Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2024 – 08:58 AM EST

PDB ID	:	4OJN
Title	:	Crystal structure of human muscle L-lactate dehydrogenase
Authors	:	Kolappan, S.; Craig, L.
Deposited on	:	2014-01-21
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

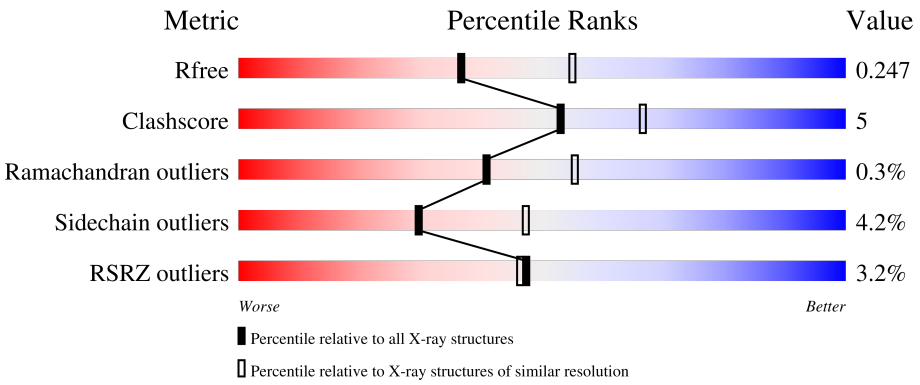
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	337	2% 89% 8%
1	B	337	2% 87% 11%
1	C	337	3% 85% 13%
1	D	337	4% 84% 14%
1	E	337	4% 84% 13%

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Mol	Chain	Length	Quality of chain
1	F	337	3% 82% 15%
1	G	337	2% 87% 11%
1	H	337	4% 82% 15%

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	1PE	H	400	-	-	X	-
3	GOL	E	402	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21736 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 L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	332	2661	1699	454	495	13	0	10	0
1	B	331	2604	1663	444	484	13	0	4	0
1	C	332	2637	1681	451	492	13	0	7	0
1	D	332	2664	1696	458	497	13	0	10	0
1	E	331	2613	1668	445	487	13	0	5	0
1	F	331	2666	1702	458	493	13	0	11	0
1	G	331	2639	1679	454	493	13	0	8	0
1	H	331	2579	1648	440	478	13	0	1	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	333	HIS	-	expression tag	UNP P00338
A	334	HIS	-	expression tag	UNP P00338
A	335	HIS	-	expression tag	UNP P00338
A	336	HIS	-	expression tag	UNP P00338
A	337	HIS	-	expression tag	UNP P00338
A	338	HIS	-	expression tag	UNP P00338
B	333	HIS	-	expression tag	UNP P00338
B	334	HIS	-	expression tag	UNP P00338
B	335	HIS	-	expression tag	UNP P00338
B	336	HIS	-	expression tag	UNP P00338
B	337	HIS	-	expression tag	UNP P00338
B	338	HIS	-	expression tag	UNP P00338
C	333	HIS	-	expression tag	UNP P00338

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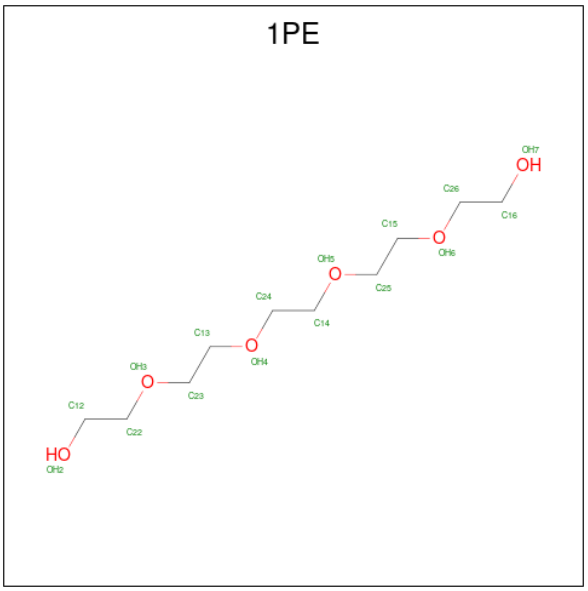
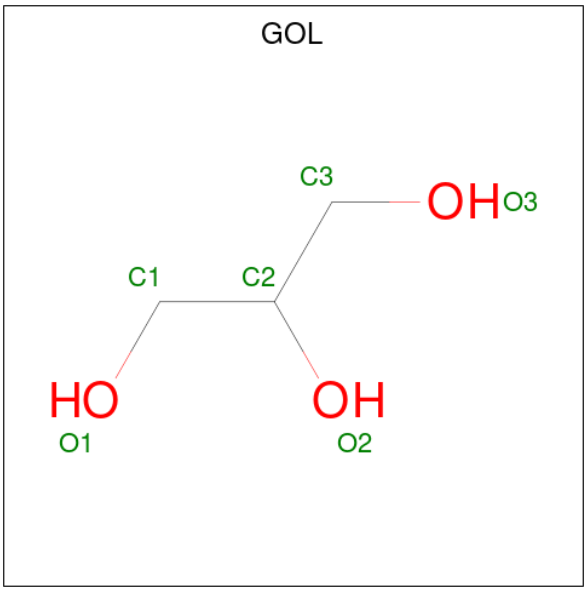
Chain	Residue	Modelled	Actual	Comment	Reference
C	334	HIS	-	expression tag	UNP P00338
C	335	HIS	-	expression tag	UNP P00338
C	336	HIS	-	expression tag	UNP P00338
C	337	HIS	-	expression tag	UNP P00338
C	338	HIS	-	expression tag	UNP P00338
D	333	HIS	-	expression tag	UNP P00338
D	334	HIS	-	expression tag	UNP P00338
D	335	HIS	-	expression tag	UNP P00338
D	336	HIS	-	expression tag	UNP P00338
D	337	HIS	-	expression tag	UNP P00338
D	338	HIS	-	expression tag	UNP P00338
E	333	HIS	-	expression tag	UNP P00338
E	334	HIS	-	expression tag	UNP P00338
E	335	HIS	-	expression tag	UNP P00338
E	336	HIS	-	expression tag	UNP P00338
E	337	HIS	-	expression tag	UNP P00338
E	338	HIS	-	expression tag	UNP P00338
F	333	HIS	-	expression tag	UNP P00338
F	334	HIS	-	expression tag	UNP P00338
F	335	HIS	-	expression tag	UNP P00338
F	336	HIS	-	expression tag	UNP P00338
F	337	HIS	-	expression tag	UNP P00338
F	338	HIS	-	expression tag	UNP P00338
G	333	HIS	-	expression tag	UNP P00338
G	334	HIS	-	expression tag	UNP P00338
G	335	HIS	-	expression tag	UNP P00338
G	336	HIS	-	expression tag	UNP P00338
G	337	HIS	-	expression tag	UNP P00338
G	338	HIS	-	expression tag	UNP P00338
H	333	HIS	-	expression tag	UNP P00338
H	334	HIS	-	expression tag	UNP P00338
H	335	HIS	-	expression tag	UNP P00338
H	336	HIS	-	expression tag	UNP P00338
H	337	HIS	-	expression tag	UNP P00338
H	338	HIS	-	expression tag	UNP P00338

