



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2018 – 01:53 AM EST

PDB ID : 1FMV  
Title : CRYSTAL STRUCTURE OF THE APO MOTOR DOMAIN OF DICTYOSTELLIUM MYOSIN II  
Authors : Bauer, C.B.; Holden, H.M.; Thoden, J.B.; Smith, R.; Rayment, I.  
Deposited on : 2000-08-18  
Resolution : 2.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

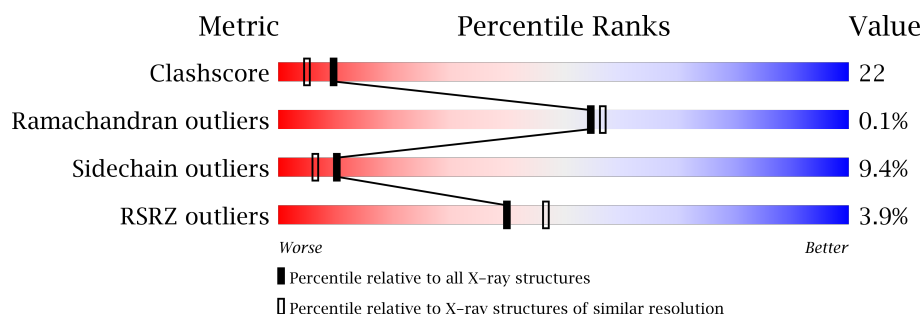
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	761	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6509 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 MYOSIN II HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	743	Total	C	N	O	S	0	5	0
			5907	3758	1020	1113	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	CYS	TYR	CONFLICT	UNP P08799
A	489	VAL	LEU	CONFLICT	UNP P08799
A	760	PRO	-	CLONING ARTIFACT	UNP P08799
A	761	ASN	-	CLONING ARTIFACT	UNP P08799

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

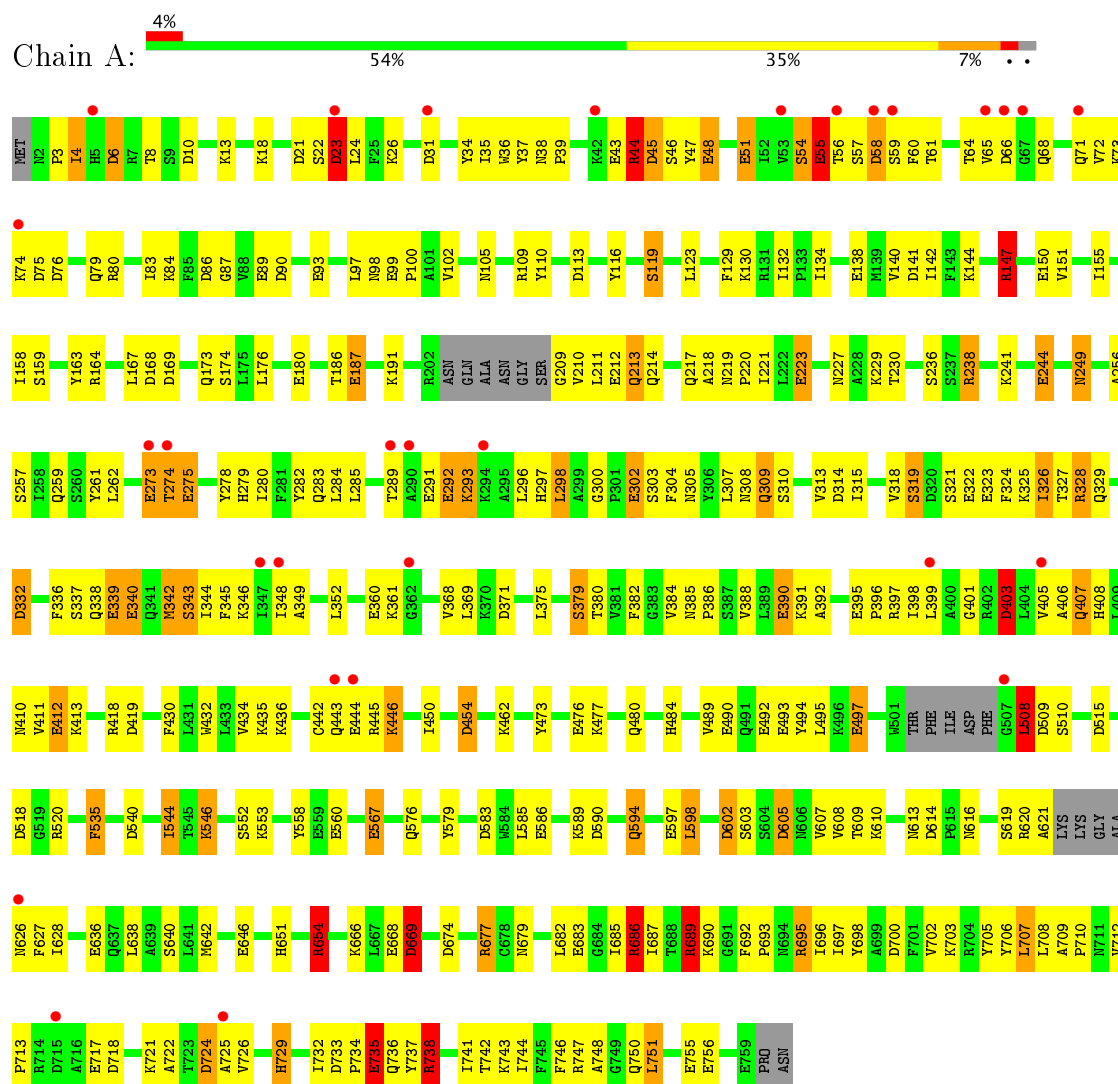
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	601	Total	O	11	0
			601	601		

### 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 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: MYOSIN II HEAVY CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.50 Å   179.70 Å   54.10 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	100.00 – 2.10 24.42 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (100.00-2.10) 96.4 (24.42-2.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 2.10 Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.196 ,   0.280 0.195 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 102.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6509	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.02	39/6041 (0.6%)	1.61	97/8161 (1.2%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	GLU	CD-OE2	7.51	1.33	1.25
1	A	275	GLU	CD-OE2	7.37	1.33	1.25
1	A	273	GLU	CD-OE2	6.90	1.33	1.25
1	A	180	GLU	CD-OE2	6.69	1.33	1.25
1	A	412	GLU	CD-OE2	6.47	1.32	1.25
1	A	497	GLU	CD-OE2	6.33	1.32	1.25
1	A	683	GLU	CD-OE2	6.25	1.32	1.25
1	A	755	GLU	CD-OE2	6.18	1.32	1.25
1	A	323	GLU	CD-OE2	6.12	1.32	1.25
1	A	444	GLU	CD-OE2	6.09	1.32	1.25
1	A	360	GLU	CD-OE2	6.08	1.32	1.25
1	A	93	GLU	CD-OE2	6.03	1.32	1.25
1	A	668	GLU	CD-OE2	6.00	1.32	1.25
1	A	492	GLU	CD-OE2	5.93	1.32	1.25
1	A	646	GLU	CD-OE2	5.79	1.32	1.25
1	A	138	GLU	CD-OE2	5.78	1.32	1.25
1	A	339	GLU	CD-OE2	5.78	1.32	1.25
1	A	340	GLU	CD-OE2	5.70	1.31	1.25
1	A	48	GLU	CD-OE2	5.67	1.31	1.25
1	A	636	GLU	CD-OE2	5.62	1.31	1.25
1	A	493	GLU	CD-OE2	5.59	1.31	1.25
1	A	244	GLU	CD-OE2	5.56	1.31	1.25
1	A	212	GLU	CD-OE2	5.55	1.31	1.25
1	A	756	GLU	CD-OE2	5.51	1.31	1.25
1	A	586	GLU	CD-OE2	5.50	1.31	1.25
1	A	490	GLU	CD-OE2	5.45	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	GLU	CD-OE2	5.42	1.31	1.25
