



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:11 PM GMT

PDB ID : 4O3U
Title : Zymogen HGF-beta/MET with Zymogen Activator Peptide ZAP2.3
Authors : Eigenbrot, C.; Landgraf, K.E.; Steffek, M.
Deposited on : 2013-12-18
Resolution : 3.04 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

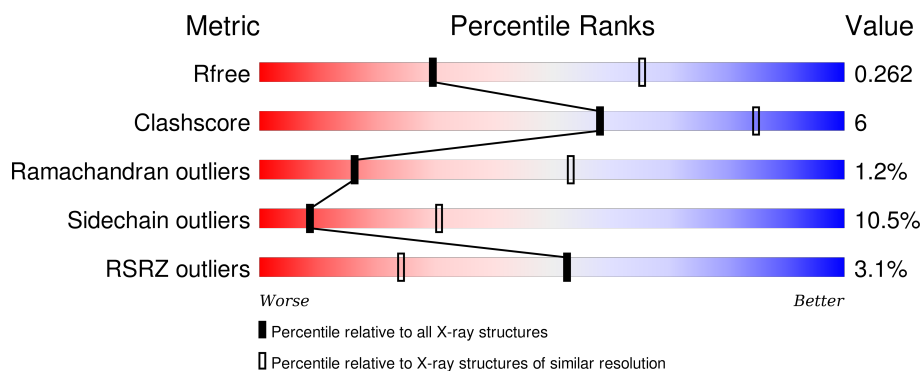
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

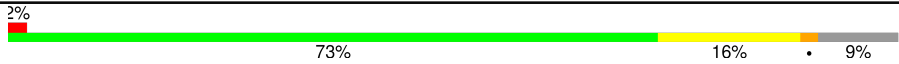


The reported resolution of this entry is 3.04 Å.

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}	91344	1995 (3.08-3.00)
Clashscore	102246	2351 (3.08-3.00)
Ramachandran outliers	100387	2272 (3.08-3.00)
Sidechain outliers	100360	2275 (3.08-3.00)
RSRZ outliers	91569	2013 (3.08-3.00)

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 $\leq 5\%$. 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	240	 2% 73% 16% 9%
2	B	551	 3% 69% 19% 9%
3	P	15	 73% 20% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5786 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 Hepatocyte growth factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	219	1703	1083	301	305	14	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	495	GLY	VAL	ENGINEERED MUTATION	UNP P14210
A	604	SER	CYS	ENGINEERED MUTATION	UNP P14210
A	729	HIS	-	EXPRESSION TAG	UNP P14210
A	730	HIS	-	EXPRESSION TAG	UNP P14210
A	731	HIS	-	EXPRESSION TAG	UNP P14210
A	732	HIS	-	EXPRESSION TAG	UNP P14210
A	733	HIS	-	EXPRESSION TAG	UNP P14210
A	734	HIS	-	EXPRESSION TAG	UNP P14210

- Molecule 2 is a protein called Hepatocyte growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	500	3969	2522	675	743	29	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	568	HIS	-	EXPRESSION TAG	UNP P08581
B	569	HIS	-	EXPRESSION TAG	UNP P08581
B	570	HIS	-	EXPRESSION TAG	UNP P08581
B	571	HIS	-	EXPRESSION TAG	UNP P08581
B	572	HIS	-	EXPRESSION TAG	UNP P08581
B	573	HIS	-	EXPRESSION TAG	UNP P08581
B	574	HIS	-	EXPRESSION TAG	UNP P08581
B	575	HIS	-	EXPRESSION TAG	UNP P08581

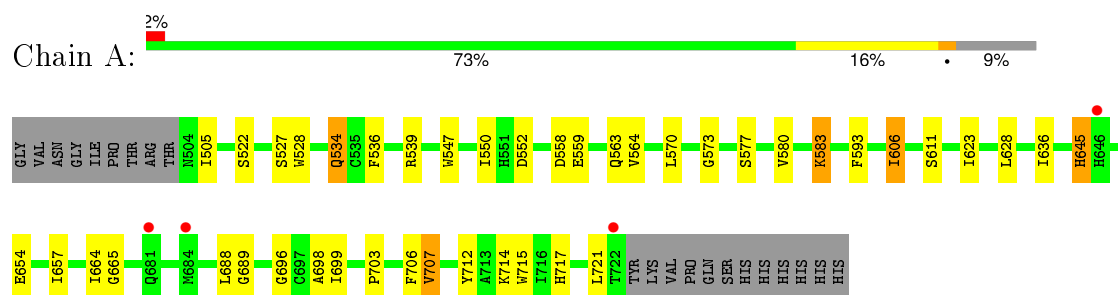
- Molecule 3 is a protein called ZAP 2.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	14	Total	C	N	O	S	0	0	0
			114	72	18	21	3			

