



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:51 PM UTC

PDB ID : 3HLM / pdb_00003hlm
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

<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

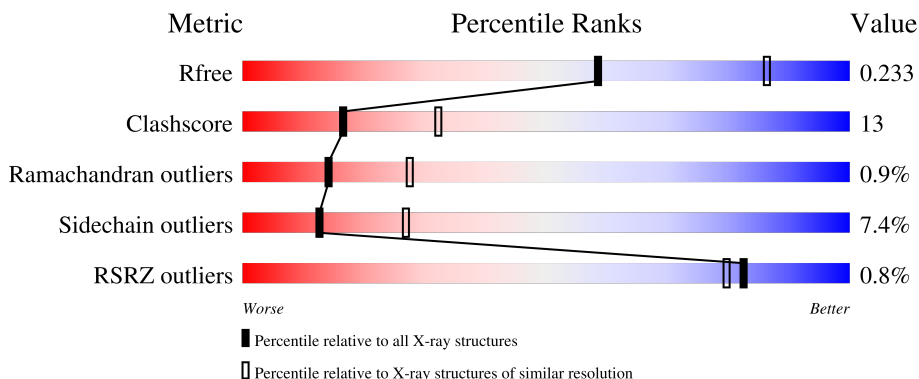
1 Overall quality at a glance i

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 ≥ 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	1	-	-	X	-

2 Entry composition [i](#)

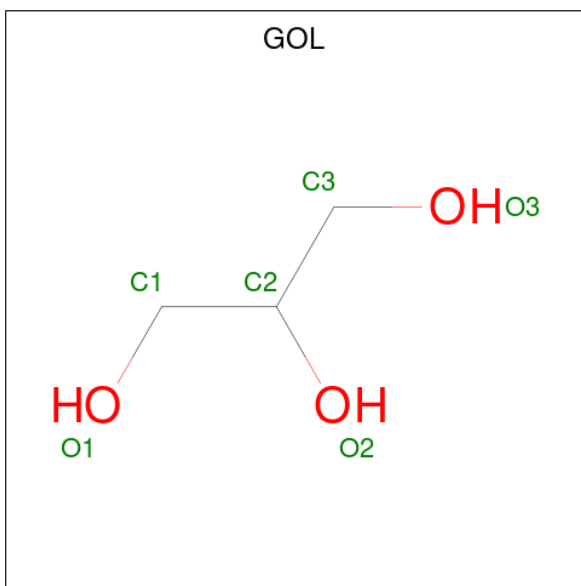
There are 3 unique types of molecules in this entry. The entry contains 13309 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: GOL) (formula: C₃H₈O₃).



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

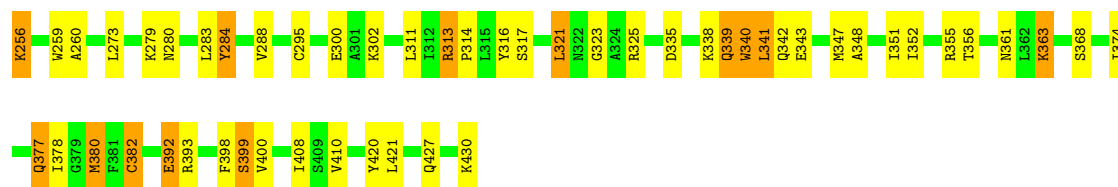
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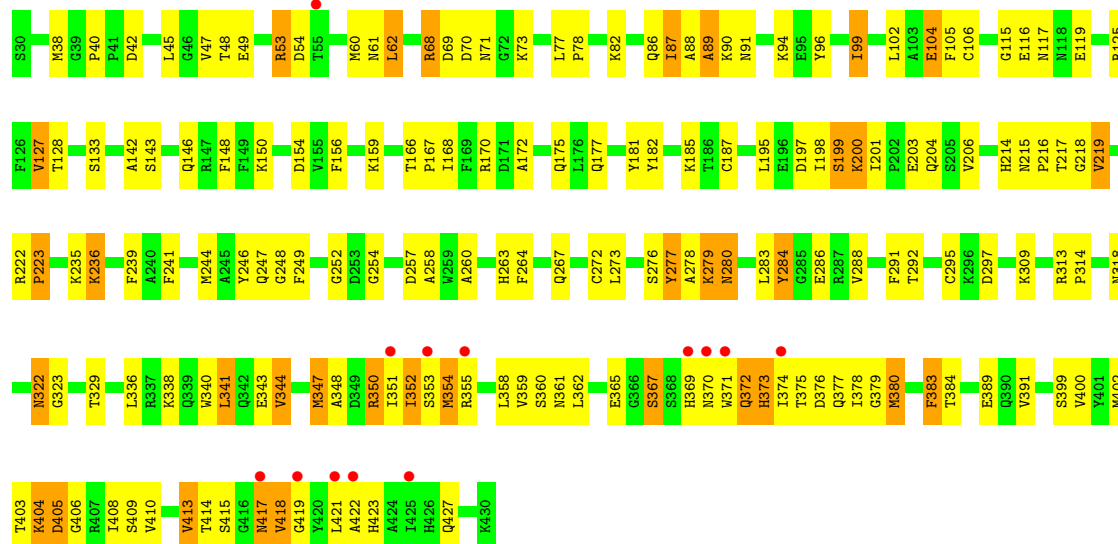
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

