



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:24 AM UTC

PDB ID : 1FMV / pdb_00001fmv
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

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

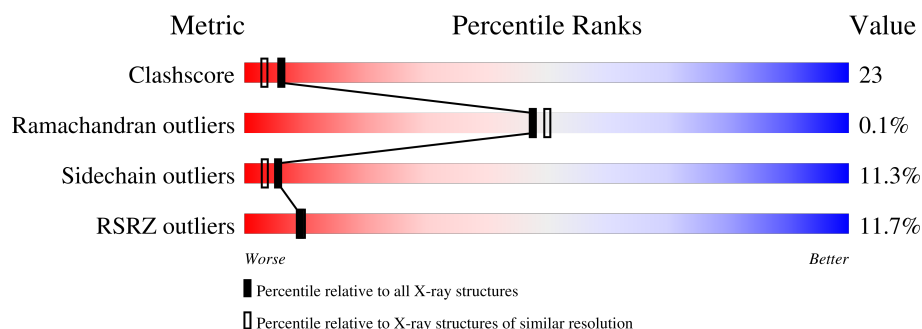
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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 (CCD ID: CL) (formula: Cl).

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

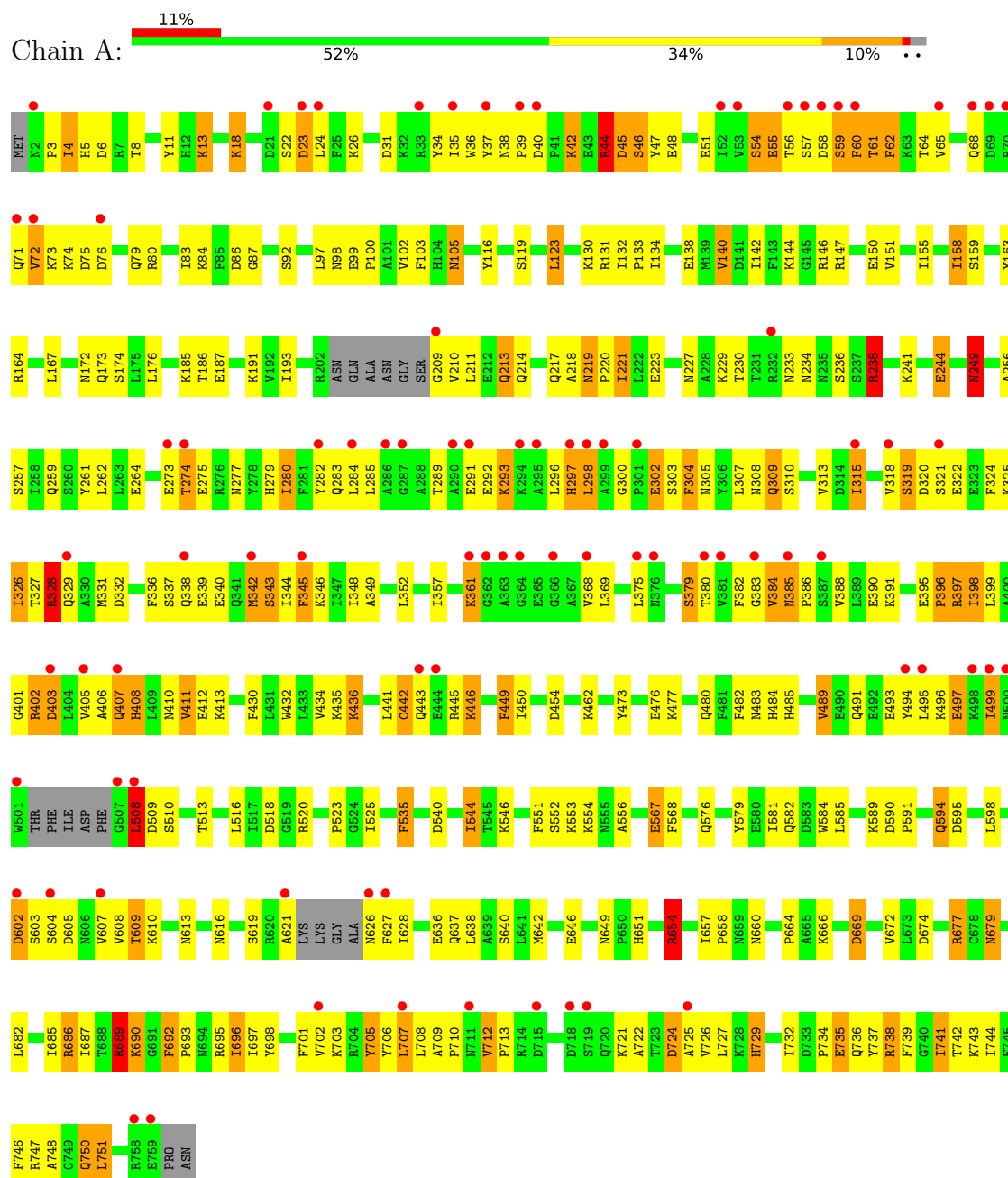
- Molecule 3 is water.

