



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:32 PM UTC

PDB ID : 2X79 / pdb_00002x79
Title : Inward facing conformation of Mhp1
Authors : Shimamura, T.; Weyand, S.; Beckstein, O.; Rutherford, N.G.; Hadden, J.M.;
Sharples, D.; Sansom, M.S.P.; Iwata, S.; Henderson, P.J.F.; Cameron, A.D.
Deposited on : 2010-02-25
Resolution : 3.80 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
Mogul : 2022.3.0, CSD as543be (2022)
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

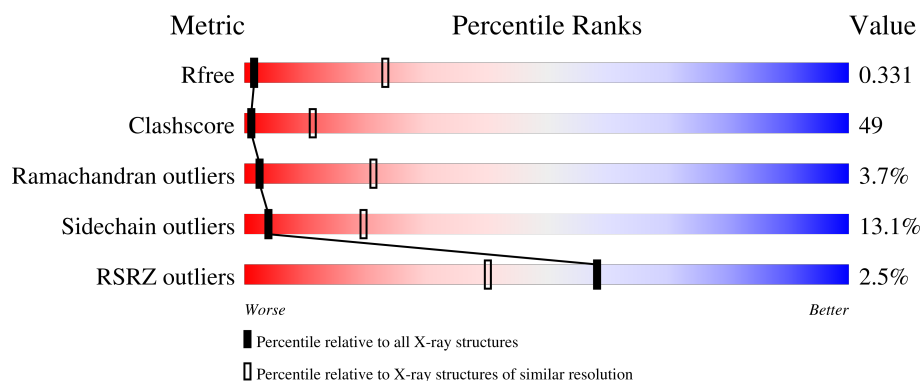
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	501	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3585 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 Hydantoin permease.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	Se	0	0	0
			3585	2380	578	605	3	19			

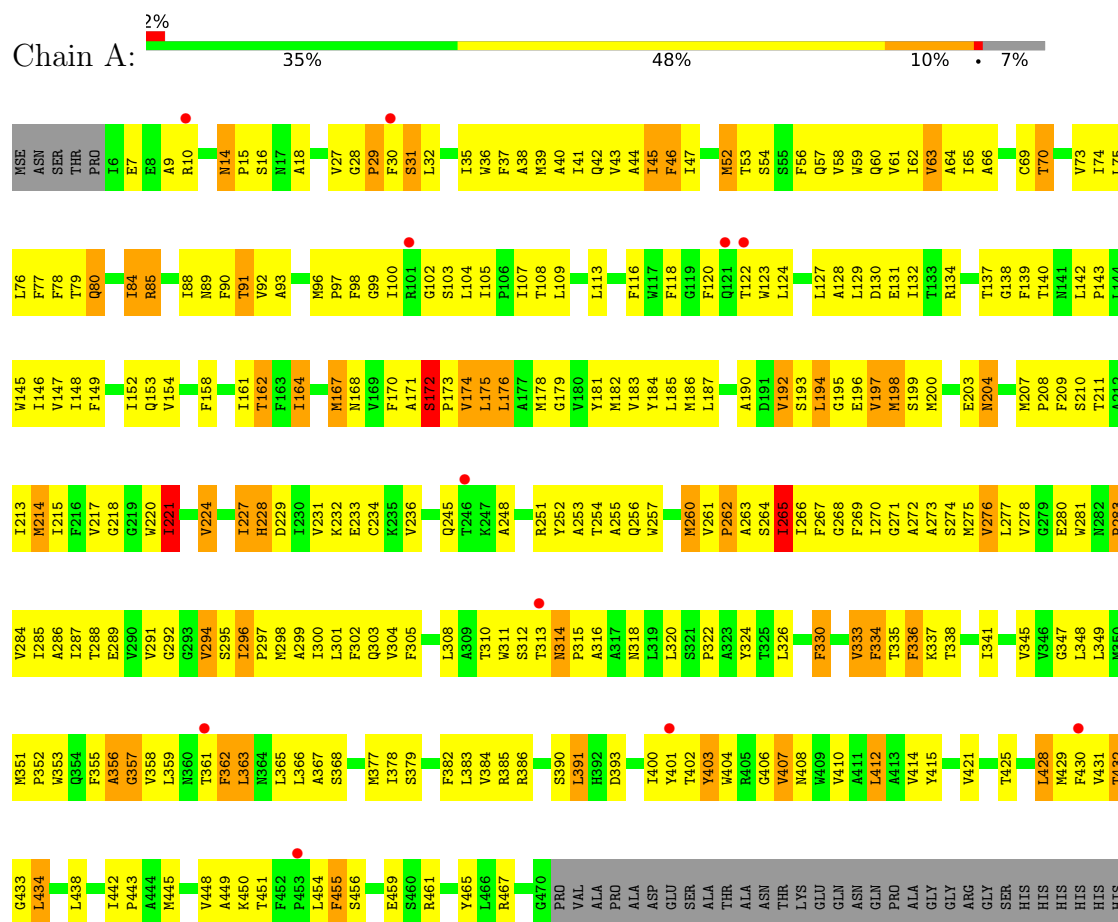
There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	489	PRO	-	expression tag	UNP D6R8X8
A	490	ALA	-	expression tag	UNP D6R8X8
A	491	GLY	-	expression tag	UNP D6R8X8
A	492	GLY	-	expression tag	UNP D6R8X8
A	493	ARG	-	expression tag	UNP D6R8X8
A	494	GLY	-	expression tag	UNP D6R8X8
A	495	SER	-	expression tag	UNP D6R8X8
A	496	HIS	-	expression tag	UNP D6R8X8
A	497	HIS	-	expression tag	UNP D6R8X8
A	498	HIS	-	expression tag	UNP D6R8X8
A	499	HIS	-	expression tag	UNP D6R8X8
A	500	HIS	-	expression tag	UNP D6R8X8
A	501	HIS	-	expression tag	UNP D6R8X8