- 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		



- 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, 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) 92.2 (29.90-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtrriage
Anisotropy	0.230	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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 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	1.49	16/3203 (0.5%)	1.28	13/4326 (0.3%)
1	B	1.44	13/3203 (0.4%)	1.24	12/4326 (0.3%)
1	C	1.58	18/3203 (0.6%)	1.33	21/4326 (0.5%)
1	D	1.29	7/3203 (0.2%)	1.23	13/4326 (0.3%)
All	All	1.46	54/12812 (0.4%)	1.27	59/17304 (0.3%)

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	64	VAL	CA-CB	8.36	1.64	1.54
1	C	351	ILE	CA-CB	8.32	1.63	1.54
1	C	168	ILE	CA-CB	8.23	1.64	1.54
1	A	64	VAL	CA-CB	8.21	1.62	1.54
1	A	127	VAL	C-O	-7.62	1.16	1.24
1	C	316	TYR	CA-C	6.95	1.60	1.52
1	A	129	VAL	C-O	-6.64	1.17	1.24
1	D	40	PRO	CA-C	6.44	1.55	1.51
1	A	128	THR	C-O	-6.32	1.16	1.24
1	C	35	HIS	CA-C	6.15	1.61	1.52
1	B	221	PRO	N-CA	-6.11	1.39	1.46
1	C	166	THR	CA-CB	6.05	1.61	1.53
1	A	321	LEU	C-O	-5.96	1.17	1.24
1	B	77	LEU	CA-C	-5.92	1.46	1.53
1	C	260	ALA	CA-C	5.85	1.60	1.52
1	C	152	SER	N-CA	-5.83	1.38	1.46
1	B	120	VAL	CA-CB	5.70	1.61	1.54
1	B	211	ALA	CA-CB	-5.68	1.44	1.53
1	B	210	HIS	C-O	-5.64	1.17	1.24
1	C	153	ARG	C-O	-5.64	1.16	1.24
1	A	75	TYR	C-O	-5.63	1.17	1.23
1	C	177	GLN	CA-C	-5.63	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	236	LYS	CA-C	5.63	1.60	1.52
1	C	207	LEU	C-O	-5.62	1.17	1.24
1	A	209	LEU	C-O	5.58	1.30	1.23
1	A	126	PHE	C-O	-5.51	1.17	1.23
1	A	259	TRP	CA-CB	5.47	1.61	1.53
1	C	382	CYS	C-O	-5.43	1.17	1.24
1	A	196	GLU	CA-C	5.40	1.59	1.52
1	C	206	VAL	C-O	-5.38	1.18	1.24
1	D	119	GLU	CA-C	5.37	1.60	1.52
1	B	245	ALA	CA-C	5.37	1.60	1.52
1	B	293	VAL	C-O	5.37	1.30	1.24
1	B	213	ALA	CA-CB	-5.36	1.45	1.53
1	C	361	ASN	C-O	-5.36	1.17	1.24
1	A	76	VAL	CA-CB	-5.33	1.47	1.54
1	D	219	VAL	CA-CB	-5.30	1.47	1.54
1	B	311	LEU	C-O	-5.30	1.17	1.24
1	A	356	THR	CA-CB	5.23	1.61	1.53
1	C	316	TYR	N-CA	5.20	1.50	1.46
1	C	400	VAL	C-O	-5.18	1.17	1.23
1	D	96	TYR	C-O	-5.14	1.17	1.23
1	C	178	GLY	C-O	5.14	1.30	1.23
1	B	166	THR	CA-CB	5.13	1.61	1.53
1	D	106	CYS	CA-C	-5.13	1.46	1.52
1	C	302	LYS	N-CA	5.13	1.52	1.46
1	B	76	VAL	CA-CB	-5.09	1.47	1.54
1	A	206	VAL	C-O	-5.07	1.18	1.24
1	B	344	VAL	CA-CB	5.06	1.59	1.54
1	A	409	SER	N-CA	-5.05	1.40	1.46
1	D	38	MET	C-O	-5.04	1.17	1.23
1	B	359	VAL	CA-CB	5.03	1.60	1.54
1	A	339	GLN	CA-C	5.02	1.59	1.52
1	A	76	VAL	C-O	-5.00	1.18	1.24

