Preliminary Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2018 – 06:19 PM JST

Deposition ID	:	D_1300006790
PDB ID	:	*(not yet assigned)*

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

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:

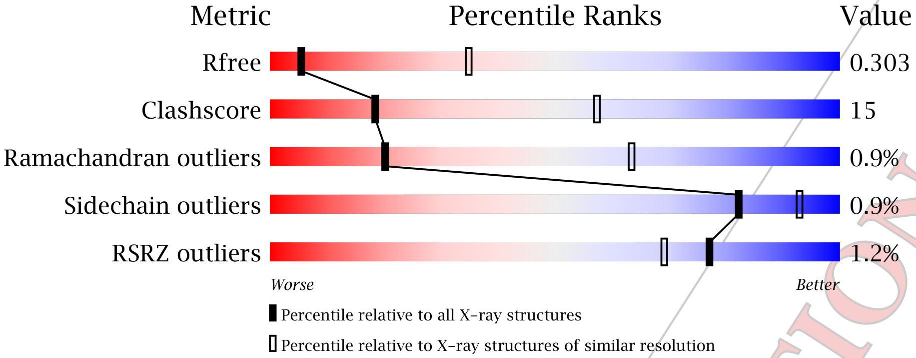
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

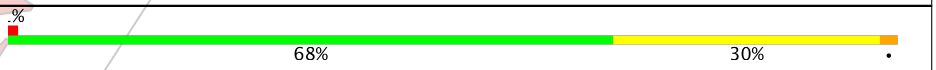
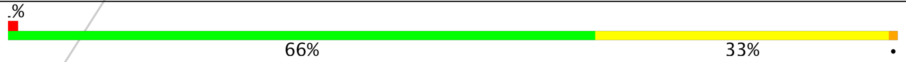
The reported resolution of this entry is 3.51 Å.

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	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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	280	
1	B	280	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4412 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	280	2205	1406	396	388	15	0	0	0
1	B	280	2205	1406	396	388	15	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

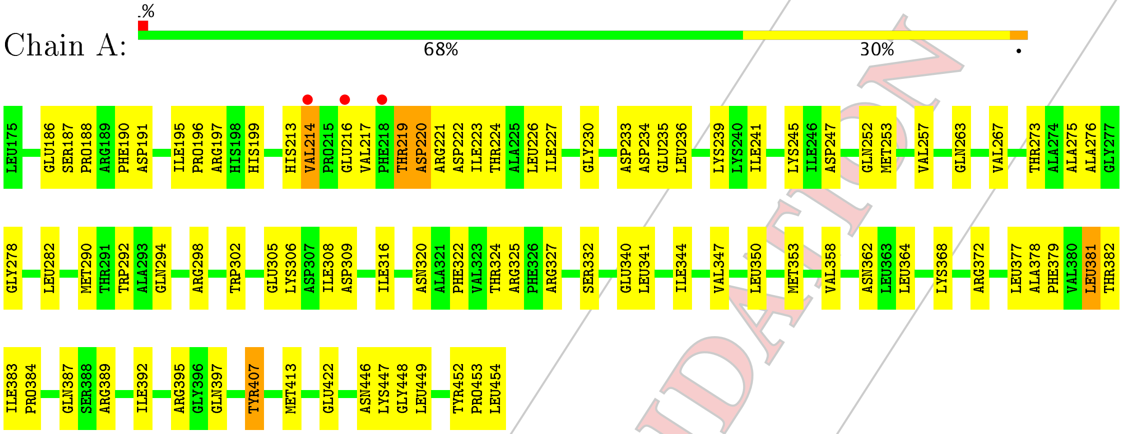
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

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.