1	A	89	GLU	CD-OE2	5.41	1.31	1.25
1	A	223	GLU	CD-OE2	5.40	1.31	1.25
1	A	717	GLU	CD-OE2	5.30	1.31	1.25
1	A	560	GLU	CD-OE2	5.29	1.31	1.25
1	A	292	GLU	CD-OE2	5.23	1.31	1.25
1	A	597	GLU	CD-OE2	5.16	1.31	1.25
1	A	187	GLU	CD-OE2	5.11	1.31	1.25
1	A	390	GLU	CD-OE2	5.06	1.31	1.25
1	A	43	GLU	CD-OE2	5.06	1.31	1.25
1	A	735	GLU	CD-OE2	5.04	1.31	1.25
1	A	567	GLU	CD-OE2	5.04	1.31	1.25
1	A	654	ARG	NE-CZ	-5.01	1.26	1.33

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	689	ARG	NE-CZ-NH1	18.89	129.74	120.30
1	A	238	ARG	NE-CZ-NH1	16.02	128.31	120.30
1	A	238	ARG	NE-CZ-NH2	-13.30	113.65	120.30
1	A	44	ARG	NE-CZ-NH1	10.99	125.80	120.30
1	A	689	ARG	NE-CZ-NH2	-10.91	114.85	120.30
1	A	45	ASP	CB-CG-OD2	-10.87	108.52	118.30
1	A	738	ARG	NE-CZ-NH1	10.71	125.65	120.30
1	A	654	ARG	CD-NE-CZ	-10.21	109.30	123.60
1	A	515	ASP	CB-CG-OD1	10.17	127.45	118.30
1	A	677	ARG	NE-CZ-NH1	-9.89	115.35	120.30
1	A	689	ARG	CD-NE-CZ	9.61	137.05	123.60
1	A	21	ASP	CB-CG-OD2	-9.49	109.76	118.30
1	A	45	ASP	CB-CG-OD1	9.43	126.79	118.30
1	A	44	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	A	169	ASP	CB-CG-OD1	8.69	126.12	118.30
1	A	6	ASP	CB-CG-OD2	-8.55	110.61	118.30
1	A	419	ASP	CB-CG-OD2	-8.44	110.71	118.30
1	A	540	ASP	CB-CG-OD1	8.22	125.70	118.30
1	A	614	ASP	CB-CG-OD1	8.21	125.69	118.30
1	A	509	ASP	CB-CG-OD1	8.08	125.57	118.30
1	A	674	ASP	CB-CG-OD2	-8.05	111.06	118.30
1	A	164	ARG	NE-CZ-NH2	8.00	124.30	120.30
1	A	515	ASP	CB-CG-OD2	-7.96	111.14	118.30
1	A	419	ASP	CB-CG-OD1	7.82	125.34	118.30
1	A	147	ARG	NE-CZ-NH1	7.80	124.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	ASP	CB-CG-OD2	-7.79	111.28	118.30
1	A	113	ASP	CB-CG-OD1	7.72	125.25	118.30
1	A	509	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	A	403	ASP	CB-CG-OD1	7.63	125.17	118.30
1	A	518	ASP	CB-CG-OD1	7.60	125.14	118.30
1	A	76	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	A	540	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	A	614	ASP	CB-CG-OD2	-7.35	111.68	118.30
1	A	620	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	A	314	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	A	169	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	A	168	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	669	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	A	738	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	A	58	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	A	695	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	654	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	10	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	A	371	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	A	54	SER	N-CA-CB	6.70	120.55	110.50