- Molecule 2 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	16	10	6	0	0
2	B	1	16	10	6	0	0
2	C	1	16	10	6	0	0
2	D	1	16	10	6	0	0
2	E	1	16	10	6	0	0
2	F	1	16	10	6	0	0
2	G	1	16	10	6	0	0
2	H	1	16	10	6	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	D	1	6	3	3	0	0
			Total	C	O		
3	D	1	6	3	3	0	0
			Total	C	O		
3	E	1	6	3	3	0	0

- Molecule 4 is water.

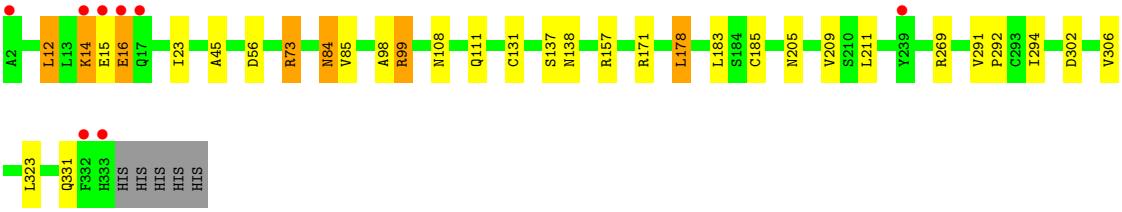
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	57	57	57	0	0
			Total	O		
4	B	66	66	66	0	0
			Total	O		
4	C	70	70	70	0	0
			Total	O		
4	D	84	84	84	0	0
			Total	O		
4	E	50	50	50	0	0
			Total	O		
4	F	66	66	66	0	0
			Total	O		
4	G	75	75	75	0	0
			Total	O		
4	H	59	59	59	0	0

3 Residue-property plots (i)

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.

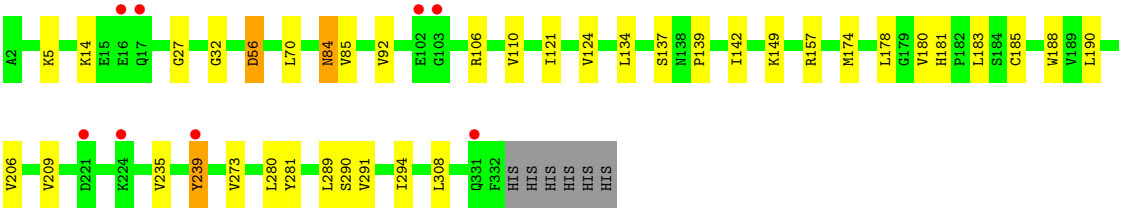
• Molecule 1: L-lactate dehydrogenase A chain

Chain A:



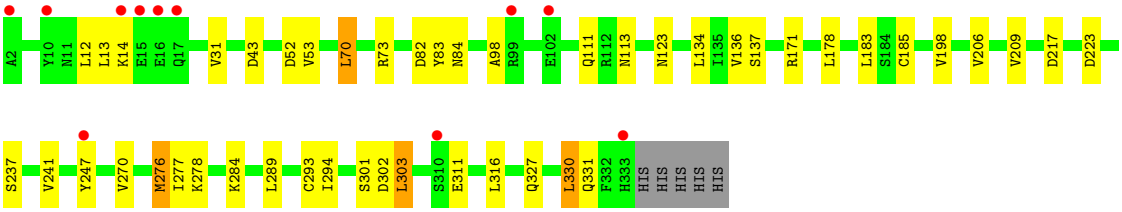
• Molecule 1: L-lactate dehydrogenase A chain

Chain B:



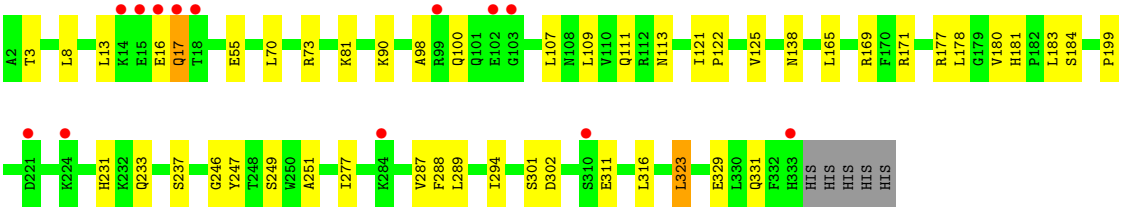
• Molecule 1: L-lactate dehydrogenase A chain

Chain C:



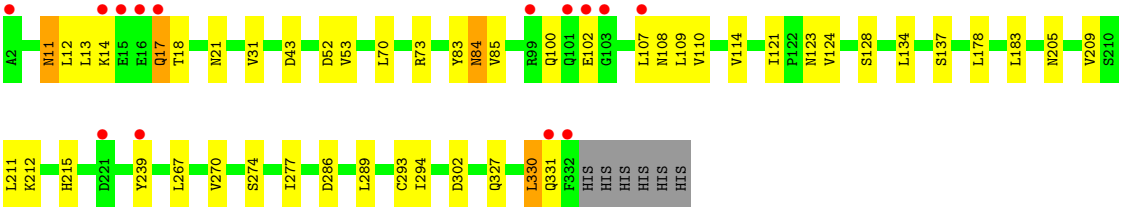
• Molecule 1: L-lactate dehydrogenase A chain

Chain D:



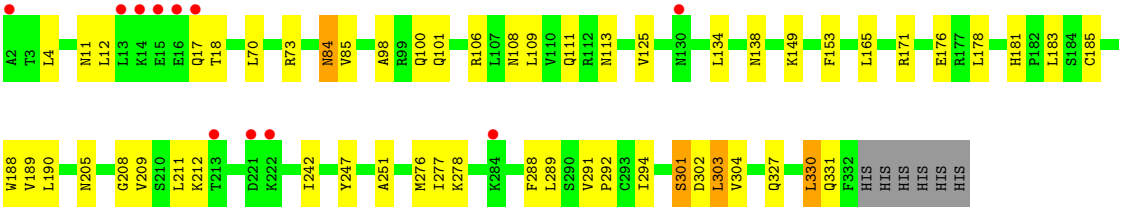
• Molecule 1: L-lactate dehydrogenase A chain

