



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:53 PM UTC

PDB ID : 3FZU / pdb_00003fzu
Title : IgG1 Fab characterized by H/D exchange
Authors : Arndt, J.; Houde, D.; Domeier, W.; Berkowitz, S.; Engen, J.R.
Deposited on : 2009-01-26
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
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

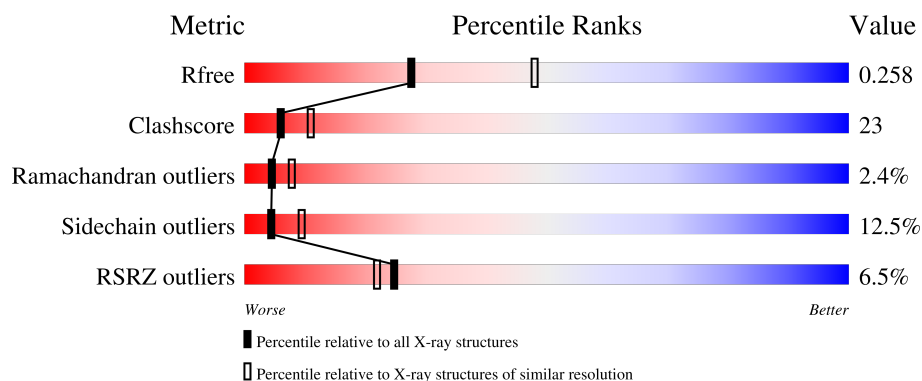
1 Overall quality at a glance

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	D	214	12% 52% 34% 11% .
1	L	214	4% 46% 43% 10% .
2	C	223	8% 58% 29% 9% .
2	H	223	2% 57% 33% 7% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6540 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 immunoglobulin IgG1 Fab, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1648	1033	277	333	5			
1	D	213	Total	C	N	O	S	0	0	0
			1630	1023	275	327	5			

- Molecule 2 is a protein called immunoglobulin IgG1 Fab, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1611	1015	273	317	6			
2	C	214	Total	C	N	O	S	0	0	0
			1596	1007	270	313	6			

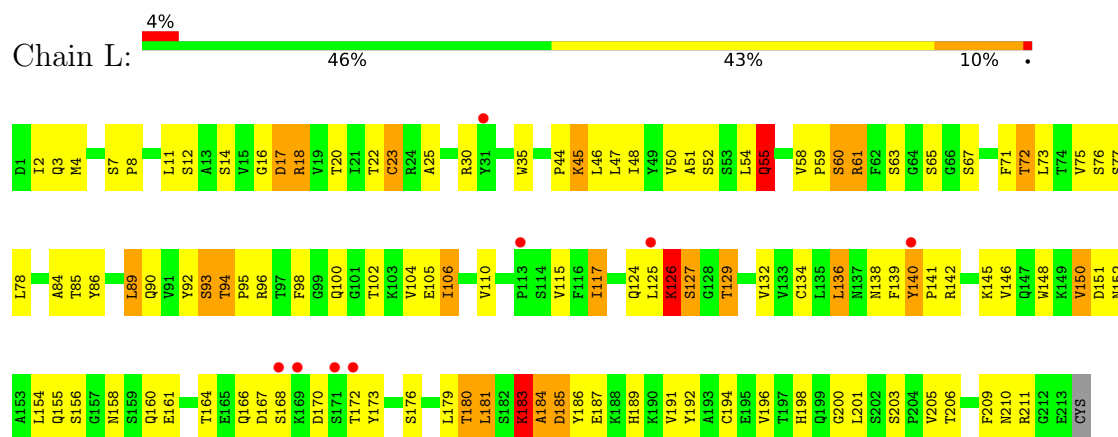
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	21	Total	O	0	0
			21	21		
3	H	12	Total	O	0	0
			12	12		
3	C	7	Total	O	0	0
			7	7		
3	D	15	Total	O	0	0
			15	15		

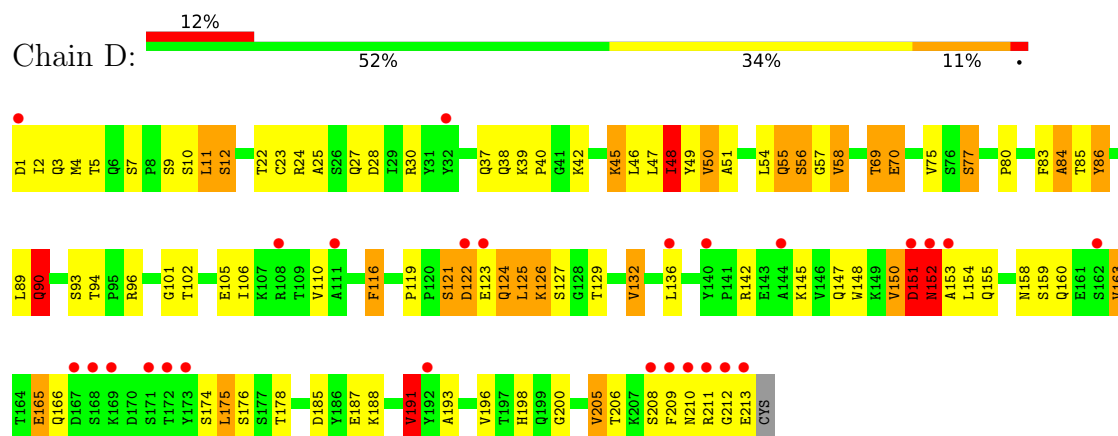
3 Residue-property plots [i](#)

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.

