



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:13 PM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

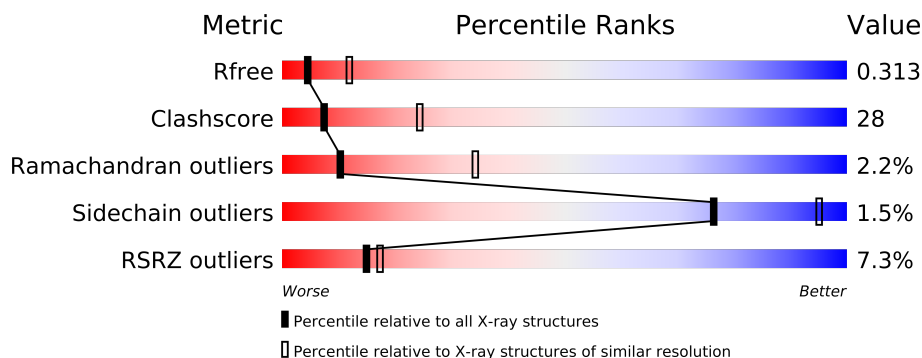
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	X	758	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6469 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MYOSIN-2 HEAVY CHAIN.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	680	ALA	GLY	ENGINEERED MUTATION	UNP P08799

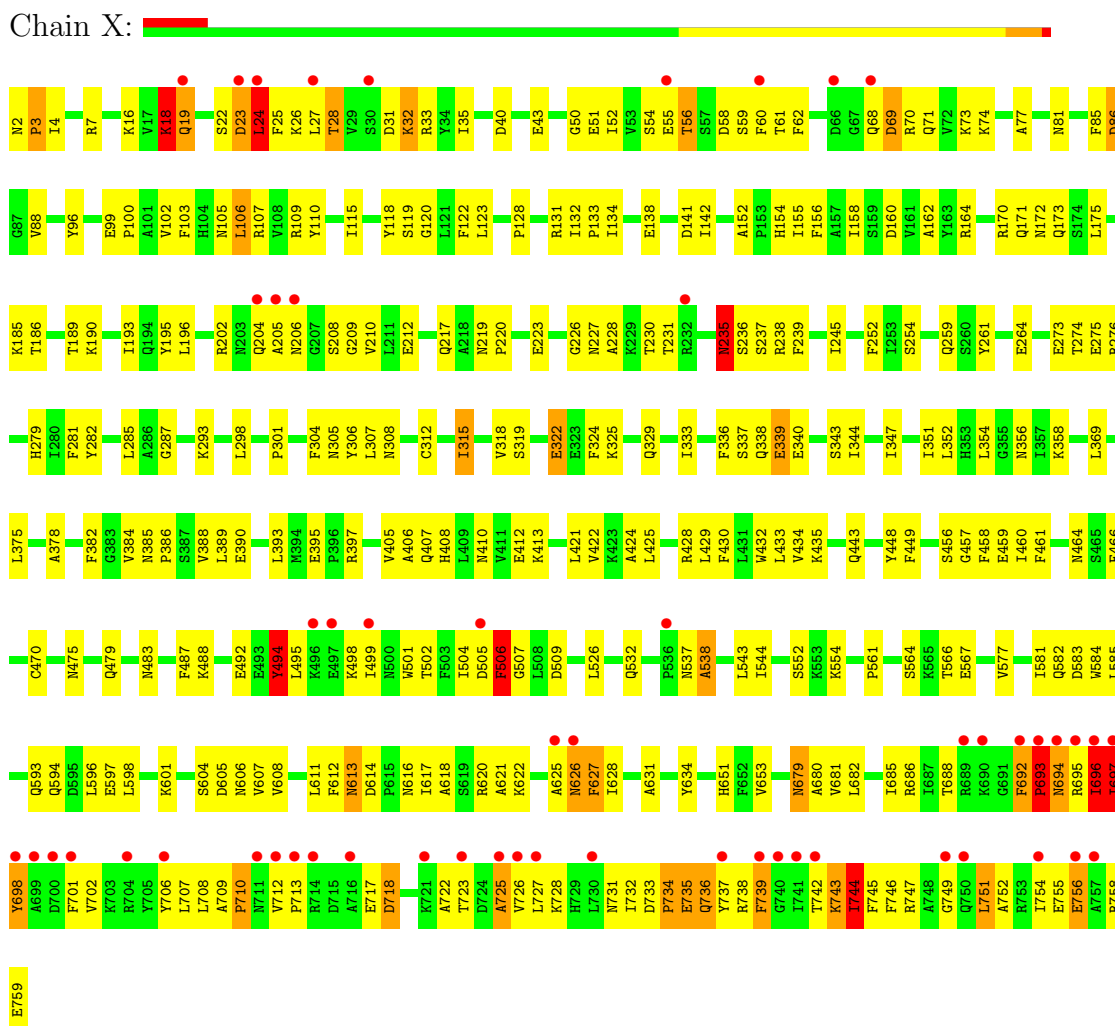
- Molecule 2 is water.

