Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 06:36 AM JST

PDB ID	:	7F5O
Title	:	Crystal structure of PTPN2 catalytic domain
Authors	:	Singh, J.P.; Lin, M.-J.; Hsu, S.-F.; Lee, C.-C.; Meng, T.-C.
Deposited on	:	2021-06-22
Resolution	:	1.70 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*
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.

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

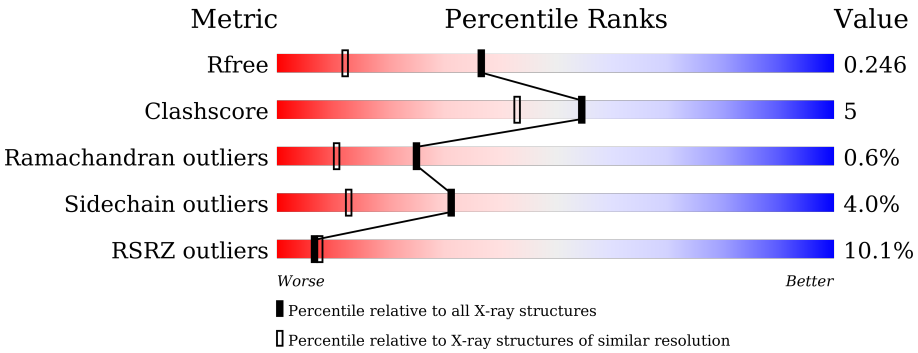
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 >=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	A	305	7% 84% 11% • •
1	B	305	13% 74% 14% • 11%
1	C	305	8% 78% 12% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7514 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 Tyrosine-protein phosphatase non-receptor type 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2408	1528	420	447	13			
1	B	271	Total	C	N	O	S	0	0	0
			2227	1411	388	416	12			
1	C	281	Total	C	N	O	S	0	0	0
			2320	1473	407	428	12			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P17706
A	-1	ASN	-	expression tag	UNP P17706
A	0	ALA	-	expression tag	UNP P17706
B	-2	SER	-	expression tag	UNP P17706
B	-1	ASN	-	expression tag	UNP P17706
B	0	ALA	-	expression tag	UNP P17706
C	-2	SER	-	expression tag	UNP P17706
C	-1	ASN	-	expression tag	UNP P17706
C	0	ALA	-	expression tag	UNP P17706

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	I	0	0
			3	3		
2	B	1	Total	I	0	0
			1	1		
2	C	2	Total	I	0	0
			2	2		

- Molecule 3 is water.

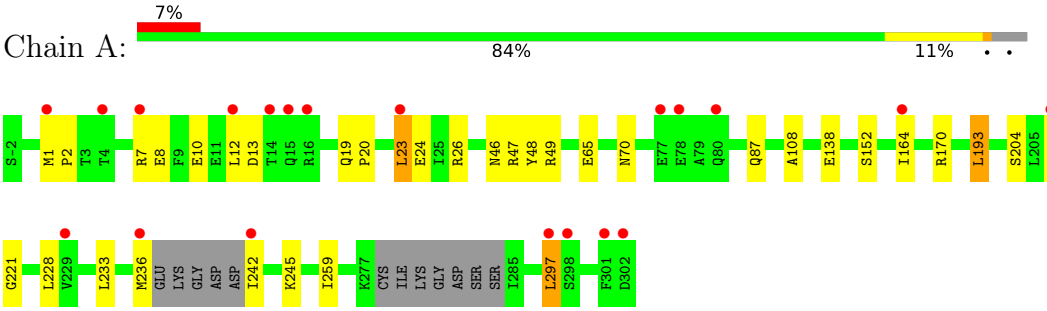
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	197	Total O 197 197	0	0
3	B	149	Total O 149 149	0	0
3	C	207	Total O 207 207	0	0

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.