Chain E:



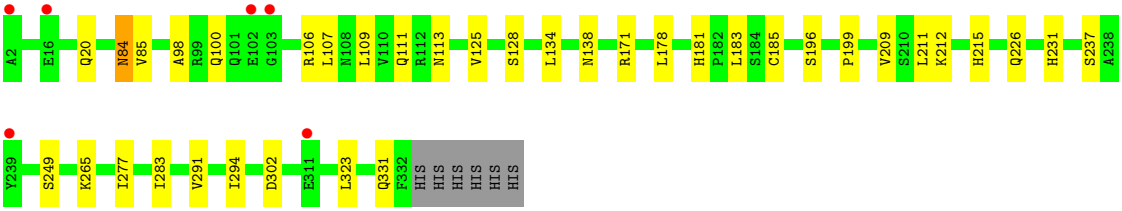
• Molecule 1: L-lactate dehydrogenase A chain

Chain F:



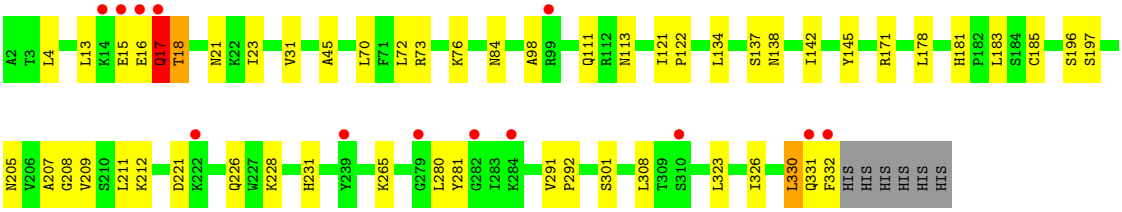
• Molecule 1: L-lactate dehydrogenase A chain

Chain G:



• Molecule 1: L-lactate dehydrogenase A chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	147.14Å 147.14Å 333.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.84 – 2.40 19.84 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.84-2.40) 99.8 (19.84-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.213 , 0.250 0.214 , 0.247	Depositor DCC
R_{free} test set	8138 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 38.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21736	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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, 0.333 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: 1PE, 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	0.47	0/2709	0.64	0/3663
1	B	0.49	0/2649	0.67	1/3584 (0.0%)
1	C	0.49	0/2682	0.67	1/3628 (0.0%)
1	D	0.47	0/2709	0.66	2/3661 (0.1%)
1	E	0.49	0/2658	0.68	0/3596
1	F	0.47	0/2711	0.65	0/3665
1	G	0.50	0/2683	0.66	0/3626
1	H	0.48	0/2624	0.68	0/3550
All	All	0.48	0/21425	0.66	4/28973 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	171	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	C	43	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	157	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	D	169	ARG	NE-CZ-NH2	5.19	122.90	120.30

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	2661	0	2733	23	0
1	B	2604	0	2681	28	0
1	C	2637	0	2707	39	0
1	D	2664	0	2735	37	0
1	E	2613	0	2686	33	0
1	F	2666	0	2749	39	0
1	G	2639	0	2712	18	0
1	H	2579	0	2661	40	0
2	A	16	0	22	4	0
2	B	16	0	22	1	0
2	C	16	0	22	2	0
2	D	16	0	22	2	0
2	E	16	0	22	4	0
2	F	16	0	22	1	0
2	G	16	0	22	2	0
2	H	16	0	22	8	0
3	D	12	0	16	1	0
3	E	6	0	8	0	0
4	A	57	0	0	0	0
4	B	66	0	0	0	0
4	C	70	0	0	4	0
4	D	84	0	0	5	0
4	E	50	0	0	1	0
4	F	66	0	0	1	0
4	G	75	0	0	2	0
4	H	59	0	0	4	0
All	All	21736	0	21864	233	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 5.

