



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:51 PM EDT

PDB ID : 6GC1 / pdb_00006gc1
Title : Crystal structure of Trx-like and NHL repeat containing domains of human NHLRC2
Authors : Biterova, E.; Uusimaa, J.; Hinttala, R.; Ruddock, L.W.
Deposited on : 2018-04-16
Resolution : 2.70 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

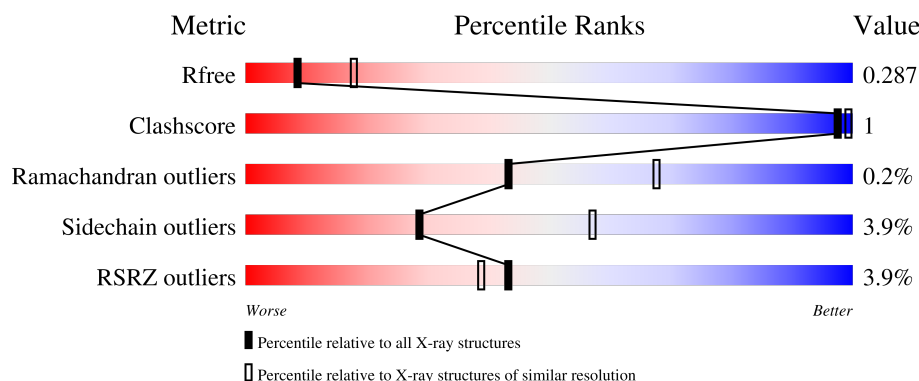
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. 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	579	2% 90% 5%
1	B	579	2% 89% 5% 6%
1	C	579	3% 89% 6% 5%
1	D	579	7% 89% 5% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17055 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 NHL repeat-containing protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4259	2710	717	816	16			
1	B	546	Total	C	N	O	S	0	0	0
			4238	2695	713	814	16			
1	C	551	Total	C	N	O	S	0	0	0
			4269	2714	719	820	16			
1	D	548	Total	C	N	O	S	0	0	0
			4252	2705	716	815	16			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q8NBF2
A	-5	HIS	-	expression tag	UNP Q8NBF2
A	-4	HIS	-	expression tag	UNP Q8NBF2
A	-3	HIS	-	expression tag	UNP Q8NBF2
A	-2	HIS	-	expression tag	UNP Q8NBF2
A	-1	HIS	-	expression tag	UNP Q8NBF2
A	0	HIS	-	expression tag	UNP Q8NBF2
B	-6	MET	-	initiating methionine	UNP Q8NBF2
B	-5	HIS	-	expression tag	UNP Q8NBF2
B	-4	HIS	-	expression tag	UNP Q8NBF2
B	-3	HIS	-	expression tag	UNP Q8NBF2
B	-2	HIS	-	expression tag	UNP Q8NBF2
B	-1	HIS	-	expression tag	UNP Q8NBF2
B	0	HIS	-	expression tag	UNP Q8NBF2
C	-6	MET	-	initiating methionine	UNP Q8NBF2
C	-5	HIS	-	expression tag	UNP Q8NBF2
C	-4	HIS	-	expression tag	UNP Q8NBF2
C	-3	HIS	-	expression tag	UNP Q8NBF2
C	-2	HIS	-	expression tag	UNP Q8NBF2
C	-1	HIS	-	expression tag	UNP Q8NBF2
C	0	HIS	-	expression tag	UNP Q8NBF2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	MET	-	initiating methionine	UNP Q8NBF2
D	-5	HIS	-	expression tag	UNP Q8NBF2
D	-4	HIS	-	expression tag	UNP Q8NBF2
D	-3	HIS	-	expression tag	UNP Q8NBF2
D	-2	HIS	-	expression tag	UNP Q8NBF2
D	-1	HIS	-	expression tag	UNP Q8NBF2
D	0	HIS	-	expression tag	UNP Q8NBF2