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: Hydantoin permease



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	173.89Å 173.89Å 74.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.39 – 3.80 33.39 – 3.80	Depositor EDS
% Data completeness (in resolution range)	90.2 (33.39-3.80) 97.2 (33.39-3.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.76Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.273 , 0.313 0.297 , 0.331	Depositor DCC
R_{free} test set	1239 reflections (9.88%)	wwPDB-VP
Wilson B-factor (Å ²)	172.7	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 215.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.169 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3585	wwPDB-VP
Average B, all atoms (Å ²)	242.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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](#)

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	0.44	0/3664	0.92	15/4977 (0.3%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	PHE	CA-C-N	6.87	126.11	118.97
1	A	330	PHE	C-N-CA	6.87	126.11	118.97
1	A	425	THR	CA-C-N	6.80	126.60	119.05
1	A	425	THR	C-N-CA	6.80	126.60	119.05
1	A	403	TYR	CB-CA-C	-6.50	109.06	116.54
1	A	172	SER	CA-C-N	6.10	125.50	118.85
1	A	172	SER	C-N-CA	6.10	125.50	118.85
1	A	14	ASN	CA-C-N	6.09	127.46	119.84
1	A	14	ASN	C-N-CA	6.09	127.46	119.84
1	A	467	ARG	CA-C-N	5.77	127.05	119.84
1	A	467	ARG	C-N-CA	5.77	127.05	119.84
1	A	336	PHE	N-CA-C	-5.72	105.56	112.54
1	A	18	ALA	CA-C-N	5.64	125.40	119.76
1	A	18	ALA	C-N-CA	5.64	125.40	119.76
1	A	265	ILE	N-CA-C	-5.50	106.46	113.22

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3585	0	3681	356	0
All	All	3585	0	3681	356	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 49.

