



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:29 PM UTC

PDB ID : 4LOG / pdb\_00004log  
Title : The crystal structure of the orphan nuclear receptor PNR ligand binding domain fused with MBP  
Authors : Tan, M.E.; Zhou, X.E.; Soon, F.-F.; Li, X.; Li, J.; Yong, E.-L.; Melcher, K.; Xu, H.E.  
Deposited on : 2013-07-12  
Resolution : 2.70 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

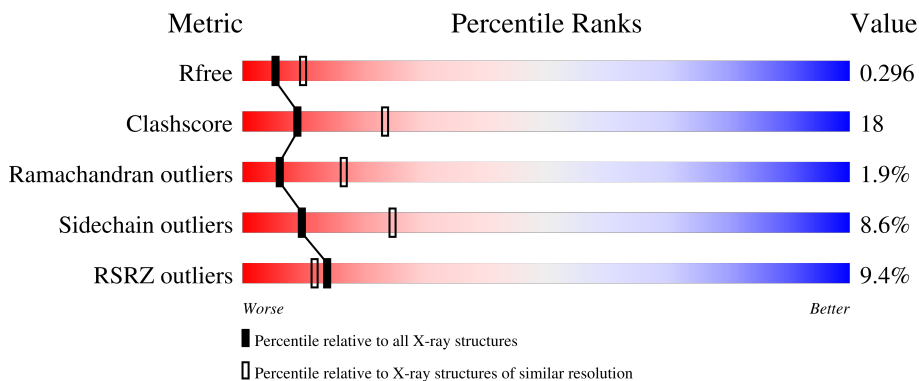
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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  $\geq 3$ , 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	574	
1	B	574	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6234 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 Maltose ABC transporter periplasmic protein and NR2E3 protein chimeric construct.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	553	Total	C	N	O	S	0	0	0
			4334	2799	712	809	14			
1	B	232	Total	C	N	O	S	0	0	0
			1838	1184	314	330	10			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP K0BGG6
A	369	ASN	-	linker	UNP K0BGG6
A	370	ALA	-	linker	UNP K0BGG6
A	371	ALA	-	linker	UNP K0BGG6
A	372	ALA	-	linker	UNP K0BGG6
A	1215	GLU	-	linker	UNP K0BGG6
A	1216	PHE	-	linker	UNP K0BGG6
A	1405	SER	CYS	engineered mutation	UNP Q8IVZ9
A	1411	HIS	-	expression tag	UNP Q8IVZ9
A	1412	HIS	-	expression tag	UNP Q8IVZ9
A	1413	HIS	-	expression tag	UNP Q8IVZ9
A	1414	HIS	-	expression tag	UNP Q8IVZ9
A	1415	HIS	-	expression tag	UNP Q8IVZ9
A	1416	HIS	-	expression tag	UNP Q8IVZ9
B	1	MET	-	initiating methionine	UNP K0BGG6
B	369	ASN	-	linker	UNP K0BGG6
B	370	ALA	-	linker	UNP K0BGG6
B	371	ALA	-	linker	UNP K0BGG6
B	372	ALA	-	linker	UNP K0BGG6
B	1215	GLU	-	linker	UNP K0BGG6
B	1216	PHE	-	linker	UNP K0BGG6
B	1405	SER	CYS	engineered mutation	UNP Q8IVZ9
B	1411	HIS	-	expression tag	UNP Q8IVZ9
B	1412	HIS	-	expression tag	UNP Q8IVZ9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1413	HIS	-	expression tag	UNP Q8IVZ9
B	1414	HIS	-	expression tag	UNP Q8IVZ9
B	1415	HIS	-	expression tag	UNP Q8IVZ9
B	1416	HIS	-	expression tag	UNP Q8IVZ9

