Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 06:02 PM JST

PDB ID	:	7WNH
Title	:	Crystal structure of Nurr1 binding to NBRE
Authors	:	Zhao, M.; Xu, T.; Wang, N.; Guo, Y.; Liu, J.
Deposited on	:	2022-01-18
Resolution	:	3.10 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:

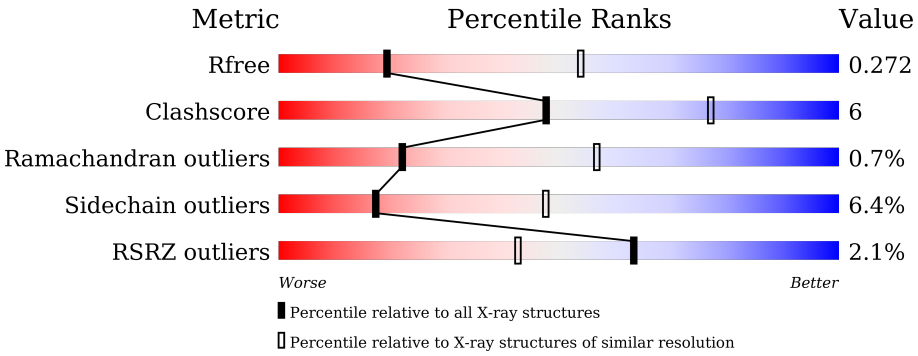
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	350	74% 13% • 12%
1	B	350	75% 13% • 11%
1	C	350	75% 14% • 11%
1	D	350	74% 15% • 10%
2	E	16	69% 31%
2	I	16	44% 50% 6%

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Mol	Chain	Length	Quality of chain
2	L	16	75% 25%
2	O	16	44% 56%
3	F	16	81% 19%
3	H	16	69% 31%
3	K	16	88% 12%
3	N	16	81% 19%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12544 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 Nuclear receptor subfamily 4 group A member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2439	1543	439	437	20			
1	B	313	Total	C	N	O	S	0	0	0
			2485	1575	448	442	20			
1	C	313	Total	C	N	O	S	0	0	0
			2484	1578	444	442	20			
1	D	316	Total	C	N	O	S	0	0	0
			2500	1582	451	447	20			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	249	MET	-	initiating methionine	UNP P43354
A	250	GLY	-	expression tag	UNP P43354
A	251	HIS	-	expression tag	UNP P43354
A	252	HIS	-	expression tag	UNP P43354
A	253	HIS	-	expression tag	UNP P43354
A	254	HIS	-	expression tag	UNP P43354
A	255	HIS	-	expression tag	UNP P43354
A	256	HIS	-	expression tag	UNP P43354
A	257	MET	-	expression tag	UNP P43354
B	249	MET	-	initiating methionine	UNP P43354
B	250	GLY	-	expression tag	UNP P43354
B	251	HIS	-	expression tag	UNP P43354
B	252	HIS	-	expression tag	UNP P43354
B	253	HIS	-	expression tag	UNP P43354
B	254	HIS	-	expression tag	UNP P43354
B	255	HIS	-	expression tag	UNP P43354
B	256	HIS	-	expression tag	UNP P43354
B	257	MET	-	expression tag	UNP P43354
C	249	MET	-	initiating methionine	UNP P43354
C	250	GLY	-	expression tag	UNP P43354
C	251	HIS	-	expression tag	UNP P43354

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Chain	Residue	Modelled	Actual	Comment	Reference
C	252	HIS	-	expression tag	UNP P43354
C	253	HIS	-	expression tag	UNP P43354
C	254	HIS	-	expression tag	UNP P43354
C	255	HIS	-	expression tag	UNP P43354
C	256	HIS	-	expression tag	UNP P43354
C	257	MET	-	expression tag	UNP P43354
D	249	MET	-	initiating methionine	UNP P43354
D	250	GLY	-	expression tag	UNP P43354
D	251	HIS	-	expression tag	UNP P43354
D	252	HIS	-	expression tag	UNP P43354
D	253	HIS	-	expression tag	UNP P43354
D	254	HIS	-	expression tag	UNP P43354
D	255	HIS	-	expression tag	UNP P43354
D	256	HIS	-	expression tag	UNP P43354
D	257	MET	-	expression tag	UNP P43354

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*CP*AP*TP*GP*AP*CP*CP*TP*TP*TP*TP*CP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	16	Total	C	N	O	P	0	0	0
			322	155	55	97	15			
2	I	16	Total	C	N	O	P	0	0	0
			322	155	55	97	15			
2	L	16	Total	C	N	O	P	0	0	0
			322	155	55	97	15			
2	O	16	Total	C	N	O	P	0	0	0
			322	155	55	97	15			