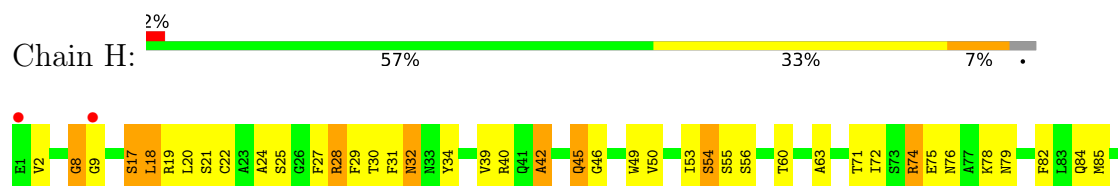
- Molecule 1: immunoglobulin IgG1 Fab, light chain

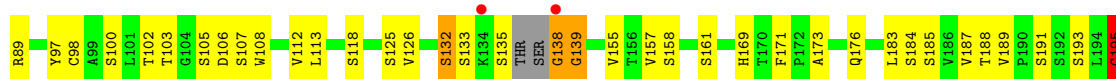


- Molecule 1: immunoglobulin IgG1 Fab, light chain

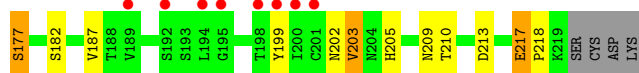
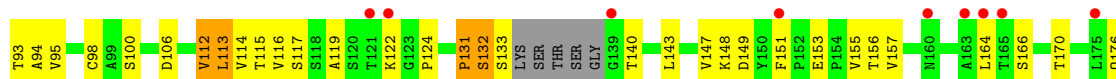
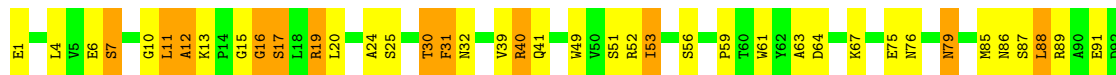


- Molecule 2: immunoglobulin IgG1 Fab, heavy chain





● Molecule 2: immunoglobulin IgG1 Fab, heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	243.05Å 61.94Å 100.85Å 90.00° 113.94° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.9 (50.00-2.50) 93.9 (50.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.261 0.220 , 0.258	Depositor DCC
R_{free} test set	2293 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.048 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6540	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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

5.1 Standard geometry

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	D	1.75	15/1665 (0.9%)	1.33	8/2264 (0.4%)
1	L	1.85	21/1683 (1.2%)	1.41	12/2285 (0.5%)
2	C	1.71	9/1634 (0.6%)	1.26	10/2226 (0.4%)
2	H	1.66	16/1649 (1.0%)	1.28	12/2246 (0.5%)
All	All	1.75	61/6631 (0.9%)	1.32	42/9021 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	H	0	2
All	All	0	3

