



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:30 pm BST

PDB ID : 2Y0R
Title : Structural basis for the allosteric interference of myosin function by mutants G680A and G680V of Dictyostelium myosin-2
Authors : Preller, M.; Bauer, S.; Adamek, N.; Fujita-Becker, S.; Fedorov, R.; Geeves, M.A.; Manstein, D.J.
Deposited on : 2010-12-07
Resolution : 2.85 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

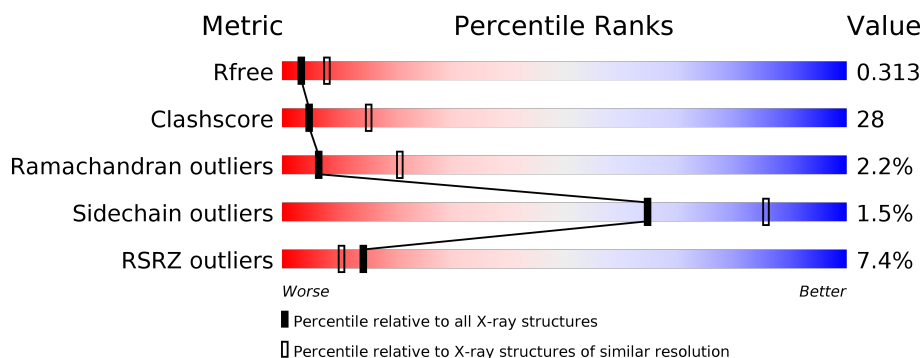
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 ≥ 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	X	758	<div> <div>7%</div> <div>59%</div> <div>36%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6469 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-2 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	758	Total	C	N	O	S	0	0	0
			6090	3868	1053	1153	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	680	ALA	GLY	engineered mutation	UNP P08799

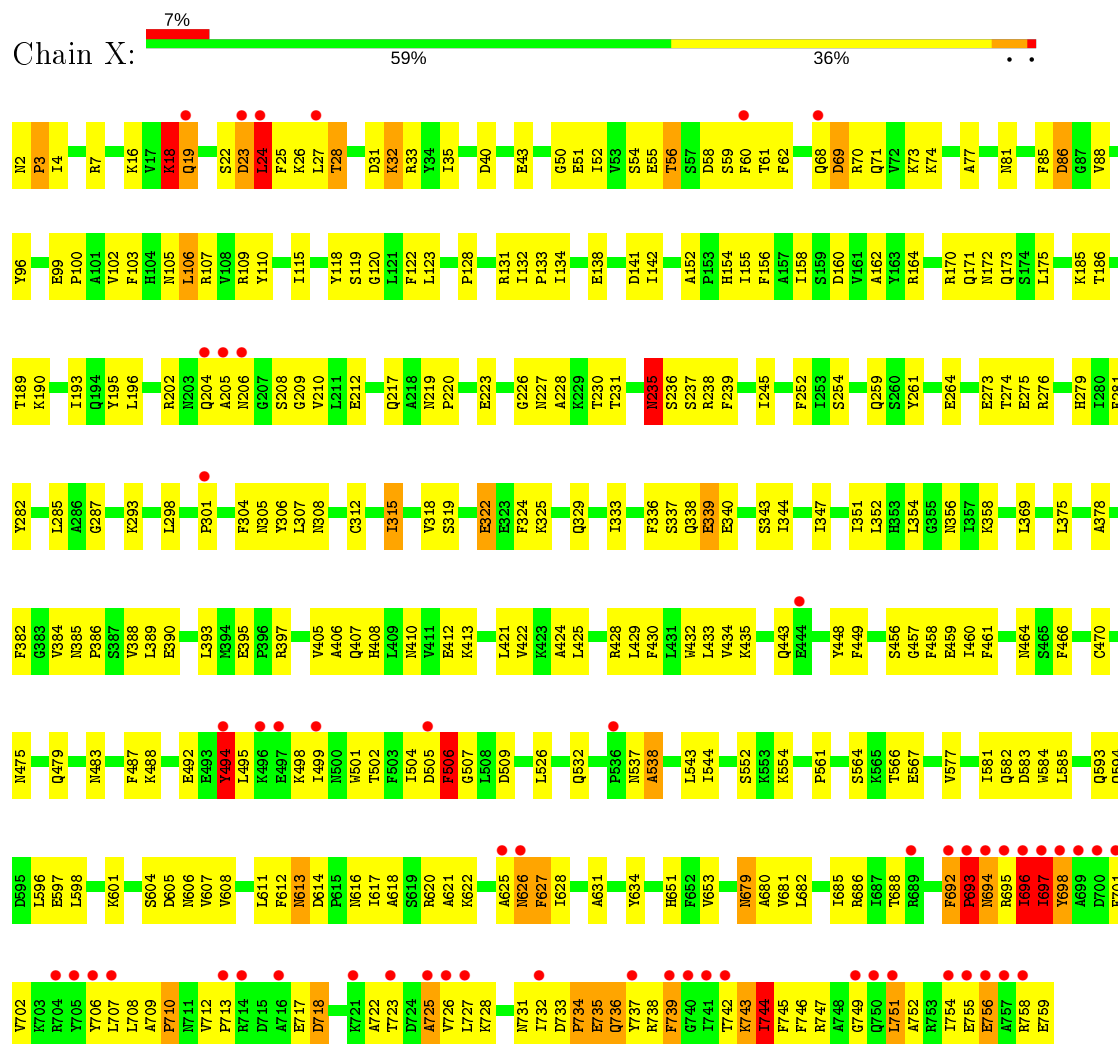
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	379	Total	O	0	0
			379	379		

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-2 HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	54.60Å 106.00Å 178.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.85 19.98 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.98-2.85) 98.3 (19.98-2.85)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.83Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.253 , 0.301 0.256 , 0.313	Depositor DCC
R_{free} test set	1241 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 69.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6469	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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	X	0.27	3/6210 (0.0%)	0.75	46/8379 (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	X	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	235	ASN	C-N	-7.33	1.17	1.34
1	X	693	PRO	N-CD	6.85	1.57	1.47
1	X	18	LYS	C-N	-5.40	1.21	1.34

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	235	ASN	C-N-CA	13.60	155.71	121.70