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	213	ALA	N-CA-C	7.51	120.41	111.02
1	D	297	ASP	N-CA-C	7.48	119.06	108.74
1	A	321	LEU	N-CA-C	6.92	118.71	111.03
1	B	385	GLY	N-CA-C	-6.87	105.76	113.79
1	D	322	ASN	N-CA-C	6.77	119.24	111.11
1	C	393	ARG	N-CA-C	6.64	118.51	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	ALA	N-CA-C	-6.63	103.98	111.07
1	A	318	ASN	N-CA-C	6.54	114.02	108.13
1	C	313	ARG	CA-C-N	-6.51	113.22	120.45
1	C	313	ARG	C-N-CA	-6.51	113.22	120.45
1	C	90	LYS	N-CA-C	-6.35	104.79	113.30
1	B	365	GLU	N-CA-C	-6.30	105.46	113.02
1	A	261	VAL	CB-CA-C	-6.15	104.00	111.88
1	C	380	MET	N-CA-C	6.10	120.56	113.18
1	A	385	GLY	N-CA-C	-6.09	106.23	115.00
1	B	288	VAL	CB-CA-C	-6.01	102.24	110.77
1	D	380	MET	N-CA-C	5.95	120.26	113.19
1	B	228	GLU	N-CA-C	5.89	117.78	111.36
1	D	318	ASN	N-CA-C	5.83	113.47	108.22
1	C	347	MET	N-CA-C	-5.82	104.94	112.68
1	A	120	VAL	N-CA-C	-5.79	104.86	110.42
1	B	418	VAL	CA-C-N	5.74	126.47	119.99
1	B	418	VAL	C-N-CA	5.74	126.47	119.99
1	D	413	VAL	N-CA-C	5.67	112.27	106.21
1	A	132	ILE	CB-CA-C	-5.66	106.88	113.22
1	A	88	ALA	N-CA-C	-5.65	105.20	111.36
1	C	180	ARG	N-CA-C	5.56	118.24	109.96
1	C	377	GLN	N-CA-C	-5.54	103.21	110.53
1	C	368	SER	N-CA-C	-5.53	105.84	112.59
1	C	39	GLY	CA-C-N	-5.51	114.70	120.38
1	C	39	GLY	C-N-CA	-5.51	114.70	120.38
1	D	218	GLY	N-CA-C	-5.49	107.09	115.00
1	B	211	ALA	N-CA-C	5.44	117.28	111.36
1	B	97	LEU	CA-C-N	-5.43	115.00	120.21
1	B	97	LEU	C-N-CA	-5.43	115.00	120.21
1	B	366	GLY	N-CA-C	5.38	125.94	113.18
1	A	97	LEU	CA-C-N	-5.38	114.09	120.11
1	A	97	LEU	C-N-CA	-5.38	114.09	120.11
1	B	335	ASP	N-CA-C	5.35	116.97	111.03
1	C	143	SER	N-CA-C	-5.35	105.62	111.82
1	C	253	ASP	N-CA-C	5.32	118.38	107.69
1	A	318	ASN	CA-C-N	5.29	125.83	120.38
1	A	318	ASN	C-N-CA	5.29	125.83	120.38
1	C	219	VAL	N-CA-C	5.29	115.71	107.99
1	C	91	ASN	N-CA-C	5.26	118.69	111.54
1	D	365	GLU	N-CA-C	-5.26	101.59	109.95
1	B	380	MET	N-CA-C	5.22	119.75	113.17
1	A	116	GLU	N-CA-C	5.22	117.39	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	177	GLN	N-CA-C	-5.20	101.52	108.86
1	D	168	ILE	N-CA-C	5.18	115.79	110.36
1	C	363	LYS	N-CA-C	-5.13	104.65	112.04
1	C	180	ARG	CB-CA-C	-5.11	102.81	110.16
1	C	321	LEU	N-CA-C	5.08	116.63	111.14
1	D	154	ASP	N-CA-C	5.08	117.89	109.46
1	C	283	LEU	N-CA-C	5.07	119.33	113.20
1	D	277	TYR	N-CA-C	-5.07	105.47	113.02
1	D	89	ALA	N-CA-C	-5.03	104.88	111.02
1	A	159	LYS	CB-CA-C	-5.00	105.22	110.17
1	D	347	MET	N-CA-C	-5.00	106.28	112.93