All (356) 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:182:MSE:HE1	1:A:287:ILE:HG23	1.29	1.11
1:A:66:ALA:HB2	1:A:265:ILE:HD11	1.28	1.09
1:A:40:ALA:HB1	1:A:264:SER:HB3	1.31	1.09
1:A:105:ILE:HD13	1:A:412:LEU:HD11	1.41	0.99
1:A:42:GLN:O	1:A:45:ILE:HG22	1.72	0.90
1:A:14:ASN:HB3	1:A:15:PRO:HD2	1.54	0.89
1:A:99:GLY:HA3	1:A:406:GLY:O	1.74	0.86
1:A:122:THR:HG23	1:A:149:PHE:HD2	1.40	0.86
1:A:186:MSE:HE1	1:A:274:SER:HA	1.59	0.85
1:A:142:LEU:HB3	1:A:143:PRO:HD3	1.59	0.84
1:A:182:MSE:HE2	1:A:291:VAL:CG1	2.08	0.83
1:A:73:VAL:HG21	1:A:257:TRP:HB2	1.62	0.81
1:A:84:ILE:HG12	1:A:231:VAL:HG13	1.62	0.80
1:A:84:ILE:HG12	1:A:231:VAL:CG1	2.12	0.79
1:A:273:ALA:O	1:A:277:LEU:HB3	1.85	0.77
1:A:287:ILE:O	1:A:291:VAL:HG22	1.85	0.77
1:A:186:MSE:HE2	1:A:277:LEU:HD23	1.67	0.76
1:A:274:SER:O	1:A:278:VAL:HB	1.85	0.75
1:A:176:LEU:HD12	1:A:176:LEU:O	1.87	0.75
1:A:42:GLN:HE21	1:A:44:ALA:HB3	1.51	0.74
1:A:122:THR:HG23	1:A:149:PHE:CD2	2.21	0.74
1:A:296:ILE:N	1:A:297:PRO:HD2	2.03	0.74
1:A:182:MSE:HE2	1:A:291:VAL:HG13	1.70	0.74
1:A:62:ILE:HG23	1:A:265:ILE:HG23	1.69	0.74
1:A:187:LEU:HD21	1:A:197:VAL:HG21	1.70	0.73
1:A:379:SER:HB2	1:A:438:LEU:HG	1.69	0.73
1:A:69:CYS:HB3	1:A:260:MSE:SE	2.39	0.72
1:A:232:LYS:O	1:A:233:GLU:HG3	1.89	0.72
1:A:36:TRP:CE3	1:A:260:MSE:HB3	2.25	0.72
1:A:99:GLY:O	1:A:103:SER:HB3	1.88	0.71
1:A:129:LEU:HD13	1:A:145:TRP:CE3	2.26	0.71
1:A:333:VAL:HB	1:A:334:PHE:CD1	2.26	0.71
1:A:454:LEU:HB2	1:A:455:PHE:CE1	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ALA:HB1	1:A:264:SER:CB	2.17	0.71
1:A:192:VAL:HG12	1:A:196:GLU:HB2	1.71	0.71
1:A:65:ILE:CG2	1:A:265:ILE:HG12	2.20	0.70
1:A:65:ILE:HG21	1:A:265:ILE:HA	1.71	0.70
1:A:32:LEU:HD23	1:A:252:TYR:HD2	1.57	0.70
1:A:224:VAL:O	1:A:227:ILE:HG13	1.92	0.70
1:A:280:GLU:HB2	1:A:286:ALA:HB2	1.74	0.70
1:A:40:ALA:HA	1:A:220:TRP:HH2	1.56	0.69
1:A:61:VAL:O	1:A:65:ILE:HG13	1.93	0.69
1:A:69:CYS:CB	1:A:261:VAL:HG22	2.22	0.69
1:A:186:MSE:CE	1:A:274:SER:HA	2.23	0.69
1:A:120:PHE:HE1	1:A:356:ALA:HB3	1.59	0.68
1:A:182:MSE:HE2	1:A:291:VAL:HG11	1.75	0.68
1:A:148:ILE:O	1:A:152:ILE:HG13	1.94	0.68
1:A:434:LEU:C	1:A:434:LEU:HD23	2.20	0.67
1:A:128:ALA:O	1:A:132:ILE:HG23	1.94	0.67
1:A:383:LEU:HD12	1:A:442:ILE:HD11	1.77	0.67
1:A:295:SER:OG	1:A:298:MSE:HB2	1.94	0.67
1:A:298:MSE:HB3	1:A:302:PHE:CE1	2.30	0.67
1:A:356:ALA:O	1:A:357:GLY:C	2.38	0.66
1:A:96:MSE:HB3	1:A:97:PRO:CD	2.25	0.66
1:A:85:ARG:HD3	1:A:85:ARG:C	2.20	0.66
1:A:14:ASN:CB	1:A:15:PRO:HD2	2.23	0.65
1:A:85:ARG:HD3	1:A:85:ARG:O	1.96	0.65
1:A:261:VAL:N	1:A:262:PRO:HD2	2.11	0.65
1:A:89:ASN:HB2	1:A:92:VAL:HG23	1.78	0.65
1:A:65:ILE:CD1	1:A:268:GLY:HA3	2.27	0.65
1:A:42:GLN:HE21	1:A:44:ALA:CB	2.09	0.65
1:A:65:ILE:HG22	1:A:265:ILE:HG12	1.78	0.64
1:A:152:ILE:CG2	1:A:311:TRP:HE1	2.10	0.64
1:A:137:THR:HB	1:A:139:PHE:CD2	2.32	0.64
1:A:236:VAL:CG2	1:A:245:GLN:HE22	2.10	0.64
1:A:59:TRP:CH2	1:A:60:GLN:HG3	2.33	0.64
1:A:176:LEU:HD11	1:A:266:ILE:HG21	1.80	0.64
1:A:221:ILE:HD11	1:A:430:PHE:CE1	2.33	0.63
1:A:152:ILE:HG22	1:A:311:TRP:HE1	1.62	0.63
1:A:363:LEU:HG	1:A:363:LEU:O	1.98	0.63