All (233) 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:C:70[A]:LEU:HD13	1:C:70[A]:LEU:O	1.21	1.30
1:B:239[A]:TYR:HD2	1:B:239[A]:TYR:N	1.52	1.07
1:C:70[A]:LEU:O	1:C:70[A]:LEU:CD1	2.06	1.02
1:C:70[A]:LEU:CD1	1:C:70[A]:LEU:C	2.30	1.00
1:C:70[A]:LEU:HD13	1:C:70[A]:LEU:C	1.79	0.99
1:C:247:TYR:CZ	4:C:568:HOH:O	2.26	0.88
1:F:149[A]:LYS:HE2	1:F:149[A]:LYS:HA	1.60	0.84
1:B:92:VAL:HG11	1:B:124:VAL:HG21	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:LEU:HD12	1:F:70:LEU:HD12	1.61	0.82
1:D:311[B]:GLU:OE1	1:D:311[B]:GLU:N	2.11	0.81
1:B:239[A]:TYR:N	1:B:239[A]:TYR:CD2	2.29	0.80
1:E:107[B]:LEU:O	1:E:107[B]:LEU:HD23	1.83	0.78
1:C:303[A]:LEU:N	1:C:303[A]:LEU:HD23	2.00	0.77
1:H:138:ASN:HD21	2:H:400:1PE:C15	1.98	0.77
1:A:183:LEU:HD12	1:B:70:LEU:HD12	1.68	0.76
1:D:107:LEU:HD11	1:D:329:GLU:HB2	1.70	0.74
1:B:239[A]:TYR:HD2	1:B:239[A]:TYR:H	0.81	0.74
1:A:183:LEU:HD11	1:B:70:LEU:O	1.88	0.74
1:H:138:ASN:HD21	2:H:400:1PE:H152	1.53	0.73
1:D:107:LEU:HD12	4:D:516:HOH:O	1.89	0.72
1:B:84:ASN:HD22	1:B:85:VAL:N	1.88	0.71
1:F:108[B]:ASN:C	1:F:108[B]:ASN:HD22	1.94	0.71
1:C:98:ALA:H	1:C:113:ASN:HD21	1.40	0.69
1:H:98:ALA:H	1:H:113:ASN:HD21	1.39	0.69
1:C:183:LEU:HD12	1:D:70:LEU:HD12	1.74	0.68
1:D:177:ARG:NH1	4:D:535:HOH:O	2.24	0.68
1:F:101[B]:GLN:OE1	1:F:101[B]:GLN:HA	1.94	0.68
1:F:171:ARG:HD3	1:F:185:CYS:O	1.95	0.67
1:D:111:GLN:HE22	1:D:331:GLN:H	1.39	0.66
1:H:171:ARG:HD3	1:H:185:CYS:O	1.96	0.66
1:D:107:LEU:CD1	4:D:516:HOH:O	2.44	0.65
1:H:138:ASN:HD22	2:H:400:1PE:H122	1.59	0.65
1:G:277:ILE:HD13	1:G:283:ILE:HD13	1.79	0.64
1:D:55:GLU:HG2	4:D:513:HOH:O	1.97	0.64
1:C:277:ILE:HD11	1:C:289:LEU:HD12	1.80	0.64
1:F:108[B]:ASN:O	1:F:108[B]:ASN:ND2	2.25	0.64
1:C:111:GLN:HE22	1:C:331[A]:GLN:H	1.45	0.64
1:G:171:ARG:HD3	1:G:185:CYS:O	1.97	0.63
1:G:138:ASN:H	2:G:400:1PE:H231	1.63	0.63
1:D:98:ALA:H	1:D:113:ASN:HD21	1.44	0.63
1:F:303:LEU:N	1:F:303:LEU:HD23	2.12	0.62
1:G:111:GLN:HE22	1:G:331:GLN:H	1.47	0.62
1:A:15:GLU:HB3	1:A:16:GLU:HA	1.81	0.62
1:E:137:SER:HA	2:E:401:1PE:H241	1.81	0.62
1:G:98:ALA:H	1:G:113:ASN:HD21	1.48	0.62
1:C:111:GLN:HE22	1:C:331[B]:GLN:H	1.47	0.62
1:C:70[A]:LEU:C	1:C:70[A]:LEU:HD12	2.19	0.61
1:C:247:TYR:CE1	4:C:568:HOH:O	2.51	0.61
1:D:311[B]:GLU:H	1:D:311[B]:GLU:CD	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107[A]:LEU:HD12	1:E:108:ASN:N	2.16	0.61
1:F:84:ASN:HD22	1:F:85:VAL:N	1.99	0.60
1:E:205:ASN:HA	1:E:211:LEU:HD13	1.83	0.60
1:E:21:ASN:HD21	1:H:21:ASN:HD21	1.49	0.60
1:A:99:ARG:H	1:A:99:ARG:NE	2.00	0.59
1:H:31:VAL:HG21	2:H:400:1PE:H142	1.85	0.59
1:B:235:VAL:O	1:B:239[A]:TYR:CZ	2.56	0.59
1:A:15:GLU:CB	1:A:16:GLU:HA	2.33	0.59
1:F:111:GLN:HE22	1:F:331:GLN:H	1.51	0.58
1:H:138:ASN:HD21	2:H:400:1PE:H151	1.68	0.58
1:C:276:MET:CE	1:C:278:LYS:H	2.15	0.58
1:A:205:ASN:HA	1:A:211:LEU:HD13	1.84	0.58
1:G:265:LYS:HE3	4:G:533:HOH:O	2.04	0.57
1:H:226:GLN:NE2	4:H:517:HOH:O	2.37	0.57
1:H:205:ASN:HA	1:H:211:LEU:HD13	1.86	0.56
1:C:276:MET:HE1	1:C:278:LYS:HB2	1.88	0.56
1:C:327:GLN:HA	1:C:330:LEU:HD22	1.87	0.56
1:F:108[B]:ASN:C	1:F:108[B]:ASN:ND2	2.59	0.55
1:A:138:ASN:HD21	2:A:400:1PE:C15	2.19	0.55
4:G:519:HOH:O	1:H:183:LEU:HD11	2.06	0.55
1:D:73[A]:ARG:NH2	4:D:524:HOH:O	2.40	0.55
1:H:138:ASN:H	2:H:400:1PE:H132	1.72	0.54
1:E:137:SER:HA	2:E:401:1PE:C24	2.37	0.54
1:G:181:HIS:CE1	1:G:183:LEU:HD13	2.42	0.54
1:B:281:TYR:CE2	1:B:308:LEU:HD12	2.43	0.54
1:E:83:TYR:CG	1:E:123:ASN:HB3	2.42	0.54
1:G:294:ILE:HD12	1:G:302:ASP:HB2	1.90	0.54
1:A:138:ASN:HD21	2:A:400:1PE:H151	1.73	0.54
1:E:121:ILE:HA	1:E:124:VAL:HG12	1.89	0.54
1:G:100:GLN:HA	1:G:109:LEU:HD13	1.89	0.54
1:E:21:ASN:ND2	1:H:21:ASN:HD21	2.07	0.53
1:F:277:ILE:HD11	1:F:289:LEU:HD12	1.90	0.53
1:F:294[A]:ILE:HD12	1:F:302:ASP:HB2	1.91	0.53
1:G:98:ALA:H	1:G:113:ASN:ND2	2.06	0.53
1:F:189:VAL:C	1:F:190:LEU:HD12	2.29	0.53
1:B:92:VAL:HG11	1:B:124:VAL:CG2	2.36	0.52
1:E:100:GLN:HB2	1:E:109:LEU:HD22	1.92	0.52
1:C:52:ASP:OD1	1:C:53:VAL:N	2.40	0.52
1:E:84:ASN:HD22	1:E:85:VAL:N	2.08	0.51
1:D:138:ASN:ND2	2:D:401:1PE:H152	2.25	0.51
1:H:111:GLN:HE22	1:H:331:GLN:H	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:ASN:HD22	1:F:84:ASN:C	2.13	0.51
1:A:291:VAL:HG22	1:A:292:PRO:HD2	1.93	0.51
1:D:233:GLN:O	1:D:237:SER:HB3	2.10	0.51
1:B:56[A]:ASP:OD2	1:B:56[A]:ASP:N	2.34	0.51
1:H:17:GLN:O	1:H:18:THR:HB	2.11	0.51
1:H:84:ASN:ND2	4:H:548:HOH:O	2.42	0.51
1:F:327:GLN:HA	1:F:330:LEU:HD22	1.92	0.50
1:F:181:HIS:CE1	1:F:183:LEU:HD13	2.46	0.50
1:H:291:VAL:HG13	1:H:292:PRO:HD2	1.93	0.50
1:A:131:CYS:O	1:A:157:ARG:NH1	2.44	0.50
1:D:16:GLU:O	1:D:17:GLN:HB3	2.12	0.50
1:F:205:ASN:HA	1:F:211:LEU:HD13	1.94	0.50
1:F:294[B]:ILE:HD12	1:F:294[B]:ILE:N	2.27	0.50
1:F:171:ARG:CD	1:F:185:CYS:O	2.58	0.49
1:A:12:LEU:HB2	1:D:301:SER:O	2.13	0.49
1:E:294:ILE:HD12	1:E:302:ASP:HB2	1.94	0.49
1:B:181:HIS:CE1	1:B:183:LEU:HD12	2.47	0.49
1:F:291:VAL:HG13	1:F:292:PRO:HD2	1.94	0.49
1:C:294:ILE:HD12	1:C:302:ASP:HB2	1.95	0.49
1:E:121:ILE:O	1:E:124:VAL:HG12	2.13	0.48
1:E:267:LEU:O	1:G:181:HIS:HB2	2.13	0.48
1:A:269:ARG:HD3	1:C:183:LEU:HD23	1.95	0.48
1:F:101[B]:GLN:OE1	1:F:101[B]:GLN:CA	2.61	0.48
1:D:90[A]:LYS:HA	1:D:90[A]:LYS:HD3	1.58	0.48
1:H:197:SER:OG	1:H:231:HIS:HE1	1.96	0.48
1:A:171:ARG:HD3	1:A:185:CYS:O	2.13	0.47
1:B:14:LYS:HE2	1:C:301:SER:O	2.14	0.47
1:C:98:ALA:H	1:C:113:ASN:ND2	2.09	0.47
1:D:184:SER:HA	3:D:402:GOL:H32	1.95	0.47
1:H:23:ILE:HD12	1:H:45:ALA:HB2	1.95	0.47
1:H:31:VAL:HG21	2:H:400:1PE:C14	2.43	0.47
1:B:180:VAL:HG12	1:B:181:HIS:O	2.14	0.47
