



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:49 PM GMT

PDB ID : 4DJZ
Title : Catalytic fragment of masp-1 in complex with its specific inhibitor developed by directed evolution on sgci scaffold
Authors : Heja, D.; Harmat, V.; Fodor, K.; Wilmanns, M.; Dobo, J.; Kekesi, K.A.; Zavodszky, P.; Gal, P.; Pal, G.
Deposited on : 2012-02-03
Resolution : 3.20 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

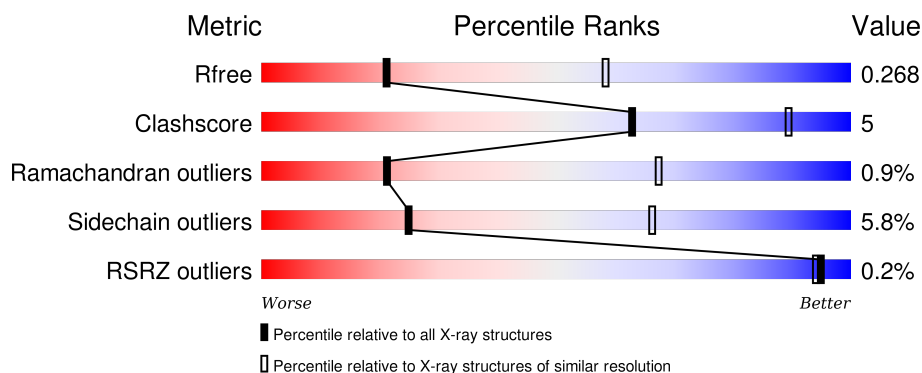
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	155	<div> <div>79%</div> <div>15%</div> <div>5%</div> </div>
1	C	155	<div> <div>84%</div> <div>12%</div> <div>5%</div> </div>
2	B	251	<div> <div>82%</div> <div>17%</div> <div>.</div> </div>
2	D	251	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>
3	H	38	<div> <div>74%</div> <div>8%</div> <div>8%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	38	 A horizontal bar chart showing the quality of chain I. The bar is divided into four segments: a long green segment (71%), a yellow segment (13%), a small orange segment (13%), and a grey segment (13%). A small black dot is located on the orange segment.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6465 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 Mannan-binding lectin serine protease 1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1099	700	180	207	12			
1	C	148	Total	C	N	O	S	0	0	0
			1096	695	181	208	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	ALA	-	EXPRESSION TAG	UNP P48740
A	295	SER	-	EXPRESSION TAG	UNP P48740
A	296	MET	-	EXPRESSION TAG	UNP P48740
A	297	THR	-	EXPRESSION TAG	UNP P48740
C	294	ALA	-	EXPRESSION TAG	UNP P48740
C	295	SER	-	EXPRESSION TAG	UNP P48740
C	296	MET	-	EXPRESSION TAG	UNP P48740
C	297	THR	-	EXPRESSION TAG	UNP P48740

- Molecule 2 is a protein called Mannan-binding lectin serine protease 1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	251	Total	C	N	O	S	0	2	0
			1918	1211	337	357	13			
2	D	251	Total	C	N	O	S	0	1	0
			1873	1186	321	353	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	499	LYS	GLU	VARIANT	UNP P48740
D	499	LYS	GLU	VARIANT	UNP P48740

- Molecule 3 is a protein called Protease inhibitor SGPI-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	34	Total	C	N	O	S	0	0	0
			241	143	43	49	6			
3	I	33	Total	C	N	O	S	0	0	0
			236	141	43	46	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	GLY	-	EXPRESSION TAG	UNP O46162
H	2	SER	-	EXPRESSION TAG	UNP O46162
H	3	GLY	-	EXPRESSION TAG	UNP O46162
H	30	PHE	ALA	ENGINEERED MUTATION	UNP O46162
H	33	ARG	LEU	ENGINEERED MUTATION	UNP O46162
H	35	LEU	ALA	ENGINEERED MUTATION	UNP O46162
H	37	TYR	PRO	ENGINEERED MUTATION	UNP O46162
I	1	GLY	-	EXPRESSION TAG	UNP O46162
I	2	SER	-	EXPRESSION TAG	UNP O46162
I	3	GLY	-	EXPRESSION TAG	UNP O46162
I	30	PHE	ALA	ENGINEERED MUTATION	UNP O46162
I	33	ARG	LEU	ENGINEERED MUTATION	UNP O46162
I	35	LEU	ALA	ENGINEERED MUTATION	UNP O46162
I	37	TYR	PRO	ENGINEERED MUTATION	UNP O46162


- Molecule 4 is water.