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 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	1239 reflections (5.05%)	DCC
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 , 42.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 24550 reflections	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.

5 Model quality i

5.1 Standard geometry i

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

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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 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	6090	0	6046	336	0
2	X	379	0	0	21	0
All	All	6469	0	6046	336	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

All (336) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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: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
1:X:24:LEU:CD1	1:X:25:PHE:H	1.87	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:532:GLN:NE2	1:X:538:ALA:HB2	1.92	0.84
1:X:24:LEU:CD1	1:X:26:LYS:N	2.38	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:738:ARG:O	1:X:744:ILE:HG21	1.96	0.66
1:X:230:THR:HA	1:X:275:GLU:HG2	1.77	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:538:ALA:O	1:X:585:LEU:HD21	2.00	0.60
1:X:27:LEU:O	1:X:28:THR:C	2.38	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:613:ASN:N	1:X:613:ASN:HD22	2.01	0.59
1:X:544:ILE:HD12	1:X:566:THR:O	2.02	0.59
1:X:132:ILE:HD12	1:X:132:ILE:N	2.18	0.59
1:X:119:SER:O	1:X:122:PHE:HB2	2.03	0.59
1:X:329:GLN:O	1:X:333:ILE:HG12	2.03	0.58
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:319:SER:HB3	1:X:322:GLU:CG	2.34	0.56
1:X:393:LEU:O	1:X:393:LEU:HD23	2.06	0.56
1:X:747:ARG:HH12	1:X:749:GLY:HA3	1.70	0.56
1:X:424:ALA:O	1:X:428:ARG:HG3	2.05	0.56
1:X:395:GLU:HA	1:X:407:GLN:O	2.05	0.56
1:X:526:LEU:HD22	1:X:631:ALA:HB1	1.86	0.56
1:X:99:GLU:N	1:X:100:PRO:HD2	2.21	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:701:PHE:O	1:X:723:THR:HG21	2.08	0.54
1:X:709:ALA:HB1	1:X:710:PRO:HD2	1.90	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:626:ASN:ND2	1:X:627:PHE:H	2.07	0.53
1:X:354:LEU:HD12	1:X:378:ALA:HB1	1.89	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:51:GLU:O	1:X:62:PHE:CA	2.57	0.53
1:X:259:GLN:HG2	1:X:261:TYR:OH	2.08	0.53
1:X:695:ARG:HG3	1:X:745:PHE:HD2	1.74	0.53
1:X:351:ILE:HG23	1:X:422:VAL:HG13	1.89	0.53
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:306:TYR:C	1:X:307:LEU:HD12	2.30	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:132:ILE:HG22	1:X:134:ILE:HG23	1.91	0.52
1:X:701:PHE:CD2	1:X:727:LEU:HD11	2.45	0.52
1:X:505:ASP:O	1:X:506:PHE:HD1	1.92	0.52
1:X:24:LEU:C	1:X:26:LYS:N	2.61	0.52
1:X:172:ASN:ND2	1:X:449:PHE:H	2.07	0.52
1:X:369:LEU:HD23	1:X:390:GLU:OE2	2.09	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:707:LEU:HD12	1:X:708:LEU:N	2.24	0.51
1:X:254:SER:C	1:X:443:GLN:HE21	2.13	0.51
1:X:228:ALA:HA	1:X:279:HIS:CE1	2.45	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:702:VAL:HA	1:X:723:THR:HG23	1.93	0.51
1:X:544:ILE:HB	1:X:581:ILE:HG13	1.92	0.51
1:X:479:GLN:HE21	1:X:483:ASN:HD21	1.59	0.51
1:X:209:GLY:O	1:X:210:VAL:HB	2.10	0.51
1:X:122:PHE:CE2	1:X:681:VAL:HA	2.45	0.51
1:X:412:GLU:HG3	1:X:413:LYS:N	2.25	0.51
1:X:238:ARG:HD3	1:X:264:GLU:OE1	2.10	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:692:PHE:HB2	1:X:746:PHE:O	2.12	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: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:696:ILE:C	1:X:696:ILE:CD1	2.79	0.49
1:X:170:ARG:HD2	1:X:448:TYR:CZ	2.47	0.49
1:X:625:ALA:O	1:X:626:ASN:O	2.30	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:758:ARG:HD2	2:X:2372:HOH:O	2.13	0.48
1:X:186:THR:O	1:X:189:THR:HG22	2.13	0.48
1:X:732:ILE:HG22	1:X:733:ASP:N	2.29	0.48
