



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:01 PM UTC

PDB ID : 4OSW / pdb_00004osw
Title : Crystal structure of the S505E mutant of TAL effector dHax3
Authors : Deng, D.; Wu, J.P.; Yan, C.Y.; Pan, X.J.; Yan, N.
Deposited on : 2014-02-13
Resolution : 2.30 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

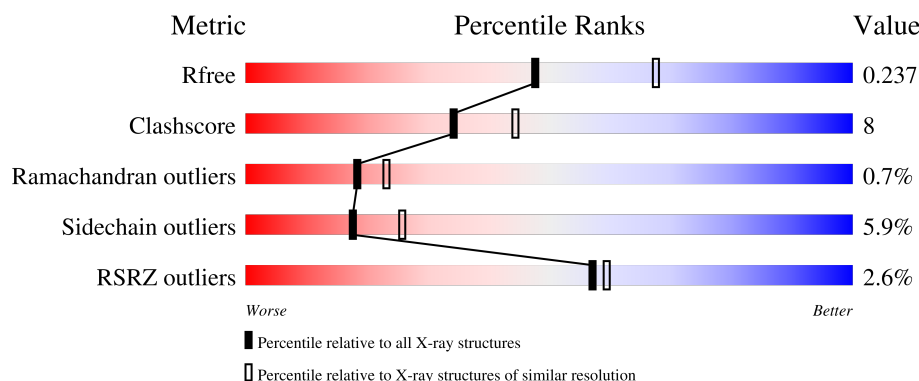
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

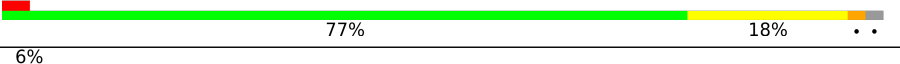
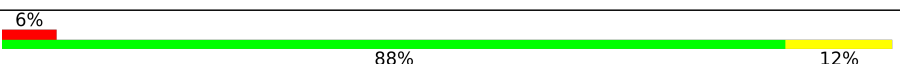
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	
1	B	499	
2	G	17	
2	I	17	
3	H	17	

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Mol	Chain	Length	Quality of chain
3	J	17	 71% 29%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8831 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	5	3	0
			3577	2237	664	664	12			
1	B	487	Total	C	N	O	S	5	3	0
			3552	2218	659	663	12			

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	GLU	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

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	J	1	Total	Mg	0	0
			1	1		

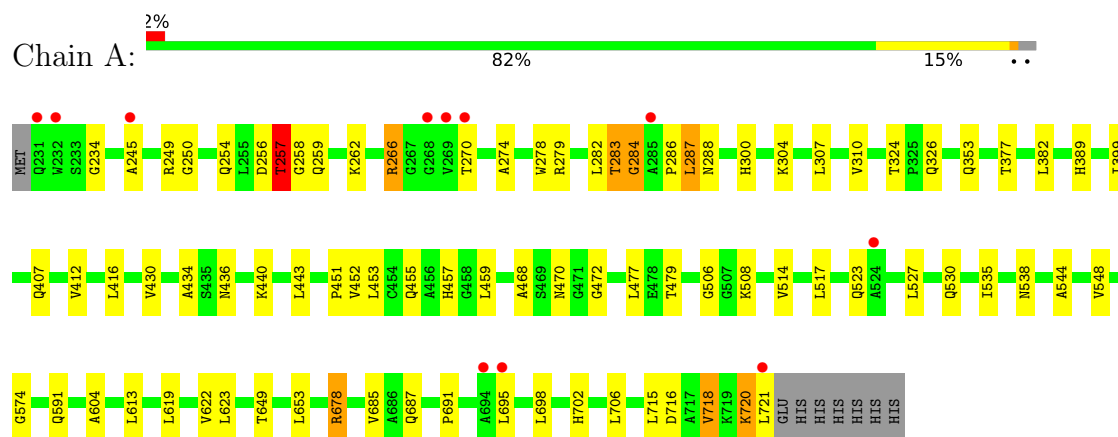
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	132	Total	O	0	0
			132	132		
5	B	118	Total	O	0	0
			118	118		
5	G	19	Total	O	0	0
			19	19		
5	H	9	Total	O	0	0
			9	9		
5	I	30	Total	O	0	0
			30	30		
5	J	11	Total	O	0	0
			11	11		