1:A:335:THR:HG22	1:A:336:PHE:N	2.14	0.63
1:A:62:ILE:HD11	1:A:269:PHE:HB2	1.79	0.63
1:A:208:PRO:HG2	1:A:211:THR:HB	1.79	0.63
1:A:40:ALA:CB	1:A:264:SER:HB3	2.21	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TRP:HB3	1:A:198:MSE:HG3	1.79	0.63
1:A:43:VAL:HG13	1:A:283:PRO:HG2	1.80	0.62
1:A:448:VAL:C	1:A:450:LYS:H	2.06	0.62
1:A:210:SER:O	1:A:214:MSE:HG2	1.99	0.62
1:A:186:MSE:HE1	1:A:274:SER:CA	2.28	0.62
1:A:355:PHE:CE2	1:A:363:LEU:HB2	2.35	0.62
1:A:385:ARG:CZ	1:A:401:TYR:HE2	2.13	0.61
1:A:221:ILE:HD11	1:A:430:PHE:HE1	1.64	0.61
1:A:214:MSE:HA	1:A:214:MSE:HE2	1.83	0.61
1:A:335:THR:HG22	1:A:336:PHE:H	1.66	0.61
1:A:96:MSE:HB3	1:A:97:PRO:HD3	1.81	0.61
1:A:442:ILE:HB	1:A:443:PRO:HD3	1.82	0.61
1:A:174:VAL:HG12	1:A:175:LEU:HD23	1.82	0.60
1:A:291:VAL:HG21	1:A:302:PHE:CD1	2.36	0.60
1:A:65:ILE:HD11	1:A:268:GLY:HA3	1.83	0.60
1:A:56:PHE:CE2	1:A:207:MSE:HE3	2.36	0.60
1:A:69:CYS:HB3	1:A:261:VAL:HG22	1.83	0.60
1:A:153:GLN:OE1	1:A:315:PRO:HG3	2.02	0.60
1:A:120:PHE:HE1	1:A:356:ALA:CB	2.14	0.59
1:A:210:SER:HB2	1:A:428:LEU:HD23	1.84	0.59
1:A:59:TRP:CZ2	1:A:60:GLN:HG3	2.36	0.59
1:A:218:GLY:HA3	1:A:368:SER:HB3	1.84	0.58
1:A:116:PHE:CE1	1:A:363:LEU:HD21	2.38	0.58
1:A:257:TRP:O	1:A:257:TRP:CE3	2.56	0.58
1:A:134:ARG:HD2	1:A:134:ARG:C	2.28	0.58
1:A:109:LEU:HD23	1:A:109:LEU:O	2.03	0.58
1:A:445:MSE:HE2	1:A:445:MSE:HA	1.85	0.58
1:A:73:VAL:HG21	1:A:257:TRP:CB	2.33	0.58
1:A:366:LEU:C	1:A:368:SER:H	2.10	0.58
1:A:378:ILE:HG22	1:A:438:LEU:HD11	1.86	0.58
1:A:29:PRO:O	1:A:255:ALA:HB1	2.03	0.58
1:A:211:THR:HG23	1:A:365:LEU:HD11	1.86	0.58
1:A:40:ALA:HA	1:A:220:TRP:CH2	2.37	0.58
1:A:186:MSE:CB	1:A:277:LEU:HD23	2.34	0.58
1:A:137:THR:HB	1:A:139:PHE:HD2	1.68	0.57
1:A:69:CYS:HB2	1:A:261:VAL:HG22	1.85	0.57
1:A:260:MSE:HG3	1:A:261:VAL:N	2.19	0.57
1:A:118:PHE:HB2	1:A:318:ASN:HB3	1.86	0.57
1:A:127:LEU:O	1:A:131:GLU:HB2	2.05	0.57
1:A:456:SER:O	1:A:459:GLU:HG2	2.04	0.57
1:A:273:ALA:O	1:A:277:LEU:CB	2.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:VAL:HG11	1:A:341:ILE:HG12	1.86	0.56
1:A:351:MSE:N	1:A:352:PRO:HD3	2.20	0.56
1:A:183:VAL:HG21	1:A:270:ILE:HG22	1.87	0.56
1:A:291:VAL:HG23	1:A:299:ALA:HA	1.86	0.56
1:A:448:VAL:C	1:A:450:LYS:N	2.60	0.56
1:A:30:PHE:C	1:A:30:PHE:CD2	2.84	0.56
1:A:76:LEU:HD22	1:A:256:GLN:OE1	2.06	0.56
1:A:182:MSE:O	1:A:186:MSE:HG3	2.06	0.56
1:A:341:ILE:O	1:A:345:VAL:HG23	2.05	0.56
1:A:84:ILE:HG23	1:A:234:CYS:HB2	1.88	0.56
1:A:410:VAL:HG21	1:A:448:VAL:CG2	2.36	0.56
1:A:64:ALA:HB2	1:A:209:PHE:CZ	2.40	0.56
1:A:186:MSE:HB2	1:A:277:LEU:HD23	1.88	0.55
1:A:181:TYR:O	1:A:181:TYR:CD1	2.60	0.55
1:A:276:VAL:O	1:A:276:VAL:HG13	2.07	0.55
1:A:32:LEU:HD11	1:A:256:GLN:HE21	1.71	0.55
1:A:105:ILE:CD1	1:A:412:LEU:HD11	2.27	0.55
1:A:236:VAL:HG23	1:A:245:GLN:HE22	1.71	0.55
1:A:32:LEU:HD21	1:A:256:GLN:HE21	1.71	0.55
1:A:314:ASN:HB3	1:A:315:PRO:HD3	1.88	0.55
1:A:43:VAL:HG21	1:A:124:LEU:HD13	1.89	0.55
1:A:192:VAL:CG1	1:A:196:GLU:HB2	2.36	0.55
1:A:88:ILE:HD12	1:A:93:ALA:HB2	1.89	0.54
1:A:296:ILE:N	1:A:297:PRO:CD	2.70	0.54
1:A:335:THR:H	1:A:338:THR:HB	1.72	0.54