1	X	206	ASN	N-CA-C	12.83	145.63	111.00
1	X	697	ILE	CB-CA-C	-11.71	88.18	111.60
1	X	235	ASN	O-C-N	-8.73	108.74	122.70
1	X	694	ASN	N-CA-C	-8.49	88.09	111.00
1	X	19	GLN	N-CA-CB	8.27	125.49	110.60
1	X	679	ASN	CB-CA-C	-7.96	94.48	110.40
1	X	86	ASP	CB-CA-C	7.95	126.30	110.40
1	X	717	GLU	N-CA-C	7.83	132.15	111.00
1	X	506	PHE	N-CA-C	-7.65	90.33	111.00
1	X	236	SER	N-CA-CB	7.44	121.66	110.50
1	X	58	ASP	CB-CA-C	7.26	124.92	110.40
1	X	506	PHE	CB-CA-C	7.07	124.54	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	68	GLN	CB-CA-C	-7.02	96.36	110.40
1	X	24	LEU	CB-CA-C	-6.92	97.05	110.20
1	X	58	ASP	N-CA-C	-6.87	92.46	111.00
1	X	206	ASN	N-CA-CB	-6.80	98.36	110.60
1	X	18	LYS	C-N-CA	6.80	138.69	121.70
1	X	315	ILE	CB-CA-C	-6.65	98.31	111.60
1	X	696	ILE	CB-CA-C	-6.46	98.67	111.60
1	X	498	LYS	N-CA-C	-6.45	93.60	111.00
1	X	33	ARG	N-CA-CB	-6.42	99.05	110.60
1	X	494	TYR	CB-CA-C	6.35	123.11	110.40
1	X	235	ASN	CB-CA-C	6.28	122.95	110.40
1	X	507	GLY	N-CA-C	-6.14	97.75	113.10
1	X	69	ASP	N-CA-CB	-6.05	99.72	110.60
1	X	205	ALA	N-CA-C	-5.98	94.85	111.00
1	X	52	ILE	N-CA-C	-5.94	94.97	111.00
1	X	236	SER	N-CA-C	-5.92	95.00	111.00
1	X	697	ILE	C-N-CA	5.91	136.47	121.70
1	X	743	LYS	CB-CA-C	5.83	122.06	110.40
1	X	567	GLU	N-CA-CB	-5.83	100.11	110.60
1	X	717	GLU	CB-CA-C	-5.82	98.77	110.40
1	X	32	LYS	CB-CA-C	-5.74	98.91	110.40
1	X	718	ASP	N-CA-CB	5.73	120.91	110.60
1	X	538	ALA	CB-CA-C	-5.71	101.54	110.10
1	X	692	PHE	CB-CA-C	5.63	121.67	110.40
1	X	679	ASN	N-CA-C	5.62	126.18	111.00
1	X	725	ALA	CB-CA-C	-5.61	101.68	110.10
1	X	86	ASP	N-CA-C	-5.57	95.96	111.00
1	X	24	LEU	C-N-CA	5.42	135.26	121.70
1	X	18	LYS	CB-CA-C	-5.42	99.56	110.40
1	X	744	ILE	N-CA-CB	5.38	123.17	110.80
1	X	52	ILE	N-CA-CB	5.36	123.14	110.80
1	X	19	GLN	N-CA-C	-5.30	96.69	111.00
1	X	627	PHE	CB-CA-C	-5.20	100.00	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	18	LYS	Peptide
1	X	235	ASN	Mainchain,Peptide
1	X	24	LEU	Peptide
1	X	697	ILE	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	X	6090	0	6046	337	0
2	X	379	0	0	21	0
All	All	6469	0	6046	337	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 28.