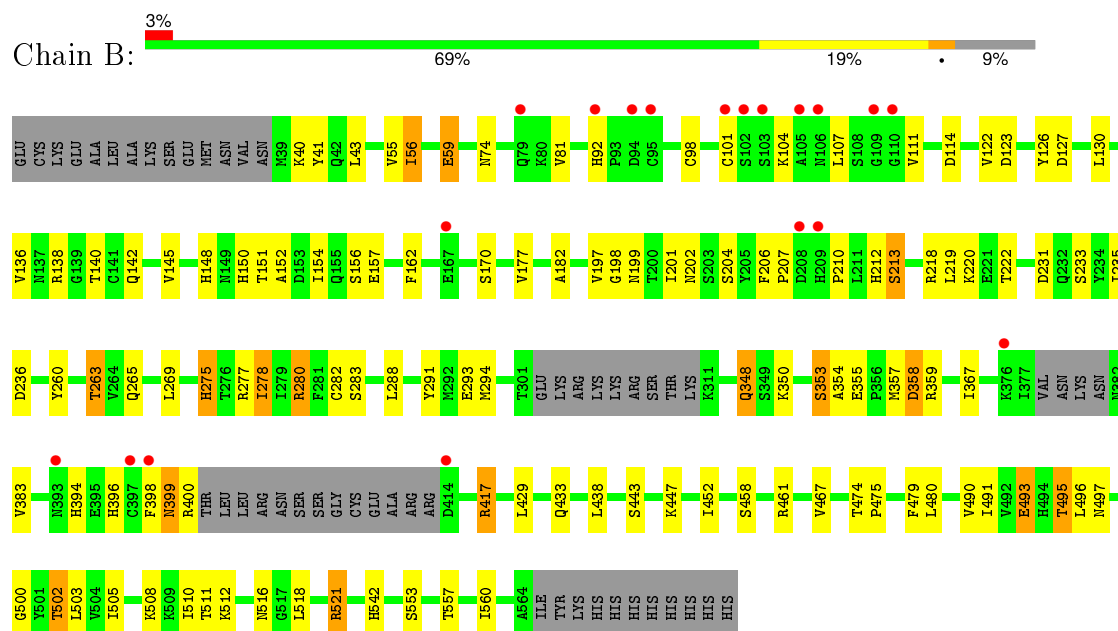
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

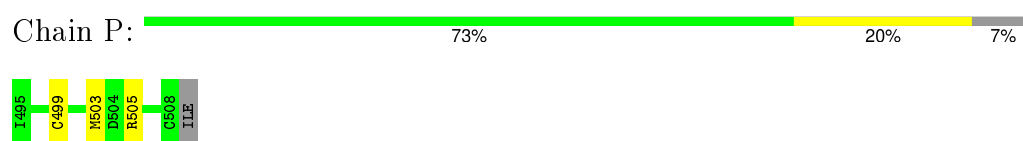
- Molecule 1: Hepatocyte growth factor



- Molecule 2: Hepatocyte growth factor receptor



- Molecule 3: ZAP 2.3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	136.10Å 139.62Å 66.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.76 – 3.04 33.81 – 3.04	Depositor EDS
% Data completeness (in resolution range)	97.5 (34.76-3.04) 97.5 (33.81-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 3.06Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.207 , 0.251 0.221 , 0.262	Depositor DCC
R_{free} test set	1007 reflections (4.32%)	DCC
Wilson B-factor (Å ²)	88.2	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.7	EDS
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 24340 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5786	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.47	0/1744	0.75	0/2362
2	B	0.48	0/4069	0.76	0/5524
3	P	0.50	0/117	0.82	0/157
All	All	0.48	0/5930	0.76	0/8043

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

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	1703	0	1688	18	0
2	B	3969	0	3816	49	0
3	P	114	0	99	1	0
All	All	5786	0	5603	67	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 6.