1:E:107[B]:LEU:HD23	1:E:107[B]:LEU:C	2.33	0.47
1:A:294[B]:ILE:HD12	1:A:294[B]:ILE:N	2.29	0.47
1:C:278:LYS:HD2	1:C:284:LYS:O	2.14	0.47
1:D:277:ILE:HD11	1:D:289:LEU:HD22	1.95	0.47
1:E:107[B]:LEU:C	1:E:107[B]:LEU:CD2	2.82	0.47
1:F:98:ALA:H	1:F:113:ASN:HD21	1.62	0.47
1:D:98:ALA:H	1:D:113:ASN:ND2	2.12	0.47
1:D:138:ASN:HD21	2:D:401:1PE:H152	1.79	0.47
1:G:215:HIS:HB2	1:H:4:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ILE:O	1:B:124:VAL:HG12	2.15	0.47
1:E:277:ILE:HG12	1:E:289:LEU:HD11	1.96	0.47
1:H:121:ILE:HB	1:H:122:PRO:HD3	1.97	0.47
1:E:239[B]:TYR:HD1	1:E:239[B]:TYR:H	1.63	0.47
1:H:196:SER:HB2	4:H:553:HOH:O	2.13	0.47
1:D:277:ILE:HD11	1:D:289:LEU:HB2	1.97	0.46
1:E:52:ASP:OD2	1:E:53:VAL:N	2.47	0.46
1:E:70:LEU:HD12	1:F:183:LEU:HD12	1.97	0.46
1:F:106:ARG:NH2	4:F:565:HOH:O	2.47	0.46
1:F:242:ILE:HG12	1:F:247:TYR:HA	1.97	0.46
1:A:137:SER:HA	2:A:400:1PE:H131	1.98	0.46
1:B:294:ILE:HD11	1:D:180:VAL:HG22	1.98	0.46
1:C:171:ARG:HD3	1:C:185:CYS:O	2.16	0.46
1:H:98:ALA:H	1:H:113:ASN:ND2	2.09	0.46
1:E:70:LEU:O	1:F:183:LEU:HD11	2.15	0.45
1:G:138:ASN:HB2	2:G:400:1PE:H122	1.97	0.45
1:B:206:VAL:O	1:B:209:VAL:HG12	2.17	0.45
1:A:98:ALA:O	2:A:400:1PE:H121	2.16	0.45
1:C:247:TYR:CE2	4:C:568:HOH:O	2.58	0.45
1:A:84:ASN:HD22	1:A:85:VAL:N	2.15	0.45
1:A:111:GLN:HE22	1:A:331:GLN:H	1.65	0.45
1:C:270:VAL:HA	1:C:293:CYS:O	2.17	0.45
1:F:125:VAL:HG12	1:F:153:PHE:CZ	2.52	0.45
1:H:16:GLU:O	1:H:17:GLN:O	2.34	0.45
1:F:188:TRP:HB3	1:F:190:LEU:HD11	1.99	0.45
1:A:178:LEU:HA	1:B:5:LYS:HE3	1.99	0.44
1:F:138:ASN:H	2:F:400:1PE:H231	1.82	0.44
1:B:137:SER:HA	2:B:400:1PE:H131	1.99	0.44
1:E:121:ILE:O	1:E:124:VAL:CG1	2.64	0.44
1:E:215:HIS:HB2	1:F:4:LEU:HD13	1.99	0.44
1:F:276:MET:HB2	1:F:288:PHE:CZ	2.52	0.44
1:B:294:ILE:CD1	1:D:180:VAL:HG22	2.48	0.44
1:E:121:ILE:HA	1:E:124:VAL:CG1	2.47	0.44
1:H:205:ASN:HD22	1:H:208:GLY:H	1.64	0.44
1:F:98:ALA:H	1:F:113:ASN:ND2	2.16	0.44
1:H:221:ASP:OD2	1:H:228:LYS:NZ	2.51	0.44
1:A:294[A]:ILE:HD12	1:A:302:ASP:HB2	1.99	0.44
1:D:199:PRO:HG3	1:D:231:HIS:CG	2.51	0.44
1:A:23:ILE:HD12	1:A:45:ALA:HB2	2.00	0.44
1:B:27:GLY:O	1:B:32:GLY:HA3	2.18	0.44
1:E:107[B]:LEU:O	1:E:107[B]:LEU:CD2	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:GLN:HA	1:F:109:LEU:HD13	1.98	0.43
1:A:306:VAL:HA	1:C:209:VAL:HG11	2.00	0.43
1:D:288:PHE:O	1:D:289:LEU:HD12	2.18	0.43
1:D:294:ILE:HD12	1:D:302:ASP:HB2	2.01	0.43
1:E:11:ASN:ND2	1:E:12:LEU:O	2.52	0.43
1:F:301:SER:OG	1:F:302:ASP:OD1	2.33	0.43
1:G:199:PRO:HG3	1:G:231:HIS:CG	2.53	0.43
1:B:110:VAL:HG21	1:B:142:ILE:HG21	1.99	0.43
1:B:188:TRP:HB3	1:B:190:LEU:HD11	2.00	0.43
1:C:276:MET:HE1	1:C:278:LYS:CB	2.48	0.43
1:D:100:GLN:HB2	1:D:109:LEU:HD22	1.99	0.43
1:F:205:ASN:HD22	1:F:208:GLY:H	1.66	0.43
1:F:292:PRO:HB2	1:F:304:VAL:HB	2.00	0.43
1:H:181:HIS:CE1	1:H:183:LEU:HD13	2.53	0.43
1:E:110:VAL:O	1:E:114:VAL:HG23	2.19	0.43
1:H:142:ILE:O	1:H:145:TYR:HB3	2.18	0.43
1:B:273:VAL:O	1:B:290:SER:HA	2.19	0.42
1:D:165:LEU:HD11	1:D:251:ALA:HB1	2.01	0.42
1:C:311[B]:GLU:CD	1:C:311[B]:GLU:H	2.22	0.42
1:G:84:ASN:ND2	1:G:85:VAL:HG23	2.34	0.42
1:D:121:ILE:HB	1:D:122:PRO:HD3	2.01	0.42
1:H:205:ASN:HA	1:H:211:LEU:CD1	2.49	0.42
1:C:136:VAL:HG12	2:C:400:1PE:H141	2.00	0.42
1:D:121:ILE:O	1:D:125:VAL:HG13	2.19	0.42
1:D:181:HIS:CE1	1:D:183:LEU:HD13	2.54	0.42
1:C:171:ARG:NH2	4:C:538:HOH:O	2.52	0.42
1:B:84:ASN:HD22	1:B:84:ASN:C	2.23	0.42
1:G:181:HIS:HE1	1:G:183:LEU:HD13	1.83	0.42
1:G:183:LEU:HD11	1:H:70:LEU:O	2.19	0.42
1:H:326:ILE:O	1:H:330:LEU:HD13	2.20	0.42
1:D:287:VAL:CG1	1:D:323:LEU:HD23	2.50	0.42
1:C:209:VAL:HG21	1:D:8:LEU:CD1	2.49	0.41
1:D:246:GLY:O	1:D:247:TYR:HB3	2.20	0.41
1:C:82:ASP:OD1	1:C:83:TYR:N	2.53	0.41
1:D:289:LEU:HD23	1:D:316:LEU:HG	2.02	0.41
1:C:206:VAL:O	1:C:209:VAL:HG22	2.20	0.41
1:C:209:VAL:CG2	1:D:8:LEU:CD1	2.99	0.41
1:E:43:ASP:O	1:H:265:LYS:NZ	2.54	0.41
1:C:302:ASP:O	1:C:303[B]:LEU:HD23	2.21	0.41
1:C:31:VAL:HG21	2:C:400:1PE:H241	2.03	0.41
1:F:188:TRP:CZ2	1:H:207:ALA:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:196:SER:N	4:H:540:HOH:O	2.50	0.41
1:H:197:SER:OG	1:H:231:HIS:CE1	2.73	0.41
1:C:198:VAL:HG21	1:C:316:LEU:CD1	2.51	0.41
1:E:31:VAL:HG21	2:E:401:1PE:H252	2.03	0.41
1:B:106:ARG:NH2	1:B:139:PRO:HB3	2.36	0.41
1:C:217:ASP:O	1:C:223:ASP:HB2	2.20	0.41
1:E:12:LEU:HB2	1:H:301:SER:O	2.21	0.41
1:E:327:GLN:HA	1:E:330:LEU:HD22	2.03	0.41
1:A:73:ARG:HE	1:A:73:ARG:HB2	1.70	0.41
2:E:401:1PE:H262	4:E:540:HOH:O	2.20	0.41
1:F:11:ASN:HA	1:G:302:ASP:OD2	2.20	0.41
1:H:137:SER:HA	2:H:400:1PE:C13	2.50	0.41
1:B:280:LEU:HD22	1:B:280:LEU:N	2.36	0.40
1:H:281:TYR:CE2	1:H:308:LEU:HD12	2.56	0.40
1:C:237:SER:O	1:C:241:VAL:HG23	2.21	0.40
1:H:280:LEU:N	1:H:280:LEU:HD22	2.36	0.40
1:B:174:MET:HG2	1:B:185:CYS:HB3	2.04	0.40
1:F:165:LEU:HD11	1:F:251:ALA:HB1	2.03	0.40
1:D:181:HIS:CE1	1:D:183:LEU:CD1	3.05	0.40
1:E:270:VAL:HA	1:E:293:CYS:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/337 (101%)	329 (97%)	9 (3%)	1 (0%)	41	55
1	B	333/337 (99%)	320 (96%)	13 (4%)	0	100	100
1	C	337/337 (100%)	331 (98%)	6 (2%)	0	100	100
1	D	340/337 (101%)	321 (94%)	18 (5%)	1 (0%)	41	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	334/337 (99%)	321 (96%)	12 (4%)	1 (0%)	41	55
1	F	340/337 (101%)	328 (96%)	12 (4%)	0	100	100
1	G	337/337 (100%)	328 (97%)	8 (2%)	1 (0%)	41	55
1	H	330/337 (98%)	317 (96%)	10 (3%)	3 (1%)	17	25
All	All	2690/2696 (100%)	2595 (96%)	88 (3%)	7 (0%)	41	55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	H	17	GLN
1	H	15	GLU
1	E	17	GLN
1	H	18	THR
1	D	249	SER
1	G	249	SER