All (337) 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:X:532:GLN:HE21	1:X:538:ALA:CB	1.31	1.44
1:X:24:LEU:HD12	1:X:25:PHE:N	1.32	1.40
1:X:532:GLN:NE2	1:X:538:ALA:HB1	1.37	1.39
1:X:23:ASP:CA	1:X:27:LEU:HD11	1.56	1.33
1:X:319:SER:CB	1:X:322:GLU:OE2	1.76	1.30
1:X:319:SER:HB3	1:X:322:GLU:OE2	1.13	1.25
1:X:319:SER:HB3	1:X:322:GLU:CD	1.58	1.23
1:X:24:LEU:CD1	1:X:25:PHE:N	2.04	1.20
1:X:532:GLN:NE2	1:X:538:ALA:CB	1.96	1.19
1:X:24:LEU:HD12	1:X:24:LEU:C	1.64	1.17
1:X:23:ASP:C	1:X:27:LEU:HD11	1.68	1.13
1:X:697:ILE:HG22	1:X:698:TYR:H	0.98	1.13
1:X:319:SER:CA	1:X:322:GLU:OE2	2.00	1.08
1:X:23:ASP:HA	1:X:27:LEU:HD11	1.13	1.08
1:X:696:ILE:HD13	1:X:697:ILE:O	1.56	1.06
1:X:24:LEU:HD12	1:X:26:LYS:N	1.71	1.04
1:X:23:ASP:HA	1:X:27:LEU:CD1	1.93	0.99
1:X:532:GLN:HE21	1:X:538:ALA:HB1	0.87	0.98
1:X:319:SER:C	1:X:322:GLU:OE2	2.02	0.98
1:X:743:LYS:O	1:X:744:ILE:CG2	2.11	0.97
1:X:24:LEU:CD1	1:X:26:LYS:H	1.81	0.94
1:X:24:LEU:HD12	1:X:26:LYS:H	1.13	0.93
1:X:697:ILE:HG22	1:X:698:TYR:N	1.79	0.92
1:X:697:ILE:CG2	1:X:698:TYR:H	1.83	0.92
1:X:23:ASP:O	1:X:27:LEU:CD1	2.21	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:24:LEU:CD1	1:X:25:PHE:H	1.87	0.87
1:X:23:ASP:C	1:X:27:LEU:CD1	2.43	0.87
1:X:743:LYS:O	1:X:744:ILE:HG23	1.76	0.85
1:X:24:LEU:CD1	1:X:26:LYS:N	2.38	0.84
1:X:532:GLN:NE2	1:X:538:ALA:HB2	1.92	0.84
1:X:728:LYS:HA	1:X:732:ILE:HB	1.58	0.83
1:X:315:ILE:O	1:X:315:ILE:HD12	1.78	0.83
1:X:743:LYS:O	1:X:744:ILE:HG22	1.79	0.82
1:X:337:SER:HB2	1:X:340:GLU:HB2	1.60	0.82
1:X:175:LEU:HD23	1:X:651:HIS:HB2	1.61	0.81
1:X:22:SER:O	1:X:23:ASP:HB2	1.80	0.81
1:X:24:LEU:O	1:X:26:LYS:N	2.15	0.80
1:X:23:ASP:O	1:X:27:LEU:HD12	1.80	0.80
1:X:712:VAL:HG11	1:X:723:THR:HG22	1.65	0.79
1:X:51:GLU:O	1:X:62:PHE:HB2	1.83	0.79
1:X:385:ASN:HB3	1:X:388:VAL:HG22	1.67	0.76
1:X:693:PRO:HD2	1:X:747:ARG:HD2	1.67	0.76
1:X:606:ASN:OD1	1:X:607:VAL:HG13	1.85	0.76
1:X:696:ILE:CD1	1:X:697:ILE:O	2.32	0.75
1:X:315:ILE:HD12	1:X:315:ILE:C	2.06	0.75
1:X:694:ASN:O	1:X:746:PHE:O	2.05	0.75
1:X:23:ASP:O	1:X:27:LEU:HD11	1.86	0.74
1:X:343:SER:HB3	1:X:607:VAL:HG21	1.71	0.72
1:X:701:PHE:HZ	1:X:751:LEU:HD21	1.52	0.72
1:X:304:PHE:HA	1:X:356:ASN:HD21	1.52	0.72
1:X:315:ILE:HD11	1:X:318:VAL:HG12	1.71	0.72
1:X:538:ALA:O	1:X:585:LEU:CD2	2.39	0.71
1:X:24:LEU:HD12	1:X:25:PHE:CA	2.19	0.71
1:X:343:SER:HB3	1:X:607:VAL:CG2	2.21	0.71
1:X:190:LYS:HG3	2:X:2142:HOH:O	1.92	0.69
1:X:306:TYR:N	2:X:2198:HOH:O	2.25	0.69
1:X:81:ASN:HD21	1:X:96:TYR:H	1.39	0.69
1:X:51:GLU:O	1:X:62:PHE:CB	2.40	0.69
1:X:626:ASN:ND2	2:X:2320:HOH:O	2.25	0.69
1:X:141:ASP:OD1	2:X:2116:HOH:O	2.10	0.68
1:X:744:ILE:O	1:X:745:PHE:HD1	1.77	0.66
1:X:85:PHE:O	1:X:86:ASP:C	2.34	0.66
1:X:230:THR:HA	1:X:275:GLU:HG2	1.77	0.66
1:X:738:ARG:O	1:X:744:ILE:HG21	1.96	0.66
1:X:738:ARG:HA	1:X:738:ARG:HE	1.61	0.65
