Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:42 am BST

PDB ID	:	4OSH
Title	:	Crystal structure of the TAL effector dHax3 with NI RVD at 2.2 angstrom resolution
Authors	:	Deng, D.; Wu, J.P.; Yan, C.Y.; Pan, X.J.; Yan, N.
Deposited on	:	2014-02-13
Resolution	:	2.20 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
https://www.wwpdb.org/validation/2017/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:

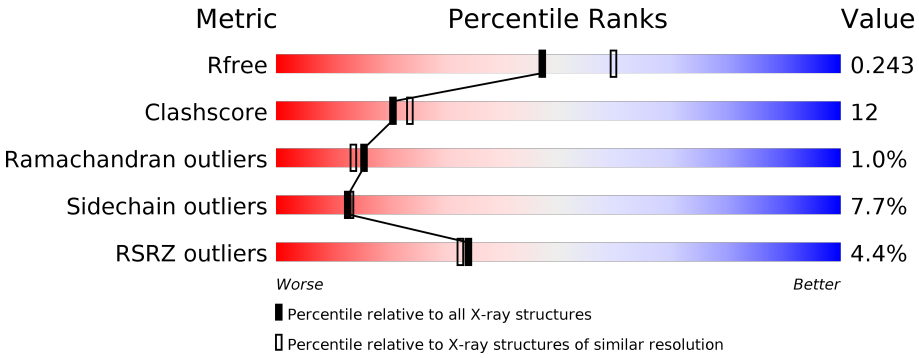
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	499	5% 75% 20%
1	B	499	3% 77% 16% 5%
2	G	17	6% 71% 6% 12% 12%
2	I	17	65% 12% 12% 12%
3	H	17	6% 47% 29% 12% 12%
3	J	17	6% 65% 24% 6% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8565 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 Hax3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	489	Total	C	N	O	S	9	0	0
			3526	2205	654	655	12			
1	A	487	Total	C	N	O	S	16	1	0
			3511	2193	651	655	12			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	230	MET	-	EXPRESSION TAG	UNP Q3ZD72
B	300	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
B	301	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
B	368	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
B	369	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
B	402	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
B	403	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
B	436	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
B	437	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
B	470	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
B	471	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
B	505	ILE	SER	ENGINEERED MUTATION	UNP Q3ZD72
B	539	GLY	SER	ENGINEERED MUTATION	UNP Q3ZD72
B	572	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
B	573	ASP	SER	ENGINEERED MUTATION	UNP Q3ZD72
B	606	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
B	607	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
B	640	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
B	641	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
B	721	LEU	-	EXPRESSION TAG	UNP Q3ZD72
B	722	GLU	-	EXPRESSION TAG	UNP Q3ZD72
B	723	HIS	-	EXPRESSION TAG	UNP Q3ZD72
B	724	HIS	-	EXPRESSION TAG	UNP Q3ZD72
B	725	HIS	-	EXPRESSION TAG	UNP Q3ZD72
B	726	HIS	-	EXPRESSION TAG	UNP Q3ZD72

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	727	HIS	-	EXPRESSION TAG	UNP Q3ZD72
B	728	HIS	-	EXPRESSION TAG	UNP Q3ZD72
A	230	MET	-	EXPRESSION TAG	UNP Q3ZD72
A	300	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
A	301	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
A	368	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
A	369	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
A	402	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
A	403	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
A	436	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
A	437	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
A	470	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
A	471	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
A	505	ILE	SER	ENGINEERED MUTATION	UNP Q3ZD72
A	539	GLY	SER	ENGINEERED MUTATION	UNP Q3ZD72
A	572	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
A	573	ASP	SER	ENGINEERED MUTATION	UNP Q3ZD72
A	606	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
A	607	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
A	640	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
A	641	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
A	721	LEU	-	EXPRESSION TAG	UNP Q3ZD72
A	722	GLU	-	EXPRESSION TAG	UNP Q3ZD72
A	723	HIS	-	EXPRESSION TAG	UNP Q3ZD72
A	724	HIS	-	EXPRESSION TAG	UNP Q3ZD72
A	725	HIS	-	EXPRESSION TAG	UNP Q3ZD72
A	726	HIS	-	EXPRESSION TAG	UNP Q3ZD72
A	727	HIS	-	EXPRESSION TAG	UNP Q3ZD72
A	728	HIS	-	EXPRESSION TAG	UNP Q3ZD72

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*TP*AP*TP*CP*TP*CP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	15	Total	C	N	O	P	0	0	0
			295	145	41	95	14			
2	I	15	Total	C	N	O	P	0	0	0
			297	144	42	96	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	15	Total	C	N	O	P	0	0	0
			318	149	70	84	15			
3	J	16	Total	C	N	O	P	0	0	0
			336	159	75	87	15			

- Molecule 4 is water.