1:X:202:ARG:HB2	1:X:212:GLU:OE2	2.14	0.48
1:X:102:VAL:HG21	1:X:682:LEU:HD12	1.96	0.48
1:X:397:ARG:HA	1:X:405:VAL:O	2.13	0.48
1:X:744:ILE:HG13	1:X:745:PHE:N	2.28	0.48
1:X:460:ILE:N	1:X:460:ILE:HD12	2.29	0.48
1:X:103:PHE:O	1:X:107:ARG:HB2	2.13	0.48
1:X:51:GLU:O	1:X:62:PHE:HA	2.14	0.48
1:X:581:ILE:HG22	1:X:582:GLN:N	2.28	0.48
1:X:226:GLY:HA3	1:X:239:PHE:CE1	2.49	0.48
1:X:726:VAL:O	1:X:726:VAL:HG12	2.14	0.47
1:X:208:SER:OG	1:X:212:GLU:HB2	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:746:PHE:CG	1:X:747:ARG:N	2.83	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:281:PHE:CD1	1:X:352:LEU:HD21	2.49	0.47
1:X:758:ARG:O	1:X:759:GLU:C	2.53	0.47
1:X:344:ILE:HD11	1:X:432:TRP:HZ3	1.80	0.47
1:X:305:ASN:HA	1:X:308:ASN:ND2	2.30	0.47
1:X:466:PHE:HB2	1:X:584:TRP:CD1	2.50	0.47
1:X:581:ILE:O	1:X:584:TRP:CD1	2.68	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
1:X:502:THR:O	1:X:504:ILE:HG12	2.15	0.46
1:X:737:TYR:HD1	1:X:739:PHE:HB2	1.80	0.46
1:X:312:CYS:O	2:X:2203:HOH:O	2.20	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:285:LEU:HD13	1:X:301:PRO:HA	1.99	0.45
1:X:196:LEU:HD12	1:X:245:ILE:HD12	2.00	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:170:ARG:HD2	1:X:448:TYR:OH	2.17	0.44
1:X:160:ASP:HB2	1:X:195:TYR:OH	2.17	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: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:162:ALA:O	1:X:173:GLN:HG3	2.18	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
1:X:384:VAL:O	1:X:386:PRO:HD3	2.19	0.43
1:X:172:ASN:HD21	1:X:448:TYR:HA	1.84	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:22:SER:HB3	1:X:23:ASP:H	1.58	0.42
1:X:707:LEU:HD13	1:X:759:GLU:CB	2.50	0.42
1:X:425:LEU:HD11	1:X:612:PHE:HZ	1.85	0.42
1:X:354:LEU:CD1	1:X:378:ALA:HB1	2.49	0.42
1:X:509:ASP:N	1:X:509:ASP:OD1	2.52	0.42
1:X:133:PRO:HB2	2:X:2107:HOH:O	2.19	0.42
1:X:254:SER:C	1:X:443:GLN:NE2	2.73	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: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: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:85:PHE:O	1:X:86:ASP:O	2.38	0.41
1:X:31:ASP:HA	1:X:756:GLU:HG2	2.02	0.41
1:X:69:ASP:N	1:X:69:ASP:OD1	2.44	0.41
1:X:733:ASP:HB2	1:X:734:PRO:CD	2.49	0.41
1:X:273:GLU:O	1:X:274:THR:HB	2.20	0.41
1:X:154:HIS:CD2	1:X:155:ILE:N	2.89	0.41
1:X:459:GLU:HB3	1:X:461:PHE:CE1	2.55	0.41
1:X:738:ARG:HA	1:X:738:ARG:NE	2.30	0.41
1:X:698:TYR:OH	1:X:742:THR:O	2.35	0.41
1:X:492:GLU:O	1:X:495:LEU:HB3	2.20	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:582:GLN:HB3	1:X:583:ASP:H	1.57	0.41
1:X:55:GLU:O	1:X:56:THR:O	2.38	0.41
1:X:276:ARG:NH2	1:X:282:TYR:CG	2.88	0.41
1:X:24:LEU:HD11	1:X:26:LYS:N	2.28	0.41
1:X:318:VAL:HG22	1:X:319:SER:N	2.36	0.41
1:X:626:ASN:CG	1:X:627:PHE:N	2.75	0.41
1:X:621:ALA:O	1:X:628:ILE:HG23	2.21	0.41
1:X:461:PHE:H	1:X:464:ASN:HD21	1.69	0.41
1:X:322:GLU:HG3	1:X:322:GLU:H	1.47	0.41
1:X:384:VAL:HG21	1:X:389:LEU:HD12	2.03	0.41
1:X:354:LEU:HD11	1:X:382:PHE:HE2	1.86	0.41
1:X:501:TRP:CG	1:X:502:THR:N	2.89	0.41
1:X:429:LEU:O	1:X:433:LEU:HG	2.20	0.41
1:X:731:ASN:O	1:X:732:ILE:HD13	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:412:GLU:HG3	1:X:413:LYS:HG3	2.03	0.40
1:X:287:GLY:HA3	1:X:324:PHE:CD2	2.56	0.40
1:X:318:VAL:HG22	1:X:319:SER:H	1.86	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:597:GLU:O	1:X:601:LYS:HB2	2.21	0.40
1:X:552:SER:O	1:X:554:LYS:HG3	2.22	0.40
1:X:35:ILE:HG22	1:X:50:GLY:HA3	2.02	0.40
1:X:343:SER:HB3	1:X:607:VAL:HG22	1.99	0.40
1:X:189:THR:O	1:X:193:ILE:HD13	2.22	0.40
1:X:488:LYS:O	1:X:492:GLU:HG2	2.21	0.40
1:X:622:LYS:C	1:X:622:LYS:HD3	2.41	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:412:GLU:HG3	1:X:413:LYS:H	1.86	0.40
1:X:204:GLN:N	1:X:204:GLN:CD	2.75	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