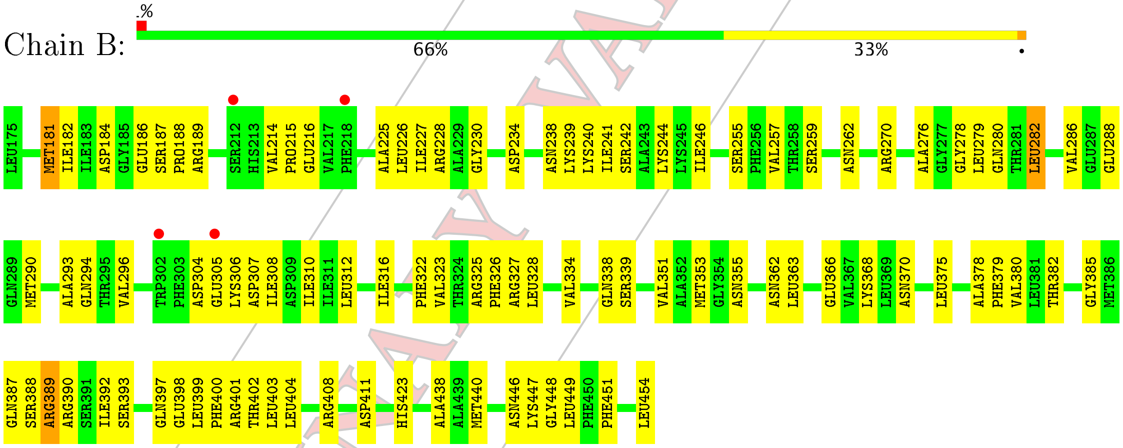
- Molecule 1:

Chain A:



- Molecule 1:

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α, β, γ	167.53Å 167.53Å 227.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.15 – 3.51 33.15 – 3.51	Depositor EDS
% Data completeness (in resolution range)	98.2 (33.15-3.51) 98.4 (33.15-3.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.38 (at 3.47Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.257 , 0.306 0.244 , 0.303	Depositor DCC
R_{free} test set	1135 reflections (4.76%)	DCC
Wilson B-factor (Å^2)	102.4	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 68.8	EDS
L-test for twinning[2]	$< \|L\| >$ = 0.55, $< L^2 >$ = 0.40	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4412	wwPDB-VP
Average B, all atoms (Å^2)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.28	0/2252	0.50	1/3043 (0.0%)
1	B	0.28	0/2252	0.51	0/3043
All	All	0.28	0/4504	0.51	1/6086 (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	A	219	THR	C-N-CA	5.34	135.06	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	2205	0	2220	69	0
1	B	2205	0	2220	74	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	4412	0	4440	132	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 15.