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	12	SER	N-CA	-7.27	1.37	1.46
2	H	46	GLY	C-O	-7.02	1.17	1.24
2	H	39	VAL	C-O	-7.00	1.16	1.24
1	L	18	ARG	C-O	-6.88	1.15	1.24
1	L	16	GLY	C-O	-6.80	1.14	1.24
1	D	38	GLN	C-O	-6.75	1.16	1.24
2	H	107	SER	C-O	-6.64	1.15	1.23
2	H	25	SER	N-CA	-6.49	1.38	1.46
1	D	84	ALA	C-O	-6.30	1.17	1.23
2	C	170	THR	C-O	-6.24	1.16	1.24
1	L	140	TYR	CA-C	-6.23	1.45	1.52
1	L	22	THR	C-O	-6.21	1.16	1.24
2	H	108	TRP	N-CA	-6.11	1.38	1.46
1	L	89	LEU	C-O	-6.03	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	110	VAL	C-O	-6.00	1.17	1.24
2	C	75	GLU	C-O	-5.98	1.17	1.24
2	C	112	VAL	CA-C	5.96	1.59	1.52
1	L	72	THR	C-O	5.94	1.30	1.24
2	H	82	PHE	N-CA	5.92	1.53	1.45
1	L	104	VAL	C-O	-5.87	1.17	1.24
2	C	53	ILE	C-O	-5.75	1.18	1.24
1	D	75	VAL	C-O	-5.75	1.17	1.24
1	L	45	LYS	CA-C	5.73	1.59	1.52
2	H	155	VAL	C-O	-5.70	1.17	1.23
1	L	23	CYS	C-O	-5.70	1.16	1.24
1	L	167	ASP	C-O	-5.66	1.17	1.23
2	C	24	ALA	CA-CB	-5.65	1.43	1.53
1	L	100	GLN	C-O	-5.64	1.16	1.24
1	L	60	SER	C-O	-5.60	1.16	1.24
1	L	115	VAL	C-O	-5.59	1.18	1.24
2	C	12	ALA	CA-CB	-5.52	1.44	1.53
1	D	165	GLU	CA-C	-5.49	1.45	1.53
1	L	94	THR	C-O	-5.48	1.17	1.23
1	D	48	ILE	C-O	-5.44	1.18	1.24
1	L	166	GLN	C-O	-5.42	1.17	1.23
2	C	51	SER	C-O	-5.40	1.17	1.23
1	D	83	PHE	C-O	-5.39	1.17	1.23
1	L	172	THR	N-CA	5.38	1.52	1.45
1	D	11	LEU	C-O	-5.36	1.17	1.23
1	L	93	SER	C-O	-5.35	1.17	1.23
1	D	70	GLU	C-O	-5.31	1.18	1.24
1	L	104	VAL	CA-C	-5.29	1.45	1.52
1	D	110	VAL	C-O	-5.28	1.18	1.24
2	H	60	THR	C-O	-5.26	1.17	1.23
2	H	29	PHE	CA-C	-5.25	1.46	1.53
1	D	25	ALA	CA-CB	-5.24	1.45	1.53
1	D	58	VAL	C-O	-5.20	1.17	1.24
1	D	191	VAL	CA-CB	5.19	1.60	1.54
2	C	39	VAL	C-O	-5.19	1.18	1.23
2	H	108	TRP	CA-C	-5.18	1.46	1.52
2	H	173	ALA	C-O	-5.18	1.17	1.23
1	D	51	ALA	C-O	-5.18	1.17	1.24
2	H	103	THR	CB-OG1	-5.15	1.35	1.43
2	H	20	LEU	C-O	-5.13	1.17	1.23
2	H	53	ILE	C-O	-5.12	1.18	1.23
1	L	17	ASP	C-O	-5.07	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	95	VAL	CA-CB	-5.07	1.48	1.54
2	H	63	ALA	CA-CB	-5.07	1.45	1.53
1	L	12	SER	C-O	5.06	1.29	1.24
1	D	86	TYR	CA-C	5.04	1.59	1.52
2	H	42	ALA	CA-CB	-5.02	1.45	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	8	GLY	N-CA-C	-8.31	98.71	112.83
2	C	15	GLY	N-CA-C	-8.25	104.14	113.79
2	C	217	GLU	CA-C-N	7.25	128.90	119.84
2	C	217	GLU	C-N-CA	7.25	128.90	119.84
1	L	145	LYS	N-CA-C	-7.17	97.55	109.24
2	H	139	GLY	N-CA-C	-6.66	106.76	114.69
1	D	121	SER	N-CA-C	-6.60	100.14	110.36
1	L	61	ARG	N-CA-CB	-6.18	100.04	110.49
2	H	217	GLU	N-CA-C	6.13	116.01	108.11
1	D	94	THR	N-CA-C	-6.10	100.12	109.64
1	L	55	GLN	CA-CB-CG	-6.00	102.10	114.10
2	H	195	GLY	CA-C-N	5.93	132.37	121.70
2	H	195	GLY	C-N-CA	5.93	132.37	121.70
1	L	44	PRO	CB-CA-C	-5.92	103.81	111.39
1	D	90	GLN	N-CA-CB	-5.71	101.13	110.21
2	C	147	VAL	CB-CA-C	-5.68	104.78	111.09
2	C	6	GLU	N-CA-C	5.67	119.21	110.42
1	L	85	THR	N-CA-C	-5.62	100.02	109.07
1	L	181	LEU	N-CA-C	5.59	117.91	109.41
1	L	138	ASN	N-CA-C	5.57	122.67	110.80
2	H	89	ARG	CB-CA-C	5.50	120.57	109.68
1	L	168	SER	N-CA-C	5.44	119.77	113.18
2	C	1	GLU	N-CA-C	-5.41	95.86	111.00
2	H	169	HIS	N-CA-C	-5.40	98.45	107.80
2	H	102	THR	CA-C-N	-5.37	113.24	120.87
2	H	102	THR	C-N-CA	-5.37	113.24	120.87
1	L	76	SER	N-CA-C	5.34	117.79	111.33
2	H	216	VAL	N-CA-C	-5.31	104.27	110.05
1	D	51	ALA	N-CA-C	5.24	121.97	110.80
2	H	210	THR	CB-CA-C	-5.22	100.67	109.50
1	D	166	GLN	N-CA-C	-5.22	101.95	110.20
2	C	177	SER	N-CA-C	-5.20	107.00	113.19
1	D	101	GLY	N-CA-C	5.19	119.14	112.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	30	ARG	CB-CA-C	-5.15	110.22	117.23
1	L	7	SER	CA-CB-OG	-5.11	100.88	111.10
1	D	27	GLN	N-CA-C	-5.11	100.97	108.79
2	C	10	GLY	N-CA-C	5.07	125.20	113.18
2	C	166	SER	N-CA-C	5.06	117.50	109.96
2	H	125	SER	N-CA-C	-5.04	102.05	110.17
2	C	7	SER	N-CA-C	-5.03	100.82	108.76
1	L	16	GLY	CA-C-N	5.02	128.82	120.94
1	L	16	GLY	C-N-CA	5.02	128.82	120.94

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	151	ASP	Peptide
2	H	138	GLY	Peptide
2	H	97	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1630	0	1581	95	0
1	L	1648	0	1613	88	0
2	C	1596	0	1558	62	0
2	H	1611	0	1570	58	0
3	C	7	0	0	1	0
3	D	15	0	0	0	0
3	H	12	0	0	1	0
3	L	21	0	0	0	0
All	All	6540	0	6322	289	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 23.