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	3128	50	0
1	B	3155	0	3128	53	0
1	C	3155	0	3128	77	0
1	D	3155	0	3129	154	0
2	A	18	0	24	4	0
2	B	12	0	16	4	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	12561	326	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 13.

All (326) 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:60:MET:HE3	1:D:417:ASN:HD21	1.03	1.08
1:D:78:PRO:HD2	1:D:343:GLU:OE2	1.56	1.06
1:D:249:PHE:HZ	1:D:380:MET:HE2	1.21	1.05
1:D:60:MET:HE3	1:D:417:ASN:ND2	1.72	1.04
1:C:81:ARG:HA	3:C:519:HOH:O	1.56	1.04
1:D:249:PHE:CZ	1:D:380:MET:HE2	1.95	1.01
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: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: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:C:60:MET:HE1	1:C:421:LEU:HD22	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:86:GLN:O	1:C:87:ILE:C	2.30	0.72
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:B:224:GLU:CD	1:B:224:GLU:H	2.00	0.69
1:C:170:ARG:HD3	3:C:494:HOH:O	1.93	0.69
1:D:249:PHE:CZ	1:D:380:MET:CE	2.74	0.68
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: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:78:PRO:HD2	1:D:343:GLU:CD	2.18	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:B:244:MET:HE2	1:B:273:LEU:HD11	1.78	0.66
1:C:78:PRO:HD2	1:C:343:GLU:CD	2.17	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:60:MET:HE2	1:B:62:LEU:HD21	1.79	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:283:LEU:O	1:D:284:TYR:C	2.40	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:C:244:MET:HE2	1:C:273:LEU:HD11	1.81	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:MET:HE2	1:C:62:LEU:HD21	1.83	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:125:ARG:O	1:D:125:ARG:HG3	2.00	0.60
1:D:404:LYS:C	1:D:406:GLY:H	2.08	0.60
1:A:389:GLU:CD	1:A:389:GLU:H	2.10	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
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:A:78:PRO:HD2	1:A:343:GLU:CD	2.28	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:D:415:SER:C	1:D:417:ASN:H	2.11	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:B:45:LEU:O	1:B:46:GLY:C	2.43	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:D:402:MET:HE2	1:D:408:ILE:HG22	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:MET:SD	1:D:421:LEU:HD13	2.45	0.56
1:D:370:ASN:C	1:D:371:TRP:CD1	2.83	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:373:HIS:O	1:D:374:ILE:C	2.48	0.56
1:D:127:VAL:O	1:D:292:THR:HA	2.05	0.56
1:D:417:ASN:OD1	1:D:417:ASN:C	2.48	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:339:GLN:O	1:C:340:TRP:C	2.50	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
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:60:MET:HE1	1:A:421:LEU:HD22	1.90	0.54
1:D:128:THR:HA	1:D:291:PHE:O	2.07	0.54
1:A:208:LEU:C	1:A:208:LEU:HD23	2.33	0.54
1:A:214:HIS:CE1	1:A:217:THR:HG23	2.43	0.54
1:B:208:LEU:C	1:B:208:LEU:HD23	2.31	0.54
1:D:288:VAL:HG22	1:D:323:GLY:HA3	1.88	0.54
1:D:389:GLU:CD	1:D:389:GLU:H	2.15	0.54
1:C:340:TRP:CZ3	1:C:341:LEU:CD1	2.91	0.54
1:A:69:ASP:C	1:A:69:ASP:OD1	2.50	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:404:LYS:C	1:D:406:GLY:N	2.66	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:373:HIS:C	1:D:375:THR:N	2.64	0.52
1:A:38:MET:HE1	1:B:302:LYS:HE2	1.91	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:244:MET:HE2	1:D:273:LEU:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:VAL:HA	1:D:362:LEU:HD12	1.92	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: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:208:LEU:HD23	1:C:208:LEU:C	2.36	0.51
