Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:15 am GMT

PDB ID	:	4IU9
Title	:	Crystal structure of a membrane transporter
Authors	:	Yan, H.; Huang, W.; Yan, C.; Gong, X.; Jiang, S.; Zhao, Y.; Wang, J.; Shi, Y.
Deposited on	:	2013-01-20
Resolution	:	3.00 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:

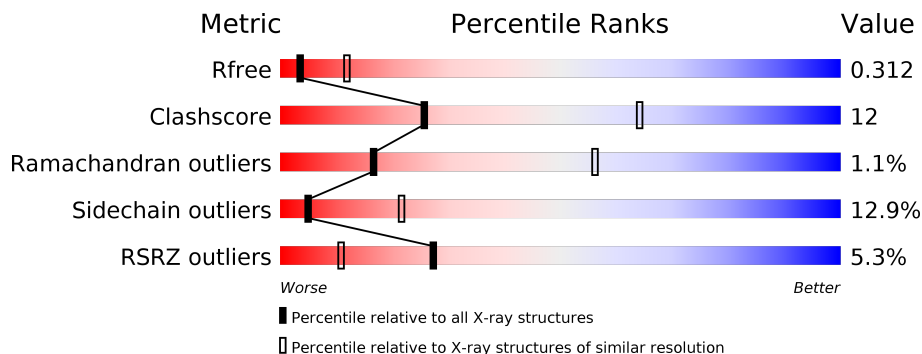|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.00 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	Percentile Ranks	Value
Rfree		0.312
Clashscore		12
Ramachandran outliers		1.1%
Sidechain outliers		12.9%
RSRZ outliers		5.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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 <=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	468	3% / 55% / 26% / • / 15%
1	B	468	6% / 63% / 24% / • / 9%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 6061 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 Nitrite extrusion protein 2.

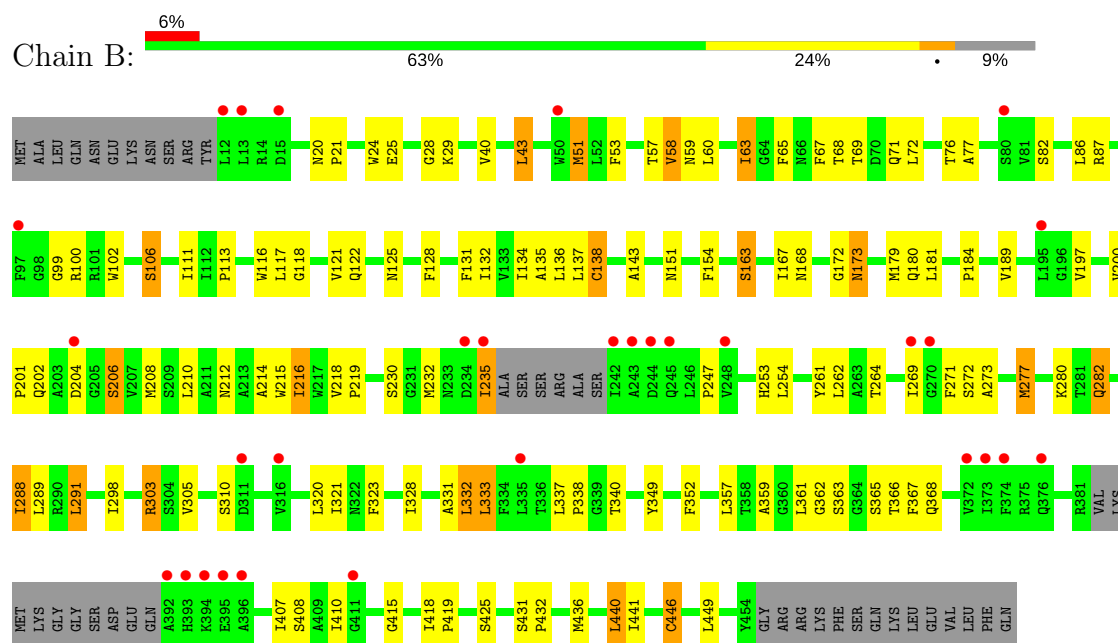| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	427	Total	C	N	O	S	0	0	0
			3129	2092	500	519	18			
1	A	396	Total	C	N	O	S	0	0	0
			2932	1966	464	484	18			

There are 12 discrepancies between the modelled and reference sequences:

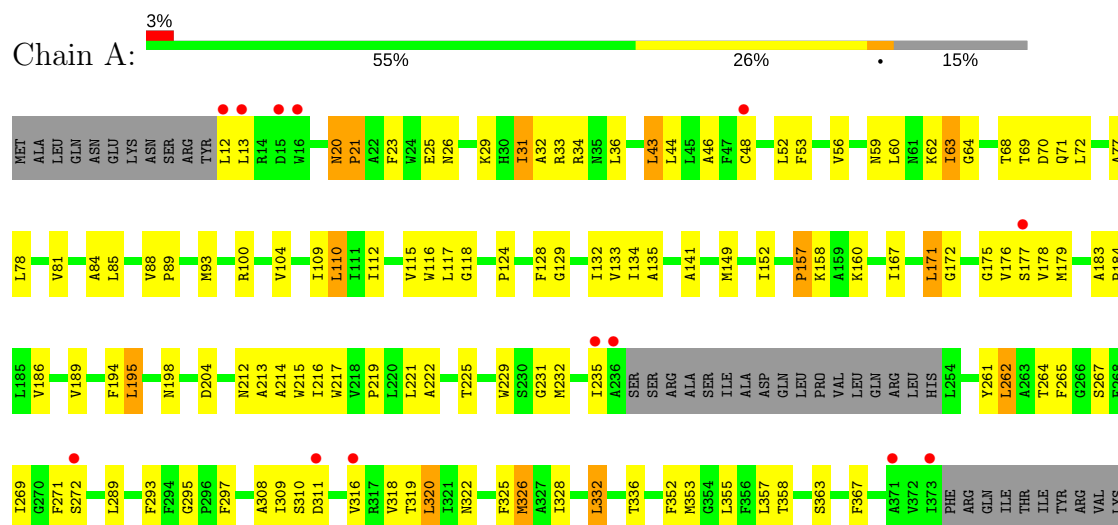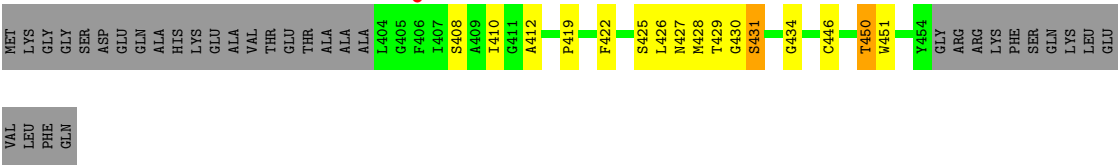| Chain	Residue	Modelled	Actual	Comment	Reference
B	463	LEU	-	EXPRESSION TAG	UNP P37758
B	464	GLU	-	EXPRESSION TAG	UNP P37758
B	465	VAL	-	EXPRESSION TAG	UNP P37758
B	466	LEU	-	EXPRESSION TAG	UNP P37758
B	467	PHE	-	EXPRESSION TAG	UNP P37758
B	468	GLN	-	EXPRESSION TAG	UNP P37758
A	463	LEU	-	EXPRESSION TAG	UNP P37758
A	464	GLU	-	EXPRESSION TAG	UNP P37758
A	465	VAL	-	EXPRESSION TAG	UNP P37758
A	466	LEU	-	EXPRESSION TAG	UNP P37758
A	467	PHE	-	EXPRESSION TAG	UNP P37758
A	468	GLN	-	EXPRESSION TAG	UNP P37758

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: Nitrite extrusion protein 2

• Molecule 1: Nitrite extrusion protein 2

MET LYS GLY GLY SER ASP GLU GLN ALA HIS LYS GLU ALA VAL THR GLU THR ALA ALA ALA **L404 G405 F406 I407 S408 A409 I410 G411 A412 P419 F422 S425 L426 N427 M428 T429 G430 S431 G434 C446 T450 W451 Y454** GLY ARG ARG LYS PHE SER GLN LYS LEU GLU

VAL LEU PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.44Å 118.21Å 127.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.84 – 3.00 39.84 – 3.00	Depositor EDS
% Data completeness (in resolution range)	76.0 (39.84-3.00) 76.2 (39.84-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.22 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.261 , 0.316 0.260 , 0.312	Depositor DCC
R_{free} test set	1404 reflections (5.15%)	DCC
Wilson B-factor (Å^2)	70.4	Xtriage
Anisotropy	1.362	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 109.0	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6061	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.43	0/3014	0.58	0/4110
1	B	0.44	0/3215	0.60	1/4388 (0.0%)
All	All	0.43	0/6229	0.59	1/8498 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	247	PRO	N-CA-CB	6.22	110.77	103.30

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	2932	0	2942	70	1
1	B	3129	0	3092	74	0
All	All	6061	0	6034	144	1

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 12.