All (289) 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)
2:C:11:LEU:HD12	2:C:12:ALA:N	1.34	1.37
1:D:150:VAL:HG23	1:D:155:GLN:NE2	1.35	1.35
1:D:121:SER:HB2	1:D:122:ASP:CB	1.67	1.22
1:D:122:ASP:CB	1:D:123:GLU:CB	2.30	1.09
1:L:124:GLN:HE21	1:L:129:THR:HG22	1.10	1.06
1:L:2:ILE:HG22	1:L:4:MET:HE3	1.35	1.06
1:L:124:GLN:NE2	1:L:129:THR:HG22	1.75	1.01
1:L:150:VAL:HG13	1:L:192:TYR:CD1	1.97	0.98
2:H:30:THR:HG23	2:H:32:ASN:HD21	1.32	0.94
1:D:150:VAL:CG2	1:D:155:GLN:NE2	2.30	0.94
2:C:11:LEU:CD1	2:C:12:ALA:N	2.30	0.93
1:D:50:VAL:HG23	1:D:50:VAL:O	1.70	0.92
2:H:30:THR:HG23	2:H:32:ASN:ND2	1.84	0.92
1:L:134:CYS:SG	1:L:194:CYS:CB	2.59	0.90
1:L:150:VAL:CG1	1:L:192:TYR:CE1	2.55	0.88
2:C:79:ASN:N	2:C:79:ASN:HD22	1.71	0.88
2:C:11:LEU:HD12	2:C:12:ALA:H	1.06	0.88
2:C:131:PRO:O	2:C:132:SER:HB2	1.74	0.86
1:D:150:VAL:HG23	1:D:155:GLN:HE21	1.34	0.86
1:L:124:GLN:HE21	1:L:129:THR:CG2	1.89	0.85
2:C:11:LEU:CD1	2:C:12:ALA:H	1.89	0.84
1:D:121:SER:CB	1:D:122:ASP:CB	2.53	0.84
1:D:4:MET:HE3	1:D:90:GLN:HG3	1.59	0.84
2:C:11:LEU:HD12	2:C:11:LEU:C	2.04	0.81
1:D:191:VAL:HG22	1:D:210:ASN:OD1	1.81	0.80
1:D:55:GLN:HE21	1:D:55:GLN:HA	1.45	0.80
1:L:136:LEU:N	1:L:136:LEU:HD12	1.96	0.79
1:L:4:MET:HE1	1:L:25:ALA:CB	2.12	0.79
2:C:157:VAL:HG22	2:C:203:VAL:HG22	1.66	0.78
2:C:131:PRO:O	2:C:132:SER:CB	2.30	0.78
2:H:32:ASN:HD22	2:H:32:ASN:H	1.31	0.77
2:H:195:GLY:CA	2:H:196:THR:HG22	2.14	0.77
2:C:30:THR:CG2	2:C:32:ASN:HB2	2.14	0.77
2:C:30:THR:HG22	2:C:32:ASN:HB2	1.67	0.76
1:D:150:VAL:HG23	1:D:155:GLN:CD	2.10	0.76
1:D:2:ILE:HG22	1:D:4:MET:HE2	1.67	0.75
2:H:195:GLY:N	2:H:196:THR:HG22	2.01	0.75
1:D:2:ILE:HG22	1:D:4:MET:CE	2.18	0.74
1:L:150:VAL:HG13	1:L:192:TYR:CE1	2.23	0.72
2:H:42:ALA:HB3	2:H:45:GLN:HG3	1.71	0.72
2:C:19:ARG:HG2	2:C:19:ARG:HH11	1.54	0.72
2:C:19:ARG:HG2	2:C:19:ARG:NH1	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:LEU:C	1:D:175:LEU:HD23	2.14	0.71
1:L:65:SER:HB3	1:L:72:THR:HG23	1.72	0.71
2:H:195:GLY:HA3	2:H:196:THR:HG22	1.72	0.71
2:C:79:ASN:HD22	2:C:79:ASN:H	1.37	0.71
2:C:30:THR:HG23	2:C:32:ASN:ND2	2.05	0.71
1:L:150:VAL:CG1	1:L:192:TYR:CD1	2.74	0.70
1:L:2:ILE:HG22	1:L:4:MET:CE	2.17	0.70
1:L:3:GLN:O	1:L:4:MET:HE2	1.90	0.70
1:D:125:LEU:C	1:D:127:SER:H	1.99	0.70
1:D:28:ASP:OD1	1:D:28:ASP:C	2.35	0.70
1:L:125:LEU:C	1:L:127:SER:H	1.99	0.69
1:D:142:ARG:HH21	1:D:163:VAL:HG11	1.57	0.69
1:D:24:ARG:NE	1:D:70:GLU:OE2	2.23	0.69
2:C:85:MET:HE1	2:C:114:VAL:HG21	1.75	0.68
1:L:124:GLN:NE2	1:L:129:THR:CG2	2.53	0.67
1:D:123:GLU:O	1:D:124:GLN:C	2.37	0.67
1:L:150:VAL:HG11	1:L:192:TYR:CE1	2.30	0.67
1:L:96:ARG:HG3	2:H:49:TRP:CD1	2.29	0.67
1:L:180:THR:O	1:L:180:THR:HG22	1.94	0.67
2:C:131:PRO:HG3	2:C:143:LEU:HB3	1.76	0.67
1:L:198:HIS:CD2	1:L:200:GLY:H	2.13	0.67
1:L:125:LEU:C	1:L:127:SER:N	2.51	0.66
2:H:195:GLY:HA3	2:H:196:THR:CB	2.24	0.66
1:D:2:ILE:HD12	1:D:93:SER:HB3	1.78	0.66
2:H:195:GLY:HA3	2:H:196:THR:CG2	2.25	0.66
2:C:119:ALA:HB3	2:C:151:PHE:CE1	2.29	0.66
1:D:50:VAL:O	1:D:50:VAL:CG2	2.41	0.66
1:D:123:GLU:O	1:D:125:LEU:N	2.29	0.65
2:H:193:SER:O	2:H:196:THR:CG2	2.45	0.65
2:C:93:THR:HG23	2:C:115:THR:HA	1.77	0.65