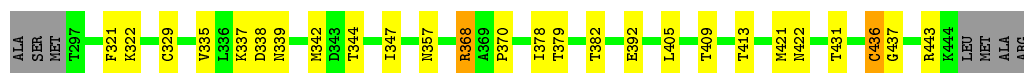
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		

3 Residue-property plots [i](#)


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: Mannan-binding lectin serine protease 1 heavy chain

Chain A: 




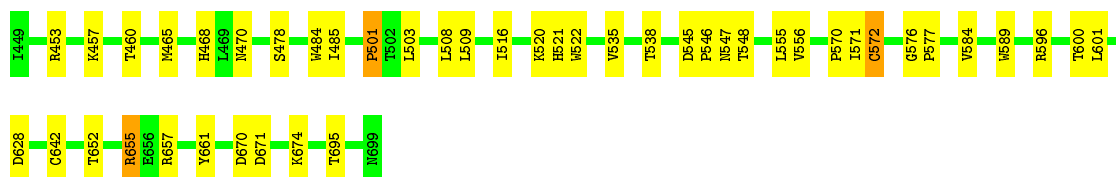
- Molecule 1: Mannan-binding lectin serine protease 1 heavy chain

Chain C: 




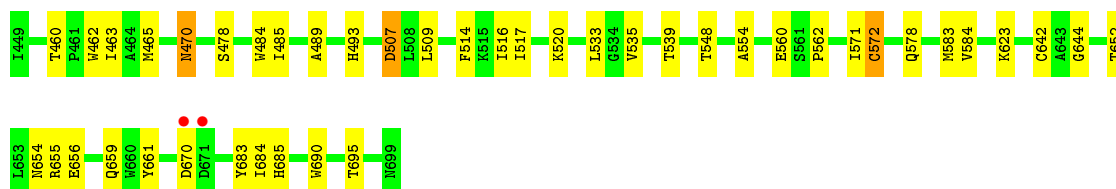
- Molecule 2: Mannan-binding lectin serine protease 1 light chain

Chain B: 



- Molecule 2: Mannan-binding lectin serine protease 1 light chain

Chain D: 

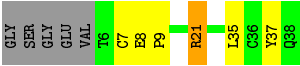


- Molecule 3: Protease inhibitor SGPI-2

Chain H: 



● Molecule 3: Protease inhibitor SGPI-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.33Å 98.40Å 155.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.91 – 3.20 46.91 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.91-3.20) 99.7 (46.91-3.20)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.228 , 0.274 0.220 , 0.268	Depositor DCC
R_{free} test set	954 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 18639 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6465	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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 [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	0.44	0/1126	0.55	0/1538
1	C	0.44	0/1123	0.56	0/1537
2	B	0.54	1/1977 (0.1%)	0.55	0/2694
2	D	0.55	2/1929 (0.1%)	0.54	0/2638
3	H	0.33	0/244	0.48	0/328
3	I	0.32	0/239	0.50	0/319
All	All	0.50	3/6638 (0.0%)	0.55	0/9054

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	589	TRP	CD2-CE2	5.10	1.47	1.41
2	D	690	TRP	CD2-CE2	5.05	1.47	1.41
2	D	462	TRP	CD2-CE2	5.01	1.47	1.41

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	A	1099	0	1010	11	0
1	C	1096	0	1002	7	0
2	B	1918	0	1796	24	0
2	D	1873	0	1708	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	241	0	205	2	0
3	I	236	0	207	4	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
All	All	6465	0	5928	65	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 5.