- Molecule 3 is a DNA chain called DNA (5'-D(*CP*CP*GP*AP*AP*AP*AP*GP*GP*TP*CP*AP*TP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	16	Total	C	N	O	P	0	0	0
			328	156	66	91	15			
3	H	16	Total	C	N	O	P	0	0	0
			328	156	66	91	15			
3	K	16	Total	C	N	O	P	0	0	0
			328	156	66	91	15			
3	N	16	Total	C	N	O	P	0	0	0
			328	156	66	91	15			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Zn 2 2	0	0
4	B	2	Total Zn 2 2	0	0
4	C	2	Total Zn 2 2	0	0
4	D	2	Total Zn 2 2	0	0

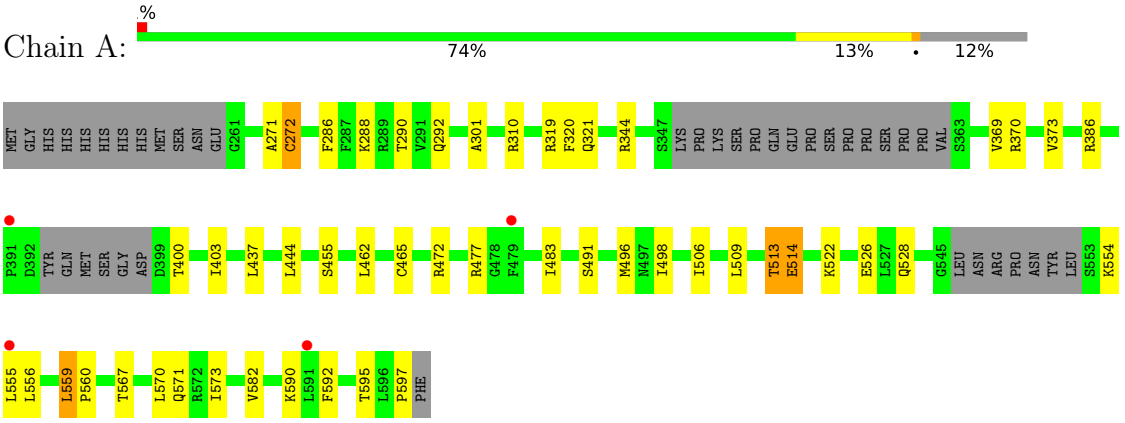
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	B	8	Total O 8 8	0	0
5	C	5	Total O 5 5	0	0
5	D	8	Total O 8 8	0	0
5	E	1	Total O 1 1	0	0
5	O	2	Total O 2 2	0	0

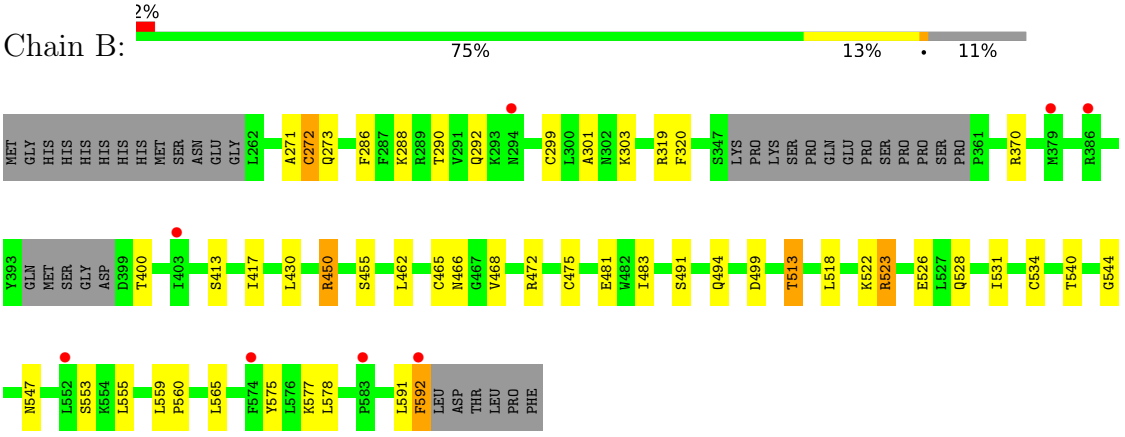
3 Residue-property plots (i)

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.