2:H:32:ASN:HD22	2:H:32:ASN:N	1.94	0.65
2:C:19:ARG:HG3	2:C:20:LEU:N	2.12	0.65
2:H:30:THR:CG2	2:H:32:ASN:HD21	2.08	0.65
1:D:150:VAL:H	1:D:155:GLN:HE21	1.45	0.65
1:D:123:GLU:O	1:D:126:LYS:N	2.30	0.64
1:L:125:LEU:O	1:L:127:SER:N	2.30	0.64
2:H:195:GLY:HA3	2:H:196:THR:HB	1.79	0.64
2:H:31:PHE:CD2	2:H:79:ASN:HA	2.33	0.64
1:L:4:MET:HE1	1:L:25:ALA:HB2	1.79	0.64
1:D:153:ALA:O	1:D:155:GLN:NE2	2.30	0.64
2:H:139:GLY:C	2:H:191:SER:HG	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ASP:O	1:D:153:ALA:N	2.30	0.63
1:L:136:LEU:N	1:L:136:LEU:CD1	2.61	0.63
2:H:18:LEU:HB2	2:H:85:MET:HE3	1.80	0.63
2:C:30:THR:HG23	2:C:32:ASN:HD22	1.63	0.63
1:D:125:LEU:O	1:D:127:SER:N	2.30	0.62
1:L:50:VAL:O	1:L:51:ALA:HB3	1.99	0.62
1:L:90:GLN:HE21	1:L:92:TYR:H	1.46	0.62
1:L:198:HIS:HD2	1:L:200:GLY:H	1.46	0.62
2:H:19:ARG:HG3	2:H:84:GLN:NE2	2.15	0.61
1:D:2:ILE:CD1	1:D:93:SER:HB3	2.30	0.61
1:D:80:PRO:HA	1:D:106:ILE:HD13	1.83	0.61
1:L:61:ARG:HG2	1:L:75:VAL:HG13	1.83	0.60
1:L:2:ILE:CG2	1:L:4:MET:HE3	2.23	0.60
2:C:30:THR:C	2:C:32:ASN:H	2.10	0.60
2:C:13:LYS:O	2:C:16:GLY:N	2.30	0.59
2:H:183:LEU:C	2:H:183:LEU:HD12	2.27	0.59
2:H:22:CYS:SG	2:H:98:CYS:CB	2.92	0.57
2:H:161:SER:H	2:H:202:ASN:HD21	1.52	0.57
1:D:125:LEU:C	1:D:127:SER:N	2.61	0.57
2:H:100:SER:O	2:H:106:ASP:HA	2.05	0.56
2:H:189:VAL:HG11	2:H:199:TYR:CE2	2.39	0.56
1:D:212:GLY:O	1:D:213:GLU:HG3	2.05	0.56
2:C:132:SER:OG	2:C:133:SER:N	2.29	0.56
2:C:148:LYS:O	2:C:149:ASP:HB2	2.04	0.55
2:H:135:SER:O	2:H:138:GLY:N	2.39	0.55
2:C:19:ARG:HH11	2:C:19:ARG:CG	2.20	0.55
2:C:4:LEU:HD13	2:C:98:CYS:SG	2.46	0.55
2:C:49:TRP:CD1	1:D:96:ARG:CG	2.90	0.55
1:D:55:GLN:HE21	1:D:55:GLN:CA	2.18	0.55
1:D:187:GLU:HA	1:D:211:ARG:CZ	2.36	0.55
2:C:209:ASN:C	2:C:209:ASN:HD22	2.13	0.55
2:C:20:LEU:HG	2:C:85:MET:HE2	1.89	0.54
2:C:30:THR:O	2:C:32:ASN:N	2.39	0.54
1:D:119:PRO:HB3	1:D:209:PHE:CZ	2.42	0.54
2:H:210:THR:HG22	2:H:211:LYS:N	2.21	0.54
1:L:8:PRO:O	1:L:102:THR:HG23	2.06	0.54
2:H:158:SER:OG	2:H:202:ASN:ND2	2.35	0.54
1:D:4:MET:HE3	1:D:90:GLN:CG	2.33	0.54
1:D:158:ASN:OD1	1:D:158:ASN:N	2.39	0.54
1:L:146:VAL:HG22	1:L:196:VAL:HG22	1.89	0.54
1:L:4:MET:HE1	1:L:25:ALA:HB1	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:183:LYS:O	1:L:184:ALA:C	2.48	0.54
1:L:46:LEU:HD23	1:L:55:GLN:HG3	1.90	0.53
1:L:134:CYS:HB2	1:L:148:TRP:CZ2	2.44	0.53
2:C:17:SER:OG	2:C:86:ASN:OD1	2.27	0.53
1:D:124:GLN:O	1:D:127:SER:N	2.41	0.53
2:H:193:SER:O	2:H:196:THR:HG22	2.08	0.53
2:C:87:SER:O	2:C:88:LEU:C	2.52	0.53
1:D:150:VAL:O	1:D:151:ASP:C	2.52	0.53
1:D:198:HIS:CD2	1:D:200:GLY:H	2.26	0.53
1:D:55:GLN:HA	1:D:55:GLN:NE2	2.20	0.52
1:D:124:GLN:O	1:D:125:LEU:C	2.51	0.52
1:D:136:LEU:HD11	1:D:196:VAL:HG21	1.91	0.52
1:D:145:LYS:HE3	1:D:147:GLN:NE2	2.25	0.52
1:D:116:PHE:N	1:D:116:PHE:CD1	2.77	0.52
1:D:193:ALA:HB2	1:D:208:SER:HB3	1.92	0.52
1:D:210:ASN:HB2	1:D:213:GLU:OE1	2.09	0.52
2:C:124:PRO:HD2	2:C:210:THR:HG21	1.92	0.52
2:C:32:ASN:HA	2:C:76:ASN:ND2	2.23	0.52
2:C:30:THR:C	2:C:32:ASN:N	2.62	0.52
2:C:49:TRP:CD1	1:D:96:ARG:HG2	2.44	0.51
1:L:61:ARG:HD2	1:L:77:SER:O	2.10	0.51
1:D:2:ILE:CG2	1:D:4:MET:CE	2.87	0.51
1:D:145:LYS:O	1:D:196:VAL:HA	2.11	0.51