1:A:300:ILE:O	1:A:304:VAL:HG23	2.06	0.54
1:A:130:ASP:OD2	1:A:140:THR:HG23	2.07	0.54
1:A:120:PHE:CE1	1:A:356:ALA:CB	2.91	0.54
1:A:181:TYR:CD1	1:A:181:TYR:C	2.84	0.54
1:A:298:MSE:HB3	1:A:302:PHE:HE1	1.71	0.54
1:A:75:LEU:O	1:A:79:THR:HG23	2.08	0.54
1:A:27:VAL:CG1	1:A:32:LEU:HB2	2.37	0.54
1:A:65:ILE:HG21	1:A:265:ILE:HG12	1.88	0.54
1:A:80:GLN:HA	1:A:227:ILE:HD13	1.89	0.54
1:A:275:MSE:HE2	1:A:281:TRP:N	2.23	0.54
1:A:105:ILE:HD13	1:A:412:LEU:CD1	2.29	0.53
1:A:124:LEU:HD23	1:A:127:LEU:HD12	1.89	0.53
1:A:38:ALA:HB1	1:A:172:SER:OG	2.09	0.53
1:A:77:PHE:O	1:A:80:GLN:HG2	2.08	0.53
1:A:248:ALA:HA	1:A:251:ARG:NH1	2.24	0.53
1:A:461:ARG:HB3	1:A:461:ARG:CZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HD11	1:A:434:LEU:CD1	2.39	0.53
1:A:213:ILE:O	1:A:217:VAL:HG23	2.09	0.53
1:A:43:VAL:HG11	1:A:124:LEU:HD11	1.90	0.53
1:A:179:GLY:O	1:A:270:ILE:HD12	2.09	0.52
1:A:378:ILE:CG2	1:A:438:LEU:HD11	2.40	0.52
1:A:32:LEU:HD23	1:A:252:TYR:CD2	2.41	0.52
1:A:41:ILE:HG23	1:A:267:PHE:CE1	2.45	0.52
1:A:52:MSE:HE2	1:A:61:VAL:HG13	1.91	0.52
1:A:122:THR:HG23	1:A:149:PHE:HB3	1.91	0.52
1:A:310:THR:O	1:A:314:ASN:HB2	2.09	0.52
1:A:14:ASN:HB3	1:A:15:PRO:CD	2.32	0.52
1:A:197:VAL:HA	1:A:200:MSE:HG3	1.92	0.52
1:A:334:PHE:CD1	1:A:334:PHE:N	2.77	0.52
1:A:9:ALA:O	1:A:10:ARG:HB3	2.08	0.51
1:A:384:VAL:HG11	1:A:445:MSE:HB3	1.92	0.51
1:A:32:LEU:HD12	1:A:32:LEU:O	2.11	0.51
1:A:178:MSE:SE	1:A:302:PHE:HD2	2.44	0.51
1:A:301:LEU:O	1:A:305:PHE:HD1	1.93	0.51
1:A:52:MSE:C	1:A:54:SER:H	2.19	0.51
1:A:378:ILE:O	1:A:382:PHE:HB2	2.11	0.51
1:A:187:LEU:CD2	1:A:197:VAL:HG21	2.40	0.51
1:A:29:PRO:HG3	1:A:252:TYR:CE2	2.46	0.51
1:A:123:TRP:O	1:A:127:LEU:HG	2.10	0.51
1:A:352:PRO:HD2	1:A:353:TRP:CZ3	2.46	0.51
1:A:181:TYR:O	1:A:184:TYR:HB3	2.11	0.51
1:A:278:VAL:HG13	1:A:289:GLU:OE1	2.11	0.51
1:A:359:LEU:O	1:A:362:PHE:N	2.30	0.51
1:A:43:VAL:HG21	1:A:124:LEU:CD1	2.41	0.50
1:A:362:PHE:N	1:A:362:PHE:CD1	2.79	0.50
1:A:118:PHE:HZ	1:A:153:GLN:HG3	1.76	0.50
1:A:333:VAL:HB	1:A:334:PHE:CE1	2.46	0.50
1:A:421:VAL:HG12	1:A:421:VAL:O	2.11	0.50
1:A:52:MSE:CE	1:A:61:VAL:HG22	2.41	0.50
1:A:73:VAL:HA	1:A:76:LEU:HD12	1.92	0.50
1:A:262:PRO:HG2	1:A:263:ALA:H	1.76	0.50
1:A:390:SER:OG	1:A:393:ASP:HB2	2.12	0.49
1:A:172:SER:N	1:A:173:PRO:CD	2.75	0.49
1:A:52:MSE:HE3	1:A:61:VAL:HG22	1.94	0.49
1:A:73:VAL:HA	1:A:76:LEU:HB2	1.95	0.49
1:A:345:VAL:O	1:A:349:LEU:HG	2.12	0.49
1:A:131:GLU:HG2	1:A:288:THR:OG1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ILE:HD13	1:A:455:PHE:C	2.37	0.49
1:A:88:ILE:CD1	1:A:93:ALA:HB2	2.43	0.49
1:A:182:MSE:O	1:A:186:MSE:N	2.37	0.49
1:A:62:ILE:HA	1:A:65:ILE:HD12	1.94	0.48
1:A:100:ILE:O	1:A:100:ILE:HG22	2.12	0.48
1:A:347:GLY:O	1:A:348:LEU:C	2.56	0.48
1:A:178:MSE:HG3	1:A:302:PHE:CD2	2.48	0.48
1:A:292:GLY:CA	1:A:299:ALA:HB2	2.43	0.48
1:A:37:PHE:C	1:A:39:MSE:H	2.21	0.48
1:A:214:MSE:O	1:A:217:VAL:HB	2.13	0.48
1:A:66:ALA:CB	1:A:265:ILE:HD11	2.20	0.48
1:A:132:ILE:HG22	1:A:303:GLN:HB2	1.96	0.48
1:A:438:LEU:HD23	1:A:438:LEU:O	2.13	0.48
1:A:362:PHE:N	1:A:362:PHE:HD1	2.11	0.48
1:A:182:MSE:HA	1:A:185:LEU:HB2	1.95	0.47
