



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:51 am GMT

PDB ID : 2X79
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

<http://wwpdb.org/validation/2016/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
Xtrriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

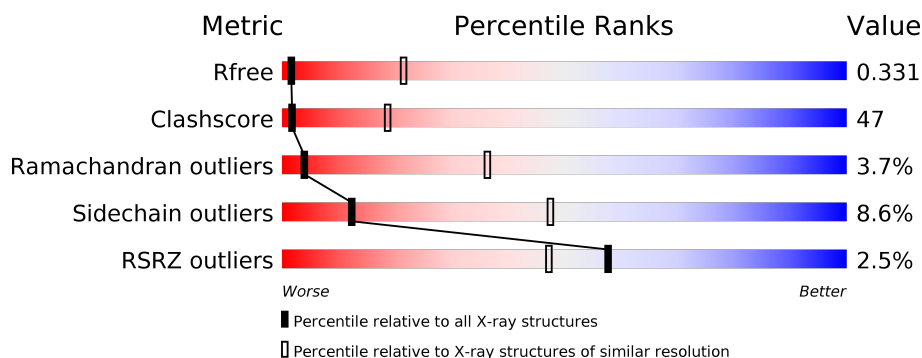
1 Overall quality at a glance

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}	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

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. 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	<div> <div>2%</div> <div> <div></div> <div>37%</div> <div>49%</div> <div>7%</div> <div>7%</div> </div> </div>

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.

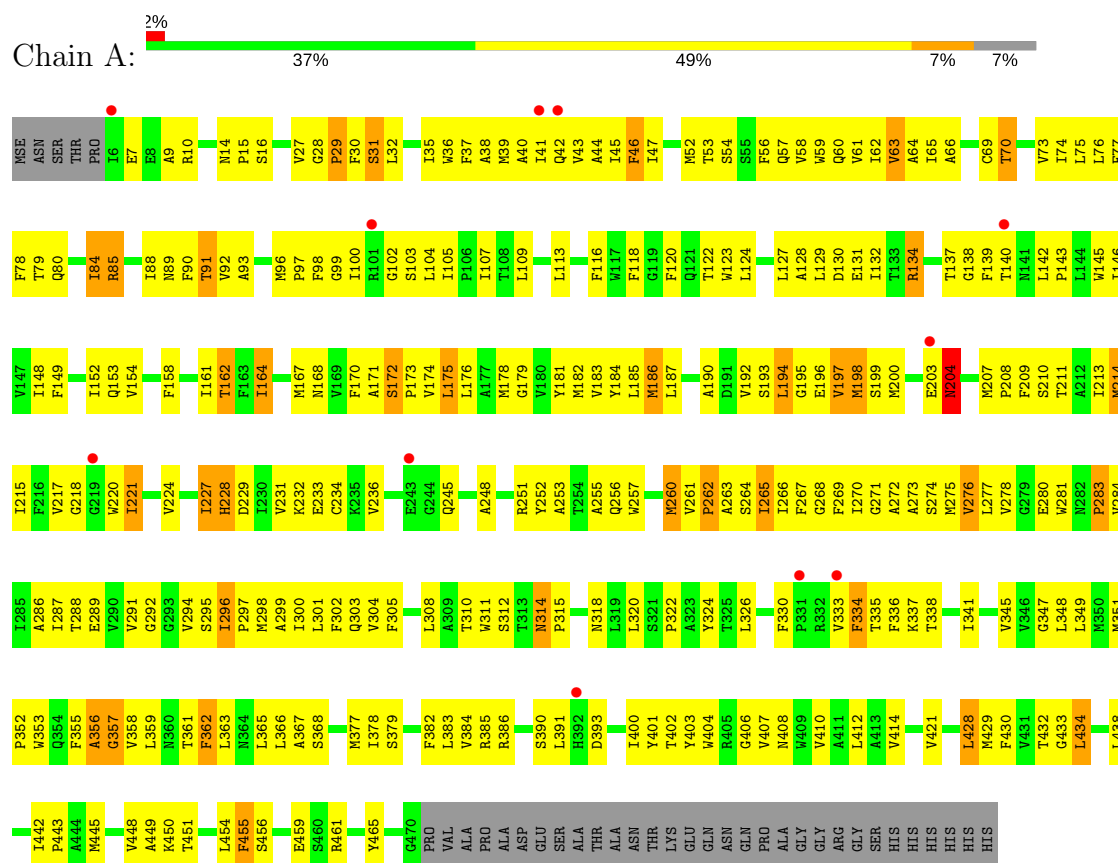
- Molecule 1 is a protein called HYDANTOIN TRANSPORT PROTEIN.