2:C:88:LEU:HB3	2:C:116:VAL:HG21	1.91	0.51
1:L:94:THR:HA	1:L:95:PRO:C	2.36	0.51
2:H:139:GLY:C	2:H:191:SER:OG	2.54	0.51
1:L:90:GLN:NE2	1:L:93:SER:H	2.09	0.50
1:L:11:LEU:HD12	1:L:11:LEU:C	2.37	0.50
2:C:40:ARG:HG2	2:C:41:GLN:N	2.26	0.50
2:H:210:THR:CG2	2:H:211:LYS:N	2.75	0.50
1:D:205:VAL:HG13	1:D:206:THR:N	2.26	0.50
2:H:32:ASN:CB	2:H:76:ASN:ND2	2.75	0.50
1:D:193:ALA:HB1	1:D:206:THR:HG23	1.93	0.50
2:H:126:VAL:CG2	2:H:203:VAL:HG21	2.42	0.50
2:C:87:SER:O	2:C:88:LEU:O	2.30	0.50
2:C:89:ARG:O	2:C:116:VAL:HG11	2.11	0.49
2:C:93:THR:O	2:C:94:ALA:HB2	2.12	0.49
1:L:61:ARG:HG2	1:L:75:VAL:CG1	2.42	0.49
1:D:150:VAL:O	1:D:151:ASP:O	2.30	0.49
1:L:89:LEU:HD13	1:L:98:PHE:CE2	2.48	0.49
1:L:65:SER:HB3	1:L:72:THR:CG2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:SER:O	1:D:77:SER:OG	2.26	0.49
1:L:150:VAL:HG11	1:L:192:TYR:HE1	1.78	0.49
1:D:187:GLU:O	1:D:211:ARG:NH2	2.46	0.49
1:L:160:GLN:HE22	2:H:176:GLN:HG2	1.77	0.48
1:D:175:LEU:HD23	1:D:176:SER:N	2.27	0.48
2:H:193:SER:O	2:H:196:THR:HG23	2.13	0.48
1:D:89:LEU:HD11	1:D:96:ARG:HB3	1.95	0.48
1:L:48:ILE:CD1	1:L:54:LEU:HD12	2.44	0.48
1:L:150:VAL:HG23	1:L:155:GLN:NE2	2.29	0.48
2:H:161:SER:N	2:H:202:ASN:HD21	2.11	0.48
1:L:50:VAL:O	1:L:51:ALA:CB	2.61	0.48
2:H:17:SER:HA	2:H:85:MET:O	2.13	0.48
1:D:175:LEU:C	1:D:175:LEU:CD2	2.84	0.48
1:L:96:ARG:HG3	2:H:49:TRP:CG	2.49	0.47
1:L:18:ARG:NH2	1:D:70:GLU:OE1	2.46	0.47
2:H:28:ARG:HE	2:H:28:ARG:HB2	1.40	0.47
2:H:2:VAL:HG21	2:H:27:PHE:CE2	2.50	0.47
2:C:113:LEU:HD13	3:C:248:HOH:O	2.15	0.47
1:D:145:LYS:HE3	1:D:147:GLN:HE22	1.79	0.47
1:L:117:ILE:HD13	1:L:209:PHE:HD1	1.80	0.47
1:L:141:PRO:O	1:L:198:HIS:HE1	1.96	0.47
1:D:4:MET:CE	1:D:90:GLN:HG3	2.38	0.47
1:L:187:GLU:O	1:L:211:ARG:NH2	2.48	0.47
2:H:32:ASN:ND2	2:H:32:ASN:H	2.07	0.47
1:L:201:LEU:HD13	1:L:205:VAL:HG23	1.97	0.47
2:C:143:LEU:HD21	2:C:199:TYR:CD1	2.50	0.46
1:L:90:GLN:NE2	1:L:92:TYR:H	2.13	0.46
2:H:196:THR:HG23	2:H:197:GLN:N	2.29	0.46
1:L:160:GLN:NE2	2:H:176:GLN:HG2	2.31	0.46
1:L:186:TYR:CE1	1:L:192:TYR:CE2	3.02	0.46
1:L:125:LEU:O	1:L:126:LYS:C	2.58	0.46
1:L:63:SER:O	1:L:73:LEU:HD12	2.16	0.46
2:H:75:GLU:OE2	2:H:78:LYS:HD2	2.16	0.46
1:D:40:PRO:CB	1:D:165:GLU:HG2	2.46	0.46
1:D:185:ASP:OD1	1:D:188:LYS:NZ	2.49	0.46
1:L:185:ASP:N	1:L:185:ASP:OD1	2.43	0.46
1:D:5:THR:O	1:D:5:THR:HG22	2.15	0.46
1:D:54:LEU:HD11	1:D:58:VAL:HG12	1.97	0.46
2:H:34:TYR:O	2:H:74:ARG:NH2	2.40	0.45
1:D:159:SER:HA	1:D:178:THR:O	2.17	0.45
1:L:67:SER:HA	1:L:71:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:24:ALA:HB1	2:H:27:PHE:HE1	1.81	0.45
1:D:148:TRP:O	1:D:155:GLN:HG2	2.17	0.45
1:L:170:ASP:C	1:L:170:ASP:OD1	2.54	0.45
1:D:119:PRO:HB3	1:D:209:PHE:CE2	2.52	0.45
1:D:152:ASN:OD1	1:D:152:ASN:N	2.47	0.45
2:C:79:ASN:N	2:C:79:ASN:ND2	2.45	0.45
1:D:37:GLN:OE1	1:D:39:LYS:HE3	2.17	0.44
1:L:158:ASN:O	1:L:179:LEU:HD12	2.17	0.44
2:C:59:PRO:HG2	2:C:61:TRP:CH2	2.52	0.44
2:C:155:VAL:HG12	2:C:205:HIS:CD2	2.53	0.44
1:D:4:MET:HE3	1:D:90:GLN:CB	2.47	0.44
1:L:84:ALA:HB3	1:L:86:TYR:CE1	2.52	0.44
2:C:30:THR:CG2	2:C:32:ASN:CB	2.91	0.44
2:C:87:SER:C	2:C:88:LEU:O	2.57	0.44
2:C:164:LEU:CD2	2:C:187:VAL:HG21	2.47	0.44
