



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 03:35 PM UTC

PDB ID : 4OTO / pdb_00004oto
Title : Crystal structure of the S505W mutant of TAL effector dHax3
Authors : Deng, D.; Wu, J.P.; Yan, C.Y.; Pan, X.J.; Yan, N.
Deposited on : 2014-02-14
Resolution : 2.59 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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.48.1

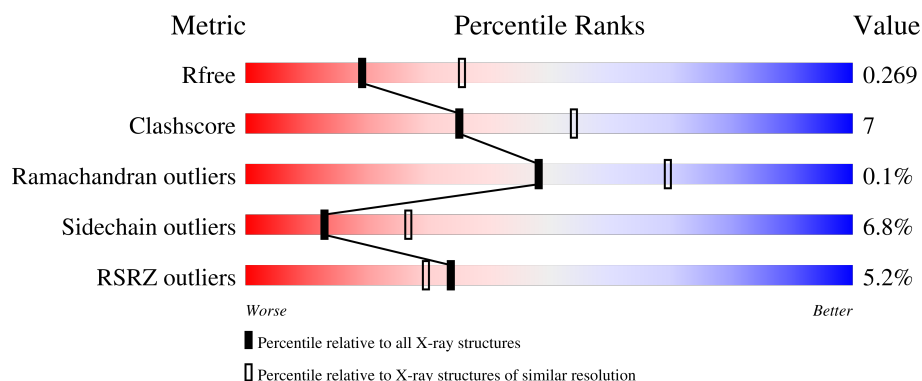
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	164625	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (2.60-2.56)

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	499	4% 75% 21% ..
1	B	499	6% 82% 14% ..
2	G	17	18% 88% 12%
2	I	17	12% 76% 24%
3	H	17	12% 65% 29% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	J	17	 76%24%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8598 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	A	491	Total	C	N	O	S	1	5	0
			3597	2250	670	665	12			
1	B	486	Total	C	N	O	S	11	8	0
			3581	2239	665	664	13			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	TRP	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	727	HIS	-	expression tag	UNP Q3ZD72
A	728	HIS	-	expression tag	UNP Q3ZD72
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	TRP	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
B	727	HIS	-	expression tag	UNP Q3ZD72
B	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	17	Total	C	N	O	P	0	0	0
			333	163	46	108	16			
2	I	17	Total	C	N	O	P	0	0	0
			334	164	46	108	16			

- 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	17	Total 357	C 169	N 80	O 92	P 16	0	0	0
3	J	17	Total 357	C 169	N 80	O 92	P 16	0	0	0

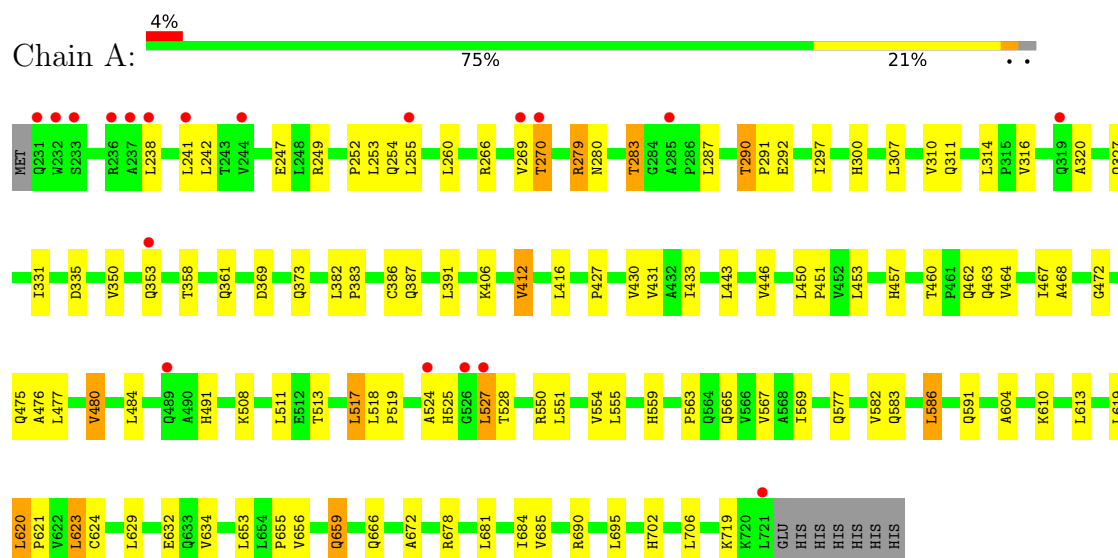
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total 10	O 10	0	0
4	B	13	Total 13	O 13	0	0
4	G	4	Total 4	O 4	0	0
4	I	9	Total 9	O 9	0	0
4	H	1	Total 1	O 1	0	0
4	J	2	Total 2	O 2	0	0

