

# Full wwPDB X-ray Structure Validation Report (i)

#### May 6, 2024 – 02:12 PM EDT

:	8SUO
:	BA.2/AZD1061/AZD3152 structure analysis
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:	2023-05-12
:	3.30 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 (i) 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 (1)) were used in the production of this report:

MolProbity		4.02b-467
	·	4.020-401
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 3.30 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.



Motric	Whole archive	Similar resolution
wiethe	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	Ι	234	77%	18%	•••
2	М	219	% 82%	16%	••
3	Н	228	80%	18%	·
4	L	215	88%	11%	) •
5	А	195	67% 3	31%	••



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# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8175 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 AZD1061 heavy chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Ι	228	Total	C 1083	N 284	0 335	${ m S}_7$	0	0	0
1	Ι	228	1709	1083	284	335	$\frac{5}{7}$	0	0	

• Molecule 2 is a protein called AZD1061 light chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	М	217	Total 1676	C 1051	N 279	O 340	S 6	0	0	0

• Molecule 3 is a protein called AZD3152 heavy chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	Н	223	Total 1670	C 1059	N 279	O 326	S 6	0	0	0

• Molecule 4 is a protein called AZD3152 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	213	Total 1570	C 980	N 261	O 323	S 6	0	0	0

• Molecule 5 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
5	А	194	Total 1550	C 1002	N 261	0 279	S 8	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	339	ASP	GLY	conflict	UNP P0DTC2
А	371	PHE	SER	conflict	UNP P0DTC2



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Chain	Residue	Modelled	Actual	Comment	Reference
А	373	PRO	SER	conflict	UNP P0DTC2
А	375	PHE	SER	conflict	UNP P0DTC2
А	376	ALA	THR	conflict	UNP P0DTC2
А	405	ASN	ASP	conflict	UNP P0DTC2
А	408	SER	ARG	conflict	UNP P0DTC2
А	417	ASN	LYS	conflict	UNP P0DTC2
А	440	LYS	ASN	conflict	UNP P0DTC2
А	477	ASN	SER	conflict	UNP P0DTC2
А	478	LYS	THR	conflict	UNP P0DTC2
А	484	ALA	GLU	conflict	UNP P0DTC2
А	493	ARG	GLN	conflict	UNP P0DTC2
А	498	ARG	GLN	conflict	UNP P0DTC2
А	501	TYR	ASN	conflict	UNP P0DTC2
А	505	HIS	TYR	conflict	UNP P0DTC2



# 3 Residue-property plots (i)

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: AZD1061 heavy chain





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	67.69Å 138.00Å 188.72Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	30.00 - 3.30	Depositor
Resolution (A)	94.36 - 2.98	EDS
% Data completeness	99.5 (30.00-3.30)	Depositor
(in resolution range)	99.6 (94.36-2.98)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.10 (at 2.96 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
B B.	0.279 , $0.332$	Depositor
II, II free	0.279 , $0.328$	DCC
$R_{free}$ test set	1864 reflections $(5.05%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	87.3	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.27, 71.5	EDS
L-test for $twinning^2$	$ < L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8175	wwPDB-VP
Average B, all atoms $(Å^2)$	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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	Bond lengths		angles
		RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	Ι	0.29	0/1751	0.52	0/2383
2	М	0.28	0/1712	0.50	0/2324
3	Н	0.31	0/1714	0.53	0/2335
4	L	0.31	0/1608	0.53	0/2192
5	А	0.26	0/1598	0.49	0/2175
All	All	0.29	0/8383	0.51	0/11409

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	Ι	1709	0	1681	37	0
2	М	1676	0	1631	27	0
3	Н	1670	0	1624	30	0
4	L	1570	0	1519	15	0
5	А	1550	0	1481	44	0
All	All	8175	0	7936	140	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 9.