All (144) 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:43:LEU:HD13	1:B:172:GLY:HA3	1.67	0.77
1:A:36:LEU:HD21	1:A:167:ILE:HG21	1.69	0.74
1:A:77:ALA:HB2	1:A:419:PRO:HB2	1.68	0.74
1:A:34:ARG:NH1	1:A:231:GLY:O	2.20	0.74
1:A:43:LEU:HD12	1:A:172:GLY:HA3	1.72	0.71
1:A:25:GLU:HA	1:A:29:LYS:HD3	1.74	0.69
1:A:48:CYS:SG	1:A:179:MET:HB3	2.37	0.65
1:A:157:PRO:HD2	1:A:160:LYS:HB2	1.78	0.64
1:B:280:LYS:HD3	1:B:288:ILE:HD11	1.80	0.64
1:A:222:ALA:HA	1:A:225:THR:HG22	1.80	0.63
1:B:261:TYR:HE2	1:B:408:SER:HA	1.63	0.63
1:A:64:GLY:HA3	1:A:124:PRO:HB3	1.82	0.62
1:B:271:PHE:CE2	1:B:418:ILE:HD13	2.35	0.61
1:A:261:TYR:HE1	1:A:408:SER:HA	1.66	0.61
1:B:118:GLY:HA3	1:B:215:TRP:NE1	2.16	0.60
1:A:71:GLN:HB3	1:A:128:PHE:CE2	2.39	0.58
1:A:81:VAL:O	1:A:85:LEU:HB2	2.04	0.58
1:A:116:TRP:CD1	1:A:134:ILE:HD11	2.39	0.57
1:A:63:ILE:HG22	1:A:64:GLY:H	1.69	0.57
1:A:29:LYS:NZ	1:A:33:ARG:HH12	2.03	0.57
1:B:40:VAL:HG23	1:B:168:ASN:HA	1.86	0.56
1:B:60:LEU:HD21	1:B:131:PHE:CE1	2.40	0.56
1:B:111:ILE:HG23	1:B:218:VAL:HG13	1.87	0.56
1:A:68:THR:N	1:A:71:GLN:OE1	2.29	0.56
1:A:110:LEU:HB3	1:A:221:LEU:HD21	1.86	0.56
1:B:310:SER:HB2	1:B:365:SER:HA	1.88	0.55
1:A:44:LEU:HD21	1:A:178:VAL:HG11	1.89	0.55
1:B:116:TRP:CD1	1:B:134:ILE:HD11	2.42	0.55
1:B:57:THR:HB	1:B:72:LEU:HD22	1.89	0.55
1:A:167:ILE:O	1:A:171:LEU:HB2	2.07	0.54
1:B:117:LEU:HD23	1:B:214:ALA:HB2	1.88	0.54
1:B:331:ALA:HB2	1:B:440:LEU:HD11	1.88	0.54
1:A:53:PHE:HE2	1:A:135:ALA:HA	1.72	0.54
1:A:264:THR:OG1	1:A:363:SER:N	2.41	0.54
1:B:71:GLN:HB3	1:B:128:PHE:CE2	2.43	0.54
1:B:106:SER:OG	1:B:106:SER:O	2.25	0.54
1:B:282:GLN:HG3	1:B:338:PRO:HD2	1.91	0.53
1:B:184:PRO:HB3	1:B:289:LEU:HB3	1.89	0.53
1:B:202:GLN:N	1:B:206:SER:O	2.41	0.53
1:A:322:ASN:O	1:A:325:PHE:N	2.38	0.53
1:B:173:ASN:OD1	1:B:303:ARG:NH1	2.42	0.53
1:A:194:PHE:CE2	1:A:195:LEU:HD13	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:CYS:O	1:A:450:THR:OG1	2.27	0.52
1:A:184:PRO:HB3	1:A:289:LEU:HD13	1.91	0.52
1:A:118:GLY:HA3	1:A:215:TRP:NE1	2.24	0.52
1:B:184:PRO:HG3	1:B:289:LEU:HD22	1.91	0.52
1:B:298:ILE:HG23	1:B:357:LEU:HD12	1.92	0.52
