Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 07:32 PM EDT

PDB ID	:	4OSS
Title	:	Crystal structure of the S505Q 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	:	2.40 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 (i) 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 (1)) were used in the production of this report:

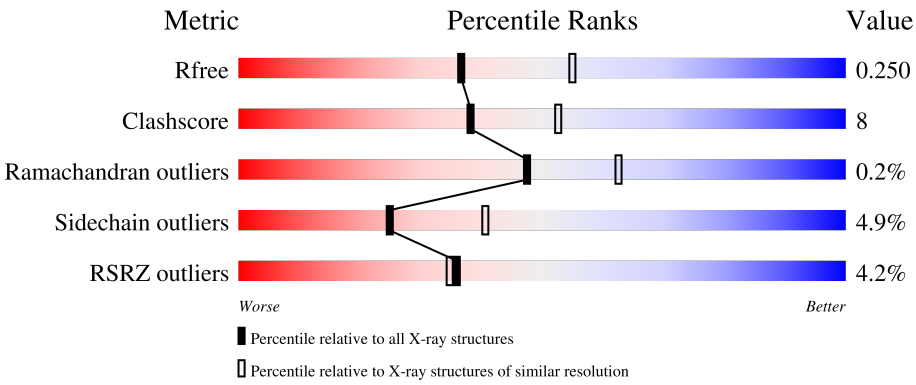
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	499	4%, 84%, 13%, ••
1	B	499	4%, 81%, 15%, ••
2	G	17	12%, 53%, 41%, 6%
2	I	17	6%, 59%, 41%
3	H	17	12%, 53%, 35%, 6%, 6%

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Mol	Chain	Length	Quality of chain
3	J	17	12% 71% 29%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8655 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
			Total	C	N	O	S			
1	A	493	3619	2263	675	669	12	0	5	0
1	B	487	3585	2238	667	667	13	0	8	0

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	GLN	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	GLN	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*GP*TP*CP*TP*CP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	G	16	315	154	44	102	15	0	0	0
			Total	C	N	O	P			
2	I	17	335	164	46	109	16	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	H	16	338	158	76	88	16	0	0	0
3	J	17	356	168	81	91	16	0	0	0

- Molecule 4 is water.

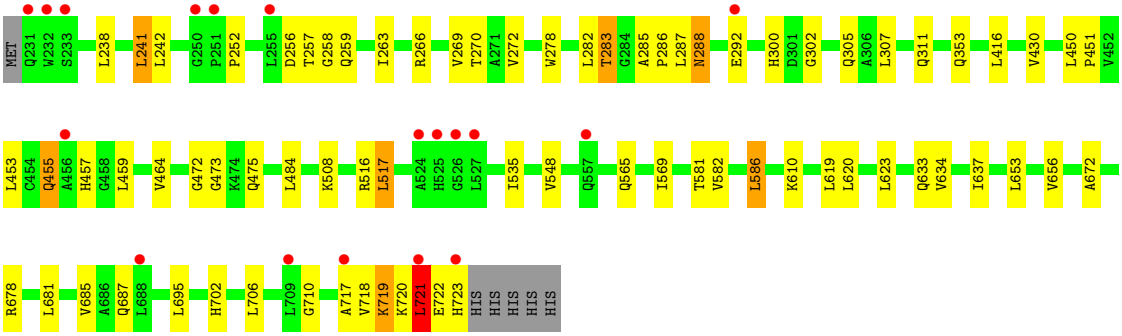
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	45	45	45	0	0
4	B	30	30	30	0	0
4	G	16	16	16	0	0
4	H	4	4	4	0	0
4	I	12	12	12	0	0

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.