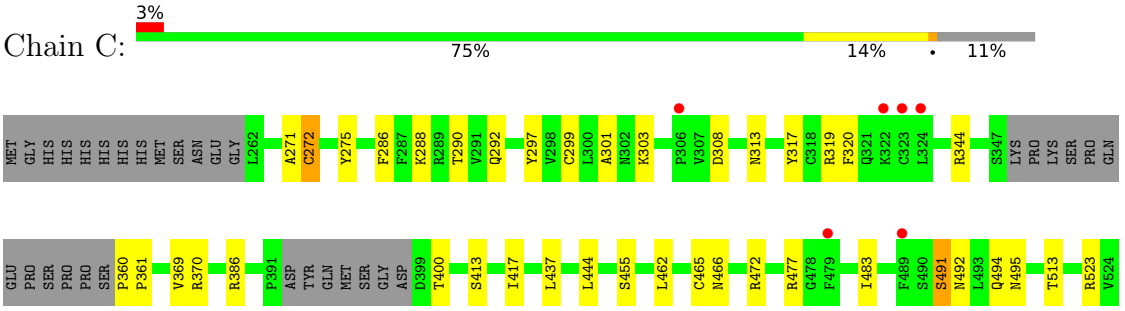
• Molecule 1: Nuclear receptor subfamily 4 group A member 2

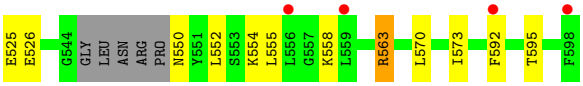


• Molecule 1: Nuclear receptor subfamily 4 group A member 2

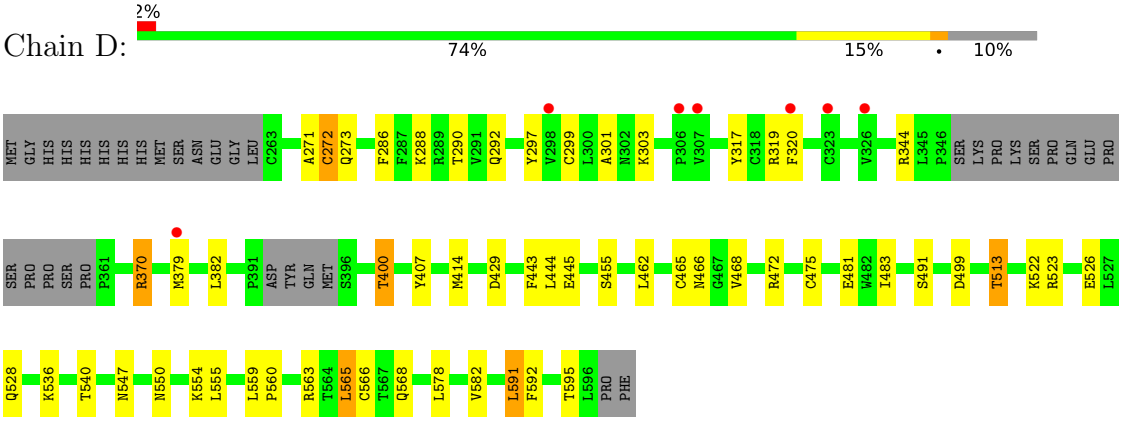


• Molecule 1: Nuclear receptor subfamily 4 group A member 2

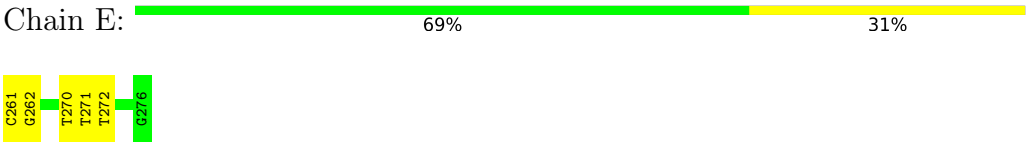




• Molecule 1: Nuclear receptor subfamily 4 group A member 2

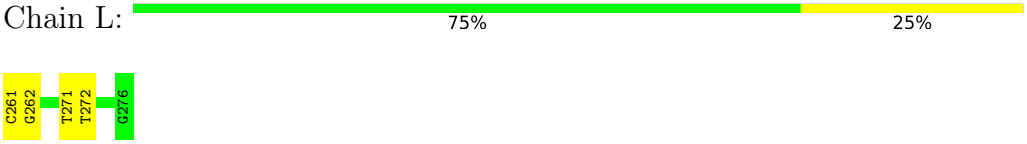


• Molecule 2: DNA (5'-D(*CP*GP*CP*AP*TP*GP*AP*CP*CP*TP*TP*TP*TP*CP*GP*G)-3')