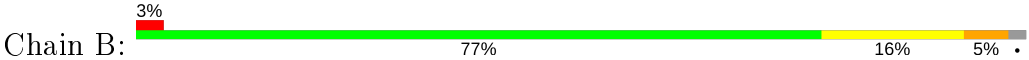
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	143	Total	O	0	0
			143	143		
4	G	26	Total	O	0	0
			26	26		
4	H	13	Total	O	0	0
			13	13		
4	A	71	Total	O	0	0
			71	71		
4	I	21	Total	O	0	0
			21	21		
4	J	8	Total	O	0	0
			8	8		

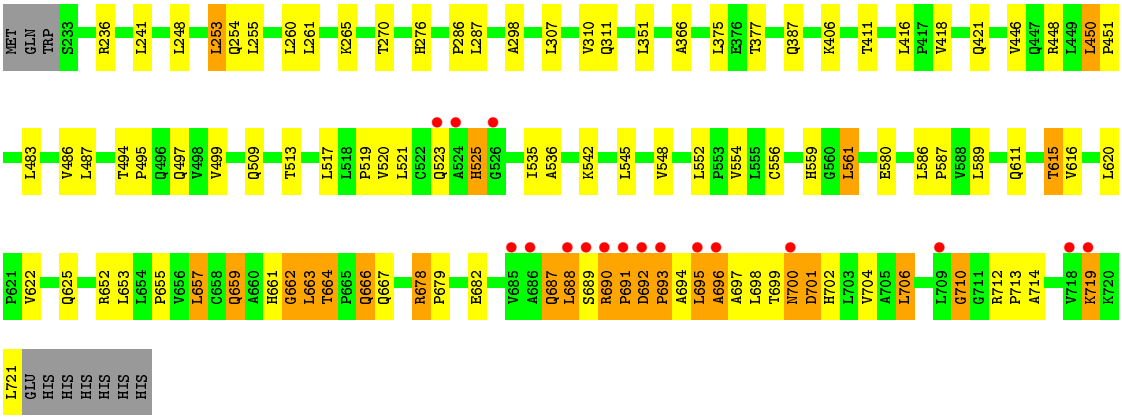
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Hax3

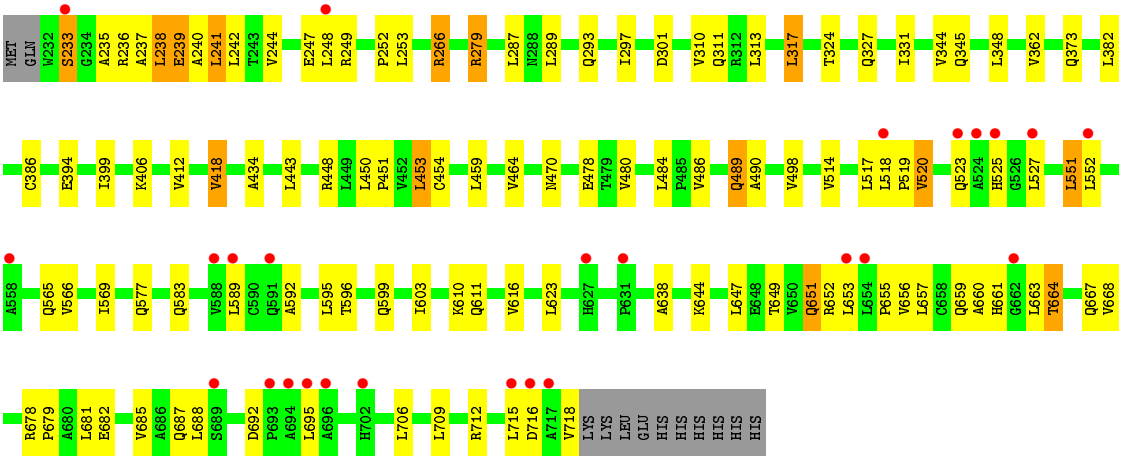
Chain B:





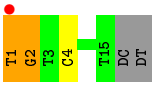
- Molecule 1: Hax3

Chain A:



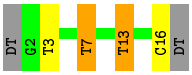
- Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*TP*AP*TP*CP*TP*CP*TP*CP*T)-3')

Chain G:



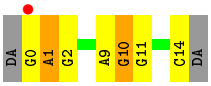
• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*TP*AP*TP*CP*TP*CP*TP*CP*T)-3')

Chain I:



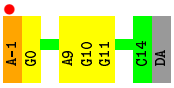
• Molecule 3: DNA (5'-D(*AP*GP*AP*GP*AP*GP*AP*TP*AP*AP*AP*GP*GP*GP*AP*CP*A)-3')

Chain H:



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

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.53Å 80.99Å 89.08Å 90.00° 103.62° 90.00°	Depositor
Resolution (Å)	36.63 – 2.20 36.63 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (36.63-2.20) 99.3 (36.63-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.205 , 0.246 0.201 , 0.243	Depositor DCC
R_{free} test set	2986 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.8	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	0.95	EDS
Total number of atoms	8565	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% 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

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	0.37	0/3560	0.54	0/4865
1	B	0.43	0/3575	0.61	0/4883
2	G	1.03	0/326	1.55	4/500 (0.8%)
2	I	0.81	0/328	1.35	2/502 (0.4%)
3	H	0.84	0/360	1.65	4/555 (0.7%)
3	J	0.70	0/381	1.38	2/588 (0.3%)
All	All	0.50	0/8530	0.82	12/11893 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	DT	O4'-C1'-N1	11.03	115.72	108.00
2	G	1	DT	C1'-O4'-C4'	-7.02	103.08	110.10
3	J	10	DG	O4'-C1'-N9	6.93	112.86	108.00
3	H	10	DG	O4'-C1'-N9	6.79	112.75	108.00
3	H	1	DA	O4'-C1'-N9	-6.08	103.75	108.00
3	H	14	DC	O4'-C1'-N1	6.08	112.25	108.00
2	G	4	DC	O4'-C1'-N1	6.04	112.23	108.00
3	H	11	DG	O4'-C1'-N9	5.56	111.89	108.00
2	I	7	DT	O4'-C1'-N1	-5.38	104.23	108.00
3	J	-1	DA	O4'-C1'-N9	5.34	111.74	108.00
2	G	2	DG	N9-C4-C5	5.23	107.49	105.40
2	I	13	DT	N3-C4-O4	5.22	123.03	119.90

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	3511	0	3653	80	3
1	B	3526	0	3684	103	0
2	G	295	0	175	2	0
2	I	297	0	173	6	0
3	H	318	0	167	6	0
3	J	336	0	179	6	0
4	A	71	0	0	2	0
4	B	143	0	0	6	0
4	G	26	0	0	0	0
4	H	13	0	0	2	0
4	I	21	0	0	6	0
4	J	8	0	0	4	0
All	All	8565	0	8031	200	3

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 12.