1	A	332	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	A	90	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	90	ASP	CB-CG-OD2	-6.58	112.37	118.30
1	A	583	ASP	CB-CG-OD1	6.45	124.11	118.30
1	A	605	ASP	CB-CG-OD2	-6.43	112.52	118.30
1	A	371	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	110	TYR	CB-CG-CD1	-6.23	117.26	121.00
1	A	44	ARG	CD-NE-CZ	6.20	132.28	123.60
1	A	583	ASP	CB-CG-OD2	-6.18	112.73	118.30
1	A	23	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	109	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	A	66	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	686	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	602	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	A	319	SER	N-CA-CB	6.01	119.51	110.50
1	A	164	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	A	119	SER	N-CA-CB	5.89	119.33	110.50
1	A	238	ARG	CA-CB-CG	-5.89	100.45	113.40
1	A	598	LEU	CA-CB-CG	-5.88	101.77	115.30
1	A	729	HIS	CA-CB-CG	-5.87	103.62	113.60
1	A	724	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	A	6	ASP	CB-CG-OD1	5.82	123.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	ALA	CB-CA-C	5.80	118.80	110.10
1	A	278	TYR	CB-CG-CD2	5.74	124.44	121.00
1	A	23	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	314	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	21	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	700	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	558	TYR	CB-CG-CD2	5.54	124.32	121.00
1	A	168	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	A	605	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	602	ASP	N-CA-CB	5.51	120.52	110.60
1	A	535	PHE	CA-CB-CG	-5.50	100.69	113.90
1	A	674	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	497	GLU	C-N-CA	-5.42	108.15	121.70
1	A	518	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	508	LEU	C-N-CA	5.38	135.16	121.70
1	A	66	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	718	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	141	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	718	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	A	733	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	418	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	180	GLU	CB-CA-C	-5.17	100.05	110.40
1	A	129	PHE	CB-CG-CD1	-5.16	117.19	120.80
1	A	3	PRO	N-CA-CB	5.14	109.46	103.30
1	A	113	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	10	ASP	CB-CG-OD1	5.13	122.91	118.30
1	A	454	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	489	VAL	N-CA-CB	5.07	122.65	111.50
1	A	76	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	590	ASP	CB-CG-OD2	-5.02	113.78	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	A	5907	0	5800	252	0
2	A	1	0	0	0	0
3	A	601	0	0	19	1
All	All	6509	0	5800	252	1

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 22.