• Molecule 2: DNA (5'-D(*CP*GP*CP*AP*TP*GP*AP*CP*CP*TP*TP*TP*TP*CP*GP*G)-3')

• Molecule 2: DNA (5'-D(*CP*GP*CP*AP*TP*GP*AP*CP*CP*TP*TP*TP*TP*CP*GP*G)-3')



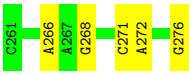
• Molecule 2: DNA (5'-D(*CP*GP*CP*AP*TP*GP*AP*CP*CP*TP*TP*TP*TP*CP*GP*G)-3')

• Molecule 3: DNA (5'-D(*CP*CP*GP*AP*AP*AP*AP*GP*GP*TP*CP*AP*TP*GP*CP*G)-3')

Chain F:

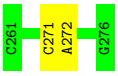
• Molecule 3: DNA (5'-D(*CP*CP*GP*AP*AP*AP*AP*GP*GP*TP*CP*AP*TP*GP*CP*G)-3')

Chain H:



• Molecule 3: DNA (5'-D(*CP*CP*GP*AP*AP*AP*AP*GP*GP*TP*CP*AP*TP*GP*CP*G)-3')

Chain K:



• Molecule 3: DNA (5'-D(*CP*CP*GP*AP*AP*AP*AP*GP*GP*TP*CP*AP*TP*GP*CP*G)-3')

Chain N:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	124.00Å 124.00Å 119.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	107.39 – 3.10 107.39 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (107.39-3.10) 99.6 (107.39-3.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.223 , 0.267 0.226 , 0.272	Depositor DCC
R_{free} test set	1762 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	77.6	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 62.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l 0.086 for h,-h-k,-l 0.021 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12544	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.41% 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: ZN

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	0.72	0/2481	0.82	0/3341
1	B	0.72	0/2531	0.83	0/3411
1	C	0.73	0/2530	0.84	0/3409
1	D	0.72	0/2545	0.85	1/3430 (0.0%)
2	E	0.60	0/359	0.95	0/552
2	I	0.59	0/359	0.94	2/552 (0.4%)
2	L	0.50	0/359	0.92	0/552
2	O	0.52	0/359	0.93	0/552
3	F	0.59	0/369	0.91	1/568 (0.2%)
3	H	0.56	0/369	0.93	2/568 (0.4%)
3	K	0.52	0/369	0.85	0/568
3	N	0.53	0/369	0.82	1/568 (0.2%)
All	All	0.69	0/12999	0.85	7/18071 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	266	DA	O5'-P-OP2	7.52	119.72	110.70
3	H	266	DA	O5'-P-OP1	-6.80	99.58	105.70
3	F	266	DA	O5'-P-OP1	-5.70	100.57	105.70
3	N	266	DA	O5'-P-OP2	5.46	117.25	110.70
2	I	276	DG	O5'-P-OP2	5.45	117.24	110.70
1	D	407	TYR	CB-CG-CD1	5.36	124.21	121.00
2	I	268	DC	C1'-O4'-C4'	-5.18	104.92	110.10