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	298/293 (102%)	286 (96%)	12 (4%)	31	49
1	B	291/293 (99%)	281 (97%)	10 (3%)	37	56
1	C	295/293 (101%)	280 (95%)	15 (5%)	24	39
1	D	298/293 (102%)	291 (98%)	7 (2%)	50	70
1	E	292/293 (100%)	275 (94%)	17 (6%)	20	32
1	F	298/293 (102%)	284 (95%)	14 (5%)	26	42
1	G	295/293 (101%)	277 (94%)	18 (6%)	18	30
1	H	288/293 (98%)	276 (96%)	12 (4%)	30	47
All	All	2355/2344 (100%)	2250 (96%)	105 (4%)	30	44

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	14	LYS
1	A	16	GLU
1	A	56[A]	ASP
1	A	56[B]	ASP
1	A	73	ARG
1	A	84	ASN
1	A	99	ARG
1	A	108	ASN
1	A	178	LEU
1	A	209	VAL
1	A	323	LEU
1	B	56[A]	ASP
1	B	56[B]	ASP
1	B	84	ASN
1	B	134	LEU
1	B	149	LYS
1	B	178	LEU
1	B	239[A]	TYR
1	B	239[B]	TYR
1	B	289	LEU
1	B	291	VAL
1	C	12	LEU
1	C	13	LEU
1	C	14	LYS
1	C	70[A]	LEU
1	C	70[B]	LEU
1	C	73	ARG
1	C	84	ASN
1	C	123	ASN
1	C	134	LEU
1	C	137	SER
1	C	178	LEU
1	C	276	MET
1	C	303[A]	LEU
1	C	303[B]	LEU
1	C	330	LEU
1	D	3	THR
1	D	13	LEU
1	D	17	GLN
1	D	81[A]	LYS
1	D	81[B]	LYS
1	D	178	LEU