1:A:76:LEU:HG	1:A:224:VAL:HG22	1.97	0.47
1:A:404:TRP:C	1:A:406:GLY:H	2.22	0.47
1:A:46:PHE:HD2	1:A:271:GLY:CA	2.28	0.47
1:A:69:CYS:SG	1:A:260:MSE:HE2	2.54	0.47
1:A:65:ILE:HD13	1:A:268:GLY:HA3	1.95	0.47
1:A:269:PHE:O	1:A:271:GLY:N	2.47	0.47
1:A:45:ILE:HD12	1:A:264:SER:HB2	1.96	0.47
1:A:197:VAL:C	1:A:199:SER:H	2.23	0.47
1:A:41:ILE:HG23	1:A:267:PHE:CZ	2.50	0.47
1:A:90:PHE:CD2	1:A:90:PHE:O	2.68	0.47
1:A:359:LEU:C	1:A:361:THR:N	2.72	0.47
1:A:455:PHE:CD1	1:A:455:PHE:N	2.83	0.47
1:A:84:ILE:HG12	1:A:231:VAL:HG11	1.94	0.46
1:A:186:MSE:HB3	1:A:277:LEU:HD23	1.97	0.46
1:A:281:TRP:O	1:A:283:PRO:HD3	2.14	0.46
1:A:330:PHE:HB3	1:A:333:VAL:HG21	1.97	0.46
1:A:46:PHE:CD2	1:A:271:GLY:HA2	2.51	0.46
1:A:167:MSE:O	1:A:171:ALA:HB2	2.15	0.46
1:A:284:VAL:HA	1:A:287:ILE:HD12	1.98	0.46
1:A:459:GLU:C	1:A:461:ARG:H	2.23	0.46
1:A:134:ARG:O	1:A:138:GLY:HA2	2.16	0.46
1:A:41:ILE:HD13	1:A:172:SER:O	2.16	0.46
1:A:116:PHE:HE1	1:A:363:LEU:HD21	1.78	0.46
1:A:291:VAL:CG2	1:A:299:ALA:HA	2.46	0.46
1:A:134:ARG:C	1:A:134:ARG:CD	2.88	0.46
1:A:161:ILE:HG22	1:A:162:THR:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:MSE:HG3	1:A:302:PHE:CE2	2.50	0.46
1:A:228:HIS:CE1	1:A:377:MSE:HE1	2.51	0.46
1:A:391:LEU:HB3	1:A:465:TYR:CD1	2.51	0.46
1:A:29:PRO:HB3	1:A:255:ALA:HB2	1.97	0.45
1:A:209:PHE:O	1:A:213:ILE:HG13	2.16	0.45
1:A:385:ARG:O	1:A:386:ARG:C	2.59	0.45
1:A:78:PHE:HD1	1:A:78:PHE:H	1.64	0.45
1:A:170:PHE:C	1:A:173:PRO:HD2	2.42	0.45
1:A:269:PHE:O	1:A:272:ALA:N	2.48	0.45
1:A:333:VAL:HB	1:A:334:PHE:HD1	1.80	0.45
1:A:36:TRP:CE3	1:A:260:MSE:CB	2.98	0.45
1:A:63:VAL:HG12	1:A:209:PHE:CZ	2.51	0.45
1:A:261:VAL:O	1:A:265:ILE:HG13	2.16	0.45
1:A:322:PRO:O	1:A:326:LEU:HG	2.16	0.45
1:A:64:ALA:HB2	1:A:209:PHE:CE1	2.51	0.45
1:A:139:PHE:CD1	1:A:139:PHE:C	2.95	0.45
1:A:203:GLU:OE1	1:A:203:GLU:HA	2.15	0.45
1:A:52:MSE:C	1:A:54:SER:N	2.74	0.45
1:A:314:ASN:CB	1:A:315:PRO:HD3	2.46	0.45
1:A:66:ALA:HA	1:A:261:VAL:HG13	1.97	0.45
1:A:149:PHE:O	1:A:153:GLN:HG2	2.16	0.45
1:A:297:PRO:O	1:A:301:LEU:HG	2.16	0.45
1:A:356:ALA:O	1:A:358:VAL:N	2.50	0.45
1:A:366:LEU:C	1:A:368:SER:N	2.74	0.45
1:A:97:PRO:O	1:A:408:ASN:ND2	2.50	0.45
1:A:385:ARG:NH2	1:A:403:TYR:OH	2.50	0.45
1:A:35:ILE:O	1:A:39:MSE:HB2	2.16	0.45
1:A:43:VAL:O	1:A:47:ILE:HG13	2.17	0.45
1:A:175:LEU:HD22	1:A:178:MSE:CE	2.47	0.45
1:A:292:GLY:N	1:A:299:ALA:HB2	2.31	0.45
1:A:410:VAL:O	1:A:414:VAL:HG23	2.17	0.44
1:A:56:PHE:HE2	1:A:207:MSE:HE3	1.79	0.44
1:A:63:VAL:HG12	1:A:209:PHE:HZ	1.83	0.44
1:A:257:TRP:O	1:A:257:TRP:CD2	2.70	0.44
1:A:220:TRP:CE2	1:A:260:MSE:HE1	2.52	0.44
1:A:260:MSE:HE3	1:A:260:MSE:HB2	1.69	0.44
1:A:269:PHE:C	1:A:271:GLY:N	2.74	0.44
1:A:43:VAL:CG1	1:A:283:PRO:HG2	2.47	0.44
1:A:59:TRP:CD2	1:A:60:GLN:N	2.87	0.43
1:A:315:PRO:O	1:A:316:ALA:C	2.59	0.43
1:A:28:GLY:O	1:A:31:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HD21	1:A:256:GLN:NE2	2.32	0.43
1:A:186:MSE:HE1	1:A:273:ALA:C	2.43	0.43
1:A:412:LEU:HD23	1:A:412:LEU:N	2.32	0.43
1:A:29:PRO:HB3	1:A:255:ALA:CB	2.48	0.43
1:A:96:MSE:CB	1:A:97:PRO:CD	2.92	0.43
1:A:174:VAL:HG11	1:A:305:PHE:CD2	2.53	0.43
