



# Full wwPDB X-ray Structure Validation Report

Nov 27, 2014 – 12:05 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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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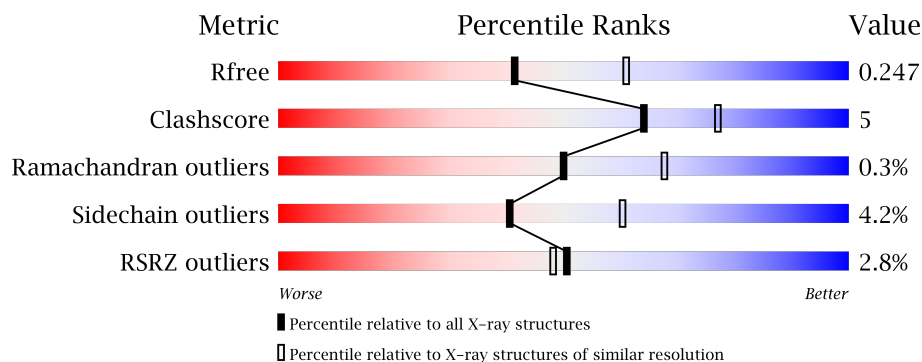
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24195  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.1.3  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24195

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	337	
1	B	337	
1	C	337	
1	D	337	
1	E	337	
1	F	337	
1	G	337	
1	H	337	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	1PE	C	400	-	X
2	1PE	D	401	-	X
3	GOL	D	402	-	X
3	GOL	D	403	-	X
3	GOL	E	402	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21736 atoms, of which 0 are hydrogen and 0 are deuterium.

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

There are 48 discrepancies between the modelled and reference sequences:

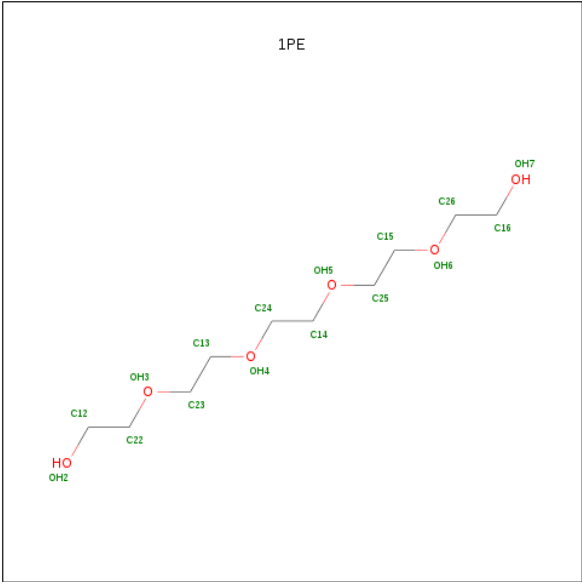
Chain	Residue	Modelled	Actual	Comment	Reference
A	333	HIS	-	EXPRESSION TAG	UNP P00338
A	334	HIS	-	EXPRESSION TAG	UNP P00338
A	335	HIS	-	EXPRESSION TAG	UNP P00338
A	336	HIS	-	EXPRESSION TAG	UNP P00338
A	337	HIS	-	EXPRESSION TAG	UNP P00338
A	338	HIS	-	EXPRESSION TAG	UNP P00338
B	333	HIS	-	EXPRESSION TAG	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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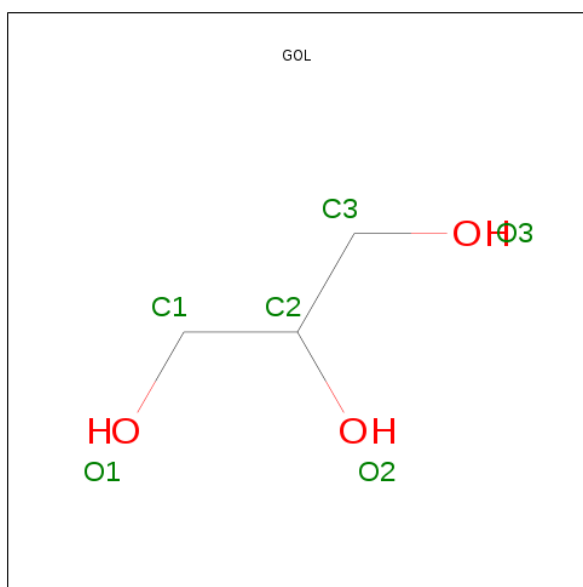
Chain	Residue	Modelled	Actual	Comment	Reference
C	334	HIS	-	EXPRESSION TAG	UNP P00338
C	335	HIS	-	EXPRESSION TAG	UNP P00338
C	336	HIS	-	EXPRESSION TAG	UNP P00338
C	337	HIS	-	EXPRESSION TAG	UNP P00338
C	338	HIS	-	EXPRESSION TAG	UNP P00338
D	333	HIS	-	EXPRESSION TAG	UNP P00338
D	334	HIS	-	EXPRESSION TAG	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<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