All (252) 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:A:293:LYS:HA	1:A:298:LEU:HD12	1.19	1.10
1:A:398:ILE:HD13	1:A:407:GLN:HG3	1.12	1.06
1:A:480:GLN:HE21	1:A:508:LEU:HD21	0.95	1.05
1:A:296:LEU:HB2	1:A:298:LEU:HD11	1.37	1.01
1:A:480:GLN:NE2	1:A:508:LEU:HD21	1.76	0.99
1:A:296:LEU:HB3	1:A:298:LEU:HD21	1.53	0.89
1:A:158:ILE:HD12	1:A:159:SER:N	1.89	0.87
1:A:97:LEU:HB2	1:A:689:ARG:HD2	1.54	0.87
1:A:296:LEU:HB2	1:A:298:LEU:CD1	2.06	0.85
1:A:398:ILE:HD13	1:A:407:GLN:CG	2.03	0.85
1:A:368:VAL:HG12	1:A:369:LEU:H	1.39	0.85
1:A:61:THR:HG23	1:A:71:GLN:HG3	1.56	0.85
1:A:397:ARG:HA	1:A:406:ALA:HA	1.60	0.84
1:A:210:VAL:O	1:A:214:GLN:HG3	1.79	0.81
1:A:293:LYS:CA	1:A:298:LEU:HD12	2.08	0.81
1:A:432:TRP:CZ2	1:A:436:LYS:HD2	2.15	0.81
1:A:45:ASP:OD2	1:A:677:ARG:NH2	2.14	0.80
1:A:329:GLN:O	1:A:332:ASP:HB2	1.82	0.78
1:A:621:ALA:CB	1:A:628:ILE:HG23	2.14	0.78
1:A:343:SER:HA	1:A:346:LYS:HB2	1.65	0.77
1:A:60:PHE:CE2	1:A:74:LYS:HG2	2.19	0.76
1:A:385:ASN:HB3	1:A:388:VAL:CG2	2.17	0.74
1:A:293:LYS:HA	1:A:298:LEU:CD1	2.10	0.74
1:A:38:ASN:ND2	1:A:44:ARG:HA	2.04	0.73
1:A:147:ARG:HG3	1:A:150:GLU:OE2	1.89	0.72
1:A:698:TYR:O	1:A:702:VAL:HG23	1.90	0.71
1:A:484[A]:HIS:NE2	1:A:508:LEU:HD22	2.05	0.71
1:A:375:LEU:HD22	1:A:386:PRO:HB3	1.73	0.70
1:A:361:LYS:CB	1:A:411:VAL:HG23	2.22	0.70
1:A:61:THR:OG1	1:A:71:GLN:HG2	1.91	0.70
1:A:249:ASN:ND2	3:A:1173:HOH:O	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:VAL:HG12	1:A:369:LEU:N	2.07	0.69
1:A:289:THR:HG23	1:A:292:GLU:OE1	1.93	0.69
1:A:594:GLN:HG3	1:A:594:GLN:O	1.93	0.68
1:A:621:ALA:HB3	1:A:628:ILE:HG23	1.76	0.68
1:A:223:GLU:HG2	1:A:227:ASN:ND2	2.10	0.67
1:A:87:GLY:H	1:A:105:ASN:ND2	1.93	0.66
1:A:59:SER:HB2	1:A:72:VAL:O	1.95	0.66
1:A:18:LYS:HB2	3:A:1103:HOH:O	1.96	0.66
1:A:229:LYS:HB2	1:A:315:ILE:HD11	1.77	0.66
1:A:296:LEU:CB	1:A:298:LEU:HD21	2.23	0.66
1:A:64:THR:HG23	1:A:68:GLN:O	1.97	0.65
1:A:435[B]:LYS:HE3	3:A:1204:HOH:O	1.96	0.65
1:A:61:THR:HG23	1:A:71:GLN:CG	2.27	0.64
1:A:249:ASN:ND2	3:A:946:HOH:O	2.31	0.64
1:A:654:ARG:NE	3:A:1435:HOH:O	2.29	0.64
1:A:336:PHE:CE2	1:A:436:LYS:HD3	2.32	0.63
1:A:39:PRO:HG3	1:A:48:GLU:HG3	1.80	0.63
1:A:594:GLN:O	1:A:598:LEU:HG	1.98	0.63
1:A:302:GLU:H	1:A:302:GLU:CD	2.02	0.62
1:A:342:MET:O	1:A:345:PHE:HB2	1.99	0.62
1:A:395:GLU:HG2	1:A:408:HIS:HA	1.81	0.62
1:A:446:LYS:NZ	3:A:1153:HOH:O	2.34	0.61
1:A:176:LEU:HD12	1:A:176:LEU:N	2.16	0.61
1:A:707:LEU:O	1:A:707:LEU:HD12	2.00	0.61
1:A:296:LEU:HB2	1:A:298:LEU:CG	2.31	0.61
1:A:293:LYS:O	1:A:297:HIS:N	2.34	0.60
1:A:654:ARG:NH1	1:A:679:ASN:O	2.35	0.60
1:A:158:ILE:HD12	1:A:159:SER:H	1.67	0.60