All (140) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:153:THR:HA	1:I:203:PRO:HA	1.47	0.96
3:H:22:CYS:HG	3:H:96:CYS:HG	1.20	0.89
4:L:152:LYS:HA	4:L:157:PRO:HA	1.54	0.87
5:A:336:CYS:HG	5:A:361:CYS:HG	0.86	0.85
2:M:139:CYS:HG	2:M:199:CYS:HG	0.92	0.85
2:M:23:CYS:HG	2:M:94:CYS:HG	1.01	0.83
5:A:391:CYS:HG	5:A:525:CYS:HG	1.20	0.79
5:A:379:CYS:HA	5:A:432:CYS:HA	1.70	0.73
4:L:137:CYS:O	4:L:138:LEU:HD23	1.88	0.72
5:A:401:VAL:HG22	5:A:509:ARG:HG2	1.75	0.67
1:I:160:VAL:HG11	1:I:168:VAL:HG21	1.79	0.65
1:I:13:LYS:HD3	1:I:131:SER:HA	1.79	0.65
3:H:213:LYS:N	3:H:214:PRO:HD2	2.13	0.64
1:I:168:VAL:HG12	1:I:218:HIS:HB2	1.81	0.63
2:M:16:GLY:HA2	2:M:83:SER:HB2	1.82	0.61
5:A:455:LEU:HD23	5:A:456:PHE:HD2	1.66	0.60
1:I:163:TYR:HE1	1:I:166:GLU:HA	1.67	0.60
2:M:206:LEU:HD13	2:M:210:VAL:HG12	1.84	0.59
3:H:22:CYS:HG	3:H:96:CYS:CB	2.16	0.58
1:I:184:PHE:CE1	2:M:169:THR:HG23	2.38	0.58
1:I:189:GLN:HE21	1:I:193:LEU:HB2	1.69	0.57
1:I:153:THR:CA	1:I:203:PRO:HA	2.31	0.56
3:H:166:TRP:HB3	3:H:171:LEU:HD23	1.87	0.56
3:H:50:SER:O	3:H:58:ILE:HA	2.06	0.56
5:A:391:CYS:CB	5:A:525:CYS:HG	2.18	0.55
5:A:418:ILE:HA	5:A:422:ASN:HB2	1.86	0.55
2:M:191:TYR:HA	2:M:197:TYR:OH	2.06	0.55
5:A:454:ARG:HA	5:A:492:LEU:HD23	1.88	0.55
1:I:157:GLY:HA3	1:I:199:VAL:HA	1.88	0.55
2:M:168:VAL:HG22	2:M:180:LEU:HD13	1.88	0.55
5:A:380:TYR:O	5:A:431:GLY:N	2.40	0.55
5:A:422:ASN:O	5:A:423:TYR:HB3	2.06	0.54
3:H:159:PRO:HD2	3:H:214:PRO:HB3	1.89	0.54
4:L:4:VAL:HB	4:L:101:GLY:HA2	1.89	0.53
5:A:403:ARG:HG2	5:A:495:TYR:HE2	1.72	0.53
3:H:212:HIS:CE1	3:H:214:PRO:HB2	2.43	0.53
1:I:204:SER:O	1:I:205:SER:C	2.48	0.52
1:I:104:TYR:O	5:A:444:LYS:HD3	2.09	0.52
5:A:453:TYR:HB3	5:A:495:TYR:CE1	2.44	0.52
4:L:135:LEU:HD12	4:L:181:LEU:HD23	1.91	0.51
2:M:113:ARG:NH1	2:M:114:THR:O	2.43	0.51
3:H:101:PHE:CE2	5:A:455:LEU:HD21	2.45	0.51