1:X:499:ILE:HD12	1:X:499:ILE:H	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:27:LEU:HB2	2:X:2029:HOH:O	1.97	0.65
1:X:712:VAL:HG23	1:X:725:ALA:HB3	1.78	0.65
1:X:131:ARG:NH1	1:X:132:ILE:O	2.29	0.65
1:X:755:GLU:O	1:X:756:GLU:HB2	1.96	0.65
1:X:274:THR:HG22	1:X:274:THR:O	1.95	0.64
1:X:122:PHE:CD2	1:X:681:VAL:HG23	2.32	0.64
1:X:227:ASN:HB3	1:X:235:ASN:O	1.97	0.64
1:X:24:LEU:C	1:X:24:LEU:CD1	2.35	0.63
1:X:696:ILE:HD12	1:X:696:ILE:O	1.98	0.63
1:X:538:ALA:O	1:X:585:LEU:HD23	1.98	0.63
1:X:701:PHE:CZ	1:X:751:LEU:HD21	2.33	0.63
1:X:24:LEU:HD12	1:X:24:LEU:O	1.99	0.63
1:X:358:LYS:HB2	2:X:2197:HOH:O	1.99	0.63
1:X:24:LEU:C	1:X:26:LYS:H	1.98	0.62
1:X:679:ASN:O	1:X:680:ALA:HB3	1.97	0.62
1:X:315:ILE:HA	2:X:2204:HOH:O	1.98	0.62
1:X:743:LYS:HD2	1:X:744:ILE:H	1.65	0.62
1:X:23:ASP:N	1:X:27:LEU:HD21	2.15	0.61
1:X:375:LEU:HD11	1:X:389:LEU:HD22	1.82	0.61
1:X:4:ILE:HB	2:X:2009:HOH:O	2.00	0.61
1:X:227:ASN:ND2	1:X:237:SER:HA	2.16	0.61
1:X:470:CYS:HB3	1:X:634:TYR:CZ	2.36	0.61
1:X:338:GLN:NE2	2:X:2217:HOH:O	2.31	0.61
1:X:594:GLN:HA	1:X:597:GLU:OE1	2.01	0.61
1:X:118:TYR:CE1	1:X:123:LEU:HD13	2.36	0.60
1:X:27:LEU:O	1:X:28:THR:C	2.38	0.60
1:X:538:ALA:O	1:X:585:LEU:HD21	2.00	0.60
1:X:77:ALA:HA	2:X:2073:HOH:O	2.02	0.60
1:X:339:GLU:HA	2:X:2216:HOH:O	2.01	0.60
1:X:2:ASN:N	1:X:3:PRO:HD3	2.17	0.60
1:X:421:LEU:HD22	1:X:596:LEU:HD23	1.83	0.60
1:X:620:ARG:HB3	1:X:628:ILE:HG12	1.83	0.59
1:X:607:VAL:HG23	1:X:608:VAL:N	2.17	0.59
1:X:31:ASP:OD1	1:X:756:GLU:O	2.21	0.59
1:X:24:LEU:HD12	1:X:25:PHE:C	2.22	0.59
1:X:692:PHE:CE2	1:X:745:PHE:HB2	2.38	0.59
1:X:544:ILE:HD12	1:X:566:THR:O	2.02	0.59
1:X:613:ASN:N	1:X:613:ASN:HD22	2.01	0.59
1:X:119:SER:O	1:X:122:PHE:HB2	2.03	0.59
1:X:132:ILE:HD12	1:X:132:ILE:N	2.18	0.59
1:X:329:GLN:O	1:X:333:ILE:HG12	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:59:SER:HA	1:X:73:LYS:HA	1.84	0.58
1:X:118:TYR:HD2	2:X:2081:HOH:O	1.84	0.58
1:X:56:THR:HA	2:X:2057:HOH:O	2.04	0.58
1:X:24:LEU:HD13	1:X:25:PHE:H	1.67	0.58
1:X:16:LYS:HE2	1:X:152:ALA:HB2	1.85	0.57
1:X:219:ASN:HB3	1:X:220:PRO:HD3	1.86	0.57
1:X:185:LYS:NZ	1:X:456:SER:HB3	2.20	0.56
1:X:239:PHE:O	2:X:2173:HOH:O	2.17	0.56
1:X:707:LEU:HD13	1:X:759:GLU:HB3	1.86	0.56
1:X:393:LEU:O	1:X:393:LEU:HD23	2.06	0.56
1:X:319:SER:HB3	1:X:322:GLU:CG	2.34	0.56
1:X:395:GLU:HA	1:X:407:GLN:O	2.05	0.56
1:X:424:ALA:O	1:X:428:ARG:HG3	2.05	0.56
1:X:747:ARG:HH12	1:X:749:GLY:HA3	1.70	0.56
1:X:99:GLU:N	1:X:100:PRO:HD2	2.21	0.56
1:X:526:LEU:HD22	1:X:631:ALA:HB1	1.86	0.56
1:X:739:PHE:HB2	1:X:744:ILE:HD13	1.87	0.56
1:X:305:ASN:HA	1:X:308:ASN:HD21	1.70	0.56
1:X:138:GLU:O	1:X:142:ILE:HG13	2.06	0.55
1:X:395:GLU:HG2	1:X:406:ALA:HB1	1.87	0.55
1:X:23:ASP:CA	1:X:27:LEU:CD1	2.52	0.55
1:X:696:ILE:C	1:X:696:ILE:HD12	2.26	0.55
1:X:202:ARG:HD3	1:X:252:PHE:CG	2.42	0.55