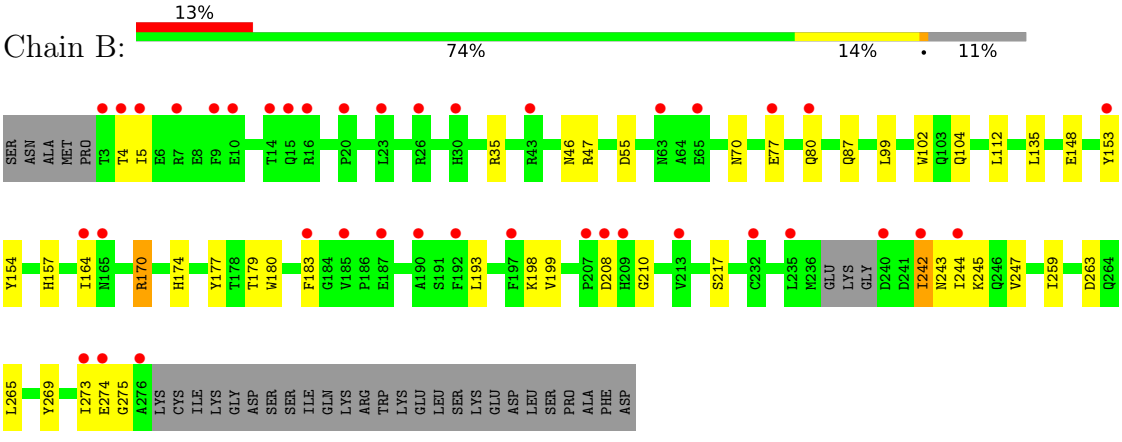
• Molecule 1: Tyrosine-protein phosphatase non-receptor type 2

Chain A:



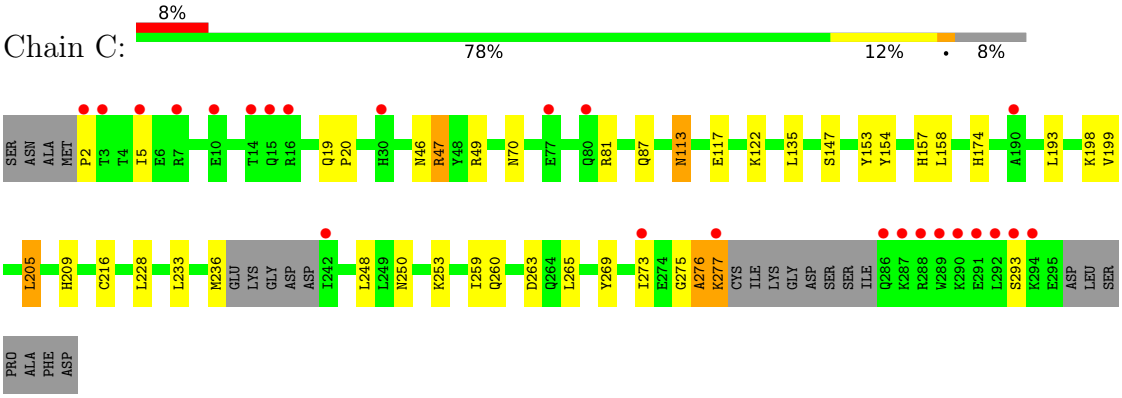
• Molecule 1: Tyrosine-protein phosphatase non-receptor type 2

Chain B:



• Molecule 1: Tyrosine-protein phosphatase non-receptor type 2

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.09Å 68.19Å 72.68Å 111.54° 102.66° 92.34°	Depositor
Resolution (Å)	24.85 – 1.70 24.84 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.0 (24.85-1.70) 95.9 (24.84-1.70)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.48 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.199 , 0.241 0.207 , 0.246	Depositor DCC
R_{free} test set	4868 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	12.3	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7514	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: IOD

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	0.80	1/2466 (0.0%)	0.91	2/3338 (0.1%)
1	B	0.72	0/2281	0.87	0/3092
1	C	0.78	0/2376	0.92	2/3214 (0.1%)
All	All	0.77	1/7123 (0.0%)	0.90	4/9644 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	GLU	CD-OE1	9.68	1.36	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2	PRO	CA-N-CD	-5.95	103.17	111.50
1	A	193	LEU	CB-CG-CD1	5.77	120.81	111.00
1	C	47	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	49	ARG	NE-CZ-NH2	5.18	122.89	120.30

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	2408	0	2360	20	0
1	B	2227	0	2167	30	0
1	C	2320	0	2277	22	0
2	A	3	0	0	2	0
2	B	1	0	0	0	0
2	C	2	0	0	1	0
3	A	197	0	0	6	0
3	B	149	0	0	7	1
3	C	207	0	0	2	1
All	All	7514	0	6804	72	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 5.