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	2439	0	2467	27	0
1	B	2485	0	2514	27	0
1	C	2484	0	2516	28	0
1	D	2500	0	2530	27	0
2	E	322	0	183	6	0
2	I	322	0	183	13	0
2	L	322	0	183	6	0
2	O	322	0	183	12	0
3	F	328	0	180	2	0
3	H	328	0	180	5	0
3	K	328	0	180	2	0
3	N	328	0	180	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	4	0	0	3	0
5	B	8	0	0	1	0
5	C	5	0	0	2	0
5	D	8	0	0	2	0
5	E	1	0	0	0	0
5	O	2	0	0	3	0
All	All	12544	0	11479	144	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 (144) 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:D:465:CYS:SG	5:D:705:HOH:O	2.09	1.09
3:H:271:DC:H2"	3:H:272:DA:C8	2.09	0.87
3:N:271:DC:H2"	3:N:272:DA:C8	2.09	0.86
3:H:276:DG:O6	2:I:261:DC:N4	2.09	0.86
2:O:266:DG:N3	5:O:301:HOH:O	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:271:DC:H2"	3:K:272:DA:C8	2.12	0.83
3:F:271:DC:H2"	3:F:272:DA:C8	2.15	0.81
1:B:540:THR:HG22	1:B:547:ASN:HA	1.65	0.78
1:B:450:ARG:NH1	5:B:701:HOH:O	2.13	0.74
1:D:370:ARG:NH1	5:D:701:HOH:O	2.22	0.72
1:D:370:ARG:NH2	2:I:276:DG:O6	2.23	0.72
1:A:509:LEU:O	5:A:701:HOH:O	2.06	0.71
2:I:271:DT:H2"	2:I:272:DT:H5'	1.73	0.71
2:O:266:DG:H1'	5:O:301:HOH:O	1.90	0.69
1:C:465:CYS:SG	5:C:705:HOH:O	2.50	0.69
1:D:540:THR:HG22	1:D:547:ASN:HA	1.72	0.69
2:L:271:DT:H2"	2:L:272:DT:H5'	1.74	0.68
1:D:591:LEU:O	1:D:595:THR:HG23	1.94	0.68
1:A:514:GLU:HB3	1:B:575:TYR:HE1	1.59	0.67
2:L:261:DC:H2"	2:L:262:DG:C8	2.29	0.67
2:I:261:DC:H2"	2:I:262:DG:C8	2.29	0.66
2:E:271:DT:H2"	2:E:272:DT:C5'	2.25	0.66
2:E:261:DC:H2"	2:E:262:DG:C8	2.30	0.66
1:B:430:LEU:CD2	1:B:523:ARG:HD2	2.25	0.65
2:I:271:DT:H2"	2:I:272:DT:C5'	2.26	0.65
3:N:271:DC:H2"	3:N:272:DA:N7	2.11	0.65
2:E:271:DT:H2"	2:E:272:DT:H5'	1.78	0.64
2:L:271:DT:H2"	2:L:272:DT:C5'	2.27	0.64
2:O:271:DT:H2"	2:O:272:DT:H5'	1.77	0.64
3:H:271:DC:H2"	3:H:272:DA:N7	2.12	0.64
3:F:271:DC:H2"	3:F:272:DA:N7	2.12	0.63
1:A:556:LEU:HA	1:A:559:LEU:HB2	1.80	0.63
1:A:444:LEU:HB3	1:A:595:THR:HG21	1.80	0.62
1:A:513:THR:OG1	1:B:578:LEU:HD22	1.98	0.62
3:K:271:DC:H2"	3:K:272:DA:N7	2.13	0.62
2:O:261:DC:H2"	2:O:262:DG:C8	2.35	0.62
2:O:271:DT:H2"	2:O:272:DT:C5'	2.30	0.62
1:C:290:THR:HG21	1:C:320:PHE:CE1	2.35	0.61
1:A:559:LEU:N	1:A:560:PRO:HD2	2.16	0.61
1:B:592:PHE:C	1:B:592:PHE:CD1	2.75	0.60
1:D:290:THR:HG21	1:D:320:PHE:CE1	2.36	0.59
1:A:465:CYS:SG	5:A:704:HOH:O	2.56	0.59
1:C:271:ALA:O	1:C:272:CYS:HB2	2.03	0.58