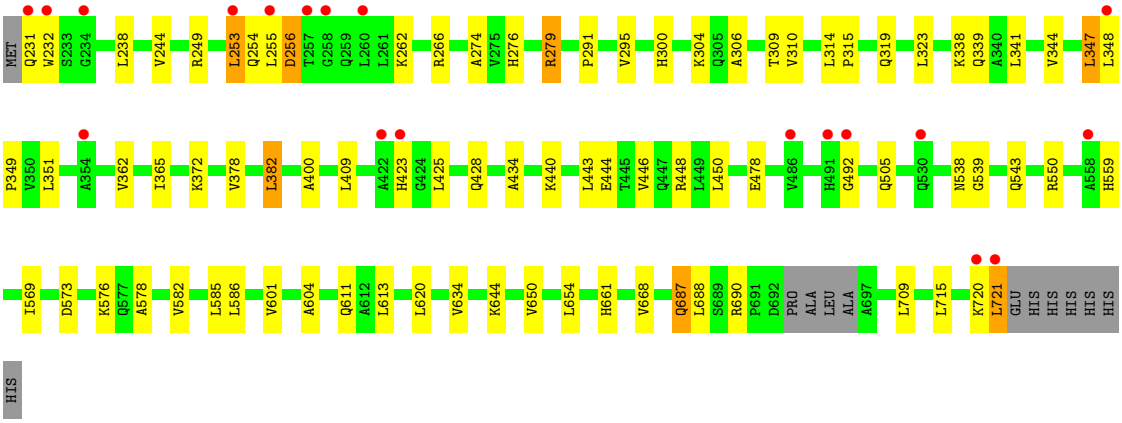
• Molecule 1: Hax3

Chain A:



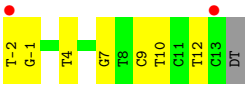
• Molecule 1: Hax3

Chain B:



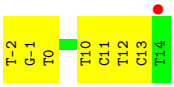
• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*TP*GP*TP*CP*TP*CP*TP*CP*T)-3')

Chain G:



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

Chain I:

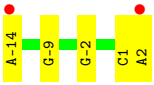


• Molecule 3: DNA (5'-D(*AP*GP*AP*GP*AP*GP*AP*CP*AP*AP*AP*GP*GP*GP*AP*CP*A)-3')

Chain H:

• Molecule 3: DNA (5'-D(*AP*GP*AP*GP*AP*GP*AP*CP*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	81.08Å 87.07Å 87.95Å 90.00° 103.00° 90.00°	Depositor
Resolution (Å)	39.50 – 2.40 39.50 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.50-2.40) 99.6 (39.50-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.219 , 0.255 0.213 , 0.250	Depositor DCC
R_{free} test set	2370 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	40.3	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 30.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8655	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.92% 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 (i)

5.1 Standard geometry (i)

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	0.38	0/3673	0.56	0/5017
1	B	0.39	0/3635	0.55	0/4961
2	G	0.70	0/348	1.51	5/534 (0.9%)
2	I	0.80	0/370	1.46	5/568 (0.9%)
3	H	0.80	0/383	1.31	2/590 (0.3%)
3	J	0.76	0/404	1.32	4/623 (0.6%)
All	All	0.47	0/8813	0.79	16/12293 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	9	DC	O4'-C1'-N1	-7.73	102.59	108.00
3	H	0	DA	O4'-C1'-N9	-7.64	102.65	108.00
3	J	-9	DG	O4'-C1'-N9	7.23	113.06	108.00
2	G	12	DT	O4'-C1'-N1	-7.08	103.04	108.00
3	J	-2	DG	O4'-C1'-N9	6.59	112.62	108.00
2	I	12	DT	N3-C4-O4	6.26	123.66	119.90
2	G	12	DT	N3-C4-O4	6.23	123.64	119.90
2	G	12	DT	C5-C4-O4	-6.13	120.61	124.90
2	I	12	DT	C5-C4-O4	-6.05	120.66	124.90
3	J	-9	DG	C3'-C2'-C1'	-6.04	95.26	102.50
2	I	12	DT	O4'-C1'-N1	-5.67	104.03	108.00
3	H	2	DA	C3'-C2'-C1'	-5.51	95.89	102.50
3	J	-14	DA	O4'-C4'-C3'	-5.32	102.37	104.50
2	I	10	DT	N3-C4-O4	5.22	123.03	119.90
2	I	0	DT	O4'-C1'-N1	-5.14	104.40	108.00
2	G	10	DT	N3-C4-O4	5.08	122.94	119.90