1:X:625:ALA:O	1:X:626:ASN:C	2.45	0.55
1:X:460:ILE:HG13	1:X:577:VAL:HG22	1.89	0.55
1:X:315:ILE:HD11	1:X:318:VAL:H	1.71	0.54
1:X:217:GLN:O	1:X:220:PRO:HD2	2.08	0.54
1:X:457:GLY:HA2	1:X:475:ASN:OD1	2.07	0.54
1:X:709:ALA:HB1	1:X:710:PRO:HD2	1.90	0.54
1:X:701:PHE:O	1:X:723:THR:HG21	2.08	0.54
1:X:695:ARG:HG3	1:X:745:PHE:CD2	2.43	0.54
1:X:614:ASP:HB3	1:X:616:ASN:OD1	2.08	0.53
1:X:354:LEU:HD12	1:X:378:ALA:HB1	1.89	0.53
1:X:626:ASN:ND2	1:X:627:PHE:H	2.07	0.53
1:X:733:ASP:HB2	1:X:734:PRO:HD2	1.91	0.53
1:X:154:HIS:CD2	1:X:156:PHE:H	2.26	0.53
1:X:24:LEU:O	1:X:27:LEU:HG	2.09	0.53
1:X:259:GLN:HG2	1:X:261:TYR:OH	2.08	0.53
1:X:51:GLU:O	1:X:62:PHE:CA	2.57	0.53
1:X:351:ILE:HG23	1:X:422:VAL:HG13	1.89	0.53
1:X:695:ARG:HG3	1:X:745:PHE:HD2	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:123:LEU:HD23	1:X:653:VAL:HG22	1.91	0.52
1:X:154:HIS:HD2	1:X:156:PHE:H	1.56	0.52
1:X:18:LYS:HD2	2:X:2021:HOH:O	2.08	0.52
1:X:132:ILE:HG22	1:X:134:ILE:HG23	1.91	0.52
1:X:306:TYR:C	1:X:307:LEU:HD12	2.30	0.52
1:X:505:ASP:O	1:X:506:PHE:HD1	1.92	0.52
1:X:701:PHE:CD2	1:X:727:LEU:HD11	2.45	0.52
1:X:24:LEU:C	1:X:26:LYS:N	2.61	0.52
1:X:369:LEU:HD23	1:X:390:GLU:OE2	2.09	0.52
1:X:172:ASN:ND2	1:X:449:PHE:H	2.07	0.52
1:X:315:ILE:CD1	1:X:315:ILE:C	2.72	0.52
1:X:744:ILE:O	1:X:745:PHE:CD1	2.61	0.52
1:X:85:PHE:C	1:X:86:ASP:O	2.46	0.52
1:X:173:GLN:NE2	2:X:2135:HOH:O	2.39	0.51
1:X:228:ALA:HA	1:X:279:HIS:CE1	2.45	0.51
1:X:254:SER:C	1:X:443:GLN:HE21	2.13	0.51
1:X:707:LEU:HD12	1:X:708:LEU:N	2.24	0.51
1:X:128:PRO:HB2	1:X:132:ILE:HD11	1.93	0.51
1:X:60:PHE:CE2	1:X:74:LYS:HG2	2.45	0.51
1:X:209:GLY:O	1:X:210:VAL:HB	2.10	0.51
1:X:479:GLN:HE21	1:X:483:ASN:HD21	1.59	0.51
1:X:544:ILE:HB	1:X:581:ILE:HG13	1.92	0.51
1:X:702:VAL:HA	1:X:723:THR:HG23	1.93	0.51
1:X:122:PHE:CE2	1:X:681:VAL:HA	2.45	0.51
1:X:238:ARG:HD3	1:X:264:GLU:OE1	2.10	0.51
1:X:412:GLU:HG3	1:X:413:LYS:N	2.25	0.51
1:X:532:GLN:HE22	1:X:538:ALA:CB	2.12	0.50
1:X:743:LYS:C	1:X:744:ILE:HG23	2.32	0.50
1:X:24:LEU:HD11	1:X:26:LYS:HG3	1.93	0.50
1:X:421:LEU:O	1:X:425:LEU:HD13	2.11	0.50
1:X:458:PHE:CZ	1:X:475:ASN:HB3	2.46	0.50
1:X:692:PHE:HB2	1:X:746:PHE:O	2.12	0.50
1:X:702:VAL:HG22	1:X:722:ALA:HB3	1.92	0.50
1:X:85:PHE:O	1:X:88:VAL:HG13	2.10	0.50
1:X:712:VAL:HG12	1:X:713:PRO:O	2.11	0.50
1:X:88:VAL:HG22	1:X:105:ASN:HD21	1.77	0.50
1:X:607:VAL:HG23	1:X:608:VAL:H	1.76	0.50
1:X:170:ARG:HD2	1:X:448:TYR:CZ	2.47	0.49
1:X:696:ILE:C	1:X:696:ILE:CD1	2.79	0.49
1:X:227:ASN:HD22	1:X:237:SER:HA	1.77	0.49
1:X:60:PHE:HE2	1:X:74:LYS:HG2	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:625:ALA:O	1:X:626:ASN:O	2.30	0.49
1:X:315:ILE:CD1	1:X:318:VAL:H	2.25	0.49
1:X:50:GLY:O	1:X:51:GLU:HG2	2.13	0.49
1:X:315:ILE:HG13	2:X:2210:HOH:O	2.11	0.49
1:X:339:GLU:CD	1:X:339:GLU:H	2.16	0.49
1:X:708:LEU:HD11	1:X:755:GLU:OE2	2.13	0.49