All (65) 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:C:382:THR:HG22	1:C:383:ARG:H	1.36	0.91
2:B:576:GLY:HA3	2:D:470:ASN:HB2	1.57	0.86
2:D:584:VAL:HG12	2:D:652:THR:HG23	1.70	0.73
2:B:584:VAL:HG12	2:B:652:THR:HG23	1.80	0.64
2:B:485:ILE:HD13	2:B:516:ILE:HG21	1.80	0.63
2:D:465:MET:HE2	2:D:517:ILE:HD12	1.80	0.62
1:A:405:LEU:HD12	1:A:431:THR:HB	1.81	0.61
2:D:460:THR:O	2:D:463:ILE:HG22	2.03	0.58
1:A:392:GLU:HG2	1:A:413:THR:HB	1.84	0.58
2:B:600:THR:HG22	2:B:601:LEU:N	2.19	0.57
2:D:485:ILE:HD13	2:D:516:ILE:HG21	1.87	0.57
2:B:501:PRO:HB3	2:B:547:ASN:OD1	2.04	0.57
1:C:382:THR:HG22	1:C:383:ARG:N	2.15	0.56
3:H:6:THR:HG22	3:H:7:CYS:H	1.70	0.56
2:D:654:ASN:HB2	2:D:661:TYR:CE2	2.42	0.54
2:B:577:PRO:HB2	3:I:37:TYR:HB3	1.91	0.53
2:D:485:ILE:CD1	2:D:516:ILE:HG21	2.38	0.53
2:D:571:ILE:HG13	2:D:572:CYS:N	2.24	0.52
2:D:465:MET:HE1	2:D:520:LYS:HE2	1.92	0.51
2:D:571:ILE:HG13	2:D:572:CYS:H	1.75	0.51
2:B:485:ILE:CD1	2:B:516:ILE:HG21	2.40	0.51
2:B:538:THR:HG22	2:B:556:VAL:HG22	1.94	0.50
3:H:9:PRO:HA	3:H:22:CYS:HB3	1.94	0.50
2:B:465:MET:HE1	2:B:520:LYS:HE2	1.95	0.49
2:B:484:TRP:CD2	2:B:695:THR:HG22	2.47	0.49
1:A:337:LYS:O	1:A:338:ASP:C	2.50	0.49
1:C:338:ASP:C	1:C:340:VAL:H	2.15	0.48
2:B:600:THR:CG2	2:B:601:LEU:N	2.77	0.47
1:A:436:CYS:HA	2:B:570:PRO:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:572:CYS:HB3	2:B:661:TYR:CD1	2.50	0.47
2:D:655:ARG:HA	2:D:656:GLU:HA	1.77	0.46
2:D:583:MET:O	2:D:652:THR:HG22	2.15	0.46
2:B:535:VAL:HG13	2:B:556:VAL:HG13	1.97	0.45
2:B:600:THR:HG22	2:B:601:LEU:O	2.16	0.45
2:D:489:ALA:HA	2:D:554:ALA:HB2	1.97	0.45
1:A:329:CYS:SG	1:A:335:VAL:HG22	2.57	0.45
1:A:370:PRO:HB2	1:A:378:ILE:HD13	1.99	0.44
1:C:443:ARG:HG2	1:C:443:ARG:H	1.62	0.44
2:B:468:HIS:C	2:B:470:ASN:N	2.71	0.44
2:D:484:TRP:CD2	2:D:695:THR:HG22	2.53	0.44
2:B:503:LEU:HD21	2:B:508:LEU:HD21	1.98	0.44
2:B:520:LYS:HE3	2:B:522:TRP:O	2.18	0.44
2:D:478:SER:O	2:D:485:ILE:HA	2.19	0.43
2:D:533:LEU:HD11	2:D:562:PRO:HB3	2.01	0.43
2:D:644:GLY:HA3	3:I:35:LEU:HG	2.00	0.43
2:B:655:ARG:HA	2:B:657:ARG:H	1.84	0.43
2:B:521:HIS:CE1	2:B:600:THR:HG23	2.53	0.42
1:A:409:THR:HG23	1:A:422:ASN:HD21	1.83	0.42
1:C:350:LEU:HD12	1:C:354:THR:HG23	2.01	0.42
2:D:578:GLN:HE22	2:D:661:TYR:HE1	1.65	0.42
2:D:683:TYR:CE2	2:D:685:HIS:HB3	2.54	0.42
1:A:321:PHE:O	1:A:322:LYS:HB2	2.20	0.42
1:C:359:ILE:H	1:C:359:ILE:HD12	1.83	0.42
1:A:347:ILE:HG22	1:A:357:ASN:HB2	2.02	0.42
1:C:314:PRO:HD2	1:C:325:VAL:HG12	2.02	0.42
3:I:8:GLU:HA	3:I:9:PRO:HD3	1.92	0.41
1:A:338:ASP:HA	1:A:339:ASN:HA	1.66	0.41
2:B:555:LEU:HD13	2:B:695:THR:HG23	2.01	0.41
2:D:623:LYS:HA	3:I:21:ARG:HH21	1.85	0.41
2:B:671:ASP:HB2	2:B:674:LYS:HD2	2.01	0.41
2:B:571:ILE:HG13	2:B:572:CYS:N	2.36	0.41
2:D:493:HIS:HB2	2:D:507:ASP:O	2.21	0.40
2:B:545:ASP:HA	2:B:546:PRO:HD3	1.90	0.40
2:D:514:PHE:CZ	2:D:535:VAL:HG21	2.56	0.40
1:A:342:MET:HG3	1:A:344:THR:O	2.21	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	Percentiles	
1	A	146/155 (94%)	138 (94%)	6 (4%)	2 (1%)	14	57
1	C	146/155 (94%)	133 (91%)	12 (8%)	1 (1%)	26	72
2	B	251/251 (100%)	235 (94%)	13 (5%)	3 (1%)	16	60
2	D	250/251 (100%)	235 (94%)	14 (6%)	1 (0%)	39	80
3	H	32/38 (84%)	27 (84%)	4 (12%)	1 (3%)	5	34
3	I	31/38 (82%)	27 (87%)	4 (13%)	0	100	100
All	All	856/888 (96%)	795 (93%)	53 (6%)	8 (1%)	21	67