All (72) 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:26:ARG:NH2	3:A:501:HOH:O	1.81	1.07
1:A:138:GLU:OE2	3:A:502:HOH:O	1.85	0.93
1:B:217:SER:CB	3:B:520:HOH:O	2.30	0.79
1:B:217:SER:CA	3:B:520:HOH:O	2.35	0.74
3:A:558:HOH:O	2:C:401:IOD:I	2.76	0.73
1:B:102:TRP:CZ3	1:B:170:ARG:HG3	2.23	0.72
1:A:1:MET:SD	1:A:7:ARG:NH2	2.62	0.72
1:C:275:GLY:O	1:C:277:LYS:N	2.21	0.72
1:B:217:SER:HA	3:B:520:HOH:O	1.91	0.71
1:B:157:HIS:HD2	1:B:174:HIS:ND1	1.89	0.70
1:C:47:ARG:H	1:C:87:GLN:HE22	1.39	0.69
1:A:23:LEU:HD12	3:A:686:HOH:O	1.93	0.68
1:B:164:ILE:HD11	3:B:626:HOH:O	1.94	0.67
1:A:47:ARG:H	1:A:87:GLN:HE22	1.45	0.62
1:B:242:ILE:HG13	1:B:247:VAL:HG21	1.80	0.61
1:B:35:ARG:HG2	1:B:55:ASP:OD2	2.00	0.61
1:B:47:ARG:H	1:B:87:GLN:HE22	1.48	0.61
1:B:217:SER:HB2	3:B:520:HOH:O	1.98	0.61
1:C:153:TYR:CE1	1:C:293:SER:HB2	2.36	0.60
1:C:157:HIS:HD2	1:C:174:HIS:ND1	2.02	0.57
1:B:153:TYR:HB2	1:B:179:THR:OG1	2.04	0.57
1:C:49:ARG:HG3	3:C:576:HOH:O	2.03	0.57
1:A:152:SER:HA	1:A:297:LEU:HD11	1.86	0.57
1:C:154:TYR:OH	1:C:198:LYS:HE3	2.05	0.57
1:A:8:GLU:O	1:A:12:LEU:HD23	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ALA:HB2	1:A:204:SER:CB	2.35	0.56
1:C:5:ILE:HG22	1:C:273:ILE:HD11	1.86	0.56
1:A:170:ARG:NH2	3:A:503:HOH:O	1.90	0.56
1:C:236:MET:HE1	1:C:276:ALA:HB2	1.87	0.56
1:B:47:ARG:H	1:B:87:GLN:NE2	2.03	0.56
1:B:242:ILE:HD11	1:B:244:ILE:HA	1.87	0.56
1:B:102:TRP:O	1:B:170:ARG:NH1	2.38	0.56
1:A:47:ARG:H	1:A:87:GLN:NE2	2.03	0.55
3:A:558:HOH:O	1:C:260:GLN:HG3	2.06	0.55
1:A:236:MET:HG2	1:A:242:ILE:HD12	1.89	0.55
1:C:19:GLN:HB3	1:C:20:PRO:HD3	1.90	0.54
1:A:24:GLU:OE2	1:A:245:LYS:NZ	2.40	0.54
1:A:108:ALA:HB2	1:A:204:SER:HB3	1.90	0.52
1:C:117:GLU:HB2	1:C:122:LYS:HE2	1.92	0.52
1:B:46:ASN:HD22	1:B:70:ASN:HD22	1.56	0.52
1:C:269:TYR:O	1:C:273:ILE:HG12	2.09	0.52
1:B:157:HIS:CD2	1:B:174:HIS:ND1	2.76	0.51
1:A:2:PRO:HD3	1:B:183:PHE:CZ	2.46	0.51
1:C:46:ASN:HD22	1:C:70:ASN:HD22	1.57	0.51
1:C:47:ARG:H	1:C:87:GLN:NE2	2.09	0.51
1:B:148:GLU:OE1	3:B:501:HOH:O	2.20	0.50
1:C:250:ASN:ND2	1:C:253:LYS:HE2	2.27	0.49
1:C:154:TYR:OH	1:C:198:LYS:CE	2.60	0.49
1:C:135:LEU:HD22	1:C:135:LEU:N	2.29	0.48
1:A:221:GLY:HA3	2:A:401:IOD:I	2.83	0.48
1:B:242:ILE:CD1	1:B:244:ILE:HG13	2.44	0.48
1:B:244:ILE:HD12	1:B:269:TYR:CE2	2.50	0.47
1:B:242:ILE:CG1	1:B:247:VAL:HG21	2.44	0.47
1:A:46:ASN:HD22	1:A:70:ASN:HD22	1.64	0.46
1:C:209:HIS:HD2	3:C:520:HOH:O	1.97	0.46
1:B:157:HIS:HE1	3:B:501:HOH:O	1.99	0.46
1:A:48:TYR:HB3	2:A:403:IOD:I	2.86	0.45
1:B:104:GLN:O	1:B:210:GLY:HA3	2.17	0.45
1:B:208:ASP:OD1	1:B:208:ASP:N	2.50	0.45
1:A:19:GLN:HB2	1:A:20:PRO:HD3	1.98	0.45
1:B:177:TYR:CD1	1:B:180:TRP:HB2	2.52	0.45
1:A:206:ASN:HB3	1:A:207:PRO:HD2	2.00	0.44
1:B:46:ASN:ND2	1:B:70:ASN:HD22	2.16	0.43
1:A:108:ALA:CB	1:A:204:SER:HB3	2.49	0.42
1:C:199:VAL:HG12	1:C:205:LEU:HD22	2.01	0.42
1:C:113:ASN:HD22	1:C:216:CYS:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:TYR:OH	1:B:198:LYS:HG3	2.20	0.41
1:B:243:ASN:OD1	1:B:245:LYS:HB3	2.20	0.41
1:B:242:ILE:C	1:B:242:ILE:HD13	2.40	0.41
1:C:147:SER:HB3	1:C:158:LEU:HB2	2.02	0.41
1:C:157:HIS:CD2	1:C:174:HIS:ND1	2.86	0.41
1:B:5:ILE:HG22	1:B:273:ILE:HD11	2.03	0.41