All (200) 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:B:661:HIS:CE1	1:B:688:LEU:HB3	1.60	1.35
1:B:664:THR:HG23	1:B:667:GLN:OE1	1.43	1.15
1:B:698:LEU:HD23	1:B:702:HIS:ND1	1.63	1.14
1:B:698:LEU:HB3	1:B:702:HIS:HB3	1.29	1.13
1:B:254:GLN:NE2	4:B:913:HOH:O	1.80	1.12
1:A:655:PRO:O	1:A:659:GLN:HB2	1.59	1.02
3:J:11:DG:N7	4:J:102:HOH:O	1.91	1.01
1:B:689:SER:O	1:B:691:PRO:HD3	1.61	1.00
1:A:486:VAL:O	1:A:490:ALA:HB3	1.62	0.98
3:J:9:DA:N7	4:J:103:HOH:O	1.99	0.94
3:J:11:DG:OP2	4:J:106:HOH:O	1.86	0.93
1:A:252:PRO:HD2	1:A:279:ARG:HG2	1.48	0.93
1:B:698:LEU:CD2	1:B:702:HIS:ND1	2.34	0.91
1:A:235:ALA:O	1:A:239:GLU:HG3	1.70	0.90
1:A:661:HIS:CD2	1:A:688:LEU:HB3	2.07	0.90
1:B:652:ARG:NH1	1:B:682:GLU:OE1	2.04	0.89
1:B:687:GLN:NE2	1:B:691:PRO:HA	1.88	0.88
2:I:16:DC:OP2	4:I:109:HOH:O	1.93	0.86
1:B:687:GLN:HE22	1:B:691:PRO:CA	1.92	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:HIS:CE1	1:B:688:LEU:CB	2.56	0.82
3:H:1:DA:P	4:H:113:HOH:O	2.40	0.79
1:A:551:LEU:HD11	1:A:583:GLN:NE2	1.97	0.79
1:B:689:SER:O	1:B:691:PRO:CD	2.30	0.79
1:B:664:THR:CG2	1:B:667:GLN:OE1	2.27	0.78
2:I:7:DT:O4	4:I:110:HOH:O	2.03	0.77
1:A:664:THR:HG22	1:A:667:GLN:H	1.50	0.76
1:B:411:THR:OG1	4:B:899:HOH:O	2.03	0.76
2:I:3:DT:OP2	4:I:114:HOH:O	2.02	0.76
1:B:698:LEU:HB3	1:B:702:HIS:CB	2.12	0.75
1:B:693:PRO:HA	1:B:696:ALA:HB3	1.67	0.75
1:B:699:THR:C	1:B:701:ASP:H	1.89	0.74
1:B:699:THR:C	1:B:701:ASP:N	2.40	0.74
3:H:1:DA:OP2	4:H:113:HOH:O	2.06	0.74
1:B:664:THR:HG23	1:B:667:GLN:CD	2.08	0.73
1:B:687:GLN:NE2	1:B:691:PRO:CA	2.50	0.72
1:B:698:LEU:HD12	1:B:698:LEU:N	2.05	0.70
2:I:16:DC:P	4:I:109:HOH:O	2.49	0.70
1:A:589:LEU:HD12	1:A:595:LEU:HD12	1.74	0.69
1:A:287:LEU:HB3	1:A:289:LEU:HD13	1.75	0.68
1:A:480:VAL:HG13	1:A:484:LEU:HD13	1.73	0.68
1:A:657:LEU:HD21	1:A:685:VAL:HG22	1.76	0.67
1:B:698:LEU:CG	1:B:702:HIS:ND1	2.57	0.66
2:I:13:DT:OP2	4:I:106:HOH:O	2.11	0.66
1:A:399:ILE:HD13	1:A:412:VAL:HG21	1.78	0.66
1:A:649:THR:OG1	1:A:678:ARG:HG3	1.96	0.66
1:B:699:THR:O	1:B:701:ASP:N	2.30	0.65
1:B:661:HIS:O	1:B:663:LEU:N	2.30	0.65
1:B:580:GLU:OE1	4:B:889:HOH:O	2.14	0.65
1:B:687:GLN:HE22	1:B:691:PRO:CB	2.11	0.64
1:A:238:LEU:HD22	1:A:242:LEU:HD11	1.80	0.64