1:A:621:ALA:HB2	1:A:628:ILE:HG12	1.84	0.60
1:A:741:ILE:HG22	1:A:742:THR:HG23	1.84	0.60
1:A:734:PRO:HA	1:A:737:TYR:CE2	2.37	0.59
1:A:187:GLU:O	1:A:191:LYS:HG2	2.01	0.59
1:A:686:ARG:O	1:A:690:LYS:HG3	2.03	0.59
1:A:585:LEU:O	1:A:589:LYS:HG3	2.03	0.59
1:A:305:ASN:HB3	3:A:1407:HOH:O	2.01	0.59
1:A:396:PRO:O	1:A:398:ILE:HD12	2.02	0.58
1:A:326:ILE:HG22	1:A:327:THR:N	2.17	0.58
1:A:305:ASN:O	1:A:309:GLN:HG2	2.03	0.58
1:A:544:ILE:HG13	1:A:544:ILE:O	2.04	0.57
1:A:55:GLU:HG3	1:A:74:LYS:NZ	2.19	0.57
1:A:713:PRO:HA	3:A:1309:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:HD11	1:A:142:ILE:CG2	2.34	0.57
1:A:324:PHE:HE2	1:A:328:ARG:NH2	2.01	0.57
1:A:436:LYS:NZ	3:A:1207:HOH:O	2.36	0.57
1:A:621:ALA:HB3	1:A:628:ILE:H	1.69	0.57
1:A:321:SER:O	1:A:325:LYS:HG3	2.05	0.57
1:A:99:GLU:HG3	3:A:1524:HOH:O	2.04	0.57
1:A:218:ALA:O	1:A:221:ILE:HB	2.06	0.56
1:A:395:GLU:HA	1:A:407:GLN:O	2.05	0.56
1:A:87:GLY:H	1:A:105:ASN:HD21	1.54	0.56
1:A:45:ASP:CG	1:A:677:ARG:HH22	2.09	0.56
1:A:259:GLN:HG2	1:A:261:TYR:CZ	2.40	0.56
1:A:34:TYR:CE1	1:A:51:GLU:HB2	2.41	0.56
1:A:693:PRO:HD2	1:A:746:PHE:O	2.06	0.56
1:A:398:ILE:CD1	1:A:407:GLN:HG3	2.08	0.56
1:A:285:LEU:O	1:A:293:LYS:NZ	2.35	0.56
1:A:300:GLY:O	1:A:303:SER:HB2	2.06	0.56
1:A:385:ASN:HB3	1:A:388:VAL:HG21	1.88	0.56
1:A:552:SER:O	1:A:553:LYS:HB2	2.06	0.56
1:A:706:TYR:HD2	1:A:712:VAL:O	1.88	0.56
1:A:732:ILE:O	1:A:734:PRO:HD3	2.05	0.56
1:A:385:ASN:OD1	1:A:386:PRO:HD2	2.06	0.55
1:A:443:GLN:HG3	1:A:445:ARG:O	2.07	0.55
1:A:741:ILE:HG22	1:A:742:THR:CG2	2.36	0.55
1:A:677:ARG:HG3	1:A:682:LEU:HD12	1.89	0.55
1:A:229:LYS:HB2	1:A:315:ILE:CD1	2.36	0.55
1:A:443:GLN:OE1	1:A:443:GLN:HA	2.06	0.55
1:A:72:VAL:HG13	1:A:73:LYS:N	2.21	0.54
1:A:735:GLU:HB3	1:A:736:GLN:OE1	2.07	0.54
1:A:692:PHE:O	1:A:695:ARG:NE	2.31	0.54
1:A:98:ASN:O	1:A:102:VAL:HG23	2.07	0.53
1:A:282:TYR:CZ	1:A:307:LEU:HD22	2.44	0.53
1:A:337:SER:OG	1:A:339:GLU:HG2	2.09	0.53
1:A:219:ASN:HB3	1:A:220:PRO:CD	2.39	0.53
1:A:273:GLU:HA	1:A:273:GLU:OE1	2.10	0.53
1:A:219:ASN:HB3	1:A:220:PRO:HD3	1.91	0.52
1:A:692:PHE:CZ	1:A:747:ARG:CZ	2.92	0.52
1:A:296:LEU:CB	1:A:298:LEU:HD11	2.25	0.52
1:A:35:ILE:O	1:A:35:ILE:HD12	2.09	0.52
1:A:722:ALA:O	1:A:725:ALA:HB3	2.10	0.52
1:A:721:LYS:O	1:A:724:ASP:HB3	2.10	0.52
1:A:59:SER:O	1:A:74:LYS:HE3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:ARG:NH1	3:A:1448:HOH:O	2.28	0.51
1:A:48:GLU:OE1	1:A:65:VAL:HG21	2.11	0.51
1:A:79:GLN:HG3	3:A:1083:HOH:O	2.10	0.51
1:A:37:TYR:OH	1:A:64:THR:HB	2.11	0.51
1:A:480:GLN:HG3	1:A:508:LEU:CD1	2.41	0.51
1:A:322:GLU:HA	1:A:325:LYS:CE	2.41	0.51
1:A:576:GLN:HB2	3:A:1276:HOH:O	2.09	0.51