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, 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: MYOSIN II HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.50Å 179.70Å 54.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.10 89.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (100.00-2.10) 96.3 (89.85-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.10Å)	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.	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 115.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6509	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.22	3/6041 (0.0%)	1.89	135/8161 (1.7%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	654	ARG	NE-CZ	-5.92	1.26	1.33
1	A	219	ASN	N-CA	-5.54	1.41	1.46
1	A	105	ASN	C-N	-5.15	1.27	1.33

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	535	PHE	CA-CB-CG	-13.11	100.69	113.80
1	A	654	ARG	CD-NE-CZ	-10.79	109.30	124.40
1	A	508	LEU	CA-C-N	10.34	135.16	120.28
1	A	508	LEU	C-N-CA	10.34	135.16	120.28
1	A	497	GLU	CA-C-N	-10.22	108.15	122.87
1	A	497	GLU	C-N-CA	-10.22	108.15	122.87
1	A	729	HIS	CA-CB-CG	-10.18	103.62	113.80
1	A	233	ASN	CA-CB-CG	9.80	122.40	112.60
1	A	689	ARG	CD-NE-CZ	9.04	137.05	124.40
1	A	674	ASP	CA-CB-CG	-8.67	103.93	112.60
1	A	508	LEU	N-CA-C	8.64	121.83	108.96
1	A	660	ASN	CA-CB-CG	-8.54	104.06	112.60
1	A	385	ASN	CA-CB-CG	-8.27	104.33	112.60
1	A	689	ARG	NE-CZ-NH1	8.24	129.74	121.50
1	A	5	HIS	CA-CB-CG	-7.88	105.92	113.80
1	A	692	PHE	O-C-N	7.86	127.85	121.17
1	A	249	ASN	CA-CB-CG	-7.85	104.75	112.60
1	A	705	TYR	N-CA-C	7.78	122.49	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	712	VAL	CA-C-O	7.61	124.75	119.20
1	A	516	LEU	CA-C-O	7.60	128.68	120.10
1	A	509	ASP	N-CA-C	7.57	120.41	111.71
1	A	408	HIS	CA-CB-CG	-7.50	106.30	113.80
1	A	45	ASP	CA-CB-CG	-7.36	105.24	112.60
1	A	105	ASN	CA-C-O	7.29	128.28	120.55
1	A	280	ILE	N-CA-C	7.13	118.75	110.62
1	A	556	ALA	N-CA-C	7.12	121.41	112.87
1	A	489	VAL	N-CA-CB	7.02	122.65	110.65
1	A	540	ASP	CA-CB-CG	6.93	119.53	112.60
1	A	60	PHE	CA-C-N	-6.89	113.28	122.99
1	A	60	PHE	C-N-CA	-6.89	113.28	122.99
1	A	238	ARG	CA-CB-CG	-6.83	100.45	114.10
1	A	238	ARG	NE-CZ-NH1	6.81	128.31	121.50
1	A	568	PHE	CA-C-N	-6.81	117.48	122.18
1	A	568	PHE	C-N-CA	-6.81	117.48	122.18
1	A	449	PHE	CA-CB-CG	-6.77	107.03	113.80
1	A	219	ASN	CA-C-O	6.75	125.35	118.73
1	A	11	TYR	N-CA-C	-6.62	103.99	111.14
1	A	602	ASP	N-CA-CB	6.59	120.52	110.70
1	A	739	PHE	CA-C-N	-6.44	115.74	122.69
1	A	739	PHE	C-N-CA	-6.44	115.74	122.69
1	A	140	VAL	CA-C-N	6.42	129.52	120.28
1	A	140	VAL	C-N-CA	6.42	129.52	120.28
1	A	712	VAL	N-CA-C	6.39	114.93	107.77
1	A	46	SER	N-CA-C	-6.39	98.83	109.24
1	A	345	PHE	CA-CB-CG	-6.37	107.43	113.80
1	A	523	PRO	CA-C-N	-6.32	116.81	122.43
1	A	523	PRO	C-N-CA	-6.32	116.81	122.43
1	A	411	VAL	N-CA-C	6.30	117.05	110.62
1	A	442	CYS	N-CA-C	6.28	119.58	110.28
1	A	238	ARG	NE-CZ-NH2	-6.17	113.65	119.20
1	A	677	ARG	NE-CZ-NH1	-6.15	115.35	121.50
1	A	750	GLN	N-CA-C	6.15	117.65	111.07
1	A	584	TRP	N-CA-CB	6.14	119.15	110.12
1	A	172	ASN	CA-CB-CG	-6.12	106.48	112.60
1	A	482	PHE	CA-CB-CG	-6.10	107.70	113.80
1	A	361	LYS	N-CA-C	6.10	118.76	107.60
1	A	234	ASN	CA-C-N	-6.01	112.93	121.83