All (67) 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:534:GLN:HE21	1:A:534:GLN:H	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:461:ARG:HG2	2:B:480:LEU:HD23	1.78	0.65
1:A:606:ILE:HD13	1:A:636:ILE:HG13	1.79	0.64
1:A:606:ILE:HD11	1:A:657:ILE:HD11	1.79	0.63
1:A:577:SER:HB3	1:A:712:TYR:CZ	2.34	0.63
2:B:130:LEU:HD23	2:B:154:ILE:HD11	1.82	0.61
2:B:263:THR:HG22	2:B:277:ARG:HB2	1.84	0.60
2:B:41:TYR:CE2	2:B:521:ARG:HB2	2.38	0.59
2:B:74:ASN:HD22	2:B:81:VAL:HG21	1.68	0.59
2:B:350:LYS:HG3	2:B:355:GLU:HG3	1.85	0.57
2:B:43:LEU:HD21	2:B:518:LEU:HD21	1.87	0.57
2:B:213:SER:HB2	2:B:236:ASP:HA	1.88	0.56
2:B:145:VAL:HB	2:B:157:GLU:HB3	1.88	0.55
2:B:98:CYS:SG	2:B:162:PHE:HB2	2.47	0.55
1:A:534:GLN:H	1:A:534:GLN:NE2	2.03	0.55
1:A:717:HIS:O	1:A:721:LEU:HB2	2.06	0.55
1:A:550:ILE:HD12	1:A:552:ASP:O	2.06	0.54
2:B:348:GLN:HE21	2:B:359:ARG:HD3	1.73	0.54
2:B:55:VAL:HG22	2:B:491:ILE:HD12	1.90	0.54
2:B:199:ASN:HB2	2:B:212:HIS:O	2.08	0.53
2:B:433:GLN:HE22	2:B:474:THR:HA	1.74	0.53
1:A:657:ILE:HG23	1:A:706:PHE:HB2	1.89	0.53
1:A:696:GLY:HA3	1:A:699:ILE:HD11	1.92	0.52
2:B:275:HIS:HD2	2:B:277:ARG:HE	1.58	0.52
2:B:358:ASP:HA	2:B:438:LEU:HB2	1.90	0.51
2:B:503:LEU:HB3	2:B:510:ILE:HD11	1.92	0.51
1:A:547:TRP:CD1	1:A:564:VAL:HB	2.46	0.51
1:A:665:GLY:O	1:A:698:ALA:HB1	2.11	0.50
2:B:263:THR:HG21	2:B:265:GLN:HE21	1.76	0.50
2:B:235:ILE:HD12	2:B:288:LEU:HD12	1.96	0.48
2:B:101:CYS:HB2	2:B:104:LYS:HB2	1.96	0.48
2:B:495:THR:HG23	2:B:500:GLY:HA2	1.95	0.48
2:B:123:ASP:OD2	2:B:126:TYR:HB2	2.14	0.47
2:B:41:TYR:HE2	2:B:521:ARG:HB2	1.79	0.47
2:B:491:ILE:O	2:B:502:THR:HA	2.14	0.47
1:A:645:HIS:HB3	1:A:703:PRO:HD3	1.97	0.46
2:B:288:LEU:O	2:B:417:ARG:NH2	2.48	0.46
1:A:528:TRP:CZ2	1:A:583:LYS:HG3	2.50	0.46
2:B:138:ARG:HH21	2:B:210:PRO:HA	1.81	0.46
2:B:55:VAL:O	2:B:56:ILE:HD12	2.16	0.46
2:B:394:HIS:HD2	2:B:396:HIS:HD2	1.63	0.45
2:B:263:THR:HG23	2:B:265:GLN:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:SER:HB2	3:P:505:ARG:CZ	2.47	0.45
2:B:59:GLU:HB3	2:B:151:THR:HG21	1.98	0.44
2:B:438:LEU:HD23	2:B:458:SER:HB3	1.99	0.44
2:B:493:GLU:O	2:B:500:GLY:HA3	2.17	0.44
2:B:399:ASN:HB3	2:B:400:ARG:H	1.63	0.44
2:B:182:ALA:HA	2:B:198:GLY:O	2.18	0.44
2:B:505:ILE:HG13	2:B:510:ILE:HD12	2.01	0.43
1:A:536:PHE:CE2	1:A:580:VAL:HG11	2.54	0.43
2:B:353:SER:OG	2:B:354:ALA:N	2.52	0.43
2:B:260:TYR:CE2	2:B:280:ARG:HG3	2.54	0.43
2:B:491:ILE:HB	2:B:503:LEU:HB2	2.01	0.43
2:B:218:ARG:HH12	2:B:220:LYS:HA	1.84	0.42
2:B:260:TYR:HD2	2:B:278:ILE:HD11	1.84	0.42
1:A:573:GLY:HA2	1:A:715:TRP:CZ2	2.54	0.42
1:A:505:ILE:H	1:A:505:ILE:HG13	1.73	0.42
2:B:92:HIS:CE1	2:B:107:LEU:HD23	2.54	0.42
2:B:461:ARG:HD3	2:B:479:PHE:C	2.40	0.42
2:B:150:HIS:NE2	2:B:152:ALA:HB3	2.34	0.42
2:B:357:MET:O	2:B:358:ASP:HB2	2.20	0.41
2:B:206:PHE:HA	2:B:207:PRO:HD3	1.92	0.41
2:B:201:ILE:HG22	2:B:202:ASN:N	2.35	0.41
2:B:433:GLN:NE2	2:B:475:PRO:HD3	2.36	0.40
2:B:429:LEU:HD23	2:B:467:VAL:CG1	2.51	0.40
2:B:291:TYR:HB3	2:B:417:ARG:HG3	2.02	0.40
1:A:689:GLY:HA2	1:A:707:VAL:O	2.21	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	217/240 (90%)	197 (91%)	19 (9%)	1 (0%)	34 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	492/551 (89%)	452 (92%)	32 (6%)	8 (2%)	12	45
3	P	12/15 (80%)	11 (92%)	1 (8%)	0	100	100
All	All	721/806 (90%)	660 (92%)	52 (7%)	9 (1%)	16	53