1:A:273:GLU:C	1:A:274:THR:HG23	2.31	0.51
1:A:99:GLU:HB2	1:A:100:PRO:HD3	1.92	0.50
1:A:249:ASN:H	1:A:249:ASN:ND2	2.07	0.50
1:A:293:LYS:HG3	3:A:1180:HOH:O	2.11	0.50
1:A:4:ILE:HD11	1:A:142:ILE:HG23	1.92	0.50
1:A:399:LEU:HD12	1:A:403:ASP:O	2.11	0.50
1:A:322:GLU:HA	1:A:325:LYS:HE3	1.92	0.50
1:A:410:ASN:OD1	1:A:413:LYS:HB2	2.11	0.49
1:A:97:LEU:CB	1:A:689:ARG:HD2	2.35	0.49
1:A:72:VAL:HG13	1:A:73:LYS:O	2.13	0.49
1:A:709:ALA:HB2	1:A:726:VAL:HA	1.94	0.49
1:A:304:PHE:O	1:A:308:ASN:ND2	2.46	0.49
1:A:495:LEU:HD12	1:A:495:LEU:O	2.12	0.49
1:A:155:ILE:HD12	1:A:158:ILE:HD11	1.93	0.49
1:A:385:ASN:HB3	1:A:388:VAL:HG23	1.92	0.49
1:A:435[A]:LYS:HZ1	1:A:616:ASN:HB3	1.78	0.49
1:A:45:ASP:O	1:A:669:ASP:HB2	2.13	0.48
1:A:385:ASN:O	1:A:388:VAL:N	2.46	0.48
1:A:703:LYS:O	1:A:703:LYS:HG2	2.11	0.48
1:A:72:VAL:CG1	1:A:73:LYS:N	2.75	0.48
1:A:83:ILE:HD12	1:A:86:ASP:OD2	2.13	0.48
1:A:609:THR:HG23	1:A:613:ASN:OD1	2.13	0.48
1:A:621:ALA:HB2	1:A:628:ILE:CG1	2.43	0.48
1:A:36:TRP:CZ2	1:A:80:ARG:HG3	2.47	0.48
1:A:343:SER:CA	1:A:346:LYS:HB2	2.42	0.48
1:A:386:PRO:O	1:A:390:GLU:HB2	2.14	0.48
1:A:442:CYS:SG	1:A:443:GLN:N	2.87	0.48
1:A:508:LEU:HD12	1:A:510:SER:H	1.79	0.48
1:A:535:PHE:N	1:A:535:PHE:CD2	2.80	0.48
1:A:280:ILE:HG13	1:A:280:ILE:O	2.14	0.48
1:A:56:THR:O	1:A:74:LYS:NZ	2.41	0.48
1:A:223:GLU:O	1:A:227:ASN:HB2	2.14	0.48
1:A:379:SER:HA	1:A:384:VAL:HG22	1.96	0.47
1:A:219:ASN:N	1:A:220:PRO:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:LYS:HD2	1:A:638:LEU:HD21	1.96	0.47
1:A:508:LEU:CD1	1:A:510:SER:H	2.28	0.47
1:A:689:ARG:HH21	1:A:748:ALA:HB1	1.78	0.47
1:A:39:PRO:HG3	1:A:48:GLU:CG	2.43	0.47
1:A:443:GLN:HB3	3:A:1171:HOH:O	2.13	0.47
1:A:710:PRO:HD3	1:A:729:HIS:CD2	2.50	0.47
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.44	0.47
1:A:99:GLU:N	1:A:100:PRO:HD2	2.30	0.47
1:A:55:GLU:HG3	1:A:74:LYS:CE	2.45	0.46
1:A:741:ILE:HA	1:A:741:ILE:HD13	1.47	0.46
1:A:382:PHE:O	1:A:603:SER:OG	2.33	0.46
1:A:59:SER:HA	1:A:74:LYS:HG3	1.97	0.46
1:A:174:SER:O	1:A:651:HIS:HD2	1.98	0.46
1:A:344:ILE:O	1:A:348:ILE:HG12	2.16	0.46
1:A:368:VAL:CG1	1:A:369:LEU:H	2.20	0.46
1:A:241:LYS:NZ	1:A:454:ASP:OD2	2.30	0.46
1:A:619:SER:HB3	1:A:626:ASN:CB	2.46	0.46
1:A:289:THR:OG1	1:A:292:GLU:HG3	2.16	0.46
1:A:324:PHE:CE2	1:A:328:ARG:NH2	2.83	0.46
1:A:446:LYS:HG2	1:A:446:LYS:O	2.15	0.45
1:A:315:ILE:HB	1:A:318:VAL:HB	1.98	0.45
1:A:435[A]:LYS:NZ	1:A:616:ASN:HB3	2.31	0.45
1:A:37:TYR:O	1:A:47:TYR:HA	2.17	0.45
1:A:382:PHE:HB3	1:A:384:VAL:HG13	1.99	0.45
1:A:4:ILE:CD1	1:A:4:ILE:N	2.80	0.45
1:A:60:PHE:CD2	1:A:74:LYS:HG2	2.51	0.45
1:A:38:ASN:ND2	1:A:46:SER:O	2.48	0.45
1:A:589:LYS:HE3	3:A:1278:HOH:O	2.16	0.44