1:C:335:ASP:O	1:C:338:LYS:HB3	2.11	0.50
1:C:125:ARG:O	1:C:125:ARG:HG3	2.11	0.50
1:D:286:GLU:CD	1:D:322:ASN:HD22	2.19	0.50
1:B:283:LEU:O	1:B:284:TYR:C	2.54	0.49
1:C:256:LYS:HE3	3:C:561:HOH:O	2.13	0.49
1:C:112:LEU:O	1:C:112:LEU:HD12	2.12	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:C:420:TYR:O	1:C:421:LEU:C	2.53	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: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: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:222:ARG:O	1:D:223:PRO:C	2.57	0.46
1:C:280:ASN:OD1	1:C:280:ASN:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:33:TRP:O	1:B:34:THR:C	2.57	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
1:B:369:HIS:HE1	1:B:429:THR:O	1.97	0.46
1:D:185:LYS:O	3:D:465:HOH:O	2.21	0.46
1:D:403:THR:OG1	1:D:405:ASP:OD1	2.30	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:164:ASN:O	1:A:165:HIS:C	2.59	0.45
1:A:313:ARG:HB3	1:A:314:PRO:HD3	1.98	0.45
1:D:90:LYS:O	1:D:91:ASN:HB3	2.15	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:112:LEU:HD12	1:C:112:LEU:C	2.41	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:C:69:ASP:OD1	1:C:69:ASP:C	2.58	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:C:146:GLN:HG3	1:C:172:ALA:O	2.17	0.45
1:D:60:MET:HE3	1:D:417:ASN:CG	2.36	0.45
1:D:69:ASP:OD1	1:D:69:ASP:C	2.60	0.44
1:D:105:PHE:CD2	1:D:105:PHE:C	2.94	0.44
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:D:246:TYR:O	1:D:247:GLN:C	2.60	0.44
1:D:415:SER:C	1:D:417:ASN:N	2.75	0.44
1:C:66:ALA:HA	1:C:380:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:402:MET:HE2	1:D:408:ILE:CG2	2.47	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:B:44:ILE:O	1:B:45:LEU:C	2.62	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
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:D:354:MET:HE3	1:D:354:MET:HB2	1.66	0.42
1:A:283:LEU:O	1:A:284:TYR:C	2.62	0.42
1:C:295:CYS:HB3	1:C:300:GLU:OE1	2.19	0.42
1:B:69:ASP:OD1	1:B:69:ASP:C	2.62	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:D:88:ALA:O	1:D:89:ALA:C	2.62	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:D:373:HIS:C	1:D:375:THR:H	2.26	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:C:190:ASP:C	1:C:190:ASP:OD1	2.62	0.42
1:D:86:GLN:HE21	1:D:86:GLN:HB3	1.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:SER:OG	1:A:279:LLP:OP2	2.29	0.41
1:D:77:LEU:HD12	1:D:77:LEU:N	2.34	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:B:364:LYS:C	1:B:366:GLY:H	2.27	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:421:LEU:O	1:D:422:ALA:C	2.64	0.41
1:A:224:GLU:HB3	1:C:224:GLU:OE2	2.21	0.41
1:B:69:ASP:HB2	2:B:1:GOL:HO3	1.82	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: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
1:A:93:ASP:OD1	1:A:93:ASP:C	2.64	0.41
1:C:321:LEU:HD22	1:C:325:ARG:NE	2.36	0.41
1:A:354:MET:HA	1:A:354:MET:HE2	2.03	0.40
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:C:118:ASN:O	1:C:119:GLU:C	2.65	0.40
1:B:42:ASP:O	1:B:43:PRO:C	2.64	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: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:A:325:ARG:O	1:A:326:ILE:C	2.65	0.40
1:B:93:ASP:OD1	1:B:93:ASP:C	2.65	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%)	24	43
1	B	398/401 (99%)	379 (95%)	18 (4%)	1 (0%)	36	55
1	C	398/401 (99%)	369 (93%)	24 (6%)	5 (1%)	9	18
1	D	398/401 (99%)	351 (88%)	41 (10%)	6 (2%)	8	16
All	All	1592/1604 (99%)	1479 (93%)	99 (6%)	14 (1%)	14	27