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	756/758 (100%)	657 (87%)	82 (11%)	17 (2%)	10	34

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

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Mol	Chain	Res	Type
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%)	76	95

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
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

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Mol	Chain	Res	Type
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 chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	X	758/758 (100%)	0.01	55 (7%) 15 17	12, 41, 106, 141	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	713	PRO	8.8
1	X	693	PRO	7.6
1	X	727	LEU	6.1
1	X	697	ILE	5.0
1	X	701	PHE	4.9
1	X	696	ILE	4.9
1	X	698	TYR	4.8
1	X	740	GLY	4.7
1	X	626	ASN	4.7
1	X	741	ILE	4.6
1	X	706	TYR	4.5
1	X	205	ALA	4.2
1	X	757	ALA	4.1
1	X	754	ILE	3.8
1	X	700	ASP	3.7
1	X	499	ILE	3.7
1	X	496	LYS	3.6
1	X	625	ALA	3.4
1	X	726	VAL	3.4
1	X	692	PHE	3.4
1	X	750	GLN	3.3
1	X	206	ASN	3.2
1	X	23	ASP	3.2
1	X	24	LEU	3.2
1	X	712	VAL	3.2
1	X	536	PRO	3.0
1	X	737	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	X	694	ASN	3.0
1	X	497	GLU	3.0
1	X	725	ALA	2.9
1	X	30	SER	2.9
1	X	505	ASP	2.9
1	X	27	LEU	2.7
1	X	711	ASN	2.7
1	X	66	ASP	2.7
1	X	695	ARG	2.6
1	X	690	LYS	2.6
1	X	699	ALA	2.5
1	X	689	ARG	2.5
1	X	749	GLY	2.4
1	X	716	ALA	2.3
1	X	55	GLU	2.3
1	X	742	THR	2.3
1	X	204	GLN	2.3
1	X	739	PHE	2.2
1	X	723	THR	2.2
1	X	721	LYS	2.2
1	X	60	PHE	2.2
1	X	756	GLU	2.2
1	X	19	GLN	2.1
1	X	714	ARG	2.1
1	X	68	GLN	2.1
1	X	704	ARG	2.1
1	X	232	ARG	2.1
1	X	730	LEU	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.