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

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



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

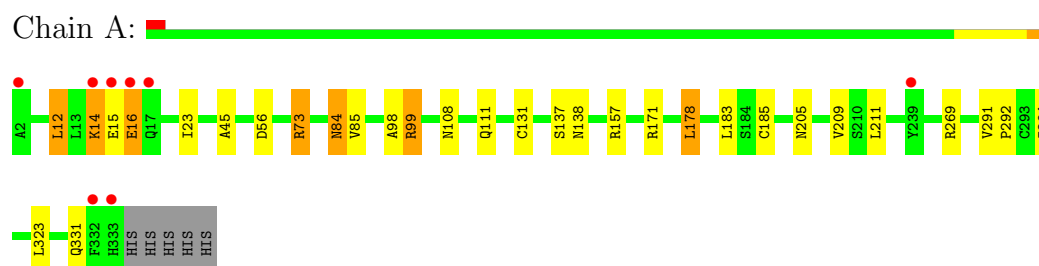
- Molecule 4 is water.

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

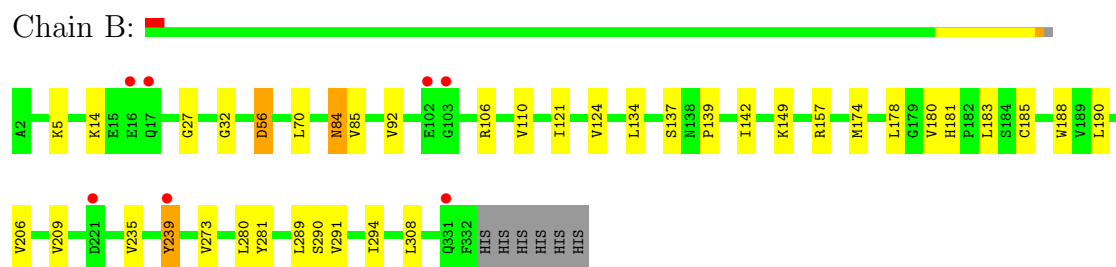
### 3 Residue-property plots

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.

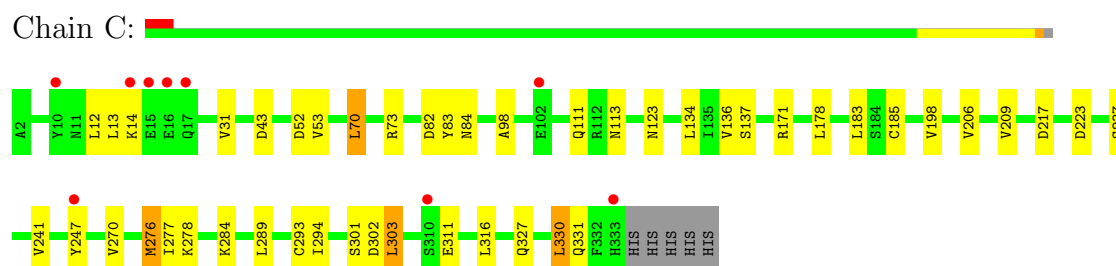
- Molecule 1: L-lactate dehydrogenase A chain



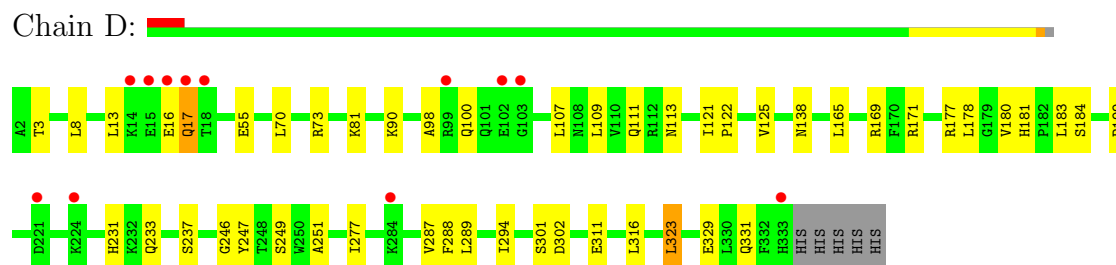
- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