1	A	234	ASN	C-N-CA	-6.01	112.93	121.83
1	A	304	PHE	CA-CB-CG	-5.99	107.81	113.80
1	A	402	ARG	CA-C-O	5.96	125.70	119.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	590	ASP	CA-C-N	5.95	125.90	119.78
1	A	590	ASP	C-N-CA	5.95	125.90	119.78
1	A	328	ARG	CA-C-O	5.92	126.83	120.55
1	A	3	PRO	N-CA-CB	5.92	109.46	103.25
1	A	690	LYS	N-CA-C	5.85	118.61	111.82
1	A	602	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	554	LYS	N-CA-CB	-5.82	103.16	110.90
1	A	483	ASN	CA-CB-CG	5.80	118.40	112.60
1	A	441	LEU	N-CA-C	5.80	120.49	112.90
1	A	61	THR	CB-CA-C	5.78	120.29	109.71
1	A	62	PHE	N-CA-C	5.77	118.17	109.23
1	A	692	PHE	CA-C-N	5.77	125.45	119.05
1	A	692	PHE	C-N-CA	5.77	125.45	119.05
1	A	92	SER	CA-C-O	5.74	126.51	119.05
1	A	513	THR	N-CA-C	-5.74	105.10	111.36
1	A	13	LYS	CB-CA-C	-5.70	101.93	110.88
1	A	164	ARG	NE-CZ-NH2	5.67	124.30	119.20
1	A	582	GLN	N-CA-C	5.66	118.56	110.24
1	A	44	ARG	CD-NE-CZ	5.63	132.28	124.40
1	A	696	ILE	CB-CA-C	-5.63	101.89	110.95
1	A	13	LYS	N-CA-C	5.62	117.08	111.07
1	A	646	GLU	CA-CB-CG	-5.61	102.89	114.10
1	A	485	HIS	CA-CB-CG	-5.61	108.19	113.80
1	A	42	LYS	CB-CA-C	5.59	119.62	110.95
1	A	219	ASN	CA-CB-CG	-5.57	107.03	112.60
1	A	604	SER	N-CA-C	-5.53	106.50	113.20
1	A	319	SER	N-CA-CB	5.53	119.51	110.39
1	A	649	ASN	N-CA-C	-5.50	100.68	109.04
1	A	701	PHE	O-C-N	5.49	127.74	122.03
1	A	595	ASP	CA-CB-CG	-5.47	107.13	112.60
1	A	535	PHE	CA-C-O	5.45	122.83	119.29
1	A	138	GLU	N-CA-C	-5.40	105.39	111.28
1	A	383	GLY	O-C-N	5.39	128.64	122.33
1	A	45	ASP	N-CA-CB	5.37	118.29	110.88
1	A	489	VAL	CB-CA-C	5.36	120.47	112.16
1	A	131	ARG	CB-CA-C	5.35	118.57	109.53
1	A	54	SER	N-CA-CB	5.35	120.55	111.57
1	A	727	LEU	O-C-N	5.35	127.58	122.07
1	A	672	VAL	O-C-N	5.34	127.66	121.94
1	A	396	PRO	CB-CA-C	-5.34	104.11	111.21
1	A	679	ASN	N-CA-C	5.33	119.42	113.02
1	A	724	ASP	CA-C-N	5.33	127.68	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	724	ASP	C-N-CA	5.33	127.68	120.65
1	A	123	LEU	N-CA-C	-5.32	99.85	108.52
1	A	497	GLU	N-CA-C	-5.31	100.77	109.80
1	A	221	ILE	CB-CA-C	-5.30	105.08	112.02
1	A	320	ASP	CB-CA-C	5.27	119.64	110.68
1	A	491	GLN	CB-CG-CD	-5.25	103.67	112.60
1	A	76	ASP	N-CA-C	-5.25	106.89	113.72
1	A	103	PHE	CA-CB-CG	-5.25	108.55	113.80
1	A	637	GLN	CA-C-O	5.25	126.03	120.10
1	A	525	ILE	CA-C-N	-5.24	112.34	120.31
1	A	525	ILE	C-N-CA	-5.24	112.34	120.31
1	A	45	ASP	CA-C-O	5.24	124.66	118.90
1	A	185	LYS	CB-CA-C	-5.24	102.66	110.88
1	A	297	HIS	N-CA-CB	-5.22	104.24	112.13
1	A	664	PRO	CB-CA-C	-5.19	103.06	110.75
1	A	244	GLU	CB-CA-C	-5.17	102.28	110.81
1	A	657	ILE	CB-CA-C	5.15	120.73	111.36
1	A	551	PHE	N-CA-C	5.15	120.95	114.31
1	A	146	ARG	CA-C-O	-5.14	115.19	121.36
1	A	133	PRO	N-CA-CB	5.12	105.83	102.25
1	A	193	ILE	CA-CB-CG2	5.10	119.18	110.50
1	A	657	ILE	O-C-N	-5.10	115.28	121.10
1	A	591	PRO	CB-CA-C	-5.08	104.73	111.23
1	A	636	GLU	N-CA-CB	-5.07	102.72	110.07
1	A	158	ILE	N-CA-CB	5.07	117.43	110.54
1	A	499	ILE	CB-CA-C	5.05	119.86	112.03
1	A	59	SER	N-CA-C	5.05	114.95	108.34
1	A	496	LYS	CA-C-O	5.04	125.59	119.49
1	A	18	LYS	CB-CA-C	5.04	118.08	109.72
1	A	277	ASN	N-CA-C	-5.03	103.42	110.35
1	A	567	GLU	CB-CG-CD	5.02	121.13	112.60
1	A	658	PRO	N-CA-CB	5.01	108.12	103.46
1	A	146	ARG	O-C-N	5.01	128.67	123.06