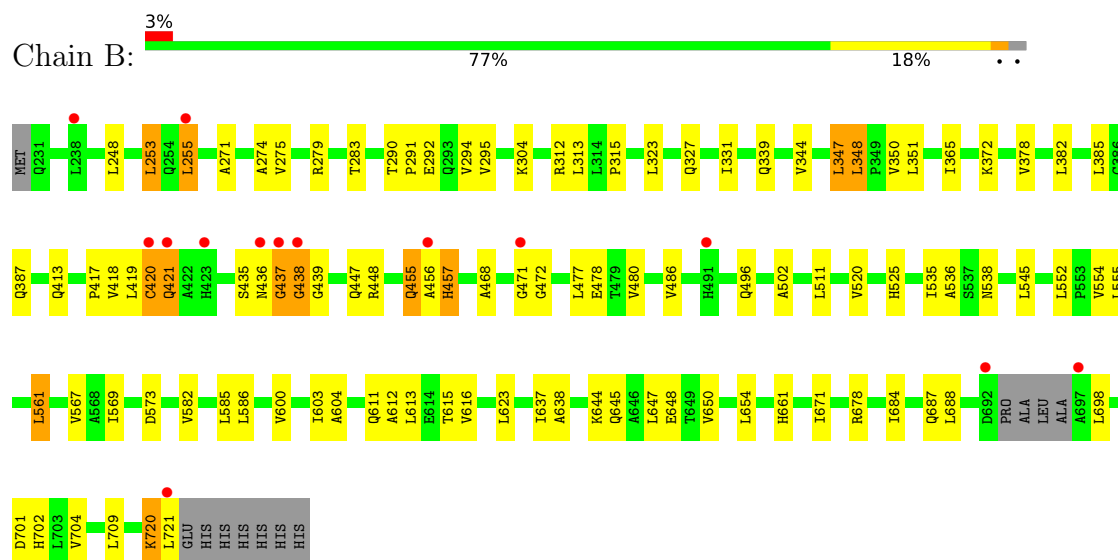
3 Residue-property plots [i](#)

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.

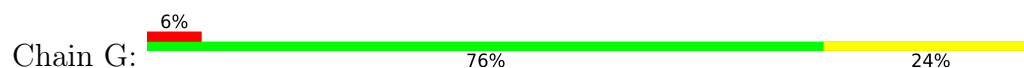
• Molecule 1: Hax3

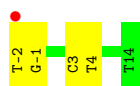


• Molecule 1: Hax3



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

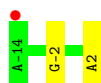
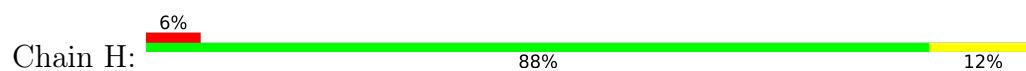




- Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*TP*AP*TP*CP*TP*CP*TP*CP*T)-3')



- 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	81.95Å 87.65Å 87.44Å 90.00° 102.55° 90.00°	Depositor
Resolution (Å)	30.86 – 2.30 30.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.86-2.30) 99.8 (30.86-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.198 , 0.243 0.196 , 0.237	Depositor DCC
R_{free} test set	2718 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.1	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	0.96	EDS
Total number of atoms	8831	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 5.66% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.55	0/3630	0.88	6/4960 (0.1%)
1	B	0.54	0/3601	0.85	3/4915 (0.1%)
2	G	0.47	0/368	1.01	0/564
2	I	0.42	0/369	1.01	0/566
3	H	0.37	0/405	0.98	0/625
3	J	0.36	0/405	0.93	1/625 (0.2%)
All	All	0.52	0/8778	0.89	10/12255 (0.1%)