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

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: HYDANTOIN TRANSPORT PROTEIN



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) 97.4 (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 0.312 , 0.331	Depositor DCC
R_{free} test set	1239 reflections (10.97%)	DCC
Wilson B-factor (Å ²)	172.7	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 153.6	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	0.90	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	0.34	0/3664	0.53	0/4977

There are no bond length outliers.

There are no bond angle outliers.

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	342	0
All	All	3585	0	3681	342	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 47.

All (342) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:176:LEU:HD12	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
1:A:192:VAL:HG12	1:A:196:GLU:HB2	1.71	0.71
1:A:40:ALA:HB1	1:A:264:SER:CB	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ILE:O	1:A:152:ILE:HG13	1.94	0.68
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:96:MSE:HB3	1:A:97:PRO:CD	2.25	0.66
1:A:14:ASN:CB	1:A:15:PRO:HD2	2.23	0.65
1:A:261:VAL:N	1:A:262:PRO:HD2	2.11	0.65
1:A:85:ARG:HD3	1:A:85:ARG:O	1.96	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:176:LEU:HD11	1:A:266:ILE:HG21	1.80	0.64
1:A:59:TRP:CH2	1:A:60:GLN:HG3	2.33	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:O	1:A:363:LEU:HG	1.98	0.63
1:A:335:THR:HG22	1:A:336:PHE:N	2.14	0.63
1:A:208:PRO:HG2	1:A:211:THR:HB	1.79	0.63
1:A:62:ILE:HD11	1:A:269:PHE:HB2	1.79	0.63
1:A:40:ALA:CB	1:A:264:SER:HB3	2.21	0.63
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: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:434:LEU:HD23	1:A:434:LEU:C	2.20	0.62
1:A:356:ALA:O	1:A:357:GLY:C	2.38	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:85:ARG:HD3	1:A:85:ARG:C	2.20	0.61
1:A:214:MSE:HE2	1:A:214:MSE:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CE3	1:A:257:TRP:O	2.56	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:378:ILE:HG22	1:A:438:LEU:HD11	1.86	0.58
1:A:73:VAL:HG21	1:A:257:TRP:CB	2.33	0.58
1:A:211:THR:HG23	1:A:365:LEU:HD11	1.86	0.58
1:A:29:PRO:O	1:A:255:ALA:HB1	2.03	0.58
1:A:448:VAL:C	1:A:450:LYS:H	2.06	0.58
1:A:186:MSE:CB	1:A:277:LEU:HD23	2.34	0.58
1:A:40:ALA:HA	1:A:220:TRP:CH2	2.37	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:127:LEU:O	1:A:131:GLU:HB2	2.05	0.57
1:A:118:PHE:HB2	1:A:318:ASN:HB3	1.86	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
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:182:MSE:O	1:A:186:MSE:HG3	2.06	0.56
1:A:76:LEU:HD22	1:A:256:GLN:OE1	2.06	0.56
1:A:341:ILE:O	1:A:345:VAL:HG23	2.05	0.56
1:A:410:VAL:HG21	1:A:448:VAL:CG2	2.36	0.56
1:A:84:ILE:HG23	1:A:234:CYS:HB2	1.88	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:CD1	1:A:181:TYR:O	2.60	0.55
1:A:276:VAL:O	1:A:276:VAL:HG13	2.07	0.55
1:A:236:VAL:HG23	1:A:245:GLN:HE22	1.71	0.55
1:A:32:LEU:HD11	1:A:256:GLN:HE21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ILE:CD1	1:A:412:LEU:HD11	2.27	0.55
1:A:314:ASN:HB3	1:A:315:PRO:HD3	1.88	0.55