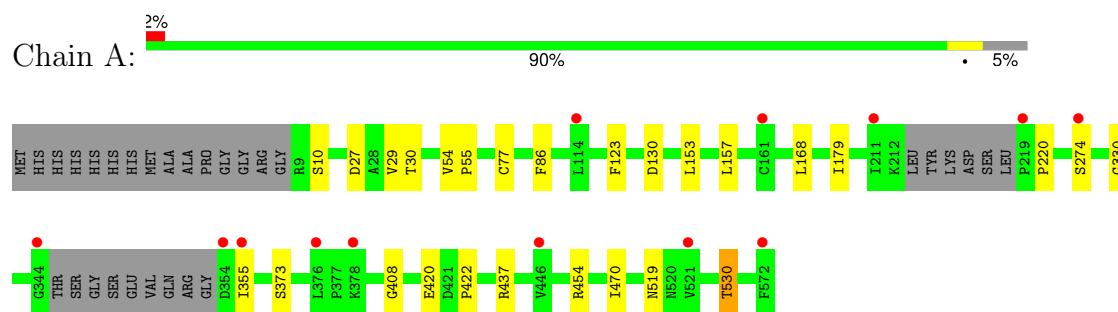
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	13	Total O 13 13	0	0
2	B	10	Total O 10 10	0	0
2	C	6	Total O 6 6	0	0
2	D	8	Total O 8 8	0	0

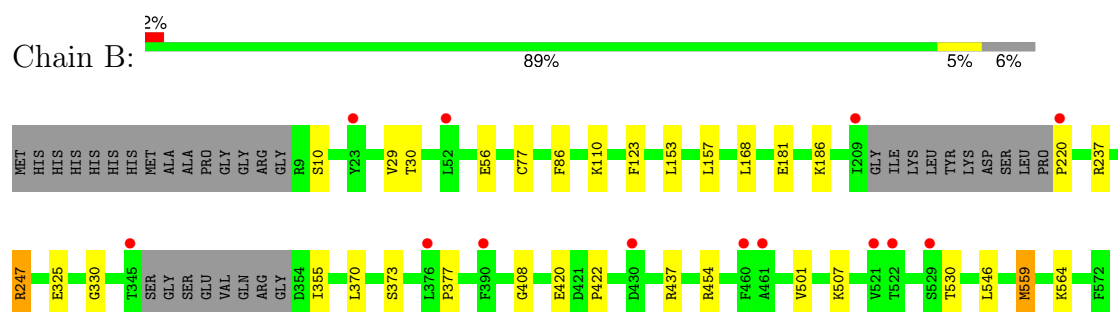
3 Residue-property plots [i](#)

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.

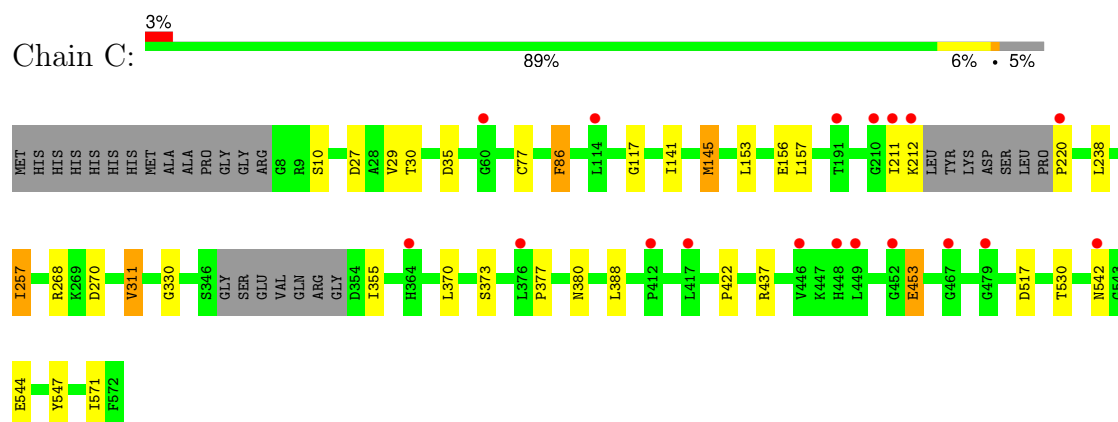
- Molecule 1: NHL repeat-containing protein 2