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	ARG
1	A	437	GLY
2	B	670	ASP
1	C	437	GLY
2	B	457	LYS
2	D	670	ASP
3	H	10	GLY
2	B	501	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	115/140 (82%)	109 (95%)	6 (5%)	29	69
1	C	116/140 (83%)	109 (94%)	7 (6%)	24	65
2	B	200/215 (93%)	190 (95%)	10 (5%)	30	71
2	D	190/215 (88%)	180 (95%)	10 (5%)	28	69
3	H	26/32 (81%)	22 (85%)	4 (15%)	3	16
3	I	25/32 (78%)	23 (92%)	2 (8%)	15	52
All	All	672/774 (87%)	633 (94%)	39 (6%)	25	66

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	ARG
1	A	379	THR
1	A	382	THR
1	A	421	MET
1	A	436	CYS
1	A	443	ARG
2	B	453	ARG
2	B	460	THR
2	B	478	SER
2	B	509	LEU
2	B	548	THR
2	B	572	CYS
2	B	596	ARG
2	B	628	ASP
2	B	642	CYS
2	B	655	ARG
1	C	301	CYS
1	C	308	VAL
1	C	368	ARG
1	C	406	ASN
1	C	417	GLN
1	C	419	VAL
1	C	436	CYS
2	D	470	ASN
2	D	507	ASP
2	D	509	LEU
2	D	539	THR

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Mol	Chain	Res	Type
2	D	548	THR
2	D	560	GLU
2	D	572	CYS
2	D	642	CYS
2	D	659	GLN
2	D	684	ILE
3	H	6	THR
3	H	7	CYS
3	H	22	CYS
3	H	38	GLN
3	I	7	CYS
3	I	21	ARG

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

Mol	Chain	Res	Type
1	C	316	GLN
1	C	406	ASN
2	D	468	HIS
2	D	470	ASN
2	D	578	GLN
3	I	38	GLN

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 [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, 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	148/155 (95%)	-0.08	0 100 100	30, 45, 70, 99	0
1	C	148/155 (95%)	-0.22	0 100 100	30, 43, 67, 82	0
2	B	251/251 (100%)	-0.33	0 100 100	24, 39, 68, 97	0
2	D	251/251 (100%)	-0.22	2 (0%) 87 80	21, 42, 77, 109	0
3	H	34/38 (89%)	-0.08	0 100 100	66, 81, 109, 122	0
3	I	33/38 (86%)	0.32	0 100 100	62, 74, 99, 102	0
All	All	865/888 (97%)	-0.20	2 (0%) 95 94	21, 44, 82, 122	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	671	ASP	2.4
2	D	670	ASP	2.3

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

There are no such residues in this entry.