1:A:32:LEU:HD21	1:A:256:GLN:HE21	1.71	0.55
1:A:448:VAL:C	1:A:450:LYS:N	2.60	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:298:MSE:HB3	1:A:302:PHE:HE1	1.71	0.54
1:A:120:PHE:CE1	1:A:356:ALA:CB	2.91	0.54
1:A:75:LEU:O	1:A:79:THR:HG23	2.08	0.54
1:A:134:ARG:HD2	1:A:134:ARG:C	2.28	0.54
1:A:65:ILE:HG21	1:A:265:ILE:HG12	1.88	0.54
1:A:275:MSE:HE2	1:A:281:TRP:N	2.23	0.54
1:A:27:VAL:CG1	1:A:32:LEU:HB2	2.37	0.54
1:A:80:GLN:HA	1:A:227:ILE:HD13	1.89	0.54
1:A:366:LEU:C	1:A:368:SER:H	2.10	0.53
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:248:ALA:HA	1:A:251:ARG:NH1	2.24	0.53
1:A:461:ARG:CZ	1:A:461:ARG:HB3	2.39	0.53
1:A:77:PHE:O	1:A:80:GLN:HG2	2.08	0.53
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:122:THR:HG23	1:A:149:PHE:HB3	1.91	0.52
1:A:41:ILE:HG23	1:A:267:PHE:CE1	2.45	0.52
1:A:32:LEU:HD23	1:A:252:TYR:CD2	2.41	0.52
1:A:52:MSE:HE2	1:A:61:VAL:HG13	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:N	1:A:334:PHE:CD1	2.77	0.52
1:A:30:PHE:CD2	1:A:30:PHE:C	2.84	0.51
1:A:9:ALA:O	1:A:10:ARG:HB3	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:123:TRP:O	1:A:127:LEU:HG	2.10	0.51
1:A:29:PRO:HG3	1:A:252:TYR:CE2	2.46	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:362:PHE:N	1:A:362:PHE:CD1	2.79	0.50
1:A:43:VAL:HG21	1:A:124:LEU:CD1	2.41	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:345:VAL:O	1:A:349:LEU:HG	2.12	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:181:TYR:CD1	1:A:181:TYR:C	2.84	0.49
1:A:131:GLU:HG2	1:A:288:THR:OG1	2.13	0.49
1:A:182:MSE:O	1:A:186:MSE:N	2.37	0.49
1:A:88:ILE:CD1	1:A:93:ALA:HB2	2.43	0.49
1:A:100:ILE:HG22	1:A:100:ILE:O	2.12	0.48
1:A:62:ILE:HA	1:A:65:ILE:HD12	1.94	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: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:46:PHE:HD2	1:A:271:GLY:CA	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:CYS:SG	1:A:260:MSE:HE2	2.54	0.47
1:A:269:PHE:O	1:A:271:GLY:N	2.47	0.47
1:A:65:ILE:HD13	1:A:268:GLY:HA3	1.95	0.47
1:A:45:ILE:HD12	1:A:264:SER:HB2	1.96	0.47
1:A:41:ILE:HG23	1:A:267:PHE:CZ	2.50	0.47
1:A:455:PHE:CD1	1:A:455:PHE:N	2.83	0.47
1:A:90:PHE:CD2	1:A:90:PHE:O	2.68	0.47
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:84:ILE:HG12	1:A:231:VAL:HG11	1.94	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:46:PHE:CD2	1:A:271:GLY:HA2	2.51	0.46
1:A:52:MSE:C	1:A:54:SER:H	2.19	0.46
1:A:134:ARG:O	1:A:138:GLY:HA2	2.16	0.46
1:A:161:ILE:HG22	1:A:162:THR:N	2.29	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: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:209:PHE:O	1:A:213:ILE:HG13	2.16	0.45
1:A:29:PRO:HB3	1:A:255:ALA:HB2	1.97	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:78:PHE:HD1	1:A:78:PHE:H	1.64	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:36:TRP:CE3	1:A:260:MSE:CB	2.98	0.45
1:A:203:GLU:OE1	1:A:203:GLU:HA	2.15	0.45
1:A:64:ALA:HB2	1:A:209:PHE:CE1	2.51	0.45
1:A:314:ASN:CB	1:A:315:PRO:HD3	2.46	0.45
1:A:149:PHE:O	1:A:153:GLN:HG2	2.16	0.45
1:A:66:ALA:HA	1:A:261:VAL:HG13	1.97	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:385:ARG:NH2	1:A:403:TYR:OH	2.50	0.45