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	TYR
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%)	321 (96%)	12 (4%)	31	58
1	B	333/333 (100%)	305 (92%)	28 (8%)	10	22
1	C	333/333 (100%)	310 (93%)	23 (7%)	14	30
1	D	333/333 (100%)	298 (90%)	35 (10%)	6	14
All	All	1332/1332 (100%)	1234 (93%)	98 (7%)	13	27

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	THR
1	A	80	VAL
1	A	82	LYS
1	A	104	GLU
1	A	107	LYS
1	A	150	LYS
1	A	224	GLU
1	A	308	LEU
1	A	333	SER
1	A	338	LYS
1	A	345	LYS
1	A	382	CYS
1	B	34	THR
1	B	44	ILE
1	B	48	THR
1	B	52	LYS
1	B	55	THR
1	B	70	ASP
1	B	79	SER
1	B	84	GLU
1	B	90	LYS
1	B	104	GLU
1	B	116	GLU
1	B	117	ASN
1	B	132	ILE
1	B	133	SER
1	B	207	LEU
1	B	224	GLU
1	B	227	LYS
1	B	311	LEU
1	B	344	VAL
1	B	360	SER
1	B	364	LYS

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Mol	Chain	Res	Type
1	B	367	SER
1	B	368	SER
1	B	374	ILE
1	B	383	PHE
1	B	387	LYS
1	B	392	GLU
1	B	396	LYS
1	C	30	SER
1	C	48	THR
1	C	70	ASP
1	C	86	GLN
1	C	87	ILE
1	C	90	LYS
1	C	99	ILE
1	C	111	GLU
1	C	123	SER
1	C	133	SER
1	C	150	LYS
1	C	207	LEU
1	C	219	VAL
1	C	224	GLU
1	C	256	LYS
1	C	311	LEU
1	C	341	LEU
1	C	342	GLN
1	C	356	THR
1	C	363	LYS
1	C	378	ILE
1	C	392	GLU
1	C	399	SER
1	D	47	VAL
1	D	53	ARG
1	D	62	LEU
1	D	68	ARG
1	D	70	ASP
1	D	71	ASN
1	D	87	ILE
1	D	99	ILE
1	D	104	GLU
1	D	127	VAL
1	D	133	SER
1	D	143	SER

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Mol	Chain	Res	Type
1	D	159	LYS
1	D	199	SER
1	D	200	LYS
1	D	223	PRO
1	D	235	LYS
1	D	338	LYS
1	D	341	LEU
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	383	PHE
1	D	400	VAL
1	D	404	LYS
1	D	409	SER
1	D	417	ASN
1	D	418	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	117	ASN
1	A	146	GLN
1	A	361	ASN
1	A	427	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
1	B	426	HIS
1	C	35	HIS
1	C	263	HIS

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Mol	Chain	Res	Type
1	C	275	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	214	HIS
1	D	263	HIS
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	2.43	7 (30%)	25,32,34	2.61	8 (32%)
1	LLP	A	279	1	23,24,25	3.30	13 (56%)	25,32,34	2.52	7 (28%)
1	LLP	C	279	1	23,24,25	3.00	12 (52%)	25,32,34	2.40	6 (24%)
1	LLP	B	279	1	23,24,25	2.82	12 (52%)	25,32,34	2.23	6 (24%)