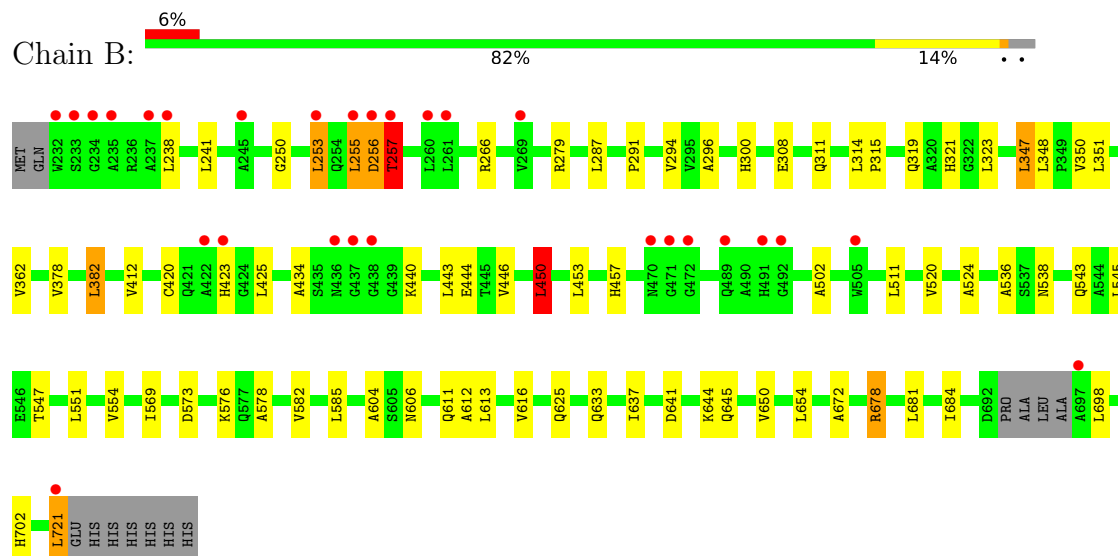
3 Residue-property plots

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.

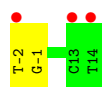
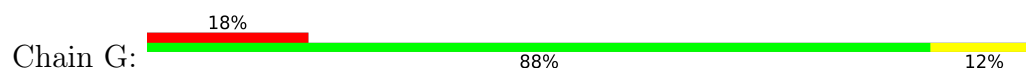
• Molecule 1: Hax3



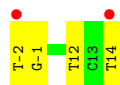
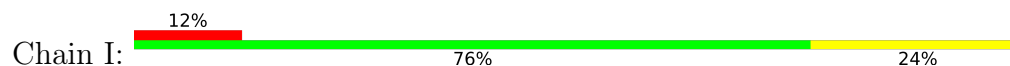
• Molecule 1: Hax3



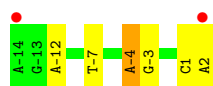
• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*TP*AP*TP*CP*TP*CP*TP*CP*T)-3')