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
5:A:392:PHE:CD2	5:A:515:PHE:HB3	2.46	0.51	
2:M:166:GLU:HB3	2:M:180:LEU:HD11	1.93	0.51	
3:H:152:CYS:SG	3:H:208:CYS:CB	2.98	0.51	
1:I:219:LYS:N	1:I:220:PRO:CD	2.74	0.51	
3:H:100:ALA:HB2	3:H:113:GLU:HB2	1.92	0.51	
3:H:213:LYS:N	3:H:214:PRO:CD	2.75	0.50	
2:M:154:LYS:HG2	2:M:159:LEU:HA	1.94	0.50	
3:H:177:THR:HG22	3:H:192:SER:OG	2.12	0.50	
1:I:162:ASP:HA	1:I:193:LEU:HB3	1.94	0.50	
1:I:199:VAL:HG21	2:M:140:LEU:HD13	1.94	0.49	
3:H:20:LEU:HD12	3:H:81:LEU:O	2.11	0.49	
2:M:194:HIS:O	2:M:216:ARG:NH2	2.44	0.49	
3:H:215:SER:O	3:H:216:ASN:HB2	2.12	0.49	
3:H:177:THR:HA	3:H:192:SER:HA	1.94	0.49	
5:A:439:ASN:O	5:A:443:SER:HB2	2.11	0.49	
1:I:104:TYR:HE1	1:I:109:VAL:HG23	1.78	0.49	
3:H:20:LEU:HD11	3:H:83:MET:HE2	1.94	0.48	
4:L:137:CYS:C	4:L:138:LEU:HD23	2.32	0.48	
5:A:379:CYS:CB	5:A:432:CYS:HG	2.25	0.48	
1:I:93:THR:HG23	1:I:128:THR:HA	1.96	0.48	
2:M:166:GLU:HA	2:M:181:SER:O	2.14	0.48	
3:H:193:VAL:HG21	4:L:138:LEU:HD12	1.95	0.48	
3:H:20:LEU:HD11	3:H:83:MET:CE	2.43	0.48	
3:H:109:TYR:HA	4:L:34:TYR:HB3	1.94	0.48	
2:M:89:VAL:HG12	2:M:110:GLU:HA	1.96	0.48	
5:A:362:VAL:HB	5:A:526:GLY:HA2	1.96	0.48	
3:H:102:PRO:O	5:A:457:ARG:O	2.32	0.47	
1:I:180:GLY:HA3	1:I:201:THR:HG22	1.96	0.47	
5:A:426:PRO:HD3	5:A:464:PHE:CE2	2.49	0.47	
3:H:159:PRO:HA	3:H:188:TYR:HE2	1.77	0.47	
1:I:162:ASP:OD1	1:I:189:GLN:NE2	2.48	0.47	
5:A:412:PRO:HB3	5:A:426:PRO:O	2.14	0.47	
5:A:448:ASN:HB3	5:A:497:PHE:HB2	1.97	0.47	
2:M:95:GLN:HB2	2:M:103:PHE:CD2	2.50	0.46	
3:H:215:SER:OG	3:H:217:THR:HB	2.16	0.46	
5:A:381:GLY:HA3	5:A:430:THR:HA	1.95	0.46	
1:I:186:ALA:HB2	1:I:196:LEU:HD23	1.98	0.46	
2:M:112:LYS:HA	2:M:145:TYR:OH	2.15	0.46	
4:L:123:PRO:HD3	4:L:135:LEU:CD2	2.46	0.46	
5:A:393:THR:HA	5:A:522:ALA:HA	1.98	0.46	
5:A:455:LEU:HD23	5:A:456:PHE:CD2	2.46	0.46	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:A:490:PHE:CG	5:A:491:PRO:HD2	2.50	0.46
4:L:145:GLY:O	4:L:167:PRO:HG2	2.16	0.46
1:I:166:GLU:HG2	1:I:167:PRO:HA	1.99	0.45
4:L:85:GLU:HG3	4:L:107:THR:HA	1.99	0.45
1:I:157:GLY:CA	1:I:199:VAL:HA	2.46	0.45
1:I:204:SER:O	1:I:206:SER:N	2.49	0.45
1:I:142:LEU:HD21	2:M:138:VAL:HG21	1.99	0.45
3:H:22:CYS:SG	3:H:96:CYS:CB	3.05	0.45
4:L:138:LEU:HD22	4:L:178:SER:HB3	1.98	0.45
1:I:186:ALA:HA	1:I:196:LEU:HB3	1.99	0.45
2:M:122:ILE:HD12	2:M:213:SER:HA	1.98	0.45
5:A:353:TRP:CD1	5:A:423:TYR:HB2	2.52	0.44
5:A:394:ASN:HB2	5:A:516:GLU:OE1	2.17	0.44
5:A:404:GLY:HA2	5:A:407:VAL:HG23	2.00	0.44
2:M:34:ASN:HD22	5:A:449:TYR:CB	2.31	0.44
1:I:142:LEU:CD2	2:M:138:VAL:HG21	2.48	0.44
1:I:85:MET:HB3	1:I:88:LEU:HD21	1.98	0.43
3:H:191:SER:HG	4:L:180:TYR:HE2	1.65	0.43
3:H:91:THR:HG23	3:H:122:THR:HA	1.99	0.43
5:A:526:GLY:N	5:A:527:PRO:HD3	2.32	0.43
2:M:39:LEU:HD13	2:M:77:PHE:CG	2.54	0.43
4:L:11:SER:HB2	4:L:109:LEU:HD11	2.00	0.43
5:A:409:GLN:HA	5:A:414:GLN:OE1	2.19	0.43
3:H:33:ALA:CB	3:H:104:TYR:HA	2.48	0.43
4:L:136:VAL:HG12	4:L:136:VAL:O	2.18	0.43
5:A:401:VAL:CG2	5:A:509:ARG:HG2	2.46	0.43
2:M:39:LEU:HD13	2:M:77:PHE:CD1	2.54	0.43
1:I:181:VAL:O	1:I:182:HIS:HD2	2.02	0.42
1:I:180:GLY:H	1:I:200:VAL:HG23	1.84	0.42
2:M:139:CYS:HG	2:M:199:CYS:CB	2.30	0.42
5:A:480:CYS:O	5:A:483:VAL:HG22	2.18	0.42
3:H:47:TRP:CZ3	4:L:97:LYS:HB2	2.54	0.42
5:A:438:SER:OG	5:A:509:ARG:HG3	2.20	0.42
1:I:213:ILE:HA	1:I:227:LYS:O	2.20	0.42
5:A:395:VAL:HA	5:A:514:SER:O	2.19	0.42
1:I:137:PRO:HA	1:I:162:ASP:O	2.19	0.41
5:A:449:TYR:OH	5:A:498:ARG:NH2	2.53	0.41
2:M:34:ASN:HD22	5:A:449:TYR:HB3	1.84	0.41
3:H:27:PHE:HD2	3:H:32:TYR:CD2	2.38	0.41
1:I:172:TRP:HB3	1:I:177:LEU:HD23	2.02	0.41
2:M:163:ASN:N	2:M:163:ASN:OD1	2.54	0.41