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	D	279	1	-	7/16/17/19	0/1/1/1
1	LLP	A	279	1	-	9/16/17/19	0/1/1/1
1	LLP	C	279	1	-	7/16/17/19	0/1/1/1
1	LLP	B	279	1	-	7/16/17/19	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	-7.95	1.18	1.36
1	A	279	LLP	O3-C3	-7.75	1.19	1.36
1	B	279	LLP	O3-C3	-7.35	1.20	1.36
1	D	279	LLP	O3-C3	-6.96	1.21	1.36
1	A	279	LLP	C3-C2	-5.53	1.35	1.41
1	D	279	LLP	CE-NZ	5.36	1.58	1.46
1	C	279	LLP	P-OP3	-5.15	1.35	1.54
1	A	279	LLP	P-OP3	-5.11	1.35	1.54
1	A	279	LLP	CE-NZ	4.82	1.57	1.46
1	C	279	LLP	C3-C2	-4.82	1.36	1.41
1	A	279	LLP	P-OP1	-4.69	1.35	1.50
1	A	279	LLP	P-OP2	-4.66	1.37	1.54
1	B	279	LLP	P-OP3	-4.44	1.38	1.54
1	B	279	LLP	P-OP2	-4.34	1.38	1.54
1	C	279	LLP	P-OP1	-4.03	1.37	1.50
1	B	279	LLP	C3-C2	-4.03	1.36	1.41
1	C	279	LLP	P-OP2	-3.98	1.40	1.54
1	C	279	LLP	CE-NZ	3.63	1.55	1.46
1	B	279	LLP	P-OP1	-3.62	1.39	1.50
1	A	279	LLP	CD-CE	3.51	1.63	1.51
1	A	279	LLP	P-OP4	-3.50	1.49	1.60
1	B	279	LLP	CE-NZ	3.50	1.54	1.46
1	D	279	LLP	C4-C4'	3.40	1.53	1.46
1	D	279	LLP	C2-N1	3.27	1.39	1.33
1	D	279	LLP	C4'-NZ	3.07	1.37	1.27
1	B	279	LLP	C4-C5	-2.94	1.37	1.42
1	A	279	LLP	C4'-NZ	2.83	1.36	1.27
1	C	279	LLP	C4-C4'	2.79	1.52	1.46
1	B	279	LLP	P-OP4	-2.76	1.51	1.60
1	C	279	LLP	C4'-NZ	2.75	1.36	1.27
1	C	279	LLP	C4-C5	-2.73	1.38	1.42
1	C	279	LLP	C4-C3	-2.70	1.36	1.41
1	C	279	LLP	P-OP4	-2.69	1.51	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	LLP	C4-C4'	2.61	1.52	1.46
1	A	279	LLP	CA-N	-2.60	1.40	1.48
1	B	279	LLP	C4-C3	-2.55	1.36	1.41
1	B	279	LLP	C4'-NZ	2.27	1.34	1.27
1	A	279	LLP	C4-C5	-2.25	1.38	1.42
1	B	279	LLP	CA-N	-2.15	1.42	1.48
1	A	279	LLP	C4-C3	-2.15	1.37	1.41
1	D	279	LLP	C6-N1	2.13	1.38	1.34
1	D	279	LLP	CD-CE	2.10	1.58	1.51
1	C	279	LLP	CD-CE	2.06	1.58	1.51
1	B	279	LLP	C4-C4'	2.04	1.51	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	279	LLP	OP4-C5'-C5	9.69	127.53	109.36
1	C	279	LLP	OP4-C5'-C5	8.93	126.10	109.36
1	B	279	LLP	OP4-C5'-C5	8.30	124.91	109.36
1	A	279	LLP	OP4-C5'-C5	6.73	121.98	109.36
1	A	279	LLP	CD-CE-NZ	6.54	128.13	110.83
1	D	279	LLP	C4-C3-C2	5.02	122.97	120.14
1	C	279	LLP	C4-C3-C2	4.85	122.87	120.14
1	A	279	LLP	OP2-P-OP4	-4.13	95.89	106.67
1	B	279	LLP	C5'-C5-C6	-3.83	113.12	119.36
1	D	279	LLP	C4-C4'-NZ	-3.38	108.42	124.04
1	B	279	LLP	C4-C4'-NZ	-3.27	108.93	124.04
1	A	279	LLP	C4-C3-C2	3.20	121.94	120.14
1	A	279	LLP	C3-C4-C5	-3.01	115.86	118.28
1	C	279	LLP	C3-C4-C5	-3.00	115.87	118.28
1	A	279	LLP	C5'-C5-C6	-2.99	114.49	119.36
1	C	279	LLP	C4-C4'-NZ	-2.92	110.56	124.04
1	D	279	LLP	OP2-P-OP1	2.68	121.26	110.83
1	B	279	LLP	OP2-P-OP4	-2.65	99.76	106.67
1	C	279	LLP	C5'-C5-C6	-2.64	115.05	119.36
1	D	279	LLP	C5'-C5-C6	-2.59	115.14	119.36
1	A	279	LLP	C4-C4'-NZ	-2.49	112.54	124.04
1	D	279	LLP	C5-C4-C4'	2.42	125.21	121.47
1	D	279	LLP	OP3-P-OP4	-2.36	100.50	106.67
1	D	279	LLP	C3-C4-C5	-2.30	116.43	118.28
1	B	279	LLP	OP3-P-OP2	2.24	116.19	107.80
1	B	279	LLP	C3-C4-C5	-2.14	116.56	118.28
1	C	279	LLP	OP2-P-OP1	2.02	118.72	110.83