1:D:445:GLU:HA	1:D:566:CYS:SG	2.43	0.58
1:A:514:GLU:CB	1:B:575:TYR:HE1	2.17	0.57
1:C:288:LYS:HG2	1:C:292:GLN:NE2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:ASN:O	1:C:554:LYS:HG2	2.05	0.57
1:A:290:THR:HG21	1:A:320:PHE:CE1	2.40	0.57
1:B:290:THR:HG21	1:B:320:PHE:CE1	2.40	0.57
2:O:262:DG:H2"	2:O:263:DC:C6	2.40	0.57
1:C:308:ASP:OD1	5:C:701:HOH:O	2.17	0.56
1:B:577:LYS:HD3	1:B:592:PHE:HE2	1.70	0.56
2:O:262:DG:H2"	2:O:263:DC:H6	1.70	0.56
1:D:559:LEU:HB2	1:D:560:PRO:HD3	1.87	0.56
1:D:466:ASN:OD1	1:D:468:VAL:HG23	2.05	0.56
1:D:271:ALA:O	1:D:272:CYS:HB2	2.07	0.55
1:C:313:ASN:HD21	2:I:266:DG:P	2.30	0.54
1:B:430:LEU:HD23	1:B:523:ARG:HD2	1.89	0.54
1:A:496:MET:CE	1:A:554:LYS:HB2	2.38	0.53
1:B:271:ALA:O	1:B:272:CYS:HB2	2.08	0.53
1:A:496:MET:HE1	1:A:554:LYS:HB2	1.91	0.53
1:C:492:ASN:HB3	1:C:558:LYS:HE3	1.91	0.53
1:A:321:GLN:HG2	1:A:526:GLU:OE2	2.09	0.52
1:A:567:THR:O	1:A:571:GLN:HG2	2.09	0.52
1:A:271:ALA:O	1:A:272:CYS:HB2	2.09	0.51
1:A:573:ILE:HG13	1:A:592:PHE:CD2	2.45	0.51
1:B:455:SER:OG	1:B:462:LEU:HA	2.09	0.51
1:B:559:LEU:HB2	1:B:560:PRO:HD3	1.93	0.51
2:E:271:DT:H2"	2:E:272:DT:H5"	1.92	0.51
1:D:288:LYS:HG2	1:D:292:GLN:NE2	2.26	0.51
1:B:578:LEU:O	1:B:578:LEU:HD23	2.11	0.50
2:L:261:DC:H2"	2:L:262:DG:H5'	1.94	0.50
1:C:455:SER:OG	1:C:462:LEU:HA	2.12	0.49
1:A:455:SER:OG	1:A:462:LEU:HA	2.11	0.49
1:C:313:ASN:OD1	2:I:265:DT:H5"	2.12	0.49
1:D:455:SER:OG	1:D:462:LEU:HA	2.12	0.49
2:E:261:DC:H2"	2:E:262:DG:H5'	1.95	0.49
1:A:288:LYS:HG2	1:A:292:GLN:NE2	2.28	0.49
1:B:413:SER:O	1:B:417:ILE:HG13	2.12	0.49
1:B:466:ASN:OD1	1:B:468:VAL:HG23	2.12	0.49
2:I:261:DC:H2"	2:I:262:DG:H5'	1.94	0.48
1:D:565:LEU:O	1:D:568:GLN:HB2	2.14	0.48
1:B:523:ARG:HG3	1:B:523:ARG:HH21	1.79	0.48
2:O:262:DG:C2'	2:O:263:DC:C6	2.96	0.48
1:C:455:SER:O	1:C:494:GLN:NE2	2.46	0.48
1:D:414:MET:HG2	1:D:443:PHE:CE1	2.49	0.48
2:O:266:DG:C1'	5:O:301:HOH:O	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LYS:HG2	1:B:292:GLN:NE2	2.29	0.47
1:D:536:LYS:O	1:D:540:THR:HG23	2.14	0.47
1:B:462:LEU:HD12	1:B:475:CYS:SG	2.54	0.47
1:C:290:THR:HG21	1:C:320:PHE:CD1	2.48	0.47
2:O:261:DC:H2"	2:O:262:DG:H5"	1.97	0.47
1:C:275:TYR:OH	3:H:268:DG:OP2	2.11	0.47
1:C:360:PRO:CB	1:C:361:PRO:HD3	2.44	0.47
1:C:360:PRO:HG2	1:C:361:PRO:HD3	1.96	0.47
1:D:299:CYS:SG	1:D:303:LYS:HA	2.55	0.47
1:B:290:THR:HG21	1:B:320:PHE:CD1	2.50	0.46