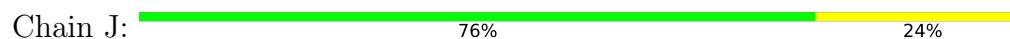
● Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*TP*AP*TP*CP*TP*CP*TP*CP*T)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.44Å 87.07Å 87.97Å 90.00° 103.24° 90.00°	Depositor
Resolution (Å)	38.42 – 2.59 38.42 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.42-2.59) 99.4 (38.42-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.219 , 0.274 0.215 , 0.269	Depositor DCC
R_{free} test set	1858 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.0	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	0.94	EDS
Total number of atoms	8598	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% 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	0.57	1/3650 (0.0%)	0.86	3/4986 (0.1%)
1	B	0.57	0/3633	0.87	7/4960 (0.1%)
2	G	0.38	0/368	0.95	0/564
2	I	0.39	0/369	1.05	1/566 (0.2%)
3	H	0.33	0/405	0.99	2/625 (0.3%)
3	J	0.31	0/405	0.88	0/625
All	All	0.54	1/8830 (0.0%)	0.89	13/12326 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	PRO	N-CD	5.34	1.55	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	12	DT	C4'-C3'-O3'	-6.56	100.16	110.00
1	B	450	LEU	CA-C-N	-5.96	112.36	118.85
1	B	450	LEU	C-N-CA	-5.96	112.36	118.85
3	H	-4	DA	C4'-C3'-O3'	5.56	118.34	110.00
3	H	-7	DT	O5'-C5'-C4'	-5.49	102.56	110.80
1	A	290	THR	CA-C-N	-5.47	113.00	119.84
1	A	290	THR	C-N-CA	-5.47	113.00	119.84
1	B	257	THR	N-CA-C	-5.32	106.29	112.89
1	B	250	GLY	CA-C-N	5.15	125.69	120.38
1	B	250	GLY	C-N-CA	5.15	125.69	120.38
1	A	684	ILE	N-CA-C	5.07	115.50	110.23
1	B	678	ARG	CA-C-N	-5.06	114.45	119.56
1	B	678	ARG	C-N-CA	-5.06	114.45	119.56