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	470	ASN	CB-CA-C	-9.22	94.88	109.72
1	A	470	ASN	N-CA-C	-8.36	95.84	108.46
1	B	420	CYS	O-C-N	-6.98	113.18	122.19
3	J	0	DA	C4'-C3'-O3'	-6.53	100.20	110.00
1	A	287	LEU	N-CA-C	5.93	118.23	111.11
1	A	472	GLY	N-CA-C	-5.53	108.00	115.36
1	A	250	GLY	CA-C-N	5.44	123.63	119.66
1	A	250	GLY	C-N-CA	5.44	123.63	119.66
1	B	457	HIS	N-CA-C	5.26	119.54	113.18
1	B	455	GLN	N-CA-C	-5.26	103.67	110.19

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	420	CYS	Mainchain,Peptide
1	B	421[B]	GLN	Peptide

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	3577	0	3711	45	0
1	B	3552	0	3687	57	0
2	G	333	0	195	12	0
2	I	334	0	198	4	0
3	H	357	0	190	3	0
3	J	357	0	190	4	0
4	A	1	0	0	1	0
4	J	1	0	0	0	0
5	A	132	0	0	11	0
5	B	118	0	0	4	0
5	G	19	0	0	0	0
5	H	9	0	0	2	0
5	I	30	0	0	3	0
5	J	11	0	0	3	0
All	All	8831	0	8171	123	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 8.