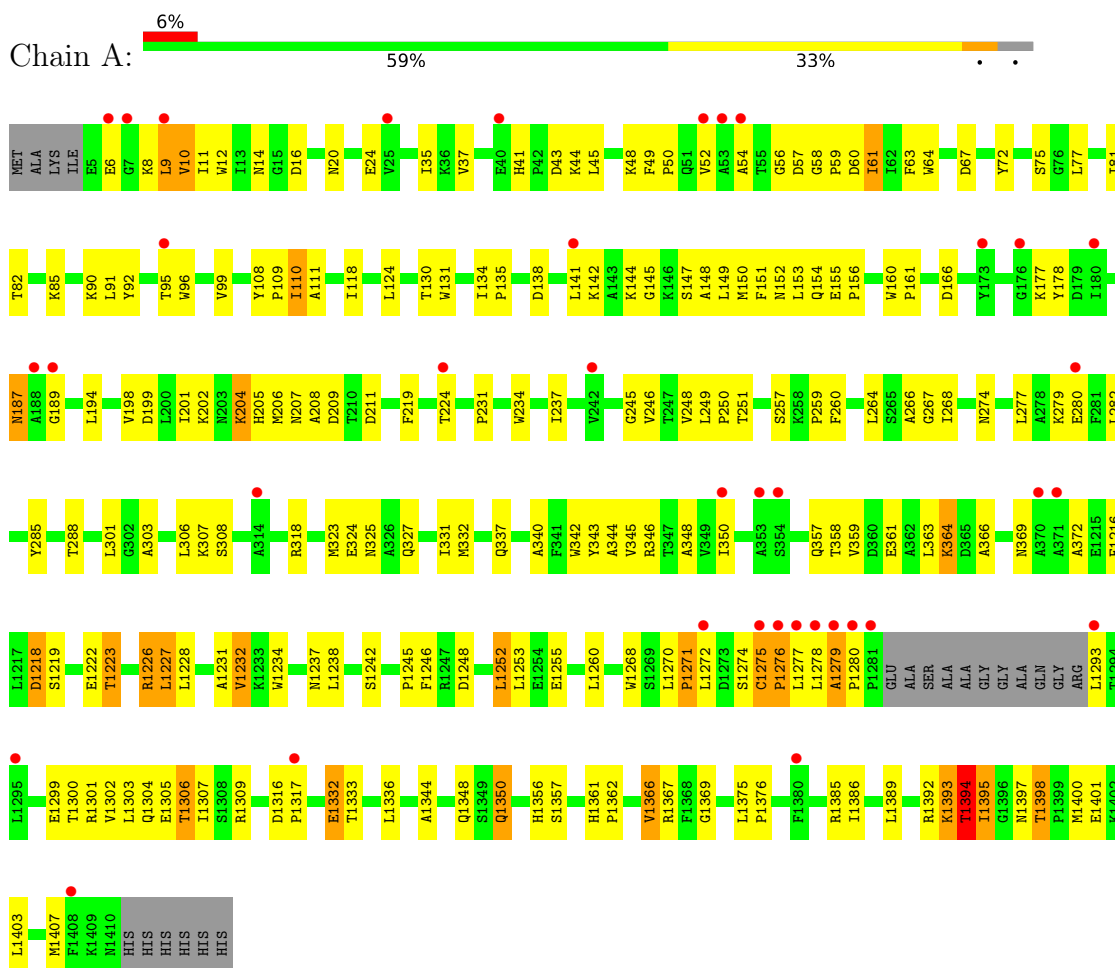
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	33	Total O 33 33	0	0
2	B	29	Total O 29 29	0	0

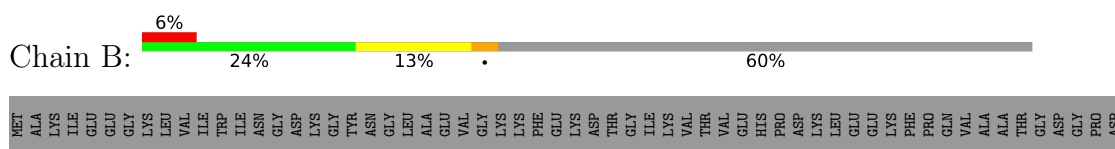
### 3 Residue-property plots

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: Maltose ABC transporter periplasmic protein and NR2E3 protein chimeric construct



- Molecule 1: Maltose ABC transporter periplasmic protein and NR2E3 protein chimeric construct





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.44Å 184.94Å 85.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-2.70) 96.5 (30.00-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.68Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.285 , 0.307 0.278 , 0.296	Depositor DCC
$R_{free}$ test set	2961 reflections (7.38%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.2	Xtrriage
Anisotropy	0.176	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 33.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.017 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6234	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.74	0/4439	0.84	0/6025
1	B	0.85	0/1879	0.95	3/2548 (0.1%)
All	All	0.78	0/6318	0.87	3/8573 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1280	PRO	N-CA-C	10.00	122.90	110.70
1	B	1279	ALA	CA-C-N	-7.82	112.33	120.38
1	B	1279	ALA	C-N-CA	-7.82	112.33	120.38

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	4334	0	4340	168	0
1	B	1838	0	1875	74	0
2	A	33	0	0	6	0
2	B	29	0	0	2	0
All	All	6234	0	6215	228	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 18.