- Molecule 1: NHL repeat-containing protein 2



- Molecule 1: NHL repeat-containing protein 2



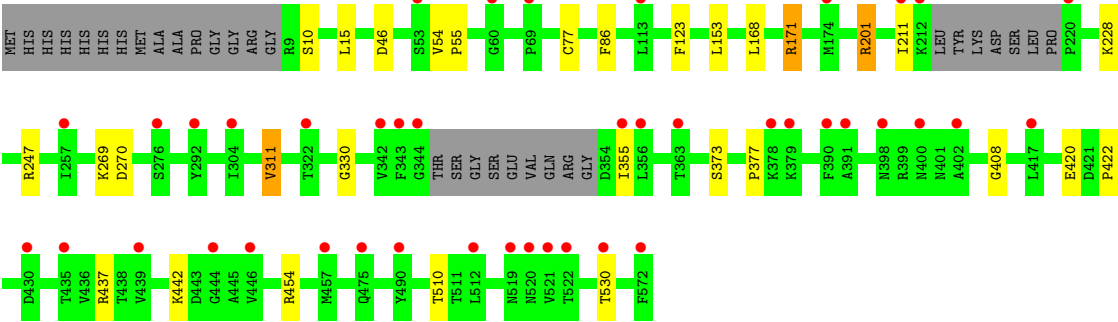
- Molecule 1: NHL repeat-containing protein 2

Chain D:

7%

89%

5% • 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.28Å 103.81Å 114.98Å 90.00° 100.77° 90.00°	Depositor
Resolution (Å)	47.77 – 2.70 47.77 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.77-2.70) 98.9 (47.77-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.246 , 0.287 0.249 , 0.287	Depositor DCC
R_{free} test set	3254 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17055	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.47% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.81	0/4352	1.03	3/5910 (0.1%)
1	B	0.82	0/4330	1.06	2/5881 (0.0%)
1	C	0.81	0/4361	1.03	2/5921 (0.0%)
1	D	0.80	0/4344	1.03	3/5898 (0.1%)
All	All	0.81	0/17387	1.04	10/23610 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	C	0	1
All	All	0	4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	201	ARG	CB-CG-CD	5.63	124.25	111.30
1	A	27	ASP	CA-CB-CG	5.56	118.16	112.60
1	D	123	PHE	CA-C-N	5.56	125.66	119.32
1	D	123	PHE	C-N-CA	5.56	125.66	119.32
1	C	453	GLU	CB-CG-CD	5.45	121.87	112.60
1	B	123	PHE	CA-C-N	5.44	125.53	119.32
1	B	123	PHE	C-N-CA	5.44	125.53	119.32
1	A	123	PHE	CA-C-N	5.27	125.33	119.32
1	A	123	PHE	C-N-CA	5.27	125.33	119.32
1	C	35	ASP	CA-CB-CG	5.09	117.69	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	237	ARG	Sidechain
1	B	247	ARG	Sidechain
1	B	454	ARG	Sidechain
1	C	437	ARG	Sidechain

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	4259	0	4225	6	0
1	B	4238	0	4198	6	0
1	C	4269	0	4233	11	0
1	D	4252	0	4218	7	0
2	A	13	0	0	0	0
2	B	10	0	0	0	0
2	C	6	0	0	0	0
2	D	8	0	0	1	0
All	All	17055	0	16874	28	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 1.