1:X:712:VAL:HG13	1:X:713:PRO:HD2	1.94	0.49
1:X:204:GLN:H	1:X:204:GLN:CD	2.16	0.48
1:X:54:SER:OG	1:X:61:THR:HB	2.13	0.48
1:X:747:ARG:NH1	1:X:749:GLY:H	2.11	0.48
1:X:186:THR:O	1:X:189:THR:HG22	2.13	0.48
1:X:758:ARG:HD2	2:X:2372:HOH:O	2.13	0.48
1:X:732:ILE:HG22	1:X:733:ASP:N	2.29	0.48
1:X:102:VAL:HG21	1:X:682:LEU:HD12	1.96	0.48
1:X:202:ARG:HB2	1:X:212:GLU:OE2	2.14	0.48
1:X:397:ARG:HA	1:X:405:VAL:O	2.13	0.48
1:X:103:PHE:O	1:X:107:ARG:HB2	2.13	0.48
1:X:460:ILE:N	1:X:460:ILE:HD12	2.29	0.48
1:X:744:ILE:HG13	1:X:745:PHE:N	2.28	0.48
1:X:226:GLY:HA3	1:X:239:PHE:CE1	2.49	0.48
1:X:581:ILE:HG22	1:X:582:GLN:N	2.28	0.48
1:X:51:GLU:O	1:X:62:PHE:HA	2.14	0.48
1:X:208:SER:OG	1:X:212:GLU:HB2	2.14	0.47
1:X:726:VAL:O	1:X:726:VAL:HG12	2.14	0.47
1:X:389:LEU:HD23	1:X:389:LEU:O	2.14	0.47
1:X:23:ASP:H	1:X:27:LEU:HD21	1.79	0.47
1:X:185:LYS:HZ1	1:X:456:SER:HB3	1.79	0.47
1:X:160:ASP:O	1:X:164:ARG:HG2	2.13	0.47
1:X:281:PHE:CD1	1:X:352:LEU:HD21	2.49	0.47
1:X:733:ASP:O	1:X:735:GLU:N	2.47	0.47
1:X:7:ARG:NH2	1:X:19:GLN:O	2.48	0.47
1:X:746:PHE:CG	1:X:747:ARG:N	2.83	0.47
1:X:344:ILE:HD11	1:X:432:TRP:HZ3	1.80	0.47
1:X:758:ARG:O	1:X:759:GLU:C	2.53	0.47
1:X:305:ASN:HA	1:X:308:ASN:ND2	2.30	0.47
1:X:581:ILE:O	1:X:584:TRP:CD1	2.68	0.47
1:X:466:PHE:HB2	1:X:584:TRP:CD1	2.50	0.47
1:X:682:LEU:CD2	1:X:686:ARG:HD2	2.45	0.47
1:X:70:ARG:O	1:X:71:GLN:HG3	2.14	0.47
1:X:718:ASP:O	1:X:722:ALA:HB2	2.15	0.46
1:X:132:ILE:HD12	1:X:132:ILE:H	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:502:THR:O	1:X:504:ILE:HG12	2.15	0.46
1:X:312:CYS:O	2:X:2203:HOH:O	2.20	0.46
1:X:737:TYR:HD1	1:X:739:PHE:HB2	1.80	0.46
1:X:561:PRO:HB2	1:X:564:SER:HB3	1.98	0.46
1:X:593:GLN:HB2	1:X:596:LEU:HD13	1.98	0.46
1:X:171:GLN:HG2	1:X:172:ASN:N	2.31	0.46
1:X:319:SER:N	1:X:322:GLU:OE2	2.48	0.45
1:X:115:ILE:HG21	1:X:128:PRO:HB3	1.97	0.45
1:X:434:VAL:HG13	2:X:2242:HOH:O	2.16	0.45
1:X:40:ASP:HB3	1:X:43:GLU:HB3	1.98	0.45
1:X:487:PHE:HZ	1:X:506:PHE:HB3	1.82	0.45
1:X:494:TYR:HA	1:X:494:TYR:HD1	1.64	0.45
1:X:698:TYR:HE1	1:X:739:PHE:CE2	2.35	0.45
1:X:315:ILE:CD1	1:X:315:ILE:O	2.59	0.45
1:X:747:ARG:NH1	1:X:749:GLY:HA3	2.32	0.45
1:X:285:LEU:HD13	1:X:301:PRO:HA	1.99	0.45
1:X:739:PHE:HB2	1:X:744:ILE:CD1	2.46	0.45
1:X:743:LYS:HZ2	1:X:745:PHE:HE1	1.65	0.45
1:X:196:LEU:HD12	1:X:245:ILE:HD12	2.00	0.44
1:X:160:ASP:HB2	1:X:195:TYR:OH	2.17	0.44
1:X:170:ARG:HD2	1:X:448:TYR:OH	2.17	0.44
1:X:337:SER:HB3	1:X:339:GLU:HG2	2.00	0.44
1:X:347:ILE:HD11	1:X:608:VAL:HB	1.99	0.44
1:X:55:GLU:O	1:X:56:THR:C	2.55	0.44
1:X:604:SER:O	1:X:605:ASP:HB2	2.18	0.44
1:X:385:ASN:HB3	1:X:388:VAL:CG2	2.44	0.44
1:X:106:LEU:HA	1:X:109:ARG:HB2	2.00	0.44
1:X:410:ASN:OD1	1:X:413:LYS:HG3	2.18	0.44
1:X:304:PHE:HA	1:X:356:ASN:ND2	2.26	0.43
1:X:679:ASN:O	1:X:680:ALA:CB	2.66	0.43
1:X:162:ALA:O	1:X:173:GLN:HG3	2.18	0.43