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)
3:B:611:HOH:O	3:C:640:HOH:O[1_445]	1.83	0.37

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	287/305 (94%)	279 (97%)	7 (2%)	1 (0%)	41 24
1	B	267/305 (88%)	254 (95%)	11 (4%)	2 (1%)	22 8
1	C	275/305 (90%)	263 (96%)	10 (4%)	2 (1%)	22 8
All	All	829/915 (91%)	796 (96%)	28 (3%)	5 (1%)	25 11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	276	ALA
1	B	259	ILE
1	A	259	ILE
1	C	259	ILE
1	B	275	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	269/279 (96%)	261 (97%)	8 (3%)	41 22
1	B	249/279 (89%)	236 (95%)	13 (5%)	23 8
1	C	259/279 (93%)	249 (96%)	10 (4%)	32 13
All	All	777/837 (93%)	746 (96%)	31 (4%)	31 13

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	13	ASP
1	A	23	LEU
1	A	164	ILE
1	A	193	LEU
1	A	228	LEU
1	A	233	LEU
1	A	297	LEU
1	B	4	THR
1	B	77	GLU
1	B	80	GLN
1	B	99	LEU
1	B	112	LEU
1	B	135	LEU
1	B	170	ARG
1	B	193	LEU
1	B	199	VAL
1	B	242	ILE
1	B	263	ASP
1	B	265	LEU
1	B	274	GLU
1	C	81	ARG
1	C	113	ASN
1	C	193	LEU
1	C	205	LEU
1	C	228	LEU

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Mol	Chain	Res	Type
1	C	233	LEU
1	C	248	LEU
1	C	263	ASP
1	C	265	LEU
1	C	277	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	46	ASN
1	A	56	HIS
1	A	63	ASN
1	A	80	GLN
1	A	87	GLN
1	A	132	GLN
1	B	46	ASN
1	B	80	GLN
1	B	87	GLN
1	B	113	ASN
1	B	132	GLN
1	B	157	HIS
1	B	165	ASN
1	C	15	GLN
1	C	46	ASN
1	C	80	GLN
1	C	87	GLN
1	C	113	ASN
1	C	125	GLN
1	C	157	HIS
1	C	165	ASN
1	C	209	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)