All (123) 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)
2:G:-2:DT:H6	2:G:-2:DT:C5'	1.38	1.35
1:A:266:ARG:HB2	5:A:1027:HOH:O	1.40	1.20
2:G:-2:DT:C5'	2:G:-2:DT:C6	2.30	1.13
2:G:-2:DT:C6	2:G:-2:DT:H5'	1.88	1.07
2:G:-2:DT:H6	2:G:-2:DT:H5'	1.15	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:-2:DT:H6	2:G:-2:DT:H5''	1.22	1.01
2:G:-2:DT:C6	2:G:-2:DT:H5''	2.07	0.84
1:A:284:GLY:O	1:A:288:ASN:ND2	2.10	0.83
1:A:324:THR:OG1	5:A:943:HOH:O	1.97	0.82
1:A:407:GLN:HB3	1:A:440:LYS:HD2	1.68	0.75
1:A:523:GLN:O	5:A:1011:HOH:O	2.05	0.75
3:H:-2:DG:N7	5:H:109:HOH:O	2.21	0.74
1:A:687:GLN:HG2	1:A:695:LEU:HD22	1.68	0.73
1:B:339:GLN:HB3	1:B:372:LYS:HD3	1.73	0.71
1:A:436:ASN:HB2	5:A:1024:HOH:O	1.90	0.70
1:A:706:LEU:HD21	1:A:718:VAL:HG21	1.74	0.69
1:B:436:ASN:O	1:B:437:GLY:C	2.34	0.69
1:B:648:GLU:OE1	5:B:832:HOH:O	2.12	0.68
3:H:-2:DG:N3	5:H:101:HOH:O	2.26	0.67
2:G:-2:DT:H3	3:H:2:DA:H2	1.43	0.67
1:A:535:ILE:HD13	1:A:548:VAL:HG21	1.76	0.66
1:A:721:LEU:O	5:A:1021:HOH:O	2.14	0.66
1:A:653:LEU:HD13	1:A:685:VAL:HG21	1.78	0.66
1:B:701:ASP:OD1	5:B:887:HOH:O	2.13	0.66
4:A:801:MG:MG	5:J:209:HOH:O	1.37	0.65
1:B:435:SER:O	1:B:436:ASN:ND2	2.30	0.65
1:A:574:GLY:HA3	5:I:127:HOH:O	1.96	0.65
2:G:-2:DT:H2''	2:G:-1:DG:H5'	1.77	0.65
3:J:-9:DG:OP2	5:J:211:HOH:O	2.16	0.62
1:A:266:ARG:HG3	1:A:300:HIS:HA	1.82	0.60
1:A:279:ARG:O	1:A:283:THR:OG1	2.20	0.59
1:B:248:LEU:HD13	1:B:255:LEU:HD22	1.87	0.57
1:B:365:ILE:HD13	1:B:378:VAL:HG21	1.85	0.57
1:B:720:LYS:NZ	1:B:720:LYS:HB3	2.19	0.57
1:B:448:ARG:NH2	1:B:478:GLU:OE1	2.36	0.57
1:A:256:ASP:O	1:A:257:THR:C	2.48	0.56
1:B:637:ILE:HD13	1:B:650:VAL:HG21	1.87	0.55
1:A:452:VAL:HG23	5:A:926:HOH:O	2.06	0.55
1:A:377:THR:OG1	5:A:954:HOH:O	2.17	0.55
2:I:13:DC:H2''	2:I:14:DT:H5''	1.90	0.54
1:A:538:ASN:HB2	5:A:1018:HOH:O	2.07	0.54
1:B:455:GLN:O	1:B:457:HIS:N	2.40	0.54
1:A:256:ASP:O	1:A:259:GLN:N	2.42	0.53
1:B:645:GLN:HB3	1:B:678:ARG:HD2	1.90	0.53
1:B:720:LYS:HB3	1:B:720:LYS:HZ3	1.73	0.53
2:G:-2:DT:H2'	2:G:-1:DG:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:VAL:HG11	1:B:447:GLN:HE21	1.74	0.52
1:B:586:LEU:HD13	1:B:600:VAL:HG11	1.91	0.52
1:B:569:ILE:HD13	1:B:582:VAL:HG21	1.93	0.51
1:B:720:LYS:NZ	1:B:720:LYS:CB	2.73	0.51
1:B:271:ALA:O	1:B:275:VAL:HG23	2.10	0.51
1:B:720:LYS:O	1:B:720:LYS:HG3	2.11	0.51
3:J:-9:DG:H2''	3:J:-8:DA:H5''	1.93	0.51
1:A:468:ALA:HB2	1:A:477:LEU:HD11	1.94	0.50
1:B:611:GLN:HB3	1:B:644:LYS:HD2	1.94	0.50
1:A:274:ALA:HB2	1:A:304:LYS:HG3	1.94	0.50
2:G:-2:DT:C6	2:G:-2:DT:C4'	2.89	0.50
2:I:9:DC:OP2	5:I:127:HOH:O	2.20	0.50
1:B:472:GLY:N	5:B:811:HOH:O	2.08	0.50
1:A:282:LEU:HA	1:A:287:LEU:HD12	1.94	0.49
1:B:436:ASN:O	1:B:437:GLY:O	2.30	0.49
1:B:661:HIS:ND1	1:B:688:LEU:HB3	2.26	0.49
1:B:253:LEU:HD21	1:B:294:VAL:HG11	1.93	0.49
1:A:702:HIS:HB3	1:B:702:HIS:CE1	2.47	0.49
1:A:389:HIS:HB3	1:A:416:LEU:HD23	1.96	0.48
1:B:419:LEU:HD21	1:B:447:GLN:HB2	1.95	0.48
1:A:716:ASP:O	1:A:720:LYS:HG2	2.14	0.48