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Mol	Chain	Res	Type
1	D	323	LEU
1	E	11	ASN
1	E	13	LEU
1	E	14	LYS
1	E	17	GLN
1	E	18	THR
1	E	73	ARG
1	E	84	ASN
1	E	102	GLU
1	E	128	SER
1	E	134	LEU
1	E	178	LEU
1	E	209	VAL
1	E	212	LYS
1	E	274	SER
1	E	286	ASP
1	E	330	LEU
1	E	331	GLN
1	F	12	LEU
1	F	17	GLN
1	F	18	THR
1	F	73	ARG
1	F	84	ASN
1	F	134	LEU
1	F	176	GLU
1	F	178	LEU
1	F	209	VAL
1	F	212	LYS
1	F	278	LYS
1	F	301	SER
1	F	303	LEU
1	F	330	LEU
1	G	20	GLN
1	G	84	ASN
1	G	106[A]	ARG
1	G	106[B]	ARG
1	G	107	LEU
1	G	125	VAL
1	G	128	SER
1	G	134	LEU
1	G	178	LEU
1	G	196	SER

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Mol	Chain	Res	Type
1	G	209	VAL
1	G	211	LEU
1	G	212	LYS
1	G	226	GLN
1	G	237[A]	SER
1	G	237[B]	SER
1	G	291	VAL
1	G	323	LEU
1	H	13	LEU
1	H	17	GLN
1	H	72	LEU
1	H	73	ARG
1	H	76	LYS
1	H	134	LEU
1	H	178	LEU
1	H	209	VAL
1	H	212	LYS
1	H	323	LEU
1	H	330	LEU
1	H	332	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	84	ASN
1	A	100	GLN
1	A	108	ASN
1	A	111	GLN
1	A	113	ASN
1	A	138	ASN
1	A	205	ASN
1	A	226	GLN
1	B	7	GLN
1	B	20	GLN
1	B	21	ASN
1	B	84	ASN
1	B	100	GLN
1	B	108	ASN
1	B	111	GLN
1	B	113	ASN
1	B	205	ASN

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Mol	Chain	Res	Type
1	B	231	HIS
1	B	327	GLN
1	C	21	ASN
1	C	84	ASN
1	C	100	GLN
1	C	111	GLN
1	C	113	ASN
1	C	231	HIS
1	D	20	GLN
1	D	100	GLN
1	D	108	ASN
1	D	111	GLN
1	D	113	ASN
1	D	138	ASN
1	D	231	HIS
1	D	298	ASN
1	E	11	ASN
1	E	20	GLN
1	E	84	ASN
1	E	100	GLN
1	E	108	ASN
1	E	111	GLN
1	E	113	ASN
1	E	164	ASN
1	E	205	ASN
1	E	231	HIS
1	E	331	GLN
1	F	7	GLN
1	F	21	ASN
1	F	84	ASN
1	F	100	GLN
1	F	111	GLN
1	F	113	ASN
1	F	205	ASN
1	F	231	HIS
1	F	297	GLN
1	F	298	ASN
1	G	7	GLN
1	G	11	ASN
1	G	20	GLN
1	G	21	ASN
1	G	111	GLN

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Mol	Chain	Res	Type
1	G	113	ASN
1	G	123	ASN
1	G	231	HIS
1	H	17	GLN
1	H	20	GLN
1	H	21	ASN
1	H	100	GLN
1	H	111	GLN
1	H	113	ASN
1	H	138	ASN
1	H	205	ASN
1	H	226	GLN
1	H	231	HIS
1	H	298	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

11 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	$\#\|Z\| > 2$
3	GOL	D	403	-	5,5,5	0.25	0	5,5,5	0.35	0
2	1PE	D	401	-	15,15,15	0.52	0	14,14,14	0.51	0
3	GOL	D	402	-	5,5,5	0.49	0	5,5,5	1.10	0
2	1PE	H	400	-	15,15,15	0.46	0	14,14,14	0.65	0
3	GOL	E	402	-	5,5,5	0.31	0	5,5,5	0.20	0
2	1PE	G	400	-	15,15,15	0.31	0	14,14,14	0.76	0
2	1PE	B	400	-	15,15,15	0.37	0	14,14,14	0.58	0
2	1PE	C	400	-	15,15,15	0.47	0	14,14,14	0.50	0
2	1PE	A	400	-	15,15,15	0.32	0	14,14,14	0.83	0
2	1PE	E	401	-	15,15,15	0.51	0	14,14,14	0.73	0
2	1PE	F	400	-	15,15,15	0.35	0	14,14,14	0.53	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
3	GOL	D	403	-	-	0/4/4/4	-
2	1PE	D	401	-	-	6/13/13/13	-
3	GOL	D	402	-	-	0/4/4/4	-
2	1PE	H	400	-	-	9/13/13/13	-
3	GOL	E	402	-	-	4/4/4/4	-
2	1PE	G	400	-	-	6/13/13/13	-
2	1PE	B	400	-	-	2/13/13/13	-
2	1PE	C	400	-	-	5/13/13/13	-
2	1PE	A	400	-	-	8/13/13/13	-
2	1PE	E	401	-	-	7/13/13/13	-
2	1PE	F	400	-	-	10/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	402	GOL	O1-C1-C2-C3
2	E	401	1PE	OH4-C13-C23-OH3
2	F	400	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
2	E	401	1PE	OH5-C14-C24-OH4
2	B	400	1PE	OH4-C13-C23-OH3
2	D	401	1PE	OH4-C13-C23-OH3
2	C	400	1PE	OH5-C14-C24-OH4
2	H	400	1PE	OH4-C13-C23-OH3
2	B	400	1PE	OH2-C12-C22-OH3
2	D	401	1PE	OH7-C16-C26-OH6
2	G	400	1PE	OH2-C12-C22-OH3
2	H	400	1PE	OH7-C16-C26-OH6
2	D	401	1PE	OH6-C15-C25-OH5
2	C	400	1PE	OH4-C13-C23-OH3
2	F	400	1PE	OH2-C12-C22-OH3
2	F	400	1PE	OH7-C16-C26-OH6
2	H	400	1PE	OH2-C12-C22-OH3
3	E	402	GOL	C1-C2-C3-O3
2	A	400	1PE	OH4-C13-C23-OH3
2	A	400	1PE	OH6-C15-C25-OH5
3	E	402	GOL	O1-C1-C2-O2
2	D	401	1PE	OH5-C14-C24-OH4
2	C	400	1PE	OH2-C12-C22-OH3
2	H	400	1PE	OH5-C14-C24-OH4
3	E	402	GOL	O2-C2-C3-O3
2	A	400	1PE	OH5-C14-C24-OH4
2	E	401	1PE	OH7-C16-C26-OH6
2	G	400	1PE	OH4-C13-C23-OH3
2	E	401	1PE	C25-C15-OH6-C26
2	C	400	1PE	C12-C22-OH3-C23
2	F	400	1PE	C23-C13-OH4-C24
2	D	401	1PE	C15-C25-OH5-C14
2	G	400	1PE	C13-C23-OH3-C22
2	E	401	1PE	C13-C23-OH3-C22
2	F	400	1PE	C14-C24-OH4-C13
2	A	400	1PE	C14-C24-OH4-C13
2	F	400	1PE	C15-C25-OH5-C14
2	A	400	1PE	C12-C22-OH3-C23
2	H	400	1PE	C24-C14-OH5-C25
2	D	401	1PE	C12-C22-OH3-C23
2	F	400	1PE	C24-C14-OH5-C25
2	H	400	1PE	C23-C13-OH4-C24
2	F	400	1PE	C16-C26-OH6-C15
2	C	400	1PE	C24-C14-OH5-C25
2	F	400	1PE	C12-C22-OH3-C23