1:A:692:PHE:CE2	1:A:747:ARG:NH1	2.85	0.44
1:A:654:ARG:HA	1:A:654:ARG:HD3	1.62	0.44
1:A:349:ALA:O	1:A:352:LEU:HB2	2.17	0.44
1:A:26:LYS:O	1:A:26:LYS:HG2	2.17	0.44
1:A:296:LEU:HA	1:A:296:LEU:HD23	1.80	0.44
1:A:23:ASP:N	1:A:23:ASP:OD1	2.51	0.44
1:A:244:GLU:O	1:A:256:ALA:HA	2.18	0.44
1:A:567:GLU:HA	1:A:579:TYR:O	2.17	0.44
1:A:284:LEU:HD12	1:A:284:LEU:HA	1.72	0.44
1:A:399:LEU:HD11	1:A:401:GLY:O	2.17	0.43
1:A:610:LYS:HA	1:A:610:LYS:HD2	1.74	0.43
1:A:209:GLY:O	1:A:213:GLN:HB2	2.18	0.43
1:A:217:GLN:O	1:A:221:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:O	1:A:297:HIS:HB2	2.17	0.43
1:A:520:ARG:HG2	3:A:1353:HOH:O	2.18	0.43
1:A:140:VAL:HG12	1:A:144:LYS:HE3	2.01	0.43
1:A:705:TYR:HB3	1:A:708:LEU:HD12	1.99	0.43
1:A:605:ASP:HB3	1:A:608:VAL:HB	2.00	0.43
1:A:116:TYR:HB3	1:A:123:LEU:HD11	2.01	0.43
1:A:473:TYR:O	1:A:476:GLU:HB2	2.18	0.43
1:A:654:ARG:HH11	1:A:654:ARG:HD2	1.24	0.43
1:A:132:ILE:HG22	1:A:134:ILE:HG23	2.00	0.43
1:A:273:GLU:O	1:A:274:THR:HG23	2.18	0.43
1:A:35:ILE:C	1:A:35:ILE:HD12	2.39	0.43
1:A:737:TYR:HB2	1:A:744:ILE:HD11	2.00	0.43
1:A:430:PHE:O	1:A:434:VAL:HG23	2.19	0.43
1:A:712:VAL:HA	1:A:713:PRO:HD3	1.85	0.42
1:A:4:ILE:CD1	1:A:142:ILE:HG23	2.49	0.42
1:A:163:TYR:CE2	1:A:167:LEU:HD11	2.54	0.42
1:A:211:LEU:HD12	1:A:211:LEU:HA	1.63	0.42
1:A:346:LYS:O	1:A:349:ALA:HB3	2.19	0.42
1:A:638:LEU:O	1:A:642:MET:HG2	2.19	0.42
1:A:6:ASP:OD1	1:A:8:THR:OG1	2.30	0.42
1:A:230:THR:HA	1:A:275:GLU:CD	2.40	0.42
1:A:480:GLN:HG3	1:A:508:LEU:HD11	2.02	0.42
1:A:293:LYS:O	1:A:296:LEU:N	2.48	0.42
1:A:18:LYS:HG3	3:A:1497:HOH:O	2.20	0.41
1:A:337:SER:OG	1:A:340:GLU:HG3	2.20	0.41
1:A:737:TYR:O	1:A:738:ARG:HD3	2.20	0.41
1:A:692:PHE:CE1	1:A:747:ARG:HG3	2.55	0.41
1:A:227:ASN:HA	1:A:236:SER:O	2.20	0.41
1:A:495:LEU:O	1:A:497:GLU:O	2.38	0.41
1:A:119:SER:OG	1:A:685:ILE:HD11	2.20	0.41
1:A:36:TRP:CE2	1:A:80:ARG:HG3	2.55	0.41
1:A:508:LEU:HD11	1:A:510:SER:CB	2.51	0.41
1:A:273:GLU:OE1	1:A:310:SER:HA	2.20	0.41
1:A:163:TYR:O	1:A:167:LEU:HG	2.20	0.41
1:A:343:SER:O	1:A:346:LYS:HB2	2.20	0.41
1:A:98:ASN:OD1	1:A:100:PRO:HG2	2.19	0.41
1:A:173:GLN:HB2	1:A:450:ILE:HG12	2.03	0.41
1:A:296:LEU:CB	1:A:298:LEU:CD2	2.97	0.41
1:A:37:TYR:O	1:A:48:GLU:N	2.48	0.41
1:A:289:THR:C	1:A:291:GLU:N	2.74	0.41
1:A:621:ALA:HB2	1:A:628:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:GLN:O	1:A:750:GLN:NE2	2.52	0.41
1:A:379:SER:HB2	1:A:386:PRO:HG3	2.03	0.41
1:A:677:ARG:HD3	1:A:677:ARG:HH11	1.55	0.41
1:A:494:TYR:HE1	1:A:695:ARG:NH2	2.18	0.41
1:A:751:LEU:HD22	1:A:751:LEU:O	2.21	0.41
1:A:687:ILE:HG21	1:A:687:ILE:HD13	1.92	0.41