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	204	SER
2	B	148	HIS
2	B	283	SER
2	B	553	SER
1	A	664	ILE
2	B	399	ASN
2	B	156	SER
2	B	233	SER
2	B	542	HIS

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	183/203 (90%)	165 (90%)	18 (10%)	10	34
2	B	451/499 (90%)	403 (89%)	48 (11%)	8	30
3	P	12/13 (92%)	10 (83%)	2 (17%)	3	12
All	All	646/715 (90%)	578 (90%)	68 (10%)	8	31

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	522	SER
1	A	527	SER
1	A	534	GLN
1	A	539	ARG
1	A	558	ASP

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Mol	Chain	Res	Type
1	A	559	GLU
1	A	563	GLN
1	A	570	LEU
1	A	583	LYS
1	A	593	PHE
1	A	606	ILE
1	A	623	ILE
1	A	628	LEU
1	A	645	HIS
1	A	654	GLU
1	A	688	LEU
1	A	707	VAL
1	A	714	LYS
2	B	40	LYS
2	B	56	ILE
2	B	59	GLU
2	B	111	VAL
2	B	114	ASP
2	B	122	VAL
2	B	127	ASP
2	B	136	VAL
2	B	140	THR
2	B	142	GLN
2	B	170	SER
2	B	177	VAL
2	B	197	VAL
2	B	213	SER
2	B	219	LEU
2	B	222	THR
2	B	231	ASP
2	B	263	THR
2	B	269	LEU
2	B	275	HIS
2	B	278	ILE
2	B	280	ARG
2	B	282	CYS
2	B	293	GLU
2	B	294	MET
2	B	348	GLN
2	B	353	SER
2	B	358	ASP
2	B	367	ILE

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Mol	Chain	Res	Type
2	B	383	VAL
2	B	398	PHE
2	B	417	ARG
2	B	443	SER
2	B	447	LYS
2	B	452	ILE
2	B	490	VAL
2	B	493	GLU
2	B	495	THR
2	B	496	LEU
2	B	497	ASN
2	B	502	THR
2	B	508	LYS
2	B	511	THR
2	B	512	LYS
2	B	516	ASN
2	B	521	ARG
2	B	557	THR
2	B	560	ILE
3	P	499	CYS
3	P	503	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	534	GLN
2	B	53	GLN
2	B	74	ASN
2	B	171	GLN
2	B	275	HIS
2	B	318	GLN
2	B	348	GLN
2	B	388	HIS
2	B	394	HIS
2	B	396	HIS
2	B	433	GLN
2	B	484	HIS
2	B	497	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 ⓘ

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	219/240 (91%)	-0.08	4 (1%) 71 43	54, 81, 126, 155	0
2	B	500/551 (90%)	0.08	19 (3%) 44 19	57, 94, 143, 173	7 (1%)
3	P	14/15 (93%)	-0.28	0 100 100	63, 79, 91, 100	0
All	All	733/806 (90%)	0.03	23 (3%) 52 24	54, 89, 138, 173	7 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	110	GLY	7.4
2	B	109	GLY	6.2
2	B	208	ASP	5.0
2	B	105	ALA	4.9
2	B	397	CYS	4.2
2	B	414	ASP	3.8
2	B	95	CYS	3.5
2	B	376	LYS	3.5
2	B	94	ASP	3.4
2	B	92	HIS	3.4
1	A	722	THR	3.3
2	B	101	CYS	3.2
1	A	646	HIS	3.1
2	B	393	ASN	3.1
2	B	106	ASN	3.0
2	B	167	GLU	2.9
2	B	79	GLN	2.5
2	B	102	SER	2.5
2	B	103	SER	2.4
1	A	684	MET	2.4
2	B	398	PHE	2.3
2	B	209	HIS	2.2
1	A	681	GLN	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 [i](#)

There are no such residues in this entry.