All (228) 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:B:1302:VAL:O	1:B:1306:THR:HG22	1.50	1.12
1:A:61:ILE:HD11	1:A:266:ALA:HB1	1.46	0.96
1:A:1275:CYS:HB2	1:A:1276:PRO:HD3	1.68	0.76
1:A:152:ASN:HD21	1:A:155:GLU:HG2	1.53	0.74
1:A:9:LEU:HD21	1:A:37:VAL:HG22	1.69	0.73
1:A:194:LEU:HD22	1:A:363:LEU:HD21	1.71	0.72
1:A:1219:SER:O	1:A:1223:THR:HG22	1.91	0.71
1:A:81:ILE:HG22	1:A:268:ILE:HD12	1.72	0.71
1:A:1253:LEU:HB3	1:A:1400:MET:HE3	1.71	0.70
1:B:1318:THR:HG23	2:B:1503:HOH:O	1.91	0.70
1:B:1278:LEU:HB2	1:B:1292:ARG:HH21	1.58	0.69
1:B:1398:THR:HG22	1:B:1401:GLU:H	1.58	0.69
1:B:1400:MET:HE2	1:B:1404:LEU:HG	1.74	0.69
1:A:1216:PHE:CG	1:A:1226:ARG:HG3	2.28	0.69
1:A:1252:LEU:HD13	1:A:1336:LEU:HD21	1.74	0.69
1:A:1357:SER:OG	1:A:1367:ARG:HD3	1.93	0.69
1:A:1350:GLN:CD	1:B:1366:VAL:HG22	2.18	0.68
1:B:1398:THR:HG22	1:B:1401:GLU:HG3	1.76	0.67
1:A:303:ALA:HB1	1:A:323:MET:HE2	1.77	0.67
1:B:341:PHE:O	1:B:345:VAL:HG23	1.95	0.66
1:A:147:SER:OG	1:A:224:THR:HG23	1.96	0.65
1:A:1393:LYS:HA	2:A:1527:HOH:O	1.95	0.65
1:B:1216:PHE:HB3	1:B:1217:LEU:HD22	1.77	0.65
1:A:130:THR:HG22	1:A:251:THR:OG1	1.98	0.64
1:A:1316:ASP:HB2	1:A:1317:PRO:HD2	1.78	0.64
1:A:1366:VAL:HG22	1:B:1350:GLN:CD	2.23	0.64
1:B:1398:THR:HG23	1:B:1400:MET:H	1.65	0.62
1:A:72:TYR:HA	1:A:77:LEU:HD12	1.81	0.61
1:A:199:ASP:HA	1:A:202:LYS:HB3	1.81	0.61
1:A:357:GLN:HE21	1:A:361:GLU:HB2	1.65	0.61
1:A:1279:ALA:H	1:A:1280:PRO:HD2	1.65	0.61
1:B:1276:PRO:HA	1:B:1292:ARG:HD2	1.81	0.61
1:A:1272:LEU:HD23	1:A:1275:CYS:SG	2.40	0.61
1:A:130:THR:HG22	1:A:251:THR:HG1	1.64	0.61
1:A:9:LEU:CD2	1:A:37:VAL:HG22	2.31	0.61
1:A:1302:VAL:O	1:A:1306:THR:HG22	2.01	0.60
1:A:151:PHE:O	1:A:153:LEU:HD23	2.01	0.60
1:A:10:VAL:HG13	1:A:59:PRO:HA	1.84	0.60
1:A:198:VAL:HG21	1:A:359:VAL:HG22	1.84	0.59
1:A:61:ILE:HD12	1:A:267:GLY:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:PRO:HG3	1:A:346:ARG:HA	1.85	0.58
1:A:138:ASP:HA	1:A:148:ALA:HB2	1.84	0.57
1:B:372:ALA:HA	1:B:1291:GLY:HA2	1.85	0.57
1:A:237:ILE:HG22	1:A:237:ILE:O	2.04	0.57
1:A:257:SER:O	1:A:259:PRO:HD3	2.05	0.57
1:A:1245:PRO:O	1:A:1248:ASP:N	2.38	0.57
1:A:1398:THR:HG22	1:A:1401:GLU:H	1.70	0.57
1:A:49:PHE:HB3	1:A:50:PRO:HD3	1.85	0.57
1:A:1316:ASP:OD1	1:A:1356:HIS:HE1	1.88	0.57
1:A:1309:ARG:NE	1:B:1332:GLU:HG2	2.20	0.56
1:A:1344:ALA:O	1:A:1348:GLN:HG3	2.06	0.56
1:A:1350:GLN:NE2	2:A:1518:HOH:O	2.38	0.56
1:B:1232:VAL:HG21	1:B:1400:MET:HE1	1.88	0.56
1:A:8:LYS:HA	1:A:35:ILE:HG23	1.89	0.56
1:A:246:VAL:HB	1:A:318:ARG:HA	1.88	0.56
1:A:91:LEU:HD12	1:A:96:TRP:CZ2	2.40	0.55
1:A:1350:GLN:NE2	1:B:1369:GLY:HA3	2.21	0.55