1:A:193:SER:O	1:A:195:GLY:N	2.52	0.43
1:A:248:ALA:O	1:A:252:TYR:HD1	2.01	0.43
1:A:35:ILE:O	1:A:35:ILE:HG22	2.18	0.43
1:A:402:THR:O	1:A:406:GLY:N	2.51	0.43
1:A:454:LEU:C	1:A:455:PHE:CG	2.95	0.43
1:A:185:LEU:HA	1:A:185:LEU:HD23	1.71	0.43
1:A:363:LEU:HA	1:A:366:LEU:HB2	2.00	0.43
1:A:429:MSE:O	1:A:433:GLY:N	2.52	0.43
1:A:193:SER:C	1:A:195:GLY:N	2.74	0.43
1:A:291:VAL:O	1:A:295:SER:N	2.51	0.43
1:A:52:MSE:HE3	1:A:52:MSE:HB3	1.98	0.43
1:A:116:PHE:CE2	1:A:352:PRO:HB3	2.54	0.43
1:A:320:LEU:O	1:A:324:TYR:HD1	2.02	0.43
1:A:361:THR:C	1:A:362:PHE:HD1	2.27	0.43
1:A:402:THR:O	1:A:406:GLY:CA	2.67	0.43
1:A:98:PHE:HB2	1:A:103:SER:HA	2.01	0.42
1:A:130:ASP:HB2	1:A:145:TRP:CD1	2.54	0.42
1:A:227:ILE:C	1:A:229:ASP:N	2.77	0.42
1:A:314:ASN:HB3	1:A:315:PRO:CD	2.49	0.42
1:A:70:THR:O	1:A:74:ILE:HG13	2.19	0.42
1:A:164:ILE:HG22	1:A:312:SER:CB	2.49	0.42
1:A:227:ILE:O	1:A:229:ASP:N	2.53	0.42
1:A:214:MSE:HA	1:A:214:MSE:CE	2.47	0.42
1:A:186:MSE:HB2	1:A:277:LEU:CD2	2.50	0.42
1:A:448:VAL:O	1:A:450:LYS:N	2.53	0.42
1:A:190:ALA:HB3	1:A:277:LEU:HD11	2.01	0.42
1:A:261:VAL:H	1:A:262:PRO:HD2	1.80	0.42
1:A:429:MSE:HE2	1:A:429:MSE:HB3	1.85	0.42
1:A:220:TRP:O	1:A:221:ILE:C	2.63	0.42
1:A:301:LEU:O	1:A:305:PHE:CD1	2.73	0.42
1:A:211:THR:O	1:A:215:ILE:HG13	2.20	0.41
1:A:275:MSE:CE	1:A:281:TRP:N	2.83	0.41
1:A:78:PHE:N	1:A:78:PHE:CD1	2.87	0.41
1:A:102:GLY:HA3	1:A:407:VAL:HG22	2.02	0.41
1:A:432:THR:O	1:A:432:THR:CG2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:HA	1:A:107:ILE:HB	2.02	0.41
1:A:287:ILE:HB	1:A:303:GLN:NE2	2.36	0.41
1:A:291:VAL:HG23	1:A:299:ALA:CA	2.49	0.41
1:A:89:ASN:HB3	1:A:91:THR:H	1.86	0.41
1:A:46:PHE:CD2	1:A:271:GLY:CA	3.04	0.41
1:A:203:GLU:O	1:A:204:ASN:HB2	2.21	0.41
1:A:179:GLY:C	1:A:270:ILE:HD12	2.46	0.41
1:A:231:VAL:C	1:A:233:GLU:H	2.28	0.41
1:A:313:THR:O	1:A:314:ASN:C	2.64	0.41
1:A:355:PHE:CD2	1:A:363:LEU:HB2	2.54	0.41
1:A:36:TRP:HZ3	1:A:260:MSE:HE3	1.85	0.41
1:A:52:MSE:O	1:A:54:SER:N	2.53	0.41
1:A:267:PHE:HA	1:A:270:ILE:HG12	2.02	0.41
1:A:292:GLY:C	1:A:294:VAL:H	2.27	0.41
1:A:46:PHE:CD1	1:A:283:PRO:HG3	2.55	0.41
1:A:186:MSE:HE1	1:A:274:SER:N	2.36	0.41
1:A:415:TYR:CD2	1:A:415:TYR:C	2.98	0.41
1:A:284:VAL:O	1:A:303:GLN:NE2	2.54	0.41
1:A:65:ILE:HG21	1:A:264:SER:O	2.21	0.40
1:A:116:PHE:CE1	1:A:363:LEU:CD2	3.03	0.40
1:A:335:THR:CG2	1:A:336:PHE:N	2.83	0.40
1:A:421:VAL:O	1:A:421:VAL:CG1	2.69	0.40
1:A:454:LEU:C	1:A:455:PHE:CD1	2.99	0.40
1:A:65:ILE:CG2	1:A:264:SER:O	2.70	0.40
1:A:73:VAL:HG13	1:A:253:ALA:O	2.21	0.40
1:A:76:LEU:O	1:A:77:PHE:C	2.65	0.40
1:A:164:ILE:H	1:A:164:ILE:HG13	1.63	0.40
1:A:391:LEU:HD12	1:A:465:TYR:HB2	2.03	0.40
1:A:36:TRP:CZ3	1:A:260:MSE:HE3	2.57	0.40
1:A:45:ILE:CD1	1:A:264:SER:HB2	2.51	0.40
1:A:46:PHE:HD2	1:A:271:GLY:HA3	1.86	0.40
1:A:58:VAL:O	1:A:58:VAL:HG12	2.22	0.40
1:A:158:PHE:CE2	1:A:337:LYS:HA	2.56	0.40
1:A:402:THR:O	1:A:406:GLY:HA2	2.21	0.40
1:A:118:PHE:CZ	1:A:153:GLN:HG3	2.55	0.40
1:A:451:THR:HG22	1:A:451:THR:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	463/501 (92%)	375 (81%)	71 (15%)	17 (4%)	2	21