Of 6 ligands modelled in this entry, 6 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 (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^{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	293/305 (96%)	0.47	22 (7%) 14 16	4, 16, 40, 53	0
1	B	271/305 (88%)	0.80	39 (14%) 2 2	9, 21, 46, 59	0
1	C	281/305 (92%)	0.47	24 (8%) 10 12	3, 15, 44, 54	0
All	All	845/915 (92%)	0.57	85 (10%) 7 8	3, 18, 44, 59	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	PHE	5.4
1	C	287	LYS	5.3
1	A	302	ASP	5.0
1	C	14	THR	4.9
1	A	298	SER	4.8
1	A	77	GLU	4.6
1	C	2	PRO	4.6
1	A	14	THR	4.3
1	B	7	ARG	4.3
1	C	291	GLU	4.1
1	C	289	TRP	3.9
1	C	30	HIS	3.9
1	A	16	ARG	3.8
1	A	208	ASP	3.7
1	A	297	LEU	3.7
1	B	240	ASP	3.6
1	A	207	PRO	3.6
1	B	16	ARG	3.6
1	B	23	LEU	3.6
1	B	153	TYR	3.5
1	B	208	ASP	3.5
1	B	30	HIS	3.5
1	A	242	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	286	GLN	3.5
1	C	293	SER	3.4
1	B	165	ASN	3.3
1	B	187	GLU	3.3
1	C	290	LYS	3.2
1	C	294	LYS	3.2
1	B	276	ALA	3.1
1	B	244	ILE	3.1
1	B	15	GLN	3.1
1	A	7	ARG	3.1
1	C	292	LEU	3.1
1	B	77	GLU	3.0
1	B	164	ILE	3.0
1	B	9	PHE	3.0
1	B	3	THR	2.9
1	B	273	ILE	2.9
1	C	15	GLN	2.9
1	C	10	GLU	2.9
1	C	190	ALA	2.9
1	A	4	THR	2.9
1	B	192	PHE	2.8
1	B	43	ARG	2.8
1	B	274	GLU	2.8
1	B	63	ASN	2.8
1	B	207	PRO	2.8
1	A	78	GLU	2.8
1	C	288	ARG	2.7
1	A	164	ILE	2.7
1	C	7	ARG	2.7
1	B	65	GLU	2.7
1	A	15	GLN	2.7
1	B	10	GLU	2.6
1	A	236	MET	2.6
1	B	80	GLN	2.6
1	B	20	PRO	2.6
1	B	185	VAL	2.5
1	B	197	PHE	2.4
1	A	80	GLN	2.4
1	B	235	LEU	2.4
1	B	14	THR	2.4
1	B	209	HIS	2.4
1	B	213	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	23	LEU	2.3
1	C	242	ILE	2.3
1	B	232	CYS	2.3
1	C	77	GLU	2.2
1	A	206	ASN	2.2
1	B	190	ALA	2.2
1	B	242	ILE	2.2
1	C	3	THR	2.2
1	A	229	VAL	2.2
1	C	273	ILE	2.2
1	B	4	THR	2.2
1	C	277	LYS	2.1
1	A	301	PHE	2.1
1	C	80	GLN	2.1
1	A	12	LEU	2.1
1	C	5	ILE	2.1
1	B	26	ARG	2.0
1	C	16	ARG	2.0
1	B	5	ILE	2.0
1	A	1	MET	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 monosaccharides in this entry.

6.4 Ligands (i)

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. 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	B-factors(Å^2)	Q<0.9
2	IOD	A	402	1/1	0.97	0.06	23,23,23,23	0
2	IOD	C	402	1/1	0.98	0.10	31,31,31,31	0
2	IOD	C	401	1/1	0.99	0.08	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	IOD	B	401	1/1	0.99	0.09	27,27,27,27	0
2	IOD	A	403	1/1	1.00	0.09	22,22,22,22	0
2	IOD	A	401	1/1	1.00	0.03	8,8,8,8	0

6.5 Other polymers (i)

There are no such residues in this entry.