1:X:688:THR:HG22	1:X:692:PHE:O	2.18	0.43
1:X:698:TYR:HE1	1:X:739:PHE:CZ	2.36	0.43
1:X:106:LEU:O	1:X:110:TYR:HB2	2.19	0.43
1:X:611:LEU:O	1:X:618:ALA:HB2	2.18	0.43
1:X:293:LYS:HA	1:X:298:LEU:HD12	2.01	0.43
1:X:617:ILE:HG22	1:X:617:ILE:O	2.18	0.43
1:X:223:GLU:O	1:X:227:ASN:HB2	2.19	0.43
1:X:231:THR:HG22	1:X:231:THR:O	2.17	0.43
1:X:315:ILE:CD1	1:X:318:VAL:HG12	2.45	0.43
1:X:594:GLN:O	1:X:598:LEU:HG	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:172:ASN:HD21	1:X:448:TYR:HA	1.84	0.43
1:X:384:VAL:O	1:X:386:PRO:HD3	2.19	0.43
1:X:384:VAL:CG2	1:X:389:LEU:HD12	2.49	0.42
1:X:336:PHE:HE2	1:X:432:TRP:CH2	2.37	0.42
1:X:430:PHE:HA	1:X:433:LEU:HD12	2.00	0.42
1:X:120:GLY:N	1:X:685:ILE:HD11	2.34	0.42
1:X:202:ARG:HD3	1:X:252:PHE:HB3	2.01	0.42
1:X:543:LEU:HD12	1:X:585:LEU:HB2	2.00	0.42
1:X:712:VAL:CG2	1:X:726:VAL:HG23	2.49	0.42
1:X:133:PRO:HB2	2:X:2107:HOH:O	2.19	0.42
1:X:22:SER:HB3	1:X:23:ASP:H	1.58	0.42
1:X:354:LEU:CD1	1:X:378:ALA:HB1	2.49	0.42
1:X:425:LEU:HD11	1:X:612:PHE:HZ	1.85	0.42
1:X:509:ASP:N	1:X:509:ASP:OD1	2.52	0.42
1:X:707:LEU:HD13	1:X:759:GLU:CB	2.50	0.42
1:X:254:SER:C	1:X:443:GLN:NE2	2.73	0.42
1:X:158:ILE:HD11	1:X:651:HIS:HB3	2.01	0.42
1:X:305:ASN:ND2	1:X:356:ASN:HA	2.35	0.42
1:X:736:GLN:HB3	1:X:737:TYR:H	1.53	0.42
1:X:747:ARG:HH12	1:X:749:GLY:CA	2.32	0.42
1:X:81:ASN:HD21	1:X:96:TYR:N	2.12	0.42
1:X:32:LYS:HB2	1:X:32:LYS:HE3	1.87	0.42
1:X:154:HIS:CD2	1:X:155:ILE:HG22	2.55	0.41
1:X:31:ASP:HA	1:X:756:GLU:HG2	2.02	0.41
1:X:85:PHE:O	1:X:86:ASP:O	2.38	0.41
1:X:69:ASP:N	1:X:69:ASP:OD1	2.44	0.41
1:X:154:HIS:CD2	1:X:155:ILE:N	2.89	0.41
1:X:273:GLU:O	1:X:274:THR:HB	2.20	0.41
1:X:459:GLU:HB3	1:X:461:PHE:CE1	2.55	0.41
1:X:733:ASP:HB2	1:X:734:PRO:CD	2.49	0.41
1:X:738:ARG:HA	1:X:738:ARG:NE	2.30	0.41
1:X:492:GLU:O	1:X:495:LEU:HB3	2.20	0.41
1:X:698:TYR:OH	1:X:742:THR:O	2.35	0.41
1:X:322:GLU:HA	1:X:325:LYS:HE3	2.01	0.41
1:X:737:TYR:CD1	1:X:739:PHE:HB2	2.56	0.41
1:X:276:ARG:NH2	1:X:282:TYR:CG	2.88	0.41
1:X:55:GLU:O	1:X:56:THR:O	2.38	0.41
1:X:582:GLN:HB3	1:X:583:ASP:H	1.57	0.41
1:X:318:VAL:HG22	1:X:319:SER:N	2.36	0.41
1:X:621:ALA:O	1:X:628:ILE:HG23	2.21	0.41
1:X:24:LEU:HD11	1:X:26:LYS:N	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:461:PHE:H	1:X:464:ASN:HD21	1.69	0.41
1:X:626:ASN:CG	1:X:627:PHE:N	2.75	0.41
1:X:322:GLU:HG3	1:X:322:GLU:H	1.47	0.41
1:X:354:LEU:HD11	1:X:382:PHE:HE2	1.86	0.41
1:X:384:VAL:HG21	1:X:389:LEU:HD12	2.03	0.41
1:X:429:LEU:O	1:X:433:LEU:HG	2.20	0.41
1:X:501:TRP:CG	1:X:502:THR:N	2.89	0.41
1:X:287:GLY:HA3	1:X:324:PHE:CD2	2.56	0.40
1:X:412:GLU:HG3	1:X:413:LYS:HG3	2.03	0.40
1:X:731:ASN:O	1:X:732:ILE:HD13	2.20	0.40
1:X:318:VAL:HG22	1:X:319:SER:H	1.86	0.40
1:X:552:SER:O	1:X:554:LYS:HG3	2.22	0.40
1:X:597:GLU:O	1:X:601:LYS:HB2	2.21	0.40
1:X:743:LYS:NZ	1:X:745:PHE:HE1	2.18	0.40