Atom-1	Atom-2	Interatomic $(\mathring{A})$	Clash
1.I.169.TVD.II	1.I.104.TVD.II		$\frac{0.41}{0.41}$
1:1:103:1 Y R:H	1:1:194:1 Y R:H	1.08	0.41
2:M:186:LEU:HD23	2:M:186:LEU:HA	1.95	0.41
3:H:30:ASP:O	3:H:53:TRP:HB2	2.21	0.41
1:I:162:ASP:HB3	1:I:193:LEU:HD13	2.03	0.41
5:A:487:ASN:HA	5:A:489:TYR:CZ	2.56	0.41
1:I:161:LYS:HG2	1:I:162:ASP:OD1	2.21	0.41
5:A:411:ALA:HB3	5:A:414:GLN:HB2	2.03	0.40
5:A:379:CYS:HB3	5:A:432:CYS:HG	1.85	0.40
1:I:33:TRP:CH2	1:I:52:LYS:HD2	2.57	0.40
1:I:73:SER:HB2	1:I:82:TYR:HB2	2.03	0.40
3:H:71:SER:OG	3:H:80:TYR:HB2	2.22	0.40
5:A:378:LYS:HD2	5:A:380:TYR:CZ	2.56	0.40
5:A:453:TYR:CZ	5:A:493:ARG:HB3	2.56	0.40
1:I:137:PRO:HA	1:I:163:TYR:HB3	2.04	0.40
2:M:122:ILE:HD11	2:M:199:CYS:CB	2.52	0.40
5:A:352:ALA:HA	5:A:466:ARG:HD3	2.03	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	Perce	entiles
1	Ι	224/234~(96%)	204 (91%)	17 (8%)	3 (1%)	12	40
2	М	215/219~(98%)	199 (93%)	16 (7%)	0	100	100
3	Н	219/228~(96%)	202~(92%)	17 (8%)	0	100	100
4	L	211/215~(98%)	197 (93%)	14 (7%)	0	100	100
5	А	192/195~(98%)	170 (88%)	22~(12%)	0	100	100
All	All	1061/1091~(97%)	972 (92%)	86 (8%)	3~(0%)	41	71