1:B:1400:MET:CE	1:B:1404:LEU:HG	2.35	0.55
1:A:1350:GLN:NE2	1:B:1366:VAL:HG22	2.21	0.55
1:A:1392:ARG:HE	1:A:1393:LYS:HE3	1.71	0.55
1:B:1279:ALA:HB3	1:B:1280:PRO:HD3	1.88	0.55
1:A:156:PRO:HB3	1:A:345:VAL:HG12	1.89	0.55
1:A:248:VAL:HA	1:A:325:ASN:HD21	1.72	0.55
1:A:344:ALA:HB1	1:A:366:ALA:HA	1.88	0.54
1:B:1221:HIS:NE2	1:B:1276:PRO:HB2	2.22	0.54
1:A:82:THR:HG23	1:A:279:LYS:NZ	2.22	0.54
1:A:160:TRP:N	1:A:161:PRO:CD	2.70	0.54
1:A:1301:ARG:CZ	1:B:1334:ARG:HH12	2.21	0.54
1:A:1309:ARG:CD	1:B:1332:GLU:HG2	2.38	0.53
1:B:1309:ARG:O	1:B:1313:LEU:HD13	2.08	0.53
1:A:1369:GLY:HA3	1:B:1350:GLN:NE2	2.24	0.53
1:B:1402:LYS:NZ	1:B:1406:ASP:CG	2.66	0.53
1:A:90:LYS:O	1:A:306:LEU:HD12	2.08	0.52
1:A:1369:GLY:HA3	1:B:1350:GLN:HE22	1.74	0.52
1:A:11:ILE:HG12	1:A:61:ILE:HG23	1.90	0.52
1:A:154:GLN:HG2	1:A:211:ASP:HA	1.90	0.52
1:A:156:PRO:HB3	1:A:345:VAL:CG1	2.40	0.52
1:A:9:LEU:HA	1:A:60:ASP:OD2	2.10	0.51
1:A:1276:PRO:HD2	1:A:1277:LEU:HD23	1.93	0.51
1:A:1393:LYS:HB2	1:A:1393:LYS:NZ	2.26	0.51
1:A:149:LEU:HD23	1:A:206:MET:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LYS:HA	1:A:204:LYS:NZ	2.25	0.51
1:B:1299:GLU:OE1	1:B:1385:ARG:HD3	2.10	0.51
1:A:274:ASN:HB3	1:A:277:LEU:HB2	1.92	0.51
1:A:1309:ARG:HD2	1:B:1332:GLU:HG2	1.91	0.51
1:A:1216:PHE:CD2	1:A:1226:ARG:HG3	2.45	0.51
1:B:1398:THR:HG23	1:B:1400:MET:N	2.25	0.50
1:B:1217:LEU:HD23	1:B:1292:ARG:HG2	1.93	0.50
1:A:1277:LEU:HD13	1:A:1303:LEU:HD22	1.92	0.50
1:A:110:ILE:HD11	1:A:301:LEU:HD13	1.94	0.50
1:A:124:LEU:HD13	1:A:141:LEU:HD11	1.93	0.50
1:A:1275:CYS:CB	1:A:1276:PRO:HD3	2.40	0.50
1:B:335:ILE:HG13	1:B:338:MET:HB2	1.94	0.50
1:A:92:TYR:HB2	1:A:95:THR:HG23	1.94	0.49
1:A:43:ASP:C	1:A:45:LEU:H	2.20	0.49
1:A:138:ASP:HB3	1:A:205:HIS:CD2	2.47	0.49
1:B:1398:THR:CG2	1:B:1401:GLU:H	2.25	0.49
1:B:1316:ASP:HB2	1:B:1317:PRO:HD2	1.96	0.48
1:A:131:TRP:CD1	1:A:250:PRO:HB2	2.49	0.48
1:A:1234:TRP:CZ2	1:A:1238:LEU:HD11	2.48	0.48
1:B:1313:LEU:N	1:B:1313:LEU:HD12	2.28	0.48
1:A:364:LYS:HA	1:A:364:LYS:HE3	1.94	0.48
1:A:1218:ASP:HB2	1:A:1222:GLU:OE2	2.13	0.48
1:A:1232:VAL:HG11	1:A:1403:LEU:HD21	1.95	0.48
1:A:248:VAL:HA	1:A:325:ASN:ND2	2.29	0.48
1:A:118:ILE:HG22	1:A:219:PHE:CZ	2.49	0.48
1:A:331:ILE:HD12	1:A:331:ILE:H	1.78	0.47
1:B:342:TRP:CD1	1:B:342:TRP:H	2.31	0.47
1:A:1277:LEU:HD12	1:A:1300:THR:HG23	1.97	0.47
1:A:50:PRO:O	1:A:54:ALA:HB2	2.14	0.47
1:A:50:PRO:HG3	1:A:72:TYR:CE1	2.50	0.47
1:A:337:GLN:HE21	1:A:340:ALA:HB3	1.80	0.47
1:B:1259:GLU:HB2	1:B:1327:VAL:HG11	1.97	0.47
1:B:1262:LEU:O	1:B:1266:ILE:HD12	2.15	0.47
1:B:1217:LEU:HD22	1:B:1217:LEU:N	2.30	0.47
1:A:156:PRO:HD3	1:A:346:ARG:HE	1.80	0.47