1:A:97:PRO:O	1:A:408:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:O	1:A:39:MSE:HB2	2.16	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:43:VAL:O	1:A:47:ILE:HG13	2.17	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:400:ILE:HD13	1:A:455:PHE:C	2.37	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:HB2	1:A:260:MSE:HE3	1.69	0.44
1:A:347:GLY:O	1:A:348:LEU:C	2.56	0.44
1:A:43:VAL:CG1	1:A:283:PRO:HG2	2.47	0.44
1:A:37:PHE:C	1:A:39:MSE:H	2.21	0.44
1:A:59:TRP:CD2	1:A:60:GLN:N	2.87	0.43
1:A:28:GLY:O	1:A:31:SER:N	2.51	0.43
1:A:32:LEU:HD21	1:A:256:GLN:NE2	2.32	0.43
1:A:412:LEU:N	1:A:412:LEU:HD23	2.32	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: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:35:ILE:HG22	1:A:35:ILE:O	2.18	0.43
1:A:402:THR:O	1:A:406:GLY:N	2.51	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:291:VAL:O	1:A:295:SER:N	2.51	0.43
1:A:116:PHE:CE2	1:A:352:PRO:HB3	2.54	0.43
1:A:52:MSE:HE3	1:A:52:MSE:HB3	1.98	0.43
1:A:320:LEU:O	1:A:324:TYR:HD1	2.02	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:314:ASN:HB3	1:A:315:PRO:CD	2.49	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:70:THR:O	1:A:74:ILE:HG13	2.19	0.42
1:A:214:MSE:CE	1:A:214:MSE:HA	2.47	0.42
1:A:186:MSE:HB2	1:A:277:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:VAL:C	1:A:199:SER:H	2.23	0.42
1:A:448:VAL:O	1:A:450:LYS:N	2.53	0.42
1:A:359:LEU:C	1:A:361:THR:N	2.72	0.42
1:A:261:VAL:H	1:A:262:PRO:HD2	1.80	0.42
1:A:190:ALA:HB3	1:A:277:LEU:HD11	2.01	0.42
1:A:429:MSE:HB3	1:A:429:MSE:HE2	1.85	0.42
1:A:301:LEU:O	1:A:305:PHE:CD1	2.73	0.42
1:A:459:GLU:C	1:A:461:ARG:H	2.23	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:102:GLY:HA3	1:A:407:VAL:HG22	2.02	0.41
1:A:432:THR:CG2	1:A:432:THR:O	2.68	0.41
1:A:78:PHE:N	1:A:78:PHE:CD1	2.87	0.41
1:A:52:MSE:C	1:A:54:SER:N	2.74	0.41
1:A:104:LEU:HA	1:A:107:ILE:HB	2.02	0.41
1:A:134:ARG:C	1:A:134:ARG:CD	2.88	0.41
1:A:291:VAL:HG23	1:A:299:ALA:CA	2.49	0.41
1:A:287:ILE:HB	1:A:303:GLN:NE2	2.36	0.41
1:A:404:TRP:C	1:A:406:GLY:H	2.22	0.41
1:A:89:ASN:HB3	1:A:91:THR:H	1.86	0.41
1:A:203:GLU:O	1:A:204:ASN:HB2	2.21	0.41
1:A:46:PHE:CD2	1:A:271:GLY:CA	3.04	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:267:PHE:HA	1:A:270:ILE:HG12	2.02	0.41
1:A:52:MSE:O	1:A:54:SER:N	2.53	0.41
1:A:186:MSE:HE1	1:A:274:SER:N	2.36	0.41
1:A:46:PHE:CD1	1:A:283:PRO:HG3	2.55	0.41
1:A:385:ARG:O	1:A:386:ARG:C	2.59	0.41
1:A:170:PHE:C	1:A:173:PRO:HD2	2.42	0.41
1:A:284:VAL:O	1:A:303:GLN:NE2	2.54	0.41
1:A:366:LEU:C	1:A:368:SER:N	2.74	0.41
1:A:116:PHE:CE1	1:A:363:LEU:CD2	3.03	0.40
1:A:139:PHE:CD1	1:A:139:PHE:C	2.95	0.40
1:A:335:THR:CG2	1:A:336:PHE:N	2.83	0.40
1:A:65:ILE:HG21	1:A:264:SER:O	2.21	0.40
1:A:421:VAL:O	1:A:421:VAL:CG1	2.69	0.40
1:A:164:ILE:HG13	1:A:164:ILE:H	1.63	0.40
1:A:391:LEU:HD12	1:A:465:TYR:HB2	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PHE:CE2	1:A:337:LYS:HA	2.56	0.40
1:A:46:PHE:HD2	1:A:271:GLY:HA3	1.86	0.40
1:A:36:TRP:CZ3	1:A:260:MSE:HE3	2.57	0.40
1:A:402:THR:O	1:A:406:GLY:HA2	2.21	0.40
1:A:45:ILE:CD1	1:A:264:SER:HB2	2.51	0.40
1:A:58:VAL:O	1:A:58:VAL:HG12	2.22	0.40
1:A:118:PHE:CZ	1:A:153:GLN:HG3	2.55	0.40
1:A:193:SER:C	1:A:195:GLY:N	2.74	0.40
1:A:451:THR:O	1:A:451:THR:HG22	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%)	4	36