1:D:151:ASP:C	1:D:153:ALA:N	2.75	0.44
1:L:14:SER:O	1:L:17:ASP:HB2	2.18	0.44
1:L:106:ILE:HD13	1:L:106:ILE:N	2.32	0.44
2:C:88:LEU:HB3	2:C:116:VAL:CG2	2.47	0.44
1:L:90:GLN:HE22	1:L:93:SER:H	1.65	0.43
2:H:72:ILE:O	3:H:226:HOH:O	2.21	0.43
1:L:89:LEU:HD13	1:L:98:PHE:CD2	2.54	0.43
2:C:100:SER:O	2:C:106:ASP:HA	2.18	0.43
1:D:37:GLN:HB2	1:D:47:LEU:HD11	2.00	0.43
1:D:46:LEU:HD21	1:D:49:TYR:HB3	2.00	0.43
1:L:142:ARG:HB2	1:L:173:TYR:CE2	2.53	0.43
2:H:40:ARG:HD3	2:H:50:VAL:CG2	2.49	0.43
1:D:85:THR:HA	1:D:102:THR:O	2.18	0.43
2:C:88:LEU:HD23	2:C:88:LEU:HA	1.63	0.43
2:H:22:CYS:HG	2:H:98:CYS:HG	0.45	0.43
2:H:206:LYS:N	2:H:207:PRO:CD	2.81	0.43
2:C:53:ILE:O	2:C:53:ILE:HG23	2.19	0.43
1:L:18:ARG:HD3	1:D:22:THR:HG21	2.00	0.43
1:D:150:VAL:O	1:D:153:ALA:HB3	2.19	0.43
1:D:84:ALA:HB3	1:D:86:TYR:CE1	2.54	0.42
2:H:132:SER:OG	2:H:133:SER:N	2.40	0.42
1:L:154:LEU:O	1:D:154:LEU:HD23	2.18	0.42
1:L:164:THR:HG23	2:H:171:PHE:CE2	2.55	0.42
2:H:78:LYS:O	2:H:79:ASN:C	2.58	0.42
1:L:78:LEU:HD21	1:L:106:ILE:HD12	2.02	0.42
1:L:154:LEU:HD23	1:D:154:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:LEU:HB2	2:H:85:MET:CE	2.47	0.42
2:H:193:SER:C	2:H:195:GLY:N	2.78	0.42
1:D:47:LEU:C	1:D:48:ILE:HG12	2.43	0.42
1:L:17:ASP:HB3	1:D:7:SER:OG	2.20	0.42
1:L:105:GLU:HG2	1:L:106:ILE:N	2.34	0.42
1:L:186:TYR:HE1	1:L:192:TYR:CE2	2.38	0.42
1:D:56:SER:HA	1:D:57:GLY:HA2	1.82	0.42
2:H:8:GLY:O	2:H:112:VAL:HG21	2.18	0.42
1:D:22:THR:CG2	1:D:23:CYS:N	2.82	0.42
1:L:151:ASP:OD2	1:L:189:HIS:ND1	2.48	0.42
2:H:40:ARG:HD3	2:H:50:VAL:HG22	2.02	0.42
2:C:63:ALA:O	2:C:64:ASP:C	2.62	0.42
2:C:176:GLN:HA	1:D:160:GLN:NE2	2.35	0.42
1:D:119:PRO:HA	1:D:132:VAL:HG13	2.01	0.42
1:D:210:ASN:CB	1:D:213:GLU:OE1	2.68	0.42
1:D:124:GLN:O	1:D:127:SER:OG	2.30	0.41
2:C:30:THR:HG23	2:C:32:ASN:H	1.85	0.41
1:D:11:LEU:C	1:D:11:LEU:HD12	2.44	0.41
1:D:69:THR:HG22	1:D:70:GLU:HG2	2.01	0.41
1:L:78:LEU:CD2	1:L:106:ILE:HD12	2.50	0.41
2:C:17:SER:HA	2:C:85:MET:O	2.19	0.41
2:C:30:THR:O	2:C:31:PHE:C	2.63	0.41
1:D:45:LYS:HA	1:D:45:LYS:HD2	1.81	0.41
1:L:71:PHE:CD1	1:L:71:PHE:N	2.89	0.41
1:L:136:LEU:CD1	1:L:136:LEU:H	2.30	0.41
2:C:205:HIS:HB3	2:C:210:THR:HB	2.01	0.41
1:L:58:VAL:O	1:L:59:PRO:C	2.61	0.41
1:L:140:TYR:CD1	1:L:141:PRO:HA	2.56	0.41
2:H:158:SER:OG	2:H:202:ASN:HB2	2.20	0.41
2:C:49:TRP:CD1	1:D:96:ARG:HG3	2.55	0.41
1:D:2:ILE:CG2	1:D:4:MET:HE1	2.51	0.41
1:L:139:PHE:CD1	1:L:139:PHE:N	2.89	0.41
1:L:136:LEU:HD21	1:L:146:VAL:CG2	2.51	0.40
2:H:54:SER:OG	2:H:55:SER:N	2.54	0.40
1:D:4:MET:HE3	1:D:90:GLN:HB2	2.03	0.40
2:H:205:HIS:CD2	2:H:207:PRO:HD2	2.56	0.40
2:C:91:GLU:CD	2:C:91:GLU:N	2.79	0.40
1:L:191:VAL:HG22	1:L:210:ASN:OD1	2.21	0.40
1:L:23:CYS:HB2	1:L:35:TRP:CH2	2.56	0.40
1:L:161:GLU:HA	1:L:176:SER:O	2.20	0.40
1:L:201:LEU:HD23	1:L:201:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:GLN:HG2	1:D:129:THR: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	D	211/214 (99%)	185 (88%)	20 (10%)	6 (3%)	4	6
1	L	211/214 (99%)	196 (93%)	11 (5%)	4 (2%)	6	11
2	C	210/223 (94%)	195 (93%)	9 (4%)	6 (3%)	3	5
2	H	213/223 (96%)	196 (92%)	13 (6%)	4 (2%)	6	11
All	All	845/874 (97%)	772 (91%)	53 (6%)	20 (2%)	4	8