1:A:486:VAL:O	1:A:490:ALA:CB	2.44	0.64
1:B:710:GLY:HA3	1:B:714:ALA:HB2	1.80	0.64
1:B:611:GLN:O	1:B:615:THR:HG23	1.98	0.63
1:B:687:GLN:HE22	1:B:691:PRO:HA	1.53	0.63
1:A:252:PRO:HD2	1:A:279:ARG:CG	2.25	0.63
1:B:695:LEU:HG	1:B:719:LYS:HB2	1.79	0.63
1:B:517:LEU:HB3	1:B:521:LEU:HD23	1.80	0.63
1:A:551:LEU:CD1	1:A:583:GLN:NE2	2.61	0.62
1:B:483:LEU:O	1:B:486:VAL:HG12	2.00	0.62
1:B:387:GLN:O	4:B:875:HOH:O	2.16	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:687:GLN:NE2	1:B:691:PRO:CB	2.63	0.61
1:A:687:GLN:HE22	1:A:692:ASP:H	1.48	0.61
1:A:638:ALA:HB2	1:A:647:LEU:HD11	1.83	0.60
1:B:695:LEU:O	1:B:697:ALA:N	2.32	0.60
1:B:664:THR:OG1	1:B:666:GLN:HG2	2.01	0.60
1:B:699:THR:O	1:B:702:HIS:N	2.33	0.59
1:B:678:ARG:HB3	1:B:679:PRO:CD	2.32	0.59
1:A:678:ARG:HB3	1:A:679:PRO:CD	2.32	0.59
1:B:698:LEU:CD1	1:B:698:LEU:N	2.66	0.59
1:A:238:LEU:HD22	1:A:242:LEU:CD1	2.33	0.58
1:A:348:LEU:HD13	1:A:362:VAL:HG11	1.84	0.58
1:A:706:LEU:HD23	1:A:715:LEU:HD12	1.83	0.58
1:B:307:LEU:O	1:B:310:VAL:HG12	2.03	0.57
1:A:577:GLN:HB3	1:A:610:LYS:HD3	1.85	0.57
1:B:678:ARG:HB3	1:B:679:PRO:HD3	1.86	0.56
1:A:678:ARG:HB3	1:A:679:PRO:HD3	1.86	0.56
1:A:235:ALA:O	1:A:239:GLU:CG	2.50	0.56
1:B:509:GLN:HB3	1:B:542:LYS:HD2	1.87	0.56
1:B:421:GLN:HG2	1:A:386:CYS:O	2.06	0.56
1:A:551:LEU:HD11	1:A:583:GLN:HE22	1.71	0.55
1:A:552:LEU:HD13	1:A:566:VAL:HG11	1.88	0.55
1:A:236:ARG:HA	1:A:239:GLU:CD	2.26	0.55
1:A:418:VAL:HG22	4:A:838:HOH:O	2.05	0.55
1:B:687:GLN:HG2	1:B:695:LEU:HD13	1.89	0.55
1:B:657:LEU:O	1:B:663:LEU:HB2	2.06	0.54
1:A:240:ALA:O	1:A:244:VAL:HG22	2.08	0.54
1:B:689:SER:C	1:B:691:PRO:HD3	2.27	0.54
1:B:692:ASP:O	1:B:695:LEU:N	2.41	0.54
1:A:252:PRO:CD	1:A:279:ARG:HG2	2.30	0.54
1:A:434:ALA:HB2	1:A:443:LEU:HD11	1.89	0.54
1:B:525:HIS:HD2	1:B:552:LEU:HD23	1.74	0.53
3:J:11:DG:P	4:J:106:HOH:O	2.58	0.53
1:B:248:LEU:HD21	1:B:276:HIS:HA	1.90	0.53
1:A:681:LEU:O	1:A:685:VAL:HG23	2.10	0.52
1:A:551:LEU:HD11	1:A:583:GLN:CD	2.30	0.52
1:B:698:LEU:HG	1:B:702:HIS:ND1	2.23	0.52
1:B:692:ASP:OD2	1:B:694:ALA:HB3	2.10	0.52
1:B:536:ALA:HB2	1:B:545:LEU:HD11	1.92	0.52
1:B:377:THR:OG1	1:B:406:LYS:HG3	2.10	0.51
1:B:698:LEU:HD23	1:B:702:HIS:CE1	2.42	0.51