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	3597	0	3744	72	0
1	B	3581	0	3714	43	1
2	G	333	0	195	1	1
2	I	334	0	198	4	0
3	H	357	0	190	5	0
3	J	357	0	190	2	0
4	A	10	0	0	1	0
4	B	13	0	0	4	0
4	G	4	0	0	0	0
4	H	1	0	0	0	0
4	I	9	0	0	0	0
4	J	2	0	0	0	0
All	All	8598	0	8231	122	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:O	1:A:254:GLN:HG2	1.54	1.07
1:B:321:HIS:O	4:B:808:HOH:O	1.85	0.93
1:A:255:LEU:HD12	1:A:260:LEU:CD2	2.03	0.89
1:A:632:GLU:O	4:A:810:HOH:O	1.96	0.82
1:A:255:LEU:HD12	1:A:260:LEU:HD23	1.67	0.77
1:A:270[A]:THR:HG21	2:I:-1:DG:H3'	1.71	0.73
1:B:434:ALA:HB2	1:B:443:LEU:HD11	1.74	0.70
1:B:543:GLN:HB3	1:B:576:LYS:HD2	1.74	0.69
1:A:254:GLN:O	1:A:254:GLN:CG	2.46	0.64
1:A:297:ILE:HD13	1:A:310:VAL:HG21	1.81	0.63
1:B:423[B]:HIS:HB3	1:B:450:LEU:HD22	1.81	0.63
1:A:255:LEU:HB2	1:A:260:LEU:HG	1.81	0.62
1:A:287:LEU:HD11	1:A:311:GLN:HA	1.81	0.62
1:A:620:LEU:HD13	1:A:634:VAL:HG11	1.82	0.61
1:B:536:ALA:HB2	1:B:545:LEU:HD11	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:THR:N	4:B:813:HOH:O	1.93	0.61
1:A:266:ARG:HG3	1:A:300:HIS:HA	1.83	0.59
3:H:-4:DA:H2''	3:H:-3:DG:O5'	2.02	0.59
1:A:653:LEU:HD13	1:A:685:VAL:HG21	1.85	0.59
1:A:253:LEU:O	1:A:254:GLN:CG	2.42	0.59
1:A:249:ARG:O	1:A:254:GLN:HB2	2.04	0.58
1:B:266:ARG:HG2	1:B:300:HIS:HA	1.86	0.57
1:A:604:ALA:HB2	1:A:613:LEU:HD11	1.85	0.57
1:A:468:ALA:HB2	1:A:477:LEU:HD11	1.86	0.57
1:B:253:LEU:HD12	1:B:291:PRO:HG3	1.87	0.57
1:B:672:ALA:HB2	1:B:681:LEU:HD11	1.86	0.56
2:I:-2:DT:H5'	2:I:-2:DT:H6	1.70	0.56
1:A:655:PRO:O	1:A:659:GLN:HB2	2.07	0.55
3:H:1:DC:H2''	3:H:2:DA:C8	2.41	0.55
1:A:450:LEU:HD13	1:A:464:VAL:HG11	1.89	0.55
1:A:672:ALA:HB2	1:A:681:LEU:HD11	1.88	0.55
1:A:238:LEU:O	1:A:242:LEU:HG	2.06	0.54
1:B:604:ALA:HB2	1:B:613:LEU:HD11	1.89	0.54
1:A:527:LEU:CD1	1:A:527:LEU:H	2.20	0.54
1:A:582:VAL:O	1:A:586:LEU:HB2	2.08	0.54
1:B:645:GLN:HB3	1:B:678:ARG:HD2	1.89	0.54
1:A:620:LEU:HB3	1:A:621:PRO:HD3	1.89	0.53
1:A:551:LEU:HA	1:A:554:VAL:HG12	1.91	0.53
1:A:491:HIS:CD2	1:A:518:LEU:HD22	2.44	0.53
3:J:1:DC:H2''	3:J:2:DA:C8	2.45	0.52
1:A:702:HIS:HB3	1:B:702:HIS:CE1	2.45	0.52
1:A:527:LEU:CD1	1:A:527:LEU:N	2.73	0.52
1:A:316:VAL:O	1:A:320:ALA:HB3	2.11	0.51
1:B:266:ARG:NH1	3:H:-3:DG:O6	2.38	0.51
1:B:348:LEU:HD23	1:B:362:VAL:HG11	1.93	0.51
1:B:257:THR:CB	4:B:813:HOH:O	2.59	0.51
1:B:721:LEU:HD12	2:I:14:DT:H71	1.92	0.50
1:A:254:GLN:O	1:A:254:GLN:HG3	2.11	0.50
1:A:460:THR:OG1	1:A:463:GLN:HG3	2.11	0.50
1:B:256:ASP:OD1	1:B:256:ASP:N	2.44	0.50
1:A:555:LEU:O	1:A:559:HIS:HB2	2.12	0.50
1:A:524:ALA:O	1:A:525:HIS:HB2	2.11	0.50
1:A:475:GLN:HB3	1:A:508:LYS:HD2	1.93	0.50
1:A:249:ARG:C	1:A:254:GLN:HA	2.37	0.50
1:A:412:VAL:HG23	1:A:443:LEU:HD11	1.93	0.50
2:G:-2:DT:H2''	2:G:-1:DG:C8	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279[A]:ARG:O	1:A:283:THR:OG1	2.22	0.49
1:A:467:ILE:HD13	1:A:480:VAL:HG21	1.94	0.49