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	342 (91%)	32 (9%)	12	47

All (32) 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	46	PHE
1	A	57	GLN
1	A	63	VAL
1	A	70	THR
1	A	84	ILE
1	A	85	ARG
1	A	91	THR
1	A	113	LEU
1	A	134	ARG
1	A	146	ILE
1	A	162	THR
1	A	164	ILE
1	A	172	SER
1	A	175	LEU
1	A	186	MSE
1	A	194	LEU
1	A	197	VAL
1	A	204	ASN

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Mol	Chain	Res	Type
1	A	214	MSE
1	A	227	ILE
1	A	260	MSE
1	A	265	ILE
1	A	276	VAL
1	A	308	LEU
1	A	334	PHE
1	A	362	PHE
1	A	428	LEU
1	A	434	LEU
1	A	455	PHE

Some 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	303	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 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](#)

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%)	-0.22	11 (2%) 58 47	179, 234, 309, 371	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	GLU	3.3
1	A	140	THR	3.3
1	A	42	GLN	3.2
1	A	203	GLU	3.1
1	A	6	ILE	2.8
1	A	392	HIS	2.7
1	A	333	VAL	2.6
1	A	101	ARG	2.5
1	A	41	ILE	2.2
1	A	219	GLY	2.2
1	A	331	PRO	2.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.