D	338	LYS	2.4
1	B	53	ARG	2.3
1	D	56	ASN	2.3
1	D	245	ALA	2.3
1	D	423	HIS	2.3
1	D	387	LYS	2.3
1	D	40	PRO	2.3
1	D	49	GLU	2.2
1	B	397	GLU	2.2
1	D	367	SER	2.2
1	B	52	LYS	2.2
1	B	273	LEU	2.2
1	D	184	PRO	2.2
1	D	380	MET	2.2
1	A	89	ALA	2.1
1	D	364	LYS	2.1
1	D	116	GLU	2.1
1	D	395	THR	2.1
1	D	46	GLY	2.0
1	D	397	GLU	2.0
1	C	244	MET	2.0
1	D	54	ASP	2.0
1	D	371	TRP	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. 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
1	LLP	B	279	24/25	0.97	0.18	-	29,36,43,47	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	D	279	24/25	0.95	0.19	-	33,51,57,59	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	B	431	6/6	0.65	0.44	12.39	49,57,60,61	0
2	GOL	A	432	6/6	0.95	0.23	6.20	33,36,37,40	0
2	GOL	C	1	6/6	0.90	0.22	4.22	61,62,62,63	0
2	GOL	B	1	6/6	0.96	0.15	3.08	39,43,44,49	0
2	GOL	A	1	6/6	0.83	0.25	2.08	36,47,51,54	0
2	GOL	A	431	6/6	0.96	0.19	1.63	40,41,43,47	0

6.5 Other polymers (i)

There are no such residues in this entry.