1:B:453:LEU:HA	1:B:457:HIS:HB2	1.94	0.49
1:B:257:THR:OG1	4:B:813:HOH:O	2.20	0.49
1:A:666:GLN:H	1:A:666:GLN:CD	2.22	0.48
1:B:611:GLN:HB3	1:B:644:LYS:HD2	1.95	0.48
1:B:698:LEU:HD23	1:B:702:HIS:CD2	2.49	0.48
1:A:527:LEU:H	1:A:527:LEU:HD13	1.77	0.47
1:B:440:LYS:NZ	1:B:444:GLU:OE2	2.48	0.47
1:A:252:PRO:HD2	1:A:279[A]:ARG:HG3	1.97	0.47
1:A:252:PRO:HG2	1:A:283:THR:HG21	1.95	0.47
1:A:416:LEU:HD13	1:A:430:VAL:HG11	1.97	0.47
1:A:518:LEU:HB3	1:A:519:PRO:HD3	1.95	0.47
1:A:619:LEU:HB3	1:A:623:LEU:HD22	1.96	0.47
1:A:577:GLN:HB3	1:A:610:LYS:HD2	1.98	0.46
1:A:450:LEU:HB3	1:A:451:PRO:HD3	1.97	0.46
1:A:472:GLY:HA3	1:A:476:ALA:HB2	1.98	0.46
3:H:-12:DA:H5'	3:H:-12:DA:H8	1.81	0.46
1:B:502:ALA:HB2	1:B:511:LEU:HD11	1.98	0.46
1:A:255:LEU:CB	1:A:260:LEU:HG	2.46	0.46
1:A:287:LEU:HD22	1:A:314:LEU:HD22	1.97	0.46
1:A:249:ARG:O	1:A:254:GLN:CB	2.64	0.46
1:A:624:CYS:HA	1:A:629:LEU:O	2.16	0.46
1:B:547:THR:OG1	1:B:576:LYS:HG3	2.16	0.45
1:A:386:CYS:HA	1:A:391:LEU:O	2.17	0.45
1:A:433:ILE:HD13	1:A:446:VAL:HG21	1.99	0.45
3:H:-12:DA:H5'	3:H:-12:DA:C8	2.52	0.45
1:B:420[B]:CYS:HA	1:B:425[B]:LEU:O	2.17	0.45
1:A:387:GLN:O	1:B:420[A]:CYS:HB3	2.16	0.45
1:B:253:LEU:HD21	1:B:294:VAL:HG11	1.98	0.45
1:B:578:ALA:O	1:B:582:VAL:HG23	2.16	0.44
1:A:565:GLN:O	1:A:569:ILE:HG13	2.17	0.44
1:B:378:VAL:O	1:B:382:LEU:HB2	2.17	0.44
1:B:551:LEU:HD23	1:B:551:LEU:HA	1.80	0.44
1:A:569:ILE:HD13	1:A:582:VAL:HG21	1.98	0.44
1:A:255:LEU:HD12	1:A:260:LEU:CG	2.47	0.44
1:A:327:GLN:O	1:A:331:ILE:HG13	2.17	0.44
1:A:527:LEU:N	1:A:527:LEU:HD12	2.32	0.43
1:A:358:THR:OG1	1:A:361:GLN:HG3	2.19	0.43
1:A:513:THR:O	1:A:517:LEU:HB2	2.19	0.43
1:B:255:LEU:HD12	1:B:255:LEU:HA	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:HIS:HB3	1:A:484:LEU:HD23	2.02	0.42
1:A:373:GLN:HB3	1:A:406:LYS:HD3	2.02	0.42
1:B:569:ILE:HD13	1:B:582:VAL:HG21	2.02	0.42
2:I:-2:DT:H5'	2:I:-2:DT:C6	2.54	0.42
1:B:347:LEU:HD12	1:B:347:LEU:HA	1.71	0.42
1:B:633:GLN:O	1:B:637:ILE:HG13	2.20	0.42
1:A:335:ASP:N	1:A:369:ASP:OD1	2.52	0.42
1:A:555:LEU:HD21	1:A:583:GLN:HB2	2.01	0.41
1:B:314:LEU:HB3	1:B:315:PRO:HD3	2.02	0.41
1:A:457:HIS:ND1	1:A:484:LEU:HD23	2.35	0.41
1:B:296:ALA:O	1:B:300:HIS:NE2	2.52	0.41
1:A:563:PRO:O	1:A:567:VAL:HG23	2.21	0.41
1:B:612:ALA:O	1:B:616:VAL:HG23	2.21	0.41
1:B:650:VAL:O	1:B:654:LEU:HB2	2.20	0.41
1:A:491:HIS:HD2	1:A:518:LEU:HD22	1.84	0.40
1:B:425[B]:LEU:HD11	1:B:446:VAL:HG11	2.03	0.40
1:B:606:ASN:HB3	1:B:641:ASP:OD2	2.21	0.40
1:A:290:THR:C	1:A:292:GLU:N	2.79	0.40
1:B:538:ASN:HB3	1:B:573:ASP:OD1	2.22	0.40
1:A:511:LEU:HD23	1:A:511:LEU:HA	1.90	0.40
1:A:427:PRO:O	1:A:431:VAL:HG23	2.22	0.40
1:B:287:LEU:HD11	1:B:311:GLN:HA	2.03	0.40
1:B:425[A]:LEU:HD11	1:B:446:VAL:HG11	2.03	0.40
3:J:-2:DG:H2''	3:J:-1:DG:H8	1.86	0.40
1:A:279[A]:ARG:HG2	1:A:280:ASN:N	2.34	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:ALA:O	2:G:-2:DT:O5'[2_344]	2.07	0.13