All (132) 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:273:THR:OG1	1:A:447:LYS:O	2.01	0.78
1:A:223:ILE:HD11	1:A:252:GLN:HB3	1.66	0.78
1:B:389:ARG:HH22	1:B:401:ARG:HD2	1.49	0.78
1:A:294:GLN:NE2	1:A:407:TYR:O	2.18	0.77
1:B:325:ARG:NH1	1:B:328:LEU:HD13	2.01	0.75
1:A:368:LYS:HE3	1:B:184:ASP:HA	1.69	0.74
1:A:290:MET:SD	1:A:382:THR:OG1	2.45	0.74
1:B:290:MET:SD	1:B:382:THR:OG1	2.47	0.71
1:B:312:LEU:O	1:B:387:GLN:NE2	2.23	0.70
1:A:219:THR:HA	1:A:220:ASP:HB2	1.76	0.68
1:A:196:PRO:HB2	1:A:199:HIS:CD2	2.29	0.68
1:B:214:VAL:HG12	1:B:216:GLU:H	1.58	0.68
1:A:379:PHE:HE1	1:A:407:TYR:HB2	1.57	0.68
1:A:213:HIS:CG	1:A:214:VAL:H	2.13	0.67
1:A:327:ARG:HH22	1:B:353:MET:HA	1.59	0.66
1:B:241:ILE:HD12	1:B:241:ILE:O	1.95	0.65
1:A:233:ASP:OD1	1:A:447:LYS:HB2	1.97	0.65
1:A:332:SER:HA	1:A:341:LEU:HD11	1.80	0.63
1:B:239:LYS:HZ1	1:B:446:ASN:HB3	1.64	0.63
1:B:280:GLN:HG3	1:B:440:MET:HB2	1.80	0.62
1:A:219:THR:HA	1:A:220:ASP:CB	2.30	0.62
1:A:275:ALA:HB1	1:B:325:ARG:NH2	2.15	0.62
1:A:340:GLU:O	1:A:344:ILE:HG12	2.01	0.60
1:B:325:ARG:HH11	1:B:328:LEU:HD13	1.65	0.59
1:B:240:LYS:HG3	1:B:454:LEU:HD13	1.85	0.58
1:B:279:LEU:HD11	1:B:326:PHE:HA	1.86	0.57
1:B:338:GLN:HG2	1:B:339:SER:H	1.70	0.57
1:A:234:ASP:OD1	1:A:235:GLU:N	2.37	0.56
1:B:307:ASP:OD1	1:B:308:ILE:N	2.38	0.56
1:A:344:ILE:HG23	1:A:377:LEU:HD11	1.89	0.55
1:B:392:ILE:HG22	1:B:393:SER:H	1.73	0.54
1:B:240:LYS:HE3	1:B:454:LEU:HD22	1.90	0.54
1:B:325:ARG:HA	1:B:328:LEU:HD12	1.88	0.54
1:A:217:VAL:HG12	1:A:219:THR:HG23	1.90	0.54
1:A:302:TRP:HE1	1:A:389:ARG:CZ	2.21	0.54
1:A:292:TRP:NE1	1:A:309:ASP:OD2	2.35	0.54
1:B:214:VAL:O	1:B:216:GLU:HG3	2.08	0.54
1:A:220:ASP:OD1	1:A:221:ARG:N	2.41	0.53
1:B:214:VAL:HG13	1:B:262:ASN:OD1	2.07	0.53
1:A:190:PHE:H	1:A:191:ASP:HA	1.73	0.53