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Mol	Chain	Res	Type	Atoms
2	E	401	1PE	OH6-C15-C25-OH5
2	G	400	1PE	C24-C14-OH5-C25
2	E	401	1PE	C16-C26-OH6-C15
2	G	400	1PE	C15-C25-OH5-C14
2	F	400	1PE	C13-C23-OH3-C22
2	H	400	1PE	C25-C15-OH6-C26
2	H	400	1PE	C16-C26-OH6-C15
2	A	400	1PE	C23-C13-OH4-C24
2	G	400	1PE	C12-C22-OH3-C23
2	A	400	1PE	C15-C25-OH5-C14
2	A	400	1PE	C24-C14-OH5-C25
2	H	400	1PE	OH6-C15-C25-OH5

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	1PE	2	0
3	D	402	GOL	1	0
2	H	400	1PE	8	0
2	G	400	1PE	2	0
2	B	400	1PE	1	0
2	C	400	1PE	2	0
2	A	400	1PE	4	0
2	E	401	1PE	4	0
2	F	400	1PE	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 (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	332/337 (98%)	-0.26	8 (2%)	59	57	25, 36, 55, 84	0
1	B	331/337 (98%)	-0.30	8 (2%)	59	57	25, 34, 50, 60	0
1	C	332/337 (98%)	-0.32	11 (3%)	46	45	23, 33, 50, 88	0
1	D	332/337 (98%)	-0.23	13 (3%)	39	38	24, 34, 52, 94	0
1	E	331/337 (98%)	-0.17	14 (4%)	36	35	24, 38, 65, 84	0
1	F	331/337 (98%)	-0.23	11 (3%)	46	45	23, 35, 52, 88	0
1	G	331/337 (98%)	-0.40	6 (1%)	68	66	23, 32, 45, 54	0
1	H	331/337 (98%)	-0.24	13 (3%)	39	38	25, 37, 56, 101	0
All	All	2651/2696 (98%)	-0.27	84 (3%)	47	46	23, 35, 54, 101	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	15	GLU	7.3
1	A	17	GLN	6.9
1	D	17	GLN	6.6
1	A	333[A]	HIS	6.2
1	H	17	GLN	5.3
1	C	16	GLU	5.1
1	F	15	GLU	5.0
1	D	16	GLU	4.9
1	F	14	LYS	4.7
1	B	103	GLY	4.7
1	C	15	GLU	4.1
1	D	103	GLY	4.1
1	C	14	LYS	4.1
1	E	17	GLN	4.0
1	F	17	GLN	3.8
1	E	331	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	15	GLU	3.7
1	D	15	GLU	3.7
1	E	102	GLU	3.7
1	E	16	GLU	3.6
1	E	103	GLY	3.3
1	F	13	LEU	3.3
1	F	222	LYS	3.3
1	C	17	GLN	3.3
1	A	14	LYS	3.3
1	D	333	HIS	3.2
1	B	102	GLU	3.2
1	B	239[A]	TYR	3.1
1	C	333	HIS	3.1
1	G	2	ALA	3.1
1	D	18	THR	2.9
1	F	130	ASN	2.9
1	A	16	GLU	2.9
1	E	99	ARG	2.9
1	H	16	GLU	2.8
1	D	284	LYS	2.8
1	B	16	GLU	2.8
1	E	15	GLU	2.8
1	A	239[A]	TYR	2.7
1	F	221	ASP	2.7
1	G	16	GLU	2.7
1	H	99	ARG	2.7
1	H	310	SER	2.6
1	H	14	LYS	2.6
1	B	331	GLN	2.6
1	E	239[A]	TYR	2.6
1	F	213	THR	2.6
1	E	14	LYS	2.5
1	G	103	GLY	2.5
1	F	2	ALA	2.5
1	B	17	GLN	2.5
1	B	221	ASP	2.5
1	D	221	ASP	2.5
1	A	2	ALA	2.4
1	H	282	GLY	2.4
1	E	2	ALA	2.4
1	D	102	GLU	2.4
1	C	10	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	239	TYR	2.4
1	C	2	ALA	2.3
1	C	247	TYR	2.3
1	H	239[A]	TYR	2.3
1	E	221	ASP	2.2
1	C	102	GLU	2.2
1	D	310	SER	2.2
1	D	224	LYS	2.2
1	C	99	ARG	2.2
1	G	311[A]	GLU	2.2
1	F	16	GLU	2.2
1	D	99	ARG	2.2
1	E	101	GLN	2.1
1	G	102	GLU	2.1
1	H	279	GLY	2.1
1	A	332	PHE	2.1
1	D	14	LYS	2.1
1	H	222	LYS	2.1
1	H	284	LYS	2.1
1	H	332	PHE	2.1
1	B	224	LYS	2.1
1	F	284	LYS	2.1
1	C	310	SER	2.0
1	E	332	PHE	2.0
1	H	331	GLN	2.0
1	E	107[A]	LEU	2.0

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

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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	E	402	6/6	0.72	0.47	67,72,72,74	0
3	GOL	D	403	6/6	0.78	0.40	62,64,64,64	0
2	1PE	E	401	16/16	0.86	0.25	37,43,66,68	0
2	1PE	F	400	16/16	0.90	0.24	37,42,59,59	0
2	1PE	G	400	16/16	0.91	0.17	32,38,47,47	0
2	1PE	H	400	16/16	0.91	0.24	37,44,52,52	0
2	1PE	A	400	16/16	0.92	0.18	35,41,58,63	0
2	1PE	C	400	16/16	0.92	0.22	37,43,56,60	0
2	1PE	D	401	16/16	0.92	0.19	42,48,58,59	0
2	1PE	B	400	16/16	0.93	0.20	35,42,55,59	0
3	GOL	D	402	6/6	0.94	0.31	35,36,43,48	0

6.5 Other polymers (i)

There are no such residues in this entry.