1:B:603:ILE:HD13	1:B:616:VAL:HG21	1.94	0.47
1:B:535:ILE:HD11	1:B:567:VAL:HG22	1.97	0.47
1:B:638:ALA:O	5:B:815:HOH:O	2.20	0.47
2:G:-2:DT:H2''	2:G:-1:DG:C5'	2.45	0.47
1:A:451:PRO:O	1:A:455:GLN:HG2	2.14	0.47
1:A:457:HIS:O	5:A:986:HOH:O	2.20	0.47
1:B:671:ILE:HD11	1:B:704:VAL:HG13	1.97	0.46
1:B:274:ALA:HB2	1:B:304:LYS:HG3	1.96	0.46
1:A:249:ARG:NH1	1:A:257:THR:OG1	2.32	0.45
1:A:256:ASP:O	1:A:258:GLY:N	2.49	0.45
1:B:615:THR:OG1	1:B:644:LYS:HG3	2.16	0.45
1:B:421[B]:GLN:HE21	1:B:421[B]:GLN:HB2	1.57	0.45
1:A:506:GLY:N	5:A:1014:HOH:O	2.35	0.45
1:B:502:ALA:HB2	1:B:511:LEU:HD11	1.99	0.45
1:B:536:ALA:HB2	1:B:545:LEU:HD11	1.98	0.44
1:B:525:HIS:HB3	1:B:552:LEU:HD22	1.99	0.44
1:A:270:THR:HG23	5:I:108:HOH:O	2.16	0.44
1:B:437:GLY:O	1:B:438:GLY:C	2.59	0.43
1:B:496[A]:GLN:CD	1:B:496[A]:GLN:H	2.26	0.43
1:B:538:ASN:HB3	1:B:573:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ALA:HB2	1:B:477:LEU:HD11	2.00	0.43
1:A:649:THR:OG1	1:A:678:ARG:HD3	2.18	0.43
1:B:438:GLY:HA2	1:B:439:GLY:HA3	1.74	0.43
1:B:344:VAL:O	1:B:348:LEU:HB2	2.19	0.43
1:B:612:ALA:O	1:B:616:VAL:HG23	2.17	0.43
3:J:1:DC:H2''	3:J:2:DA:C8	2.54	0.43
2:G:3:DC:H2''	2:G:4:DT:O5'	2.19	0.43
1:A:604:ALA:HB2	1:A:613:LEU:HD11	2.01	0.42
1:B:555:LEU:HB3	1:B:561:LEU:HD23	2.01	0.42
1:B:312:ARG:O	1:B:315:PRO:HD2	2.19	0.42
1:A:434:ALA:HB2	1:A:443:LEU:HD11	2.01	0.42
1:A:687:GLN:O	1:A:691:PRO:HA	2.20	0.42
1:B:327:GLN:O	1:B:331:ILE:HG13	2.20	0.42
1:B:638:ALA:HB2	1:B:647:LEU:HD11	2.01	0.42
1:A:479:THR:OG1	1:A:508:LYS:HG3	2.20	0.42
1:A:399:ILE:HD13	1:A:412:VAL:HG21	2.01	0.42
1:B:347:LEU:HA	1:B:350:VAL:HG12	2.00	0.42
1:A:278[B]:TRP:HD1	1:A:282:LEU:HD11	1.84	0.42
1:A:530:GLN:CD	1:A:530:GLN:H	2.27	0.42
1:B:417:PRO:O	1:B:421[A]:GLN:HG2	2.19	0.42
1:A:416:LEU:HD13	1:A:430:VAL:HG11	2.02	0.41
1:A:245:ALA:O	1:A:249:ARG:HG3	2.19	0.41
1:B:437:GLY:O	1:B:471:GLY:HA2	2.20	0.41
1:B:604:ALA:HB2	1:B:613:LEU:HD11	2.03	0.41
1:B:721:LEU:HA	2:I:14:DT:H72	2.02	0.41
1:B:623:LEU:HD23	1:B:623:LEU:HA	1.90	0.41
1:B:253:LEU:HD13	1:B:283:THR:HG21	2.02	0.41
1:A:266:ARG:HD2	1:A:266:ARG:HA	1.70	0.41
1:A:262:LYS:HG3	5:J:208:HOH:O	2.19	0.41
1:B:291:PRO:O	1:B:295:VAL:HG23	2.20	0.41
1:B:385:LEU:HD21	1:B:413:GLN:HB2	2.03	0.41
1:B:290:THR:OG1	1:B:292:GLU:HG2	2.21	0.40
2:I:-2:DT:H2''	2:I:-1:DG:C8	2.56	0.40
1:A:544:ALA:O	1:A:548:VAL:HG23	2.22	0.40
3:J:2:DA:OP2	3:J:2:DA:H2'	2.22	0.40
1:A:698:LEU:HA	5:A:905:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	492/499 (99%)	465 (94%)	23 (5%)	4 (1%)	16	20
1	B	486/499 (97%)	465 (96%)	18 (4%)	3 (1%)	21	27
All	All	978/998 (98%)	930 (95%)	41 (4%)	7 (1%)	18	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	437	GLY
1	B	438	GLY
1	B	456	ALA
1	A	234	GLY
1	A	257	THR
1	A	284	GLY
1	A	286	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	376/383 (98%)	354 (94%)	22 (6%)	18	26
1	B	375/383 (98%)	353 (94%)	22 (6%)	18	26
All	All	751/766 (98%)	707 (94%)	44 (6%)	18	26