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:B:294:GLN:NE2	1:B:404:LEU:O	2.41	0.53
1:A:247:ASP:OD2	1:A:298:ARG:NH2	2.43	0.52
1:B:389:ARG:HG2	1:B:397:GLN:HG2	1.92	0.52
1:B:279:LEU:H	1:B:440:MET:HA	1.74	0.51
1:B:186:GLU:HB3	1:B:187:SER:C	2.31	0.51
1:B:270:ARG:NH1	1:B:288:GLU:OE2	2.43	0.51
1:A:316:ILE:HD13	1:A:384:PRO:HB3	1.91	0.51
1:B:446:ASN:O	1:B:449:LEU:N	2.43	0.51
1:A:353:MET:CE	1:B:353:MET:HB3	2.42	0.50
1:B:323:VAL:HG11	1:B:351:VAL:HB	1.94	0.50
1:A:197:ARG:HH12	1:B:408:ARG:HB2	1.77	0.50
1:A:358:VAL:O	1:A:362:ASN:ND2	2.44	0.50
1:B:293:ALA:HA	1:B:296:VAL:HG22	1.93	0.50
1:A:413:MET:HG3	1:A:452:TYR:OH	2.12	0.49
1:B:385:GLY:O	1:B:389:ARG:HG3	2.13	0.49
1:A:377:LEU:O	1:A:381:LEU:HD12	2.13	0.49
1:B:181:MET:SD	1:B:182:ILE:HG13	2.52	0.49
1:A:378:ALA:O	1:A:382:THR:HG23	2.13	0.49
1:A:213:HIS:CD2	1:A:214:VAL:H	2.30	0.48
1:B:215:PRO:HD2	1:B:262:ASN:OD1	2.13	0.48
1:B:230:GLY:HA2	1:B:449:LEU:O	2.13	0.48
1:A:197:ARG:NH1	1:B:408:ARG:HB2	2.29	0.48
1:A:186:GLU:O	1:A:187:SER:OG	2.22	0.48
1:B:362:ASN:OD1	1:B:363:LEU:N	2.46	0.48
1:A:383:ILE:O	1:A:387:GLN:HG3	2.12	0.48
1:B:226:LEU:HD23	1:B:227:ILE:HD13	1.96	0.48
1:A:190:PHE:N	1:A:191:ASP:HA	2.29	0.48
1:A:275:ALA:HB1	1:B:325:ARG:CZ	2.44	0.48
1:B:382:THR:HA	1:B:400:PHE:CD1	2.49	0.48
1:A:327:ARG:NH2	1:B:353:MET:HA	2.26	0.48
1:A:379:PHE:CE1	1:A:407:TYR:HB2	2.45	0.48
1:B:234:ASP:OD2	1:B:238:ASN:ND2	2.44	0.47
1:B:389:ARG:O	1:B:390:ARG:HG3	2.14	0.47
1:B:447:LYS:HA	1:B:448:GLY:HA2	1.62	0.47
1:A:353:MET:HA	1:B:327:ARG:NH2	2.29	0.47
1:B:334:VAL:HA	1:B:423:HIS:CD2	2.50	0.47
1:A:196:PRO:HB2	1:A:199:HIS:HD2	1.80	0.46
1:B:366:GLU:N	1:B:366:GLU:OE1	2.47	0.46
1:A:213:HIS:CG	1:A:214:VAL:N	2.81	0.46
1:B:305:GLU:N	1:B:306:LYS:HA	2.30	0.46
1:B:304:ASP:C	1:B:306:LYS:HA	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:LYS:HG2	1:B:370:ASN:H	1.80	0.46
1:A:320:ASN:O	1:A:324:THR:HG23	2.15	0.46
1:A:347:VAL:HA	1:A:350:LEU:HD12	1.97	0.45
1:A:282:LEU:HD13	1:A:322:PHE:HA	1.98	0.45
1:B:188:PRO:CB	1:B:189:ARG:HA	2.47	0.45
1:A:305:GLU:HA	1:A:306:LYS:HA	1.47	0.45
1:A:223:ILE:HD11	1:A:252:GLN:CB	2.42	0.45
1:A:447:LYS:HA	1:A:448:GLY:HA2	1.67	0.45
1:A:187:SER:N	1:A:188:PRO:HD3	2.32	0.44
1:B:322:PHE:CE2	1:B:380:VAL:HG21	2.52	0.44
1:A:392:ILE:HG23	1:A:397:GLN:HG2	1.98	0.44
1:A:223:ILE:HG23	1:A:226:LEU:HD23	2.00	0.44
1:B:225:ALA:HA	1:B:228:ARG:HG2	1.99	0.44
1:B:379:PHE:HE2	1:B:411:ASP:HB3	1.82	0.44
1:A:223:ILE:HD13	1:A:253:MET:HA	2.00	0.44
1:B:379:PHE:HD1	1:B:403:LEU:HD23	1.83	0.44
1:B:255:SER:O	1:B:259:SER:N	2.51	0.43
1:A:372:ARG:NH1	1:A:422:GLU:OE1	2.45	0.43
1:B:278:GLY:O	1:B:282:LEU:HD12	2.19	0.43
1:A:263:GLN:O	1:A:267:VAL:HG23	2.19	0.43
1:A:220:ASP:O	1:A:224:THR:HG23	2.17	0.43
1:B:325:ARG:HH21	1:B:438:ALA:C	2.21	0.43
1:A:395:ARG:HG2	1:A:395:ARG:H	1.60	0.43
1:B:288:GLU:HG3	1:B:451:PHE:CZ	2.53	0.43
1:A:364:LEU:HD11	1:A:381:LEU:HD13	2.01	0.43
1:B:388:SER:O	1:B:390:ARG:N	2.52	0.42
1:A:221:ARG:HA	1:A:222:ASP:HA	1.56	0.42
1:A:257:VAL:HG21	1:A:292:TRP:CZ2	2.53	0.42
1:B:399:LEU:HG	1:B:403:LEU:HD13	2.00	0.42
1:A:278:GLY:HA2	1:A:325:ARG:HD2	2.01	0.42
1:B:241:ILE:HD11	1:B:451:PHE:HD2	1.84	0.42
1:A:239:LYS:HZ3	1:A:449:LEU:HB3	1.84	0.42
1:B:257:VAL:HG13	1:B:310:ILE:HB	2.01	0.42
1:A:227:ILE:O	1:A:230:GLY:N	2.49	0.41
1:A:358:VAL:HG12	1:A:362:ASN:HD21	1.85	0.41
1:B:282:LEU:O	1:B:286:VAL:HG23	2.21	0.41
1:B:398:GLU:O	1:B:402:THR:OG1	2.24	0.41
1:A:276:ALA:O	1:B:276:ALA:HB1	2.19	0.41
1:B:316:ILE:H	1:B:316:ILE:HD12	1.85	0.41
1:B:353:MET:O	1:B:355:ASN:N	2.49	0.41
1:A:453:PRO:O	1:A:454:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ILE:HD13	1:B:246:ILE:HG12	2.03	0.41
1:A:332:SER:HA	1:A:341:LEU:CD1	2.48	0.41
1:A:241:ILE:HD11	1:A:245:LYS:HD3	2.03	0.41
1:A:446:ASN:O	1:A:449:LEU:HB2	2.20	0.41
1:A:236:LEU:HA	1:A:236:LEU:HD23	1.88	0.41
1:B:242:SER:HB3	1:B:244:LYS:HE2	2.02	0.40
1:A:195:ILE:HD11	1:B:375:LEU:HD21	2.02	0.40
1:B:378:ALA:O	1:B:382:THR:HG23	2.21	0.40
1:B:282:LEU:HD22	1:B:322:PHE:N	2.37	0.40
1:B:239:LYS:NZ	1:B:449:LEU:O	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	278/280 (99%)	258 (93%)	16 (6%)	4 (1%)	13	53
1	B	278/280 (99%)	238 (86%)	39 (14%)	1 (0%)	38	77
All	All	556/560 (99%)	496 (89%)	55 (10%)	5 (1%)	20	63