1:A:696:ILE:O	1:A:743:LYS:HB3	2.21	0.41
1:A:297:HIS:N	1:A:297:HIS:ND1	2.69	0.40
1:A:326:ILE:CG2	1:A:327:THR:N	2.83	0.40
1:A:546:LYS:NZ	3:A:1015:HOH:O	2.54	0.40
1:A:279:HIS:O	1:A:283:GLN:HG3	2.22	0.40
1:A:605:ASP:OD2	1:A:607:VAL:N	2.44	0.40
1:A:147:ARG:HB2	1:A:150:GLU:HG3	2.03	0.40
1:A:35:ILE:HG22	1:A:79:GLN:HA	2.03	0.40
1:A:59:SER:CA	1:A:74:LYS:HG3	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1461:HOH:O	3:A:1465:HOH:O 3_556	1.97	0.23

## 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	740/761 (97%)	694 (94%)	45 (6%)	1 (0%)	55 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	THR



### 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	634/665 (95%)	575 (91%)	59 (9%)	10 7

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	13	LYS
1	A	22	SER
1	A	23	ASP
1	A	24	LEU
1	A	31	ASP
1	A	44	ARG
1	A	54	SER
1	A	55	GLU
1	A	57	SER
1	A	58	ASP
1	A	75	ASP
1	A	84	LYS
1	A	130	LYS
1	A	147	ARG
1	A	151	VAL
1	A	186	THR
1	A	213	GLN
1	A	238	ARG
1	A	249	ASN
1	A	257	SER
1	A	262	LEU
1	A	293	LYS
1	A	298	LEU
1	A	302	GLU
1	A	309	GLN
1	A	313	VAL
1	A	319	SER
1	A	326	ILE
1	A	328	ARG

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Mol	Chain	Res	Type
1	A	338	GLN
1	A	342	MET
1	A	343	SER
1	A	379	SER
1	A	380	THR
1	A	391	LYS
1	A	403	ASP
1	A	405	VAL
1	A	407	GLN
1	A	412	GLU
1	A	446	LYS
1	A	462	LYS
1	A	508	LEU
1	A	544	ILE
1	A	546	LYS
1	A	594	GLN
1	A	602	ASP
1	A	627	PHE
1	A	640	SER
1	A	654	ARG
1	A	666	LYS
1	A	669	ASP
1	A	686	ARG
1	A	689	ARG
1	A	697	ILE
1	A	707	LEU
1	A	735	GLU
1	A	738	ARG
1	A	751	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	5	HIS
1	A	38	ASN
1	A	79	GLN
1	A	105	ASN
1	A	234	ASN
1	A	249	ASN
1	A	283	GLN
1	A	308	ASN

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Mol	Chain	Res	Type
1	A	338	GLN
1	A	439	ASN
1	A	480	GLN
1	A	491	GLN
1	A	662	GLN
1	A	720	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	743/761 (97%)	-0.14	29 (3%)	40 47	7, 30, 74, 98	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	362	GLY	5.3
1	A	53	VAL	5.2
1	A	290	ALA	4.2
1	A	507	GLY	3.9
1	A	444	GLU	3.7
1	A	725	ALA	3.6
1	A	56	THR	3.6
1	A	405	VAL	3.5
1	A	273	GLU	3.4
1	A	23	ASP	3.3
1	A	443	GLN	3.3
1	A	31	ASP	3.0
1	A	66	ASP	2.9
1	A	65	VAL	2.8
1	A	289	THR	2.7
1	A	58	ASP	2.7
1	A	348	ILE	2.7
1	A	715	ASP	2.7
1	A	294	LYS	2.6
1	A	42	LYS	2.6
1	A	274	THR	2.5
1	A	5	HIS	2.4
1	A	59	SER	2.4
1	A	399	LEU	2.3
1	A	626	ASN	2.1
1	A	67	GLY	2.1
1	A	74	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	71	GLN	2.1
1	A	347	ILE	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	A	800	1/1	0.98	0.05	-	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.