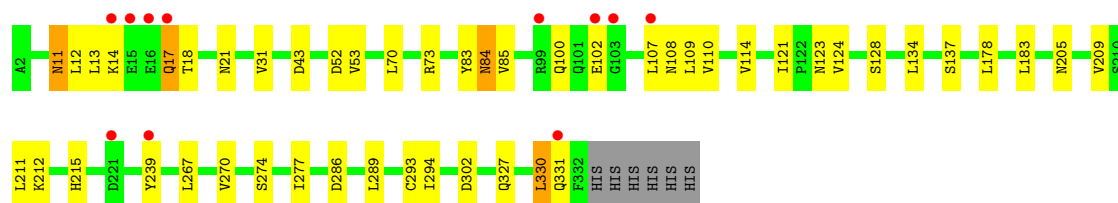
- Molecule 1: L-lactate dehydrogenase A chain





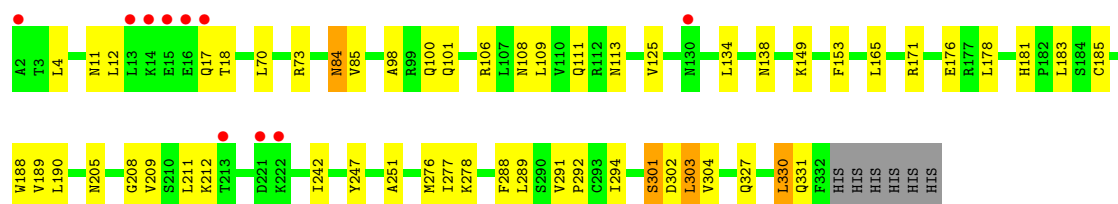
- Molecule 1: L-lactate dehydrogenase A chain

Chain E:



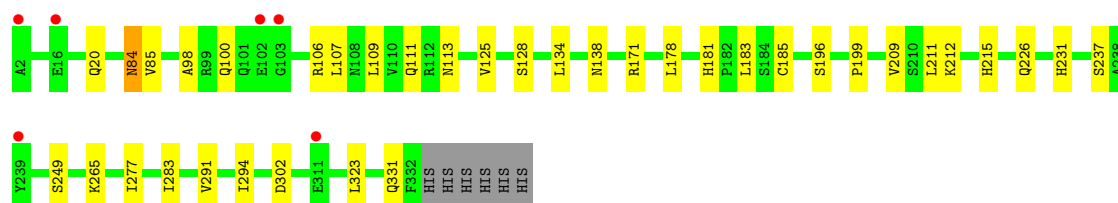
- Molecule 1: L-lactate dehydrogenase A chain

Chain F:



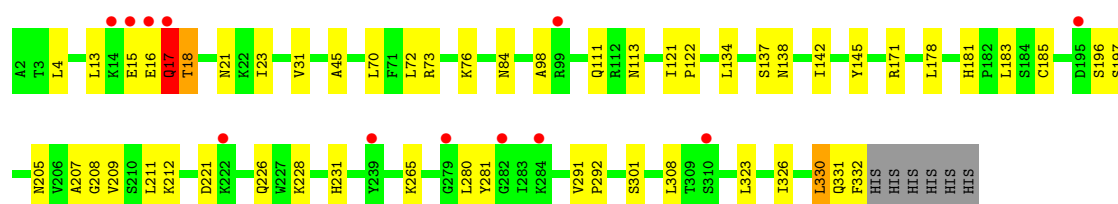
- Molecule 1: L-lactate dehydrogenase A chain

Chain G:



- Molecule 1: L-lactate dehydrogenase A chain

Chain H:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 24.0	EDS
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 162753 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21736	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 1PE