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	VAL
1	A	216	GLU
1	A	220	ASP
1	B	389	ARG
1	A	308	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	235/235 (100%)	233 (99%)	2 (1%)	82	93
1	B	235/235 (100%)	233 (99%)	2 (1%)	82	93
All	All	470/470 (100%)	466 (99%)	4 (1%)	82	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	381	LEU
1	A	407	TYR
1	B	181	MET
1	B	282	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
1	A	213	HIS
1	B	417	ASN
1	B	446	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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	280/280 (100%)	-0.27	3 (1%)	80	72	71, 98, 171, 238	0
1	B	280/280 (100%)	-0.12	4 (1%)	75	67	83, 114, 190, 267	0
All	All	560/560 (100%)	-0.20	7 (1%)	77	69	71, 107, 186, 267	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	305	GLU	3.4
1	A	218	PHE	3.3
1	B	218	PHE	2.9
1	A	214	VAL	2.6
1	B	212	SER	2.6
1	A	216	GLU	2.4
1	B	302	TRP	2.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	**Type**	**Chain**	**Res**	**Atoms**	**RSCC**	**RSR**	**LLDF**	**B-factors(Å^2)**	**Q<0.9**
2	ZN	A	500	1/?	0.98	0.03	-2.34	92,92,92,92	0
2	ZN	B	500	1/?	0.99	0.02	-3.18	78,78,78,78	0

6.5 Other polymers ⓘ

There are no such residues in this entry.