1:B:1216:PHE:CB	1:B:1217:LEU:HD22	2.44	0.47
1:B:1215:GLU:O	1:B:1216:PHE:C	2.58	0.46
1:A:1268:TRP:HZ3	1:A:1275:CYS:HB3	1.80	0.46
1:A:1272:LEU:HD23	1:A:1275:CYS:HG	1.78	0.46
1:B:1226:ARG:O	1:B:1230:MET:HB2	2.15	0.46
1:A:1403:LEU:O	1:A:1407:MET:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:PHE:CE2	1:A:266:ALA:HB2	2.51	0.46
1:A:1385:ARG:NH2	1:A:1389:LEU:HD21	2.30	0.46
1:B:1218:ASP:O	1:B:1222:GLU:HG2	2.16	0.46
1:B:1353:LEU:HD23	1:B:1368:PHE:CE1	2.50	0.46
1:A:1276:PRO:HD2	1:A:1277:LEU:CD2	2.45	0.46
1:B:368:THR:O	1:B:372:ALA:HB2	2.16	0.46
1:A:166:ASP:O	1:A:189:GLY:HA3	2.16	0.45
1:A:1227:LEU:HD13	1:A:1227:LEU:HA	1.80	0.45
1:B:372:ALA:HB1	1:B:1291:GLY:C	2.41	0.45
1:A:1350:GLN:OE1	1:B:1366:VAL:HG22	2.15	0.45
1:B:338:MET:O	1:B:341:PHE:HB2	2.15	0.45
1:A:348:ALA:HB2	1:A:366:ALA:HB2	1.99	0.45
1:B:1295:LEU:HB3	1:B:1300:THR:OG1	2.17	0.45
1:B:1400:MET:HE1	1:B:1403:LEU:HD22	1.97	0.45
1:A:350:ILE:HD12	2:A:1515:HOH:O	2.17	0.45
1:A:1278:LEU:HD23	1:A:1278:LEU:H	1.81	0.45
1:B:1316:ASP:HB2	1:B:1317:PRO:CD	2.47	0.45
1:A:1270:LEU:HB2	1:A:1271:PRO:HD3	1.99	0.45
1:A:151:PHE:O	1:A:153:LEU:CD2	2.65	0.45
1:B:1402:LYS:NZ	1:B:1406:ASP:OD2	2.49	0.45
1:A:1218:ASP:OD1	1:A:1218:ASP:N	2.50	0.44
1:A:1277:LEU:HD23	1:A:1277:LEU:N	2.33	0.44
1:A:1299:GLU:OE1	1:A:1389:LEU:HD11	2.17	0.44
1:A:150:MET:HB2	1:A:224:THR:HG21	1.99	0.44
1:A:249:LEU:HD12	1:A:259:PRO:HG3	1.99	0.44
1:A:1245:PRO:O	1:A:1246:PHE:C	2.59	0.44
1:B:1381:ILE:HD11	1:B:1386:ILE:HD13	1.99	0.44
1:A:63:PHE:O	1:A:64:TRP:HB2	2.17	0.44
1:A:82:THR:HG23	1:A:82:THR:O	2.18	0.44
1:A:1301:ARG:O	1:A:1304:GLN:HG2	2.17	0.44
1:A:1332:GLU:HG2	1:B:1309:ARG:HD2	1.99	0.44
1:B:348:ALA:HB2	1:B:366:ALA:HB2	1.99	0.44
1:A:54:ALA:HA	1:A:77:LEU:HD21	1.99	0.44
1:A:145:GLY:HA2	2:A:1525:HOH:O	2.17	0.44
1:A:118:ILE:HA	1:A:245:GLY:O	2.18	0.44
1:A:1332:GLU:HG2	1:B:1309:ARG:CD	2.48	0.44
1:B:1313:LEU:N	1:B:1313:LEU:CD1	2.81	0.44
1:A:1385:ARG:O	1:A:1386:ILE:C	2.61	0.44
1:B:1269:SER:HA	1:B:1272:LEU:HD22	1.99	0.43
1:A:201:ILE:HD13	1:A:208:ALA:HB2	2.00	0.43
1:A:14:ASN:ND2	1:A:16:ASP:OD1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LYS:HG2	1:A:178:TYR:H	1.83	0.43
1:A:357:GLN:CD	1:A:358:THR:H	2.25	0.43
1:A:153:LEU:HD21	2:A:1503:HOH:O	2.18	0.43
1:A:207:ASN:C	1:A:209:ASP:H	2.26	0.43
1:A:268:ILE:N	2:A:1501:HOH:O	2.40	0.43
1:A:344:ALA:HB1	1:A:366:ALA:CA	2.48	0.43
1:B:1336:LEU:HD13	1:B:1342:VAL:HG21	2.01	0.43
1:A:110:ILE:HG13	1:A:111:ALA:N	2.32	0.43
1:A:187:ASN:HD22	1:A:187:ASN:HA	1.63	0.43
1:A:231:PRO:HA	1:A:234:TRP:CE2	2.53	0.43
1:A:337:GLN:HE21	1:A:340:ALA:CB	2.32	0.43