1:D:290:THR:HG21	1:D:320:PHE:CD1	2.51	0.46
1:B:513:THR:HA	1:B:528:GLN:NE2	2.30	0.46
1:A:290:THR:HG21	1:A:320:PHE:CD1	2.51	0.46
1:A:498:ILE:HD11	1:A:555:LEU:HD13	1.98	0.46
1:D:578:LEU:HD23	1:D:578:LEU:O	2.15	0.46
1:B:286:PHE:CD2	1:B:319:ARG:HD3	2.51	0.45
1:C:444:LEU:HB3	1:C:595:THR:HG21	1.98	0.45
1:A:528:GLN:NE2	5:A:701:HOH:O	2.43	0.45
1:B:299:CYS:SG	1:B:303:LYS:HA	2.57	0.45
1:C:299:CYS:SG	1:C:303:LYS:HA	2.57	0.45
1:C:462:LEU:HD13	1:C:483:ILE:HD11	1.99	0.44
1:D:513:THR:HA	1:D:528:GLN:NE2	2.32	0.44
1:D:286:PHE:CD2	1:D:319:ARG:HD3	2.53	0.44
1:B:455:SER:O	1:B:494:GLN:NE2	2.49	0.44
1:C:286:PHE:CD2	1:C:319:ARG:HD3	2.53	0.44
1:D:462:LEU:HD12	1:D:475:CYS:SG	2.57	0.44
1:C:526:GLU:HG2	1:D:429:ASP:HB3	2.00	0.44
1:A:513:THR:HA	1:A:528:GLN:NE2	2.33	0.43
2:I:261:DC:C2'	2:I:262:DG:C8	3.00	0.43
1:C:313:ASN:ND2	2:I:266:DG:OP1	2.50	0.43
1:C:573:ILE:HG13	1:C:592:PHE:CD2	2.53	0.43
1:C:413:SER:O	1:C:417:ILE:HG13	2.19	0.42
1:A:462:LEU:HD13	1:A:483:ILE:HD11	2.01	0.42
1:C:369:VAL:HG11	2:O:276:DG:C5	2.54	0.42
2:L:271:DT:H2"	2:L:272:DT:H5"	2.00	0.42
1:A:286:PHE:CD2	1:A:319:ARG:HD3	2.55	0.42
1:A:506:ILE:HG13	1:A:555:LEU:CD2	2.49	0.42
1:C:360:PRO:HB2	1:C:361:PRO:HD3	2.01	0.42
1:D:550:ASN:O	1:D:554:LYS:HG3	2.20	0.42
1:A:369:VAL:O	1:A:373:VAL:HG23	2.20	0.42
1:D:297:TYR:HB2	1:D:317:TYR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:SER:O	1:C:495:ASN:ND2	2.53	0.41
1:B:531:ILE:O	1:B:534:CYS:HB3	2.20	0.41
1:D:379:MET:HA	1:D:382:LEU:HD21	2.03	0.41
1:D:462:LEU:HD13	1:D:483:ILE:HD11	2.02	0.41
2:I:270:DT:C6	2:I:271:DT:H72	2.56	0.41
1:A:403:ILE:HG21	1:A:582:VAL:HG13	2.02	0.41
1:A:573:ILE:HG13	1:A:592:PHE:CG	2.56	0.41
1:B:462:LEU:HD13	1:B:483:ILE:HD11	2.03	0.41
2:I:271:DT:H2"	2:I:272:DT:H5"	1.98	0.41
3:H:276:DG:N1	2:I:261:DC:N3	2.41	0.41
2:L:261:DC:C2'	2:L:262:DG:C8	3.01	0.41
2:E:270:DT:C6	2:E:271:DT:H72	2.57	0.40
2:O:268:DC:C2	2:O:269:DC:C5	3.09	0.40
1:B:544:GLY:O	1:D:400:THR:HG22	2.20	0.40
1:C:297:TYR:HB2	1:C:317:TYR:HA	2.02	0.40
1:C:563:ARG:HD3	1:C:563:ARG:HA	1.71	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	301/350 (86%)	278 (92%)	21 (7%)	2 (1%)	22	57
1	B	307/350 (88%)	281 (92%)	24 (8%)	2 (1%)	22	57
1	C	305/350 (87%)	281 (92%)	22 (7%)	2 (1%)	22	57
1	D	310/350 (89%)	281 (91%)	27 (9%)	2 (1%)	25	59
All	All	1223/1400 (87%)	1121 (92%)	94 (8%)	8 (1%)	22	57