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	265	0
2	A	1	0	0	0	0
3	A	601	0	0	19	1
All	All	6509	0	5800	265	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 23.

All (265) 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:61:THR:HG23	1:A:71:GLN:HG3	1.56	0.85
1:A:368:VAL:HG12	1:A:369:LEU:H	1.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:THR:OG1	1:A:71:GLN:HG2	1.91	0.70
1:A:361:LYS:CB	1:A:411:VAL:HG23	2.22	0.70
1:A:249:ASN:ND2	3:A:1173:HOH:O	2.24	0.69
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:O	1:A:594:GLN:HG3	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:59:SER:HB2	1:A:72:VAL:O	1.95	0.66
1:A:87:GLY:H	1:A:105:ASN:ND2	1.93	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:302:GLU:H	1:A:302:GLU:CD	2.02	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: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:N	1:A:176:LEU:HD12	2.16	0.61
1:A:707:LEU:HD12	1:A:707:LEU:O	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:45:ASP:CG	1:A:677:ARG:HH22	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ASN:O	1:A:309:GLN:HG2	2.03	0.58
1:A:55:GLU:HG3	1:A:74:LYS:NZ	2.19	0.57
1:A:544:ILE:O	1:A:544:ILE:HG13	2.04	0.57
1:A:713:PRO:HA	3:A:1309:HOH:O	2.04	0.57
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:99:GLU:HG3	3:A:1524:HOH:O	2.04	0.57
1:A:321:SER:O	1:A:325:LYS:HG3	2.05	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:34:TYR:CE1	1:A:51:GLU:HB2	2.41	0.56
1:A:259:GLN:HG2	1:A:261:TYR:CZ	2.40	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:273:GLU:C	1:A:274:THR:HG23	2.31	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:OE1	1:A:273:GLU:HA	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:35:ILE:HD12	1:A:35:ILE:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:CB	1:A:298:LEU:HD11	2.25	0.52
1:A:435[A]:LYS:HZ1	1:A:616:ASN:HB3	1.75	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
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:331:MET:HE1	1:A:345:PHE:CZ	2.45	0.51
1:A:99:GLU:HB2	1:A:100:PRO:HD3	1.92	0.50
1:A:249:ASN:ND2	1:A:249:ASN:H	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:97:LEU:CB	1:A:689:ARG:HD2	2.35	0.49
1:A:410:ASN:OD1	1:A:413:LYS:HB2	2.11	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:O	1:A:495:LEU:HD12	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:45:ASP:O	1:A:669:ASP:HB2	2.13	0.48
1:A:83:ILE:HD12	1:A:86:ASP:OD2	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: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:56:THR:O	1:A:74:LYS:NZ	2.41	0.48
1:A:280:ILE:O	1:A:280:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLU:O	1:A:227:ASN:HB2	2.14	0.48
1:A:35:ILE:HD12	1:A:35:ILE:C	2.39	0.47
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
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:72:VAL:CG1	1:A:73:LYS:N	2.75	0.47
1:A:230:THR:HA	1:A:275:GLU:CD	2.40	0.47