There are no chirality outliers.

All (30) 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	C5-C4-C4'-NZ
1	D	279	LLP	C4-C4'-NZ-CE
1	D	279	LLP	CA-CB-CG-CD
1	C	279	LLP	CD-CE-NZ-C4'
1	C	279	LLP	C4-C4'-NZ-CE
1	D	279	LLP	CD-CE-NZ-C4'
1	B	279	LLP	CD-CE-NZ-C4'
1	A	279	LLP	CA-CB-CG-CD
1	B	279	LLP	C5-C4-C4'-NZ

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	279	LLP	2	0
1	A	279	LLP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	1	-	5,5,5	0.36	0	5,5,5	0.79	0
2	GOL	A	1	-	5,5,5	0.62	0	5,5,5	1.75	2 (40%)
2	GOL	A	431	-	5,5,5	0.49	0	5,5,5	0.69	0
2	GOL	B	431	-	5,5,5	1.01	0	5,5,5	1.16	1 (20%)
2	GOL	A	432	-	5,5,5	0.77	0	5,5,5	1.05	0
2	GOL	C	1	-	5,5,5	0.30	0	5,5,5	0.78	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	1	-	-	4/4/4/4	-
2	GOL	A	1	-	-	2/4/4/4	-
2	GOL	A	431	-	-	4/4/4/4	-
2	GOL	B	431	-	-	2/4/4/4	-
2	GOL	A	432	-	-	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	-2.40	99.26	109.18
2	B	431	GOL	O2-C2-C3	2.17	118.15	109.18
2	A	1	GOL	C3-C2-C1	2.12	119.56	111.80

There are no chirality outliers.

All (18) 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	431	GOL	O2-C2-C3-O3
2	A	432	GOL	O1-C1-C2-C3
2	A	432	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	GOL	4	0
2	A	1	GOL	2	0
2	A	432	GOL	2	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, 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	400/401 (99%)	-0.71	0 100 100	17, 31, 44, 53	0
1	B	400/401 (99%)	-0.55	0 100 100	20, 34, 63, 84	0
1	C	400/401 (99%)	-0.44	0 100 100	18, 33, 50, 61	0
1	D	400/401 (99%)	0.14	13 (3%) 49 45	20, 53, 85, 91	0
All	All	1600/1604 (99%)	-0.39	13 (0%) 82 80	17, 35, 73, 91	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	353	SER	3.2
1	D	419	GLY	3.0
1	D	422	ALA	2.7
1	D	351	ILE	2.7
1	D	425	ILE	2.3
1	D	355	ARG	2.2
1	D	421	LEU	2.2
1	D	369	HIS	2.1
1	D	370	ASN	2.1
1	D	55	THR	2.1
1	D	417	ASN	2.0
1	D	371	TRP	2.0
1	D	374	ILE	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, 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(\AA^2)	Q<0.9
1	LLP	A	279	24/25	0.93	0.10	18,28,35,38	0
1	LLP	D	279	24/25	0.93	0.10	33,51,57,59	0
1	LLP	C	279	24/25	0.94	0.09	18,27,41,43	0
1	LLP	B	279	24/25	0.95	0.09	29,36,43,47	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(\AA^2)	Q<0.9
2	GOL	B	431	6/6	0.70	0.22	49,57,60,61	0
2	GOL	C	1	6/6	0.75	0.21	61,62,62,63	0
2	GOL	A	1	6/6	0.80	0.17	36,47,51,54	0
2	GOL	A	431	6/6	0.93	0.08	40,41,43,47	0
2	GOL	B	1	6/6	0.93	0.08	39,43,44,49	0
2	GOL	A	432	6/6	0.94	0.15	33,36,37,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.