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	132	SER
2	H	196	THR
2	C	132	SER
1	D	124	GLN
1	D	152	ASN
1	L	52	SER
2	H	195	GLY
1	D	122	ASP
1	D	126	LYS
1	L	126	LYS
2	C	31	PHE
1	D	125	LEU
1	D	151	ASP
1	L	183	LYS

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Mol	Chain	Res	Type
1	L	184	ALA
2	C	16	GLY
2	C	218	PRO
2	C	88	LEU
2	C	131	PRO
2	H	9	GLY

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	D	184/190 (97%)	160 (87%)	24 (13%)	4	8
1	L	189/190 (100%)	167 (88%)	22 (12%)	5	11
2	C	178/187 (95%)	154 (86%)	24 (14%)	4	8
2	H	179/187 (96%)	158 (88%)	21 (12%)	5	11
All	All	730/754 (97%)	639 (88%)	91 (12%)	4	9

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	THR
1	L	30	ARG
1	L	45	LYS
1	L	47	LEU
1	L	55	GLN
1	L	60	SER
1	L	106	ILE
1	L	117	ILE
1	L	126	LYS
1	L	127	SER
1	L	129	THR
1	L	132	VAL
1	L	136	LEU
1	L	150	VAL
1	L	152	ASN

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Mol	Chain	Res	Type
1	L	156	SER
1	L	180	THR
1	L	181	LEU
1	L	183	LYS
1	L	185	ASP
1	L	203	SER
1	L	206	THR
2	H	17	SER
2	H	18	LEU
2	H	21	SER
2	H	28	ARG
2	H	32	ASN
2	H	45	GLN
2	H	54	SER
2	H	56	SER
2	H	71	THR
2	H	74	ARG
2	H	105	SER
2	H	113	LEU
2	H	118	SER
2	H	157	VAL
2	H	184	SER
2	H	185	SER
2	H	187	VAL
2	H	188	THR
2	H	200	ILE
2	H	203	VAL
2	H	206	LYS
2	C	7	SER
2	C	11	LEU
2	C	17	SER
2	C	19	ARG
2	C	25	SER
2	C	30	THR
2	C	40	ARG
2	C	52	ARG
2	C	56	SER
2	C	67	LYS
2	C	79	ASN
2	C	112	VAL
2	C	113	LEU
2	C	117	SER

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Mol	Chain	Res	Type
2	C	122	LYS
2	C	140	THR
2	C	153	GLU
2	C	156	THR
2	C	177	SER
2	C	182	SER
2	C	202	ASN
2	C	203	VAL
2	C	213	ASP
2	C	217	GLU
1	D	1	ASP
1	D	3	GLN
1	D	9	SER
1	D	10	SER
1	D	12	SER
1	D	42	LYS
1	D	45	LYS
1	D	48	ILE
1	D	50	VAL
1	D	55	GLN
1	D	56	SER
1	D	69	THR
1	D	77	SER
1	D	90	GLN
1	D	105	GLU
1	D	116	PHE
1	D	132	VAL
1	D	150	VAL
1	D	152	ASN
1	D	163	VAL
1	D	174	SER
1	D	175	LEU
1	D	191	VAL
1	D	205	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	90	GLN
1	L	124	GLN
1	L	152	ASN
1	L	198	HIS

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Mol	Chain	Res	Type
2	H	32	ASN
2	H	33	ASN
2	H	84	GLN
2	H	202	ASN
2	C	32	ASN
2	C	79	ASN
2	C	84	GLN
2	C	176	GLN
2	C	209	ASN
1	D	55	GLN
1	D	147	GLN
1	D	155	GLN
1	D	160	GLN
1	D	189	HIS
1	D	198	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 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	D	213/214 (99%)	0.64	26 (12%) 8 7	27, 39, 49, 54	0
1	L	213/214 (99%)	0.33	8 (3%) 44 39	24, 37, 48, 52	0
2	C	214/223 (95%)	0.29	17 (7%) 18 16	6, 24, 47, 52	0
2	H	217/223 (97%)	0.17	5 (2%) 61 57	18, 34, 45, 54	0
All	All	857/874 (98%)	0.36	56 (6%) 25 22	6, 36, 48, 54	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	171	SER	4.0
1	D	212	GLY	3.9
1	D	140	TYR	3.6
2	C	121	THR	3.6
1	D	122	ASP	3.6
1	D	210	ASN	3.5
1	D	123	GLU	3.3
1	D	151	ASP	3.3
1	D	168	SER	3.3
2	C	163	ALA	3.2
1	D	144	ALA	2.9
2	H	1	GLU	2.9
2	C	198	THR	2.8
2	C	151	PHE	2.8
1	D	167	ASP	2.7
1	D	153	ALA	2.7
2	C	200	ILE	2.7
2	C	122	LYS	2.6
1	D	172	THR	2.6
2	C	164	LEU	2.6
1	L	169	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	173	TYR	2.6
1	D	192	TYR	2.6
1	D	169	LYS	2.5
1	L	171	SER	2.5
2	H	138	GLY	2.5
2	C	192	SER	2.5
1	L	113	PRO	2.4
2	C	195	GLY	2.4
2	H	219	LYS	2.4
1	D	211	ARG	2.4
1	L	168	SER	2.3
1	D	209	PHE	2.3
2	H	9	GLY	2.3
2	C	139	GLY	2.3
1	L	172	THR	2.2
2	C	175	LEU	2.2
1	D	108	ARG	2.2
2	C	201	CYS	2.2
1	L	31	TYR	2.2
1	D	162	SER	2.2
1	L	125	LEU	2.2
1	L	140	TYR	2.1
1	D	32	TYR	2.1
1	D	213	GLU	2.1
2	C	189	VAL	2.1
1	D	136	LEU	2.1
2	C	160	ASN	2.1
2	C	194	LEU	2.1
1	D	1	ASP	2.1
2	H	134	LYS	2.0
2	C	165	THR	2.0
1	D	111	ALA	2.0
1	D	152	ASN	2.0
1	D	208	SER	2.0
2	C	199	TYR	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.