1:X:751:LEU:HG	1:X:754:ILE:HD11	2.03	0.40
1:X:189:THR:O	1:X:193:ILE:HD13	2.22	0.40
1:X:343:SER:HB3	1:X:607:VAL:HG22	1.99	0.40
1:X:488:LYS:O	1:X:492:GLU:HG2	2.21	0.40
1:X:35:ILE:HG22	1:X:50:GLY:HA3	2.02	0.40
1:X:622:LYS:C	1:X:622:LYS:HD3	2.41	0.40
1:X:204:GLN:N	1:X:204:GLN:CD	2.75	0.40
1:X:412:GLU:HG3	1:X:413:LYS:H	1.86	0.40
1:X:692:PHE:HA	1:X:747:ARG:HD2	2.03	0.40
1:X:755:GLU:O	1:X:756:GLU:CB	2.66	0.40
1:X:743:LYS:HD2	1:X:744:ILE:N	2.35	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	X	756/758 (100%)	657 (87%)	82 (11%)	17 (2%)	6 21

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	23	ASP
1	X	56	THR
1	X	626	ASN
1	X	735	GLU
1	X	736	GLN
1	X	744	ILE
1	X	756	GLU
1	X	706	TYR
1	X	752	ALA
1	X	28	THR
1	X	696	ILE
1	X	710	PRO
1	X	751	LEU
1	X	3	PRO
1	X	537	ASN
1	X	734	PRO
1	X	693	PRO

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	X	662/662 (100%)	652 (98%)	10 (2%)	65 86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	106	LEU
1	X	322	GLU
1	X	339	GLU
1	X	408	HIS
1	X	435	LYS
1	X	494	TYR
1	X	506	PHE
1	X	613	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	698	TYR
1	X	739	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	5	HIS
1	X	71	GLN
1	X	79	GLN
1	X	81	ASN
1	X	105	ASN
1	X	154	HIS
1	X	172	ASN
1	X	188	ASN
1	X	217	GLN
1	X	227	ASN
1	X	234	ASN
1	X	279	HIS
1	X	283	GLN
1	X	305	ASN
1	X	309	GLN
1	X	356	ASN
1	X	439	ASN
1	X	464	ASN
1	X	472	ASN
1	X	483	ASN
1	X	511	GLN
1	X	532	GLN
1	X	550	HIS
1	X	613	ASN
1	X	626	ASN
1	X	637	GLN
1	X	649	ASN
1	X	662	GLN
1	X	720	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	235:ASN	C	236:SER	N	1.17

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	X	758/758 (100%)	-0.01	56 (7%)	14 10	12, 41, 106, 141	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	693	PRO	7.6
1	X	713	PRO	6.4
1	X	727	LEU	6.3
1	X	757	ALA	5.8
1	X	706	TYR	5.7
1	X	697	ILE	5.2
1	X	205	ALA	5.1
1	X	23	ASP	4.3
1	X	726	VAL	4.3
1	X	741	ILE	4.2
1	X	698	TYR	4.1
1	X	626	ASN	4.1
1	X	625	ALA	4.1
1	X	701	PHE	4.1
1	X	740	GLY	4.0
1	X	750	GLN	4.0
1	X	696	ILE	3.9
1	X	496	LYS	3.8
1	X	692	PHE	3.8
1	X	27	LEU	3.7
1	X	700	ASP	3.7
1	X	754	ILE	3.4
1	X	694	ASN	3.4
1	X	689	ARG	3.3
1	X	206	ASN	3.2
1	X	725	ALA	3.1
1	X	24	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	X	536	PRO	3.0
1	X	499	ILE	2.9
1	X	505	ASP	2.8
1	X	714	ARG	2.7
1	X	737	TYR	2.7
1	X	723	THR	2.7
1	X	704	ARG	2.6
1	X	707	LEU	2.5
1	X	204	GLN	2.5
1	X	497	GLU	2.5
1	X	758	ARG	2.4
1	X	695	ARG	2.4
1	X	705	TYR	2.4
1	X	742	THR	2.3
1	X	301	PRO	2.3
1	X	756	GLU	2.3
1	X	755	GLU	2.3
1	X	68	GLN	2.2
1	X	721	LYS	2.2
1	X	699	ALA	2.2
1	X	494	TYR	2.2
1	X	739	PHE	2.1
1	X	19	GLN	2.1
1	X	732	ILE	2.1
1	X	751	LEU	2.1
1	X	716	ALA	2.1
1	X	444	GLU	2.0
1	X	749	GLY	2.0
1	X	60	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.