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	CYS
1	B	272	CYS
1	C	272	CYS
1	D	272	CYS
1	D	301	ALA
1	C	301	ALA
1	B	301	ALA
1	A	301	ALA

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	269/308 (87%)	253 (94%)	16 (6%)	19	50
1	B	274/308 (89%)	255 (93%)	19 (7%)	15	45
1	C	275/308 (89%)	259 (94%)	16 (6%)	20	51
1	D	276/308 (90%)	257 (93%)	19 (7%)	15	45
All	All	1094/1232 (89%)	1024 (94%)	70 (6%)	17	48

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	ARG
1	A	344	ARG
1	A	370	ARG
1	A	386	ARG
1	A	400	THR
1	A	437	LEU
1	A	472	ARG
1	A	477	ARG
1	A	491	SER
1	A	513	THR
1	A	514	GLU
1	A	522	LYS
1	A	559	LEU
1	A	570	LEU

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Mol	Chain	Res	Type
1	A	590	LYS
1	A	597	PRO
1	B	273	GLN
1	B	370	ARG
1	B	400	THR
1	B	450	ARG
1	B	465	CYS
1	B	472	ARG
1	B	481	GLU
1	B	491	SER
1	B	499	ASP
1	B	513	THR
1	B	518	LEU
1	B	522	LYS
1	B	523	ARG
1	B	526	GLU
1	B	553	SER
1	B	555	LEU
1	B	565	LEU
1	B	591	LEU
1	B	592	PHE
1	C	344	ARG
1	C	370	ARG
1	C	386	ARG
1	C	400	THR
1	C	437	LEU
1	C	466	ASN
1	C	472	ARG
1	C	477	ARG
1	C	491	SER
1	C	513	THR
1	C	523	ARG
1	C	525	GLU
1	C	552	LEU
1	C	555	LEU
1	C	563	ARG
1	C	570	LEU
1	D	273	GLN
1	D	344	ARG
1	D	370	ARG
1	D	400	THR
1	D	444	LEU

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Mol	Chain	Res	Type
1	D	472	ARG
1	D	481	GLU
1	D	491	SER
1	D	499	ASP
1	D	513	THR
1	D	522	LYS
1	D	523	ARG
1	D	526	GLU
1	D	555	LEU
1	D	563	ARG
1	D	565	LEU
1	D	582	VAL
1	D	591	LEU
1	D	592	PHE

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	269	ASN
1	A	292	GLN
1	A	316	GLN
1	A	388	GLN
1	A	495	ASN
1	A	528	GLN
1	B	269	ASN
1	B	292	GLN
1	B	316	GLN
1	B	388	GLN
1	B	471	HIS
1	B	495	ASN
1	B	528	GLN
1	C	269	ASN
1	C	292	GLN
1	C	466	ASN
1	C	495	ASN
1	D	269	ASN
1	D	292	GLN
1	D	471	HIS
1	D	495	ASN
1	D	528	GLN
1	D	571	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 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

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

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	309/350 (88%)	0.03	4 (1%) 77 59	52, 84, 131, 188	0
1	B	313/350 (89%)	0.15	8 (2%) 56 33	60, 86, 129, 183	0
1	C	313/350 (89%)	0.17	10 (3%) 47 25	54, 88, 147, 178	0
1	D	316/350 (90%)	0.07	7 (2%) 62 41	49, 85, 138, 180	0
2	E	16/16 (100%)	-0.53	0 100 100	61, 74, 86, 93	0
2	I	16/16 (100%)	-0.75	0 100 100	75, 90, 103, 104	0
2	L	16/16 (100%)	-0.68	0 100 100	72, 91, 114, 116	0
2	O	16/16 (100%)	-0.79	0 100 100	77, 93, 112, 115	0
3	F	16/16 (100%)	-0.55	0 100 100	50, 76, 92, 97	0
3	H	16/16 (100%)	-0.72	0 100 100	69, 91, 111, 117	0
3	K	16/16 (100%)	-0.86	0 100 100	75, 92, 113, 113	0
3	N	16/16 (100%)	-0.76	0 100 100	70, 92, 117, 118	0
All	All	1379/1528 (90%)	0.03	29 (2%) 63 43	49, 86, 136, 188	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	323	CYS	4.3
1	B	592	PHE	4.2
1	D	320	PHE	3.6
1	B	379	MET	3.5
1	C	592	PHE	3.1
1	B	552	LEU	3.1
1	D	306	PRO	2.9
1	D	326	VAL	2.9
1	D	379	MET	2.8
1	C	559	LEU	2.7
1	C	324	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	489	PHE	2.7
1	D	307	VAL	2.6
1	B	574	PHE	2.6
1	C	306	PRO	2.5
1	A	555	LEU	2.5
1	A	479	PHE	2.4
1	C	479	PHE	2.4
1	B	583	PRO	2.4
1	A	591	LEU	2.3
1	A	391	PRO	2.3
1	C	556	LEU	2.3
1	C	598	PHE	2.2
1	B	294	ASN	2.2
1	C	322	LYS	2.1
1	B	386	ARG	2.0
1	D	323	CYS	2.0
1	B	403	ILE	2.0
1	D	298	VAL	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
4	ZN	C	602	1/1	0.84	0.07	181,181,181,181	0
4	ZN	D	602	1/1	0.93	0.14	188,188,188,188	0
4	ZN	A	602	1/1	0.96	0.11	105,105,105,105	0
4	ZN	D	601	1/1	0.97	0.14	112,112,112,112	0
4	ZN	C	601	1/1	0.98	0.17	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	A	601	1/1	0.99	0.19	81,81,81,81	0
4	ZN	B	602	1/1	0.99	0.13	91,91,91,91	0
4	ZN	B	601	1/1	1.00	0.16	92,92,92,92	0

6.5 Other polymers (i)

There are no such residues in this entry.