All (3) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	Ι	205	SER
1	Ι	204	SER
1	Ι	162	ASP

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Ι	190/195~(97%)	188 (99%)	2(1%)	73 85
2	М	190/192~(99%)	186 (98%)	4 (2%)	53 75
3	Н	184/184~(100%)	183 (100%)	1 (0%)	88 93
4	L	177/179~(99%)	173 (98%)	4 (2%)	50 73
5	А	166/167~(99%)	161 (97%)	5(3%)	41 68
All	All	907/917~(99%)	891 (98%)	16 (2%)	59 78

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Ι	98	CYS
1	Ι	199	VAL
2	М	59	THR
2	М	95	GLN
2	М	159	LEU
2	М	175	ASP
3	Н	120	THR
4	L	22	CYS
4	L	28	ASP
4	L	32	TYR
4	L	89	TYR
5	А	403	ARG
5	А	434	ILE
5	А	438	SER
5	А	458	LYS
5	А	525	CYS



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	Ι	182	HIS
1	Ι	210	GLN
1	Ι	222	ASN
4	L	40	GLN
4	L	197	GLN
5	А	505	HIS

#### 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 monosaccharides 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,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	Ι	228/234~(97%)	0.11	7 (3%) 49 48	78, 122, 154, 174	0
2	М	217/219~(99%)	-0.12	3 (1%) 75 75	74, 126, 149, 184	0
3	Н	223/228~(97%)	-0.09	1 (0%) 92 93	37, 110, 142, 166	0
4	L	213/215~(99%)	-0.13	0 100 100	30, 104, 134, 210	0
5	А	194/195~(99%)	0.03	13 (6%) 17 17	105, 152, 230, 272	0
All	All	1075/1091~(98%)	-0.04	24 (2%) 62 60	30, 121, 190, 272	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	А	520	ALA	6.0
1	Ι	212	TYR	4.7
5	А	450	ASN	4.1
5	А	521	PRO	3.9
5	А	518	LEU	3.8
5	А	410	ILE	3.5
5	А	522	ALA	3.2
5	А	425	LEU	3.2
5	А	515	PHE	3.2
1	Ι	177	LEU	3.0
5	А	519	HIS	2.9
1	Ι	179	SER	2.7
5	А	356	LYS	2.7
1	Ι	167	PRO	2.7
1	Ι	121	TRP	2.5
5	А	514	SER	2.5
5	А	517	LEU	2.5
5	А	513	LEU	2.4
1	Ι	175	GLY	2.3
1	Ι	180	GLY	2.3



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Mol	Chain	Res	Type	RSRZ
2	М	21	ILE	2.3
2	М	151	VAL	2.3
2	М	86	ALA	2.1
3	Н	30	ASP	2.1

## 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 monosaccharides 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.