1:B:687:GLN:O	1:B:687:GLN:NE2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:HG2	1:A:249:ARG:HH11	1.76	0.50
1:B:486:VAL:HG13	1:B:487:LEU:N	2.25	0.50
1:B:559:HIS:HB3	1:B:586:LEU:HD23	1.91	0.50
1:B:692:ASP:O	1:B:693:PRO:C	2.49	0.50
1:B:692:ASP:O	1:B:692:ASP:OD2	2.30	0.50
3:J:-1:DA:H1'	3:J:0:DG:H5'	1.94	0.50
3:H:1:DA:H1'	3:H:2:DG:H5"	1.94	0.49
1:A:266:ARG:NH1	3:J:9:DA:OP2	2.44	0.49
1:B:690:ARG:O	1:B:691:PRO:O	2.30	0.49
1:B:698:LEU:CD2	1:B:702:HIS:CE1	2.96	0.49
1:A:373:GLN:HB3	1:A:406:LYS:HD2	1.94	0.49
1:B:666:GLN:H	1:B:666:GLN:CD	2.16	0.49
1:B:450:LEU:HB3	1:B:451:PRO:HD3	1.95	0.48
1:A:525:HIS:ND1	1:A:552:LEU:HD23	2.28	0.48
1:A:287:LEU:HD11	1:A:311:GLN:HA	1.95	0.48
1:B:706:LEU:HD22	1:B:714:ALA:HB1	1.96	0.48
1:A:661:HIS:NE2	1:A:688:LEU:HB3	2.26	0.47
2:G:1:DT:H4'	2:G:2:DG:H5'	1.95	0.47
1:B:698:LEU:HB3	1:B:702:HIS:CG	2.50	0.47
1:B:663:LEU:HD21	1:B:704:VAL:CG2	2.45	0.47
1:B:513:THR:OG1	1:B:542:LYS:HG3	2.15	0.47
1:A:596:THR:N	1:A:599:GLN:OE1	2.32	0.47
1:B:495:PRO:O	1:B:499:VAL:HG23	2.15	0.47
1:A:324:THR:HG23	1:A:327:GLN:H	1.78	0.47
1:A:651:GLN:HB2	1:A:651:GLN:HE21	1.59	0.46
1:B:253:LEU:HB3	1:B:255:LEU:HG	1.97	0.46
1:B:697:ALA:C	1:B:698:LEU:HD12	2.35	0.46
2:I:16:DC:O5'	4:I:109:HOH:O	2.20	0.46
1:B:525:HIS:CD2	1:B:552:LEU:HD23	2.51	0.46
1:B:661:HIS:O	1:B:662:GLY:C	2.52	0.46
1:B:664:THR:O	1:B:667:GLN:HB2	2.16	0.46
1:B:661:HIS:C	1:B:663:LEU:N	2.69	0.45
1:A:489:GLN:H	1:A:489:GLN:HG3	1.53	0.45
1:B:286:PRO:HD2	4:B:885:HOH:O	2.16	0.45
1:B:366:ALA:HB2	1:B:375:LEU:HD11	1.98	0.45
1:A:448:ARG:NH2	1:A:478:GLU:OE2	2.49	0.45
1:A:649:THR:HG1	1:A:678:ARG:HG3	1.81	0.45
1:B:448:ARG:HD2	4:B:915:HOH:O	2.17	0.45
1:A:518:LEU:HB3	1:A:519:PRO:HD3	1.99	0.45
1:A:519:PRO:O	1:A:523:GLN:HG2	2.16	0.45
1:A:668:VAL:HG13	1:A:681:LEU:HD21	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:CYS:HA	1:B:561:LEU:O	2.17	0.45
3:H:0:DG:H1'	3:H:1:DA:H5'	1.99	0.45
1:B:657:LEU:HA	1:B:657:LEU:HD12	1.85	0.44
1:A:454:CYS:HA	1:A:459:LEU:O	2.17	0.44
1:B:486:VAL:CG1	1:B:487:LEU:N	2.80	0.44
1:A:611:GLN:HB3	1:A:644:LYS:HD2	1.99	0.44
1:B:661:HIS:ND1	1:B:688:LEU:HG	2.32	0.44
1:A:712:ARG:HG3	1:A:716:ASP:OD1	2.16	0.44