1:A:598:LEU:HA	1:A:598:LEU:HD23	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:59:SER:HA	1:A:74:LYS:HG3	1.97	0.46
1:A:382:PHE:O	1:A:603:SER:OG	2.33	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:289:THR:C	1:A:291:GLU:N	2.74	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:4:ILE:N	1:A:4:ILE:CD1	2.80	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: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:446:LYS:O	1:A:446:LYS:HG2	2.15	0.44
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:HD23	1:A:296:LEU:HA	1.80	0.44
1:A:23:ASP:OD1	1:A:23:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:284:LEU:HD12	1.72	0.44
1:A:399:LEU:HD11	1:A:401:GLY:O	2.17	0.43
1:A:610:LYS:HD2	1:A:610:LYS:HA	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
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:304:PHE:C	1:A:308:ASN:ND2	2.77	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:223:GLU:HG2	1:A:227:ASN:CG	2.43	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: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:375:LEU:HD23	1:A:375:LEU:C	2.45	0.42
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:HA	1:A:211:LEU:HD12	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: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:692:PHE:CE1	1:A:747:ARG:HG3	2.55	0.41
1:A:737:TYR:O	1:A:738:ARG:HD3	2.20	0.41
1:A:62:PHE:CD1	1:A:62:PHE:C	2.97	0.41
1:A:227:ASN:HA	1:A:236:SER:O	2.20	0.41
1:A:473:TYR:OH	1:A:518:ASP:OD2	2.36	0.41
1:A:495:LEU:O	1:A:497:GLU:O	2.38	0.41
1:A:36:TRP:CE2	1:A:80:ARG:HG3	2.55	0.41
1:A:119:SER:OG	1:A:685:ILE:HD11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:GLN:HG3	1:A:445:ARG:C	2.45	0.41
1:A:449:PHE:CD1	1:A:449:PHE:C	2.98	0.41
1:A:6:ASP:C	1:A:8:THR:H	2.28	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:40:ASP:C	1:A:42:LYS:N	2.75	0.41
1:A:98:ASN:OD1	1:A:100:PRO:HG2	2.19	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:37:TYR:O	1:A:48:GLU:N	2.48	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:379:SER:HB2	1:A:386:PRO:HG3	2.03	0.41
1:A:494:TYR:HE1	1:A:695:ARG:NH2	2.18	0.41
1:A:621:ALA:HB2	1:A:628:ILE:CD1	2.50	0.41
1:A:677:ARG:HH11	1:A:677:ARG:HD3	1.55	0.41
1:A:750:GLN:O	1:A:750:GLN:NE2	2.52	0.41
1:A:751:LEU:HD22	1:A:751:LEU:O	2.21	0.41
1:A:273:GLU:O	1:A:274:THR:OG1	2.36	0.41
1:A:687:ILE:HD13	1:A:687:ILE:HG21	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:238:ARG:HH11	1:A:264:GLU:CD	2.29	0.40
1:A:546:LYS:NZ	3:A:1015:HOH:O	2.54	0.40
1:A:6:ASP:C	1:A:8:THR:N	2.79	0.40
1:A:279:HIS:O	1:A:283:GLN:HG3	2.22	0.40
1:A:296:LEU:C	1:A:297:HIS:ND1	2.80	0.40
1:A:605:ASP:OD2	1:A:607:VAL:N	2.44	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
1:A:147:ARG:HB2	1:A:150:GLU:HG3	2.03	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%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	634/665 (95%)	563 (89%)	71 (11%)	6	3