1:A:343:TYR:HE1	1:A:369:ASN:ND2	2.17	0.43
1:A:1304:GLN:HA	1:A:1307:ILE:HD12	2.00	0.43
1:B:1275:CYS:HB2	1:B:1276:PRO:HD2	2.01	0.43
1:B:1220:ILE:N	2:B:1506:HOH:O	2.41	0.43
1:B:1400:MET:HE2	1:B:1404:LEU:CG	2.45	0.42
1:A:44:LYS:HB2	1:A:48:LYS:HE3	2.02	0.42
1:A:110:ILE:HG23	1:A:264:LEU:O	2.18	0.42
1:A:1366:VAL:HG22	1:B:1350:GLN:NE2	2.34	0.42
1:A:161:PRO:HG3	1:A:259:PRO:HA	2.02	0.42
1:A:249:LEU:CD1	1:A:259:PRO:HG3	2.49	0.42
1:A:1302:VAL:O	1:A:1306:THR:CG2	2.68	0.42
1:B:1327:VAL:O	1:B:1330:LYS:NZ	2.34	0.42
1:A:260:PHE:HB3	1:A:332:MET:HE2	2.00	0.42
1:A:323:MET:HG3	1:A:327:GLN:OE1	2.19	0.42
1:A:343:TYR:HE1	1:A:369:ASN:HD22	1.66	0.42
1:A:1255:GLU:HG3	1:A:1333:THR:CG2	2.50	0.42
1:A:110:ILE:HD12	1:A:110:ILE:O	2.20	0.42
1:B:1260:LEU:HD11	1:B:1328:LEU:HD13	2.01	0.42
1:A:1394:THR:C	1:A:1395:ILE:HD12	2.45	0.42
1:A:1361:HIS:N	1:A:1362:PRO:HD3	2.35	0.41
1:A:369:ASN:O	1:A:372:ALA:HB3	2.19	0.41
1:A:285:TYR:O	1:A:288:THR:OG1	2.34	0.41
1:B:1331:PRO:HG3	1:B:1343:GLU:HA	2.02	0.41
1:A:14:ASN:HB2	1:A:64:TRP:HZ3	1.85	0.41
1:A:61:ILE:HD11	1:A:266:ALA:CB	2.33	0.41
1:A:12:TRP:CH2	1:A:52:VAL:HG21	2.55	0.41
1:A:307:LYS:O	1:A:308:SER:C	2.63	0.41
1:A:1228:LEU:O	1:A:1231:ALA:HB3	2.20	0.41
1:A:1367:ARG:HH11	1:A:1367:ARG:HG3	1.84	0.41
1:A:54:ALA:HA	1:A:77:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:TYR:CD2	1:A:282:LEU:HD13	2.56	0.41
1:A:134:ILE:N	1:A:135:PRO:CD	2.83	0.41
1:B:1331:PRO:HD2	1:B:1332:GLU:OE2	2.21	0.41
1:A:20:ASN:O	1:A:24:GLU:HG2	2.21	0.41
1:A:118:ILE:HG12	1:A:246:VAL:HG22	2.02	0.41
1:A:342:TRP:CE3	1:A:342:TRP:HA	2.56	0.41
1:A:1316:ASP:OD2	1:A:1316:ASP:C	2.63	0.41
1:A:1375:LEU:N	1:A:1376:PRO:CD	2.84	0.41
1:B:1319:GLU:CD	1:B:1367:ARG:HH21	2.29	0.41
1:B:1315:VAL:HA	1:B:1319:GLU:OE1	2.21	0.41
1:B:1375:LEU:N	1:B:1376:PRO:CD	2.84	0.41
1:B:1257:TRP:CG	1:B:1258:SER:N	2.89	0.40
1:A:99:VAL:HG21	1:A:109:PRO:HD3	2.03	0.40
1:B:1400:MET:HE3	1:B:1400:MET:O	2.20	0.40
1:A:142:LYS:HZ2	1:A:147:SER:HA	1.86	0.40
1:B:358:THR:HG22	1:B:359:VAL:H	1.85	0.40
1:A:43:ASP:O	1:A:45:LEU:N	2.48	0.40
1:A:1303:LEU:HD23	1:A:1303:LEU:O	2.22	0.40
1:B:363:LEU:O	1:B:367:GLN:HB2	2.22	0.40
1:B:1301:ARG:O	1:B:1305:GLU:HB2	2.22	0.40
1:A:57:ASP:CG	1:A:58:GLY:H	2.30	0.40
1:A:75:SER:HB2	1:A:77:LEU:HG	2.03	0.40
1:A:82:THR:HG23	1:A:279:LYS:HZ2	1.85	0.40
1:A:142:LYS:NZ	1:A:147:SER:HA	2.37	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	549/574 (96%)	488 (89%)	53 (10%)	8 (2%)	<b>8</b>   <b>22</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	228/574 (40%)	199 (87%)	22 (10%)	7 (3%)	3	8
All	All	777/1148 (68%)	687 (88%)	75 (10%)	15 (2%)	6	17