1:B:687:GLN:HE22	1:B:692:ASP:H	1.65	0.44
1:B:692:ASP:C	1:B:692:ASP:OD2	2.57	0.43
1:B:661:HIS:NE2	1:B:688:LEU:HB3	2.20	0.43
1:A:655:PRO:O	1:A:659:GLN:N	2.45	0.43
1:B:700:ASN:O	1:B:704:VAL:HG23	2.18	0.43
1:A:484:LEU:HD12	1:A:498:VAL:HG11	2.01	0.43
3:H:9:DA:H2"	3:H:10:DG:O5'	2.18	0.43
1:A:565:GLN:O	1:A:569:ILE:HG13	2.19	0.43
1:B:298:ALA:HB2	1:B:307:LEU:HD11	2.00	0.43
1:B:535:ILE:HD13	1:B:548:VAL:HG21	2.01	0.43
1:B:687:GLN:NE2	1:B:691:PRO:HB3	2.34	0.43
1:B:519:PRO:O	1:B:523:GLN:HG2	2.19	0.42
1:B:687:GLN:O	1:B:691:PRO:CA	2.67	0.42
1:A:237:ALA:O	1:A:241:LEU:HD22	2.19	0.42
1:B:687:GLN:O	1:B:691:PRO:HA	2.19	0.42
1:A:313:LEU:HB3	1:A:317:LEU:HD22	2.02	0.42
1:A:331:ILE:HD13	1:A:344:VAL:HG21	2.02	0.42
1:A:652:ARG:NH2	1:A:682:GLU:OE2	2.50	0.42
1:B:270:THR:HG21	2:G:2:DG:H5"	2.01	0.42
1:A:656:VAL:O	1:A:660:ALA:HB3	2.19	0.42
1:B:652:ARG:HD2	1:B:653:LEU:CD2	2.49	0.41
3:H:9:DA:H2'	3:H:10:DG:C8	2.55	0.41
1:A:551:LEU:CD1	1:A:583:GLN:HE22	2.32	0.41
1:A:603:ILE:HD13	1:A:616:VAL:HG21	2.03	0.41
1:B:712:ARG:HB3	1:B:713:PRO:HD3	2.02	0.41
1:A:517:LEU:HA	1:A:520:VAL:HG13	2.03	0.41
1:A:450:LEU:N	1:A:451:PRO:HD2	2.36	0.41
1:A:611:GLN:HB3	1:A:644:LYS:CD	2.50	0.41
1:A:661:HIS:CB	1:A:688:LEU:HD13	2.50	0.41
1:B:494:THR:OG1	1:B:497:GLN:HG2	2.20	0.41
1:A:293:GLN:O	1:A:297:ILE:HG13	2.21	0.41
1:B:655:PRO:O	1:B:659:GLN:HB2	2.21	0.41
1:B:663:LEU:HD21	1:B:704:VAL:HG21	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:LEU:HB3	1:B:587:PRO:HD3	2.02	0.41
1:A:450:LEU:HD23	1:A:464:VAL:HG11	2.03	0.41
1:A:453:LEU:HA	1:A:453:LEU:HD13	1.89	0.41
1:A:657:LEU:O	1:A:663:LEU:HB2	2.21	0.41
1:B:616:VAL:O	1:B:620:LEU:HB2	2.21	0.41
1:B:706:LEU:HA	1:B:706:LEU:HD23	1.86	0.41
1:A:653:LEU:HD13	1:A:685:VAL:HG21	2.03	0.40
1:B:307:LEU:O	1:B:311:GLN:HG3	2.21	0.40
1:A:484:LEU:CD1	1:A:498:VAL:HG11	2.51	0.40
1:A:657:LEU:HA	1:A:657:LEU:HD23	1.93	0.40
1:B:699:THR:O	1:B:700:ASN:C	2.59	0.40
1:B:695:LEU:HB2	1:B:719:LYS:HG3	2.02	0.40
1:A:247:GLU:O	1:A:279:ARG:NH1	2.54	0.40
1:A:470:ASN:HB2	4:A:831:HOH:O	2.21	0.40
1:A:253:LEU:HG	1:A:279:ARG:HG3	2.02	0.40
1:A:655:PRO:O	1:A:659:GLN:CB	2.49	0.40
1:A:297:ILE:HD13	1:A:310:VAL:HG21	2.04	0.40