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	494/499 (99%)	469 (95%)	24 (5%)	1 (0%)	44	64
1	B	490/499 (98%)	465 (95%)	25 (5%)	0	100	100
All	All	984/998 (99%)	934 (95%)	49 (5%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	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	379/383 (99%)	347 (92%)	32 (8%)	9	18
1	B	377/383 (98%)	355 (94%)	22 (6%)	17	34
All	All	756/766 (99%)	702 (93%)	54 (7%)	13	25

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	LEU
1	A	247	GLU
1	A	269[A]	VAL
1	A	269[B]	VAL
1	A	270[A]	THR
1	A	270[B]	THR
1	A	279[A]	ARG
1	A	279[B]	ARG
1	A	283	THR
1	A	307	LEU
1	A	350	VAL
1	A	353	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	382	LEU
1	A	412	VAL
1	A	453	LEU
1	A	462	GLN
1	A	480	VAL
1	A	517	LEU
1	A	527	LEU
1	A	528	THR
1	A	550	ARG
1	A	586	LEU
1	A	591	GLN
1	A	620	LEU
1	A	623	LEU
1	A	656	VAL
1	A	659	GLN
1	A	678	ARG
1	A	690	ARG
1	A	695	LEU
1	A	706	LEU
1	A	719	LYS
1	B	238	LEU
1	B	241	LEU
1	B	253	LEU
1	B	255	LEU
1	B	256	ASP
1	B	257	THR
1	B	279	ARG
1	B	308	GLU
1	B	319	GLN
1	B	323	LEU
1	B	347	LEU
1	B	350	VAL
1	B	351	LEU
1	B	382	LEU
1	B	412	VAL
1	B	450	LEU
1	B	520	VAL
1	B	554	VAL
1	B	585	LEU
1	B	625	GLN
1	B	684	ILE
1	B	721	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	ASN
1	A	293	GLN
1	A	300	HIS
1	A	334	HIS
1	A	339	GLN
1	A	373	GLN
1	A	421	GLN
1	A	423	HIS
1	A	491	HIS
1	A	577	GLN
1	A	593	HIS
1	A	640	HIS
1	A	651	GLN
1	B	288	ASN
1	B	339	GLN
1	B	353	GLN
1	B	368	HIS
1	B	373	GLN
1	B	389	HIS
1	B	436	ASN
1	B	441	GLN
1	B	462	GLN
1	B	475	GLN
1	B	491	HIS
1	B	538	ASN
1	B	577	GLN
1	B	606	ASN
1	B	617	GLN
1	B	702	HIS

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 [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	491/499 (98%)	0.20	19 (3%) 44 39	14, 38, 76, 172	16 (3%)
1	B	486/499 (97%)	0.31	28 (5%) 30 26	15, 42, 79, 110	19 (3%)
2	G	17/17 (100%)	-0.38	3 (17%) 4 4	27, 29, 92, 150	0
2	I	17/17 (100%)	-0.42	2 (11%) 10 9	23, 25, 106, 119	0
3	H	17/17 (100%)	0.13	2 (11%) 10 9	37, 48, 114, 116	0
3	J	17/17 (100%)	0.39	0 100 100	37, 47, 107, 128	0
All	All	1045/1066 (98%)	0.23	54 (5%) 34 30	14, 41, 79, 172	35 (3%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	471	GLY	7.4
1	B	472	GLY	7.2
1	A	237	ALA	5.9
1	B	436	ASN	5.8
1	B	423[A]	HIS	4.5
1	B	260	LEU	4.2
1	A	721	LEU	4.1
1	B	232	TRP	4.1
1	B	437	GLY	4.0
1	B	470	ASN	4.0
1	A	231	GLN	4.0
1	A	524	ALA	3.9
2	I	-2	DT	3.9
1	A	232	TRP	3.6
2	G	-2	DT	3.4
1	A	269[A]	VAL	3.4
1	B	255	LEU	3.4
1	B	235	ALA	3.3
1	B	257	THR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	H	2	DA	3.2
1	B	238	LEU	3.2
1	B	697	ALA	3.1
1	B	253	LEU	3.1
2	G	14	DT	3.0
1	B	234	GLY	2.9
1	A	526	GLY	2.9
1	A	233	SER	2.8
1	A	255	LEU	2.7
1	B	422[A]	ALA	2.7
1	B	261	LEU	2.7
1	B	256	ASP	2.7
1	A	270[A]	THR	2.7
1	B	489	GLN	2.6
1	A	319	GLN	2.5
1	A	236	ARG	2.5
3	H	-14	DA	2.5
1	B	237	ALA	2.5
1	B	492	GLY	2.5
1	B	505	TRP	2.4
1	A	353	GLN	2.4
1	B	233	SER	2.4
1	A	244	VAL	2.4
1	B	438	GLY	2.4
2	I	14	DT	2.3
1	B	491	HIS	2.3
1	B	245	ALA	2.3
1	A	527	LEU	2.3
1	A	238	LEU	2.3
1	A	241	LEU	2.2
1	A	285	ALA	2.2
2	G	13	DC	2.2
1	B	269	VAL	2.1
1	A	489	GLN	2.1
1	B	721	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.