1:A:261:TYR:CE1	1:A:408:SER:HA	2.44	0.52
1:A:177:SER:OG	1:A:297:PHE:HB2	2.09	0.51
1:A:426:LEU:O	1:A:430:GLY:HA2	2.11	0.51
1:B:100:ARG:HD3	1:B:232:MET:O	2.10	0.51
1:B:102:TRP:O	1:B:106:SER:HB3	2.10	0.51
1:A:328:ILE:O	1:A:332:LEU:HB2	2.10	0.51
1:B:53:PHE:CE2	1:B:135:ALA:HA	2.46	0.51
1:A:183:ALA:HB1	1:A:213:ALA:HB1	1.92	0.51
1:B:113:PRO:HG3	1:B:137:LEU:HB3	1.92	0.51
1:A:320:LEU:HG	1:A:450:THR:HB	1.92	0.50
1:B:154:PHE:HB3	1:B:235:ILE:HD11	1.93	0.50
1:A:422:PHE:O	1:A:426:LEU:HB2	2.12	0.50
1:B:432:PRO:O	1:B:436:MET:HG3	2.12	0.49
1:A:189:VAL:O	1:A:212:ASN:ND2	2.45	0.49
1:B:269:ILE:HG22	1:B:415:GLY:HA3	1.95	0.49
1:B:362:GLY:O	1:B:366:THR:HG22	2.13	0.48
1:A:100:ARG:HD3	1:A:232:MET:O	2.12	0.48
1:B:59:ASN:HB3	1:B:208:MET:HE3	1.96	0.48
1:A:425:SER:HB2	1:A:434:GLY:HA3	1.95	0.48
1:B:51:MET:HE2	1:B:269:ILE:HG23	1.95	0.48
1:B:323:PHE:CE2	1:B:446:CYS:HB3	2.48	0.48
1:B:122:GLN:OE1	1:B:197:VAL:HA	2.12	0.48
1:A:31:ILE:HG13	1:A:32:ALA:N	2.30	0.47
1:A:78:LEU:HD11	1:A:132:ILE:HD13	1.95	0.47
1:B:99:GLY:HA3	1:B:151:ASN:OD1	2.14	0.47
1:B:425:SER:OG	1:B:431:SER:O	2.18	0.47
1:A:214:ALA:O	1:A:215:TRP:HD1	1.97	0.47
1:A:88:VAL:HB	1:A:89:PRO:HD3	1.95	0.47
1:A:46:ALA:O	1:A:141:ALA:HB1	2.15	0.47
1:A:217:TRP:O	1:A:221:LEU:HB2	2.15	0.47
1:B:216:ILE:O	1:B:219:PRO:HD2	2.15	0.47
1:A:186:VAL:HG11	1:A:216:ILE:HG21	1.97	0.46
1:B:134:ILE:O	1:B:138:CYS:HB2	2.16	0.46
1:B:163:SER:O	1:B:167:ILE:HD12	2.16	0.46
1:B:359:ALA:O	1:B:363:SER:HB2	2.16	0.46
1:B:51:MET:HE3	1:B:273:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:TYR:CE2	1:B:408:SER:HA	2.46	0.46
1:B:189:VAL:O	1:B:212:ASN:ND2	2.49	0.46
1:B:407:ILE:HA	1:B:410:ILE:HG22	1.98	0.46
1:A:216:ILE:O	1:A:219:PRO:HD2	2.15	0.45
1:A:175:GLY:HA2	1:A:178:VAL:HG12	1.98	0.45
1:B:303:ARG:HD3	1:B:363:SER:HB3	1.97	0.45
1:A:269:ILE:HA	1:A:272:SER:HB2	1.99	0.45
1:A:13:LEU:HD12	1:A:235:ILE:HG12	1.98	0.45
1:B:76:THR:HB	1:B:273:ALA:HB1	1.99	0.45
1:B:201:PRO:O	1:B:202:GLN:HG3	2.16	0.45
1:B:333:LEU:HA	1:B:333:LEU:HD23	1.80	0.45
1:B:261:TYR:CD2	1:B:407:ILE:HG22	2.51	0.45
1:A:36:LEU:HA	1:A:152:ILE:HD11	1.99	0.45