All (3) 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)
1:A:233:SER:OG	1:A:523:GLN:CB[2_655]	1.67	0.53
1:A:233:SER:CB	1:A:523:GLN:CB[2_655]	1.96	0.24
1:A:233:SER:OG	1:A:523:GLN:CA[2_655]	2.18	0.02

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	486/499 (97%)	458 (94%)	26 (5%)	2 (0%)	34 37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	487/499 (98%)	466 (96%)	13 (3%)	8 (2%)	9 7
All	All	973/998 (98%)	924 (95%)	39 (4%)	10 (1%)	15 14

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	690	ARG
1	B	691	PRO
1	B	662	GLY
1	B	696	ALA
1	B	700	ASN
1	A	279	ARG
1	B	525	HIS
1	A	592	ALA
1	B	710	GLY
1	B	693	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	370/383 (97%)	346 (94%)	24 (6%)	17 19
1	B	372/383 (97%)	339 (91%)	33 (9%)	9 9
All	All	742/766 (97%)	685 (92%)	57 (8%)	13 13

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	236	ARG
1	B	241	LEU
1	B	253	LEU
1	B	260	LEU
1	B	261	LEU
1	B	265	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	287	LEU
1	B	351	LEU
1	B	416	LEU
1	B	418	VAL
1	B	446	VAL
1	B	450	LEU
1	B	520	VAL
1	B	554	VAL
1	B	561	LEU
1	B	589	LEU
1	B	615	THR
1	B	622	VAL
1	B	625	GLN
1	B	657	LEU
1	B	659	GLN
1	B	663	LEU
1	B	664	THR
1	B	666	GLN
1	B	678	ARG
1	B	687	GLN
1	B	688	LEU
1	B	692	ASP
1	B	695	LEU
1	B	701	ASP
1	B	706	LEU
1	B	719	LYS
1	B	721	LEU
1	A	233	SER
1	A	238	LEU
1	A	239	GLU
1	A	241	LEU
1	A	248	LEU
1	A	266	ARG
1	A	301	ASP
1	A	317	LEU
1	A	345	GLN
1	A	382	LEU
1	A	394	GLU
1	A	418	VAL
1	A	453	LEU
1	A	489	GLN
1	A	514	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	520	VAL
1	A	527	LEU
1	A	551	LEU
1	A	623	LEU
1	A	651	GLN
1	A	664	THR
1	A	695	LEU
1	A	709	LEU
1	A	718	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	334	HIS
1	B	353	GLN
1	B	368	HIS
1	B	387	GLN
1	B	457	HIS
1	B	525	HIS
1	B	593	HIS
1	B	666	GLN
1	B	687	GLN
1	A	276	HIS
1	A	280	ASN
1	A	368	HIS
1	A	462	GLN
1	A	583	GLN
1	A	625	GLN
1	A	651	GLN
1	A	687	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

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	487/499 (97%)	0.24	26 (5%) 26 25	22, 46, 87, 116	13 (2%)
1	B	489/499 (97%)	-0.07	17 (3%) 44 42	17, 32, 72, 120	9 (1%)
2	G	15/17 (88%)	-0.56	1 (6%) 17 16	23, 26, 39, 99	0
2	I	15/17 (88%)	-0.54	0 100 100	27, 34, 50, 72	0
3	H	15/17 (88%)	-0.19	1 (6%) 17 16	27, 38, 59, 91	0
3	J	16/17 (94%)	-0.19	1 (6%) 20 19	37, 45, 83, 124	0
All	All	1037/1066 (97%)	0.06	46 (4%) 34 32	17, 39, 83, 124	22 (2%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	696	ALA	5.3
1	A	695	LEU	5.0
1	B	700	ASN	4.6
1	B	693	PRO	4.6
1	A	588	VAL	4.3
1	B	524	ALA	3.9
1	B	685	VAL	3.8
1	B	689	SER	3.8
1	B	686	ALA	3.7
1	A	716	ASP	3.6
1	B	695	LEU	3.3
3	J	-1	DA	3.3
1	A	717	ALA	3.2
1	B	691	PRO	3.2
1	B	688	LEU	3.2
1	A	248	LEU	3.2
1	B	709	LEU	3.1
1	A	591	GLN	3.1
1	A	527	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	654	LEU	2.9
1	A	589	LEU	2.9
1	A	523	GLN	2.7
1	A	627	HIS	2.6
1	A	518	LEU	2.6
1	B	690	ARG	2.5
1	B	718	VAL	2.5
1	A	552	LEU	2.5
2	G	1	DT	2.5
1	A	693	PRO	2.5
1	A	233	SER	2.5
1	B	526	GLY	2.4
1	A	702	HIS	2.4
1	B	719	LYS	2.4
1	A	524	ALA	2.3
1	A	558	ALA	2.3
1	A	631	PRO	2.3
1	A	653	LEU	2.2
1	A	525	HIS	2.2
1	A	689	SER	2.2
1	B	696	ALA	2.2
1	B	523	GLN	2.1
1	A	662	GLY	2.1
1	A	694	ALA	2.1
1	B	692	ASP	2.0
1	A	715	LEU	2.0
3	H	0	DG	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 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.