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(°)	Ideal(°)
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 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (233) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:70[A]:LEU:O	1:C:70[A]:LEU:HD13	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:92:VAL:HG11	1:B:124:VAL:HG21	1.58	0.83
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:HD23	1:E:107[B]:LEU:O	1.83	0.78
1:C:303[A]:LEU:HD23	1:C:303[A]:LEU:N	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:HD22	1:F:108[B]:ASN:C	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:HA	1:F:101[B]:GLN:OE1	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:247:TYR:CE1	4:C:568:HOH:O	2.51	0.61
1:C:70[A]:LEU:HD12	1:C:70[A]:LEU:C	2.19	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	Distance(Å)	Clash(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
1:F:84:ASN:HD22	1:F:84:ASN:C	2.13	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:CA	1:F:101[B]:GLN:OE1	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:31:VAL:HG21	2:H:400:1PE:C14	2.43	0.47
1:H:23:ILE:HD12	1:H:45:ALA:HB2	1.95	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:N	1:A:294[B]:ILE:HD12	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:138:ASN:HD21	2:D:401:1PE:H152	1.79	0.47
1:D:98:ALA:H	1:D:113:ASN:ND2	2.12	0.47
1:G:215:HIS:HB2	1:H:4:LEU:HD13	1.95	0.47
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:111:GLN:HE22	1:A:331:GLN:H	1.65	0.45
1:A:84:ASN:HD22	1:A:85:VAL:N	2.15	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:H	1:C:311[B]:GLU:CD	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:C	1:B:84:ASN:HD22	2.23	0.42
1:G:181:HIS:HE1	1:G:183:LEU:HD13	1.83	0.42
1:H:326:ILE:O	1:H:330:LEU:HD13	2.20	0.42
1:G:183:LEU:HD11	1:H:70:LEU:O	2.19	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:217:ASP:O	1:C:223:ASP:HB2	2.20	0.41
1:B:106:ARG:NH2	1:B:139:PRO:HB3	2.36	0.41
1:E:327:GLN:HA	1:E:330:LEU:HD22	2.03	0.41
1:E:12:LEU:HB2	1:H:301:SER:O	2.21	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

### 5.3.1 Protein backbone ⓘ

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%)	50	68
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%)	50	68
1	E	334/337 (99%)	321 (96%)	12 (4%)	1 (0%)	50	68
1	F	340/337 (101%)	328 (96%)	12 (4%)	0	100	100
1	G	337/337 (100%)	328 (97%)	8 (2%)	1 (0%)	50	68
1	H	330/337 (98%)	317 (96%)	10 (3%)	3 (1%)	25	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2690/2696 (100%)	2595 (96%)	88 (3%)	7 (0%)	50	68

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 ⓘ

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%)	42	63
1	B	291/293 (99%)	281 (97%)	10 (3%)	49	70
1	C	295/293 (101%)	280 (95%)	15 (5%)	33	50
1	D	298/293 (102%)	291 (98%)	7 (2%)	63	82
1	E	292/293 (100%)	275 (94%)	17 (6%)	28	43
1	F	298/293 (102%)	284 (95%)	14 (5%)	36	54
1	G	295/293 (101%)	277 (94%)	18 (6%)	26	40
1	H	288/293 (98%)	276 (96%)	12 (4%)	40	60
All	All	2355/2344 (100%)	2250 (96%)	105 (4%)	40	57

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

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Mol	Chain	Res	Type
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
1	D	323	LEU
1	E	11	ASN
1	E	13	LEU

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Mol	Chain	Res	Type
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
1	G	209	VAL
1	G	211	LEU
1	G	212	LYS

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Mol	Chain	Res	Type
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

Some 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
1	B	231	HIS
1	B	327	GLN
1	C	21	ASN

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Mol	Chain	Res	Type
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
1	G	113	ASN
1	G	123	ASN
1	G	231	HIS