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	GLY
1	A	168	ASN
1	A	228	HIS
1	A	194	LEU
1	A	449	ALA
1	A	53	THR
1	A	204	ASN
1	A	283	PRO
1	A	294	VAL
1	A	314	ASN
1	A	356	ALA
1	A	198	MSE
1	A	367	ALA
1	A	29	PRO
1	A	262	PRO
1	A	296	ILE
1	A	221	ILE

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	374/382 (98%)	325 (87%)	49 (13%)	4 20

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	16	SER
1	A	31	SER
1	A	45	ILE
1	A	46	PHE
1	A	52	MSE
1	A	57	GLN
1	A	63	VAL
1	A	70	THR
1	A	80	GLN
1	A	84	ILE
1	A	85	ARG
1	A	91	THR
1	A	108	THR
1	A	113	LEU
1	A	146	ILE
1	A	147	VAL
1	A	162	THR
1	A	164	ILE
1	A	167	MSE
1	A	172	SER
1	A	174	VAL
1	A	175	LEU
1	A	176	LEU
1	A	192	VAL
1	A	194	LEU
1	A	197	VAL
1	A	214	MSE
1	A	221	ILE
1	A	224	VAL
1	A	227	ILE
1	A	254	THR
1	A	260	MSE
1	A	265	ILE
1	A	276	VAL
1	A	285	ILE
1	A	308	LEU
1	A	333	VAL

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Mol	Chain	Res	Type
1	A	334	PHE
1	A	362	PHE
1	A	363	LEU
1	A	391	LEU
1	A	407	VAL
1	A	412	LEU
1	A	428	LEU
1	A	431	VAL
1	A	432	THR
1	A	434	LEU
1	A	455	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	204	ASN
1	A	228	HIS
1	A	245	GLN
1	A	256	GLN
1	A	360	ASN
1	A	364	ASN

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](#)

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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	446/501 (89%)	-0.05	11 (2%) 58 40	179, 234, 309, 371	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	313	THR	3.6
1	A	121	GLN	3.5
1	A	361	THR	2.5
1	A	401	TYR	2.4
1	A	122	THR	2.4
1	A	246	THR	2.4
1	A	10	ARG	2.3
1	A	453	PRO	2.2
1	A	430	PHE	2.1
1	A	101	ARG	2.1
1	A	30	PHE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.