All (28) 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:141:ILE:HG21	1:C:145:MET:HE3	1.71	0.71
1:C:257:ILE:HD11	1:C:571:ILE:HG23	1.76	0.66
1:D:46:ASP:OD1	1:D:171:ARG:NH2	2.38	0.57
1:C:117:GLY:HA3	1:C:145:MET:HE2	1.89	0.53
1:D:408:GLY:O	1:D:437:ARG:NH2	2.42	0.51
1:A:54:VAL:HG12	1:A:55:PRO:O	2.12	0.50
1:B:408:GLY:O	1:B:437:ARG:NH2	2.42	0.49
1:A:408:GLY:O	1:A:437:ARG:NH2	2.42	0.48
1:B:29:VAL:HG23	1:B:30:THR:HG23	1.97	0.47
1:B:56:GLU:HB2	1:D:15:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:VAL:HG12	1:D:55:PRO:O	2.15	0.46
1:C:86:PHE:CE1	1:C:145:MET:HE1	2.51	0.45
1:A:454:ARG:NH1	1:C:517:ASP:OD1	2.46	0.44
1:C:29:VAL:HG23	1:C:30:THR:HG23	1.98	0.44
1:D:270:ASP:HA	1:D:311:VAL:CG1	2.48	0.44
1:C:238:LEU:HD11	1:C:547:TYR:CE2	2.53	0.43
1:A:29:VAL:HG23	1:A:30:THR:HG23	2.00	0.43
1:C:257:ILE:N	1:C:257:ILE:CD1	2.81	0.43
1:C:270:ASP:HA	1:C:311:VAL:CG1	2.49	0.43
1:C:542:ASN:HB2	1:C:544:GLU:HG2	2.01	0.43
1:A:168:LEU:HD12	1:A:168:LEU:N	2.34	0.42
1:B:355:ILE:HG22	1:B:370:LEU:HA	2.00	0.42
1:B:546:LEU:HD23	1:B:559:MET:HE2	2.01	0.42
1:C:355:ILE:HG22	1:C:370:LEU:HA	2.00	0.41
1:D:168:LEU:HD12	1:D:168:LEU:N	2.35	0.41
1:D:269:LYS:NZ	2:D:601:HOH:O	2.52	0.40
1:A:519:ASN:O	1:A:530:THR:HG21	2.22	0.40
1:B:168:LEU:N	1:B:168:LEU:HD12	2.36	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	543/579 (94%)	519 (96%)	22 (4%)	2 (0%)	30	54
1	B	540/579 (93%)	517 (96%)	22 (4%)	1 (0%)	43	68
1	C	545/579 (94%)	521 (96%)	23 (4%)	1 (0%)	43	68
1	D	542/579 (94%)	518 (96%)	23 (4%)	1 (0%)	43	68
All	All	2170/2316 (94%)	2075 (96%)	90 (4%)	5 (0%)	43	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	GLY
1	B	330	GLY
1	C	330	GLY
1	D	330	GLY
1	A	220	PRO

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	472/495 (95%)	458 (97%)	14 (3%)	36	66
1	B	470/495 (95%)	450 (96%)	20 (4%)	26	54
1	C	473/495 (96%)	452 (96%)	21 (4%)	25	53
1	D	471/495 (95%)	452 (96%)	19 (4%)	28	56
All	All	1886/1980 (95%)	1812 (96%)	74 (4%)	28	57

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	77	CYS
1	A	86	PHE
1	A	130	ASP
1	A	153	LEU
1	A	157	LEU
1	A	179	ILE
1	A	274	SER
1	A	355	ILE
1	A	373	SER
1	A	420	GLU
1	A	422	PRO
1	A	470	ILE
1	A	530	THR
1	B	10	SER
1	B	77	CYS
1	B	86	PHE

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Mol	Chain	Res	Type
1	B	110	LYS
1	B	153	LEU
1	B	157	LEU
1	B	181	GLU
1	B	186	LYS
1	B	220	PRO
1	B	247	ARG
1	B	325	GLU
1	B	373	SER
1	B	377	PRO
1	B	420	GLU
1	B	422	PRO
1	B	501	VAL
1	B	507	LYS
1	B	530	THR
1	B	559	MET
1	B	564	LYS
1	C	10	SER
1	C	27	ASP
1	C	77	CYS
1	C	86	PHE
1	C	145	MET
1	C	153	LEU
1	C	156	GLU
1	C	157	LEU
1	C	211	ILE
1	C	212	LYS
1	C	220	PRO
1	C	257	ILE
1	C	268	ARG
1	C	311	VAL
1	C	373	SER
1	C	377	PRO
1	C	380	ASN
1	C	388	LEU
1	C	422	PRO
1	C	453	GLU
1	C	530	THR
1	D	10	SER
1	D	77	CYS
1	D	86	PHE
1	D	153	LEU