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
2	1PE	A	400	-	15,15,15	0.33	0	14,14,14	0.84	0
2	1PE	B	400	-	15,15,15	0.39	0	14,14,14	0.60	0
2	1PE	C	400	-	15,15,15	0.49	0	14,14,14	0.51	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	1PE	D	401	-	15,15,15	0.53	0	14,14,14	0.52	0
3	GOL	D	402	-	5,5,5	0.43	0	5,5,5	1.14	1 (20%)
3	GOL	D	403	-	5,5,5	0.19	0	5,5,5	0.33	0
2	1PE	E	401	-	15,15,15	0.53	0	14,14,14	0.74	0
3	GOL	E	402	-	5,5,5	0.24	0	5,5,5	0.30	0
2	1PE	F	400	-	15,15,15	0.36	0	14,14,14	0.53	0
2	1PE	G	400	-	15,15,15	0.33	0	14,14,14	0.76	0
2	1PE	H	400	-	15,15,15	0.47	0	14,14,14	0.64	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	1PE	A	400	-	-	0/13/13/13	0/0/0/0
2	1PE	B	400	-	-	0/13/13/13	0/0/0/0
2	1PE	C	400	-	-	0/13/13/13	0/0/0/0
2	1PE	D	401	-	-	0/13/13/13	0/0/0/0
3	GOL	D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	D	403	-	-	0/4/4/4	0/0/0/0
2	1PE	E	401	-	-	0/13/13/13	0/0/0/0
3	GOL	E	402	-	-	0/4/4/4	0/0/0/0
2	1PE	F	400	-	-	0/13/13/13	0/0/0/0
2	1PE	G	400	-	-	0/13/13/13	0/0/0/0
2	1PE	H	400	-	-	0/13/13/13	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	GOL	O3-C3-C2	2.11	119.73	110.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	332/337 (98%)	-0.21	8 (2%)	56	54	25, 36, 55, 84	0
1	B	331/337 (98%)	-0.27	7 (2%)	60	58	25, 34, 50, 60	0
1	C	332/337 (98%)	-0.27	9 (2%)	52	49	23, 33, 50, 88	0
1	D	332/337 (98%)	-0.19	12 (3%)	41	39	24, 34, 52, 94	0
1	E	331/337 (98%)	-0.13	11 (3%)	44	42	24, 38, 65, 84	0
1	F	331/337 (98%)	-0.20	10 (3%)	48	45	23, 35, 52, 88	0
1	G	331/337 (98%)	-0.35	6 (1%)	65	63	23, 32, 45, 54	0
1	H	331/337 (98%)	-0.20	12 (3%)	41	39	25, 37, 56, 101	0
All	All	2651/2696 (98%)	-0.23	75 (2%)	50	48	23, 35, 54, 101	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	15	GLU	7.1
1	A	17	GLN	6.7
1	D	17	GLN	5.9
1	A	333[A]	HIS	5.5
1	D	16	GLU	5.0
1	F	15	GLU	5.0
1	H	17	GLN	4.6
1	C	16	GLU	4.5
1	F	14	LYS	4.5
1	B	103	GLY	4.3
1	E	17	GLN	3.9
1	D	103	GLY	3.8
1	C	14	LYS	3.7
1	C	15	GLU	3.7
1	E	331	GLN	3.6
1	F	17	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	13	LEU	3.5
1	C	17	GLN	3.5
1	D	15	GLU	3.5
1	E	103	GLY	3.4
1	A	15	GLU	3.3
1	E	16	GLU	3.2
1	H	16	GLU	3.2
1	A	14	LYS	3.1
1	B	239[A]	TYR	3.0
1	B	102	GLU	3.0
1	E	102	GLU	3.0
1	C	333	HIS	2.9
1	E	99	ARG	2.8
1	D	333	HIS	2.8
1	G	2	ALA	2.8
1	D	284	LYS	2.8
1	E	15	GLU	2.8
1	F	222	LYS	2.8
1	F	130	ASN	2.8
1	B	16	GLU	2.7
1	D	18	THR	2.7
1	F	221	ASP	2.6
1	G	16	GLU	2.6
1	A	2	ALA	2.5
1	D	102	GLU	2.5
1	H	14	LYS	2.5
1	C	10	TYR	2.5
1	E	239[A]	TYR	2.5
1	H	310	SER	2.5
1	A	16	GLU	2.5
1	F	2	ALA	2.5
1	B	331	GLN	2.5
1	G	239	TYR	2.5
1	F	16	GLU	2.5
1	E	14	LYS	2.4
1	H	99	ARG	2.4
1	A	239[A]	TYR	2.3
1	B	17	GLN	2.3
1	D	221	ASP	2.3
1	C	102	GLU	2.3
1	D	224	LYS	2.3
1	H	222	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	311[A]	GLU	2.2
1	F	213	THR	2.2
1	E	221	ASP	2.2
1	C	247	TYR	2.2
1	G	102	GLU	2.2
1	D	99	ARG	2.2
1	H	284	LYS	2.2
1	H	282	GLY	2.1
1	B	221	ASP	2.1
1	C	310	SER	2.1
1	D	14	LYS	2.1
1	H	195	ASP	2.1
1	G	103	GLY	2.0
1	H	279	GLY	2.0
1	H	239[A]	TYR	2.0
1	E	107[A]	LEU	2.0
1	A	332	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	D	403	6/6	0.35	18.57	62,64,64,64	0
3	GOL	D	402	6/6	0.33	8.63	35,36,43,48	0
2	1PE	D	401	16/16	0.19	6.64	42,48,58,59	0
2	1PE	C	400	16/16	0.22	5.86	37,43,56,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	E	402	6/6	0.49	2.53	67,72,72,74	0
2	1PE	B	400	16/16	0.19	1.28	35,42,55,59	0
2	1PE	F	400	16/16	0.22	1.07	37,42,59,59	0
2	1PE	H	400	16/16	0.22	1.04	37,44,52,52	0
2	1PE	G	400	16/16	0.17	0.93	32,38,47,47	0
2	1PE	E	401	16/16	0.24	0.88	37,43,66,68	0
2	1PE	A	400	16/16	0.19	0.83	35,41,58,63	0

## 6.5 Other polymers

There are no such residues in this entry.