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1276	PRO
1	B	362	ALA
1	B	1281	PRO
1	A	1275	CYS
1	B	1277	LEU
1	B	1279	ALA
1	A	1279	ALA
1	A	1394	THR
1	A	1395	ILE
1	A	1274	SER
1	B	1280	PRO
1	B	1396	GLY
1	B	359	VAL
1	A	1271	PRO
1	A	56	GLY

### 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	459/472 (97%)	426 (93%)	33 (7%)	13	32
1	B	201/472 (43%)	177 (88%)	24 (12%)	5	13
All	All	660/944 (70%)	603 (91%)	57 (9%)	10	25

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	9	LEU
1	A	10	VAL
1	A	41	HIS
1	A	61	ILE
1	A	67	ASP
1	A	85	LYS
1	A	110	ILE
1	A	144	LYS
1	A	187	ASN
1	A	204	LYS
1	A	280	GLU
1	A	324	GLU
1	A	364	LYS
1	A	1218	ASP
1	A	1223	THR
1	A	1226	ARG
1	A	1227	LEU
1	A	1232	VAL
1	A	1237	ASN
1	A	1242	SER
1	A	1252	LEU
1	A	1260	LEU
1	A	1293	LEU
1	A	1305	GLU
1	A	1306	THR
1	A	1332	GLU
1	A	1350	GLN
1	A	1366	VAL
1	A	1393	LYS
1	A	1394	THR
1	A	1397	ASN
1	A	1398	THR
1	B	334	ASN
1	B	342	TRP
1	B	358	THR
1	B	363	LEU
1	B	367	GLN
1	B	1215	GLU
1	B	1227	LEU
1	B	1230	MET
1	B	1233	LYS
1	B	1266	ILE