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Mol	Chain	Res	Type
1	D	171	ARG
1	D	201	ARG
1	D	211	ILE
1	D	228	LYS
1	D	247	ARG
1	D	311	VAL
1	D	355	ILE
1	D	373	SER
1	D	377	PRO
1	D	420	GLU
1	D	422	PRO
1	D	442	LYS
1	D	454	ARG
1	D	510	THR
1	D	530	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	131	ASN
1	A	487	ASN
1	B	40	GLN
1	B	43	GLN
1	B	131	ASN
1	B	155	GLN
1	B	400	ASN
1	B	476	HIS
1	B	508	ASN
1	C	40	GLN
1	C	131	ASN
1	C	380	ASN
1	C	395	ASN
1	C	400	ASN
1	C	487	ASN
1	D	40	GLN
1	D	50	GLN
1	D	131	ASN
1	D	155	GLN
1	D	395	ASN
1	D	400	ASN
1	D	411	GLN

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Mol	Chain	Res	Type
1	D	487	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 oligosaccharides 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	549/579 (94%)	0.41	13 (2%) 59 56	36, 54, 82, 102	0
1	B	546/579 (94%)	0.60	13 (2%) 59 56	37, 59, 81, 134	0
1	C	551/579 (95%)	0.70	18 (3%) 49 45	42, 64, 91, 122	0
1	D	548/579 (94%)	0.93	42 (7%) 19 17	41, 71, 99, 164	0
All	All	2194/2316 (94%)	0.66	86 (3%) 43 39	36, 62, 92, 164	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	521	VAL	5.4
1	B	521	VAL	4.7
1	D	430	ASP	3.7
1	C	412	PRO	3.6
1	D	220	PRO	3.5
1	D	211	ILE	3.5
1	C	220	PRO	3.5
1	B	209	ILE	3.4
1	D	435	THR	3.4
1	C	479	GLY	3.4
1	D	304	ILE	3.3
1	D	391	ALA	3.2
1	A	219	PRO	3.2
1	D	522	THR	3.2
1	A	211	ILE	3.2
1	D	417	LEU	3.2
1	D	344	GLY	3.2
1	D	444	GLY	3.1
1	B	220	PRO	3.0
1	B	522	THR	3.0
1	D	257	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	521	VAL	2.9
1	C	191	THR	2.9
1	C	210	GLY	2.8
1	D	355	ILE	2.8
1	B	390	PHE	2.8
1	D	174	MET	2.7
1	D	457	MET	2.7
1	D	490	TYR	2.7
1	B	345	THR	2.7
1	D	530	THR	2.6
1	B	376	LEU	2.6
1	D	356	LEU	2.6
1	D	402	ALA	2.6
1	C	452	GLY	2.6
1	B	460	PHE	2.5
1	D	400	ASN	2.5
1	A	354	ASP	2.5
1	D	378	LYS	2.5
1	C	467	GLY	2.5
1	D	60	GLY	2.5
1	D	446	VAL	2.5
1	D	322	THR	2.4
1	D	292	TYR	2.4
1	D	572	PHE	2.4
1	D	379	LYS	2.4
1	B	461	ALA	2.4
1	D	113	LEU	2.4
1	C	212	LYS	2.4
1	D	390	PHE	2.4
1	D	342	VAL	2.3
1	D	53	SER	2.3
1	D	439	VAL	2.3
1	A	378	LYS	2.2
1	B	529	SER	2.2
1	A	376	LEU	2.2
1	B	52	LEU	2.2
1	A	572	PHE	2.2
1	C	364	HIS	2.2
1	D	519	ASN	2.2
1	C	60	GLY	2.2
1	C	449	LEU	2.2
1	A	274	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	430	ASP	2.2
1	A	355	ILE	2.2
1	D	343	PHE	2.2
1	D	212	LYS	2.1
1	D	475	GLN	2.1
1	D	520	ASN	2.1
1	C	542	ASN	2.1
1	D	398	ASN	2.1
1	A	344	GLY	2.1
1	D	69	PRO	2.1
1	C	417	LEU	2.1
1	C	211	ILE	2.1
1	C	446	VAL	2.1
1	D	363	THR	2.0
1	C	114	LEU	2.0
1	C	376	LEU	2.0
1	D	512	LEU	2.0
1	A	161	CYS	2.0
1	A	446	VAL	2.0
1	D	276	SER	2.0
1	A	114	LEU	2.0
1	C	448	HIS	2.0
1	B	23	TYR	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 oligosaccharides 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.