All (71) 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

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Mol	Chain	Res	Type
1	A	58	ASP
1	A	72	VAL
1	A	75	ASP
1	A	84	LYS
1	A	130	LYS
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	315	ILE
1	A	319	SER
1	A	326	ILE
1	A	328	ARG
1	A	338	GLN
1	A	342	MET
1	A	343	SER
1	A	357	ILE
1	A	379	SER
1	A	380	THR
1	A	384	VAL
1	A	391	LYS
1	A	397	ARG
1	A	398	ILE
1	A	402	ARG
1	A	403	ASP
1	A	405	VAL
1	A	407	GLN
1	A	412	GLU
1	A	436	LYS
1	A	446	LYS
1	A	462	LYS
1	A	489	VAL
1	A	493	GLU
1	A	499	ILE

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Mol	Chain	Res	Type
1	A	508	LEU
1	A	544	ILE
1	A	581	ILE
1	A	594	GLN
1	A	602	ASP
1	A	609	THR
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	741	ILE
1	A	751	LEU

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

Mol	Chain	Res	Type
1	A	2	ASN
1	A	5	HIS
1	A	38	ASN
1	A	105	ASN
1	A	188	ASN
1	A	234	ASN
1	A	249	ASN
1	A	283	GLN
1	A	309	GLN
1	A	338	GLN
1	A	439	ASN
1	A	480	GLN
1	A	491	GLN
1	A	532	GLN
1	A	550	HIS
1	A	649	ASN
1	A	662	GLN
1	A	720	GLN
1	A	729	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	A	743/761 (97%)	0.41	87 (11%) 9 9	7, 30, 74, 98	5 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	VAL	5.8
1	A	621	ALA	5.6
1	A	363	ALA	5.0
1	A	501	TRP	4.9
1	A	715	ASP	4.3
1	A	368	VAL	4.1
1	A	40	ASP	4.1
1	A	725	ALA	4.0
1	A	59	SER	4.0
1	A	500	ASN	3.9
1	A	39	PRO	3.9
1	A	380	THR	3.9
1	A	627	PHE	3.6
1	A	507	GLY	3.5
1	A	315	ILE	3.5
1	A	23	ASP	3.5
1	A	209	GLY	3.4
1	A	508	LEU	3.4
1	A	290	ALA	3.4
1	A	362	GLY	3.4
1	A	494	TYR	3.3
1	A	364	GLY	3.3
1	A	273	GLU	3.3
1	A	626	ASN	3.2
1	A	405	VAL	3.1
1	A	274	THR	3.0
1	A	294	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	381	VAL	3.0
1	A	361	LYS	3.0
1	A	375	LEU	2.9
1	A	72	VAL	2.9
1	A	387	SER	2.9
1	A	318	VAL	2.8
1	A	37	TYR	2.8
1	A	385	ASN	2.8
1	A	366	GLY	2.8
1	A	57	SER	2.7
1	A	711	ASN	2.7
1	A	58	ASP	2.7
1	A	295	ALA	2.7
1	A	376	ASN	2.7
1	A	52	ILE	2.7
1	A	498	LYS	2.7
1	A	2	ASN	2.6
1	A	298	LEU	2.6
1	A	69	ASP	2.6
1	A	329	GLN	2.6
1	A	301	PRO	2.6
1	A	33	ARG	2.6
1	A	407	GLN	2.6
1	A	65	VAL	2.5
1	A	758	ARG	2.5
1	A	602	ASP	2.5
1	A	383	GLY	2.5
1	A	718	ASP	2.5
1	A	68	GLN	2.5
1	A	76	ASP	2.4
1	A	444	GLU	2.4
1	A	299	ALA	2.4
1	A	443	GLN	2.4
1	A	702	VAL	2.4
1	A	286	ALA	2.4
1	A	495	LEU	2.4
1	A	604	SER	2.4
1	A	287	GLY	2.4
1	A	35	ILE	2.4
1	A	403	ASP	2.3
1	A	71	GLN	2.2
1	A	321	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	291	GLU	2.2
1	A	24	LEU	2.2
1	A	56	THR	2.2
1	A	345	PHE	2.2
1	A	342	MET	2.2
1	A	607	VAL	2.2
1	A	707	LEU	2.2
1	A	499	ILE	2.1
1	A	232	ARG	2.1
1	A	21	ASP	2.1
1	A	284	LEU	2.1
1	A	338	GLN	2.1
1	A	70	ARG	2.1
1	A	297	HIS	2.1
1	A	60	PHE	2.1
1	A	759	GLU	2.0
1	A	719	SER	2.0
1	A	282	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	A	800	1/1	0.97	0.05	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.