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Mol	Chain	Res	Type
1	B	1277	LEU
1	B	1282	GLU
1	B	1290	GLN
1	B	1298	MET
1	B	1303	LEU
1	B	1306	THR
1	B	1318	THR
1	B	1332	GLU
1	B	1366	VAL
1	B	1381	ILE
1	B	1384	GLU
1	B	1393	LYS
1	B	1394	THR
1	B	1398	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	20	ASN
1	A	51	GLN
1	A	154	GLN
1	A	187	ASN
1	A	205	HIS
1	A	220	ASN
1	A	284	ASN
1	A	337	GLN
1	A	357	GLN
1	A	367	GLN
1	A	1221	HIS
1	A	1267	GLN
1	A	1350	GLN
1	A	1356	HIS
1	A	1360	HIS
1	A	1364	GLN
1	B	357	GLN
1	B	1267	GLN
1	B	1290	GLN
1	B	1341	HIS
1	B	1346	GLN
1	B	1350	GLN
1	B	1356	HIS

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Mol	Chain	Res	Type
1	B	1364	GLN
1	B	1397	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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	553/574 (96%)	0.54	37 (6%) 24 21	21, 59, 99, 161	0
1	B	232/574 (40%)	0.66	37 (15%) 5 4	21, 50, 112, 148	7 (3%)
All	All	785/1148 (68%)	0.58	74 (9%) 14 12	21, 57, 104, 161	7 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	ILE	6.1
1	A	1276	PRO	5.8
1	B	342	TRP	4.8
1	B	1276	PRO	4.8
1	B	1268	TRP	4.8
1	B	1215	GLU	4.6
1	B	1216	PHE	4.6
1	B	1278	LEU	4.5
1	B	363	LEU	4.3
1	A	1277	LEU	4.3
1	B	337	GLN	4.2
1	B	336	PRO	4.2
1	A	1295	LEU	4.2
1	A	354	SER	4.1
1	B	356	ARG	4.0
1	B	1217	LEU	4.0
1	B	1281	PRO	4.0
1	B	1293	LEU	4.0
1	B	359	VAL	3.9
1	B	333	PRO	3.9
1	A	1293	LEU	3.8
1	B	335	ILE	3.8
1	A	1281	PRO	3.7
1	B	331	ILE	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	242	VAL	3.6
1	A	54	ALA	3.6
1	B	334	ASN	3.4
1	A	1272	LEU	3.3
1	B	341	PHE	3.3
1	A	1280	PRO	3.3
1	A	370	ALA	3.3
1	A	1278	LEU	3.2
1	B	1280	PRO	3.2
1	A	6	GLU	3.1
1	B	360	ASP	3.1
1	B	1289	ALA	3.1
1	B	1298	MET	3.0
1	B	371	ALA	2.9
1	A	1279	ALA	2.9
1	B	355	GLY	2.8
1	B	332	MET	2.8
1	B	1282	GLU	2.8
1	B	1314	ALA	2.7
1	A	314	ALA	2.7
1	B	1275	CYS	2.6
1	A	9	LEU	2.5
1	B	1277	LEU	2.5
1	A	95	THR	2.5
1	B	364	LYS	2.4
1	A	280	GLU	2.4
1	A	189	GLY	2.4
1	B	1291	GLY	2.4
1	A	224	THR	2.4
1	A	371	ALA	2.3
1	A	53	ALA	2.3
1	B	1221	HIS	2.3
1	A	188	ALA	2.3
1	A	353	ALA	2.3
1	A	173	TYR	2.2
1	A	7	GLY	2.2
1	A	1380	PHE	2.2
1	A	40	GLU	2.2
1	B	367	GLN	2.2
1	A	350	ILE	2.2
1	A	1275	CYS	2.1
1	A	25	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	352	ALA	2.1
1	B	1292	ARG	2.1
1	A	141	LEU	2.1
1	A	176	GLY	2.1
1	A	1408	PHE	2.1
1	B	358	THR	2.1
1	A	52	VAL	2.1
1	A	1317	PRO	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.