1:B:58:VAL:HG22	1:B:277:MET:HG2	1.99	0.45
1:A:293:PHE:C	1:A:295:GLY:H	2.20	0.45
1:A:29:LYS:HZ2	1:A:33:ARG:HH12	1.65	0.44
1:A:56:VAL:O	1:A:60:LEU:HG	2.17	0.44
1:A:129:GLY:O	1:A:132:ILE:HB	2.17	0.44
1:B:60:LEU:HA	1:B:60:LEU:HD12	1.84	0.44
1:B:20:ASN:HA	1:B:21:PRO:HD3	1.85	0.44
1:A:271:PHE:CE2	1:A:355:LEU:HD22	2.53	0.43
1:B:128:PHE:CE1	1:B:132:ILE:HD11	2.54	0.43
1:A:12:LEU:HD23	1:A:13:LEU:N	2.33	0.43
1:B:337:LEU:HD11	1:B:436:MET:SD	2.58	0.43
1:B:102:TRP:CG	1:B:102:TRP:O	2.71	0.43
1:B:116:TRP:CG	1:B:134:ILE:HD11	2.53	0.43
1:B:77:ALA:HB2	1:B:419:PRO:HB2	2.01	0.43
1:B:25:GLU:HA	1:B:29:LYS:HD3	2.00	0.43
1:A:308:ALA:C	1:A:310:SER:H	2.21	0.43
1:A:308:ALA:O	1:A:310:SER:N	2.51	0.43
1:A:427:ASN:HB3	1:A:428:MET:H	1.70	0.43
1:A:20:ASN:HA	1:A:21:PRO:HD2	1.81	0.42
1:B:63:ILE:HG22	1:B:65:PHE:CD2	2.54	0.42
1:A:59:ASN:HA	1:A:62:LYS:HE3	2.01	0.42
1:B:118:GLY:HA3	1:B:215:TRP:CD1	2.54	0.42
1:B:24:TRP:CE2	1:B:29:LYS:HB3	2.55	0.42
1:B:261:TYR:HA	1:B:264:THR:HG1	1.85	0.42
1:A:20:ASN:O	1:A:23:PHE:N	2.53	0.42
1:A:129:GLY:O	1:A:133:VAL:HG23	2.20	0.42
1:A:293:PHE:C	1:A:295:GLY:N	2.74	0.42
1:A:326:MET:HG2	1:A:358:THR:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:ILE:HA	1:B:441:ILE:HD13	1.75	0.41
1:A:104:VAL:HG21	1:A:229:TRP:CE3	2.56	0.41
1:B:67:PHE:HE1	1:B:128:PHE:HB2	1.85	0.41
1:A:262:LEU:HD12	1:A:410:ILE:O	2.21	0.41
1:A:84:ALA:HB2	1:A:412:ALA:HB3	2.02	0.41
1:A:117:LEU:HB2	1:A:134:ILE:HG21	2.03	0.41
1:B:328:ILE:O	1:B:332:LEU:HB2	2.21	0.41
1:B:87:ARG:HG2	1:B:143:ALA:HA	2.03	0.41
1:B:179:MET:C	1:B:181:LEU:H	2.24	0.41
1:B:291:LEU:HD13	1:B:349:TYR:CE2	2.56	0.41
1:A:319:THR:O	1:A:322:ASN:HB3	2.20	0.40
1:B:333:LEU:HD13	1:B:436:MET:HE1	2.03	0.40
1:A:264:THR:HG23	1:A:265:PHE:H	1.87	0.40
1:B:184:PRO:HB3	1:B:289:LEU:HD13	2.02	0.40
1:B:43:LEU:HD23	1:B:43:LEU:HA	1.87	0.40
1:B:58:VAL:CG2	1:B:277:MET:HG2	2.52	0.40
1:A:100:ARG:HG3	1:A:232:MET:HB2	2.04	0.40
1:B:184:PRO:CB	1:B:289:LEU:HB3	2.51	0.40
1:B:323:PHE:CD2	1:B:446:CYS:HB3	2.57	0.40
1:B:271:PHE:CD2	1:B:418:ILE:HG21	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ASN:OD1	1:A:431:SER:OG[2_555]	2.04	0.16