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	257	THR
1	A	266	ARG
1	A	283	THR
1	A	307	LEU
1	A	310	VAL
1	A	326	GLN
1	A	353	GLN
1	A	382	LEU
1	A	453	LEU
1	A	459	LEU
1	A	514	VAL
1	A	517	LEU
1	A	527	LEU
1	A	591	GLN
1	A	619	LEU
1	A	622	VAL
1	A	623	LEU
1	A	678	ARG
1	A	715	LEU
1	A	718	VAL
1	A	720	LYS
1	B	253	LEU
1	B	255	LEU
1	B	279	ARG
1	B	313	LEU
1	B	323	LEU
1	B	347	LEU
1	B	348	LEU
1	B	351	LEU
1	B	382	LEU
1	B	387	GLN
1	B	480	VAL
1	B	486	VAL
1	B	520	VAL
1	B	554	VAL
1	B	561	LEU
1	B	585	LEU
1	B	654	LEU
1	B	684	ILE
1	B	687	GLN
1	B	698	LEU
1	B	709	LEU

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Mol	Chain	Res	Type
1	B	720	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	HIS
1	A	355	HIS
1	A	373	GLN
1	A	387	GLN
1	A	407	GLN
1	A	457	HIS
1	A	491	HIS
1	A	543	GLN
1	A	549	GLN
1	A	559	HIS
1	A	577	GLN
1	A	611	GLN
1	A	640	HIS
1	A	645	GLN
1	A	661	HIS
1	A	674	ASN
1	B	368	HIS
1	B	373	GLN
1	B	436	ASN
1	B	447	GLN
1	B	470	ASN
1	B	475	GLN
1	B	538	ASN
1	B	543	GLN
1	B	559	HIS
1	B	606	ASN
1	B	611	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 [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](#)

Of 2 ligands modelled in this entry, 2 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 [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%)	-0.14	11 (2%) 62 64	20, 38, 76, 148	14 (2%)
1	B	487/499 (97%)	0.05	14 (2%) 53 56	24, 44, 74, 108	12 (2%)
2	G	17/17 (100%)	-0.52	1 (5%) 28 30	30, 34, 89, 96	0
2	I	17/17 (100%)	-0.78	0 100 100	25, 30, 76, 78	0
3	H	17/17 (100%)	0.06	1 (5%) 28 30	40, 49, 92, 105	0
3	J	17/17 (100%)	-0.22	0 100 100	36, 48, 74, 80	0
All	All	1046/1066 (98%)	-0.06	27 (2%) 57 59	20, 42, 76, 148	26 (2%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	438	GLY	8.7
1	B	437	GLY	3.4
1	A	524	ALA	3.3
1	B	436	ASN	3.2
1	B	721	LEU	3.1
1	B	697	ALA	3.0
1	B	491	HIS	2.9
1	B	238	LEU	2.9
1	B	421[A]	GLN	2.9
1	B	456	ALA	2.9
1	A	232	TRP	2.8
1	A	694	ALA	2.8
1	B	471	GLY	2.6
1	B	420	CYS	2.5
1	A	695	LEU	2.5
1	A	231	GLN	2.3
1	A	269	VAL	2.3
3	H	-14	DA	2.3
1	A	285	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	692	ASP	2.3
1	A	270	THR	2.3
1	A	721	LEU	2.2
1	A	268	GLY	2.2
2	G	-2	DT	2.2
1	B	423	HIS	2.2
1	B	255	LEU	2.1
1	A	245	ALA	2.1

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](#)

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, 95th 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	MG	A	801	1/1	0.69	0.13	93,93,93,93	0
4	MG	J	101	1/1	0.83	0.13	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.