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	A	390/468 (83%)	339 (87%)	45 (12%)	6 (2%)	12	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	421/468 (90%)	361 (86%)	57 (14%)	3 (1%)	25	67
All	All	811/936 (87%)	700 (86%)	102 (13%)	9 (1%)	17	56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28	GLY
1	B	58	VAL
1	A	157	PRO
1	A	158	LYS
1	A	309	ILE
1	A	21	PRO
1	B	180	GLN
1	A	316	VAL
1	A	63	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	293/371 (79%)	259 (88%)	34 (12%)	6	26
1	B	304/371 (82%)	261 (86%)	43 (14%)	4	18
All	All	597/742 (80%)	520 (87%)	77 (13%)	5	22

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	43	LEU
1	B	51	MET
1	B	63	ILE
1	B	68	THR
1	B	69	THR
1	B	82	SER
1	B	86	LEU

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Mol	Chain	Res	Type
1	B	106	SER
1	B	121	VAL
1	B	125	ASN
1	B	136	LEU
1	B	138	CYS
1	B	163	SER
1	B	173	ASN
1	B	200	VAL
1	B	204	ASP
1	B	206	SER
1	B	210	LEU
1	B	216	ILE
1	B	230	SER
1	B	235	ILE
1	B	253	HIS
1	B	254	LEU
1	B	262	LEU
1	B	272	SER
1	B	277	MET
1	B	282	GLN
1	B	288	ILE
1	B	291	LEU
1	B	303	ARG
1	B	305	VAL
1	B	320	LEU
1	B	321	ILE
1	B	332	LEU
1	B	333	LEU
1	B	340	THR
1	B	352	PHE
1	B	361	LEU
1	B	367	PHE
1	B	368	GLN
1	B	440	LEU
1	B	446	CYS
1	B	449	LEU
1	A	20	ASN
1	A	31	ILE
1	A	43	LEU
1	A	52	LEU
1	A	69	THR
1	A	70	ASP

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Mol	Chain	Res	Type
1	A	72	LEU
1	A	93	MET
1	A	109	ILE
1	A	110	LEU
1	A	112	ILE
1	A	115	VAL
1	A	149	MET
1	A	171	LEU
1	A	176	VAL
1	A	195	LEU
1	A	198	ASN
1	A	204	ASP
1	A	262	LEU
1	A	267	SER
1	A	311	ASP
1	A	318	VAL
1	A	320	LEU
1	A	326	MET
1	A	332	LEU
1	A	336	THR
1	A	352	PHE
1	A	353	MET
1	A	357	LEU
1	A	367	PHE
1	A	429	THR
1	A	431	SER
1	A	450	THR
1	A	451	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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	A	396/468 (84%)	-0.07	14 (3%)	44	19	94, 124, 174, 219	0
1	B	427/468 (91%)	0.18	30 (7%)	17	6	91, 121, 186, 290	0
All	All	823/936 (87%)	0.06	44 (5%)	27	11	91, 122, 179, 290	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	242	ILE	5.6
1	B	244	ASP	5.5
1	A	236	ALA	5.0
1	B	394	LYS	4.7
1	A	406	PHE	4.7
1	B	311	ASP	4.6
1	B	245	GLN	3.9
1	B	235	ILE	3.8
1	B	204	ASP	3.8
1	B	396	ALA	3.7
1	A	15	ASP	3.7
1	B	392	ALA	3.6
1	A	13	LEU	3.5
1	B	12	LEU	3.5
1	B	270	GLY	3.5
1	B	373	ILE	3.1
1	B	248	VAL	3.1
1	B	376	GLN	3.0
1	B	243	ALA	2.9
1	B	15	ASP	2.9
1	B	13	LEU	2.7
1	B	374	PHE	2.6
1	B	50	TRP	2.6
1	A	316	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	12	LEU	2.5
1	A	311	ASP	2.5
1	B	411	GLY	2.5
1	A	177	SER	2.5
1	B	335	LEU	2.5
1	A	235	ILE	2.5
1	B	316	VAL	2.4
1	B	395	GLU	2.4
1	A	16	TRP	2.3
1	B	195	LEU	2.3
1	A	48	CYS	2.3
1	B	372	VAL	2.3
1	B	234	ASP	2.2
1	A	373	ILE	2.2
1	B	80	SER	2.2
1	B	97	PHE	2.1
1	B	269	ILE	2.1
1	A	371	ALA	2.1
1	A	272	SER	2.1
1	B	393	HIS	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 carbohydrates 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.