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	3619	0	3761	59	0
1	B	3585	0	3720	48	0
2	G	315	0	186	6	0
2	I	335	0	198	6	0
3	H	338	0	177	8	0
3	J	356	0	189	1	0
4	A	45	0	0	18	0
4	B	30	0	0	6	0
4	G	16	0	0	4	0
4	H	4	0	0	3	0
4	I	12	0	0	5	0
All	All	8655	0	8231	125	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 (125) 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:473:GLY:HA2	4:A:843:HOH:O	1.52	1.09
1:A:702:HIS:HE1	4:B:829:HOH:O	1.33	1.08
1:A:473:GLY:CA	4:A:843:HOH:O	2.06	1.03
1:A:516:ARG:CD	4:A:841:HOH:O	2.08	1.02
1:A:516:ARG:NE	4:A:841:HOH:O	1.96	0.99
1:A:472:GLY:O	4:A:843:HOH:O	1.82	0.96
1:A:472:GLY:C	4:A:843:HOH:O	2.06	0.93
1:B:428:GLN:O	4:B:823:HOH:O	1.86	0.90
2:G:4:DT:OP1	4:G:111:HOH:O	1.90	0.89
1:A:720:LYS:C	4:A:824:HOH:O	2.12	0.88
1:B:505:GLN:NE2	2:G:7:DG:O6	2.07	0.88
2:I:13:DC:O5'	4:I:107:HOH:O	1.91	0.87
1:A:516:ARG:HD3	4:A:841:HOH:O	1.69	0.85
1:A:719:LYS:O	4:A:824:HOH:O	1.95	0.85
1:A:719:LYS:C	4:A:824:HOH:O	2.16	0.84
3:H:-7:DC:OP1	4:H:102:HOH:O	1.96	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:112:HOH:O	3:H:2:DA:C2	2.28	0.83
3:H:-7:DC:P	4:H:102:HOH:O	2.36	0.82
1:B:687:GLN:NE2	4:B:828:HOH:O	2.13	0.80
1:B:539:GLY:O	4:B:813:HOH:O	2.01	0.79
1:A:720:LYS:CA	4:A:824:HOH:O	2.31	0.77
2:I:13:DC:OP2	4:I:107:HOH:O	2.02	0.77
3:H:-8:DA:O3'	4:H:102:HOH:O	2.04	0.76
2:G:-2:DT:O2	4:G:112:HOH:O	2.04	0.75
2:I:13:DC:P	4:I:107:HOH:O	2.45	0.73
2:I:11:DC:OP2	4:I:104:HOH:O	2.06	0.73
1:B:611:GLN:HB3	1:B:644:LYS:HD2	1.72	0.70
1:A:473:GLY:N	4:A:843:HOH:O	2.15	0.70
1:A:257:THR:N	4:A:834:HOH:O	2.24	0.70
1:A:722:GLU:OE1	1:A:722:GLU:C	2.30	0.69
2:I:13:DC:H2'	4:I:107:HOH:O	1.91	0.69
1:A:706:LEU:HD21	1:A:718:VAL:HG21	1.74	0.69
1:B:604:ALA:O	4:B:801:HOH:O	2.10	0.68
1:A:258:GLY:N	4:A:834:HOH:O	1.96	0.65
4:G:112:HOH:O	3:H:2:DA:H2	1.71	0.64
1:A:720:LYS:O	1:A:723:HIS:N	2.30	0.63
1:A:569:ILE:HD13	1:A:582:VAL:HG21	1.79	0.63
1:B:654:LEU:HD13	1:B:668:VAL:HG11	1.82	0.62
1:A:720:LYS:O	1:A:722:GLU:N	2.33	0.62
1:A:653:LEU:HD13	1:A:685:VAL:HG21	1.81	0.62
1:A:719:LYS:O	1:A:723:HIS:HD2	1.83	0.61
1:B:661:HIS:CD2	1:B:688:LEU:HB3	2.35	0.61
1:B:256:ASP:OD1	1:B:256:ASP:N	2.33	0.60
1:B:274:ALA:HB2	1:B:304:LYS:HG3	1.82	0.59
1:A:695:LEU:HD11	1:A:719:LYS:HD2	1.86	0.58
1:B:604:ALA:HB2	1:B:613:LEU:HD11	1.83	0.58
1:A:720:LYS:N	4:A:824:HOH:O	2.31	0.58
1:B:434:ALA:HB2	1:B:443:LEU:HD11	1.86	0.57
1:A:450:LEU:HD13	1:A:464:VAL:HG11	1.87	0.56
3:H:1:DC:H2"	3:H:2:DA:C8	2.40	0.56
1:B:538:ASN:HB3	1:B:573:ASP:OD1	2.05	0.55
1:B:309:THR:OG1	1:B:338:LYS:HG3	2.06	0.55
1:A:451:PRO:O	1:A:455:GLN:HG2	2.08	0.54
1:A:720:LYS:O	4:A:824:HOH:O	2.18	0.54
1:B:559:HIS:HB3	1:B:586:LEU:HD23	1.89	0.54
1:B:425[B]:LEU:HD11	1:B:446:VAL:HG11	1.89	0.54
1:B:425[A]:LEU:HD11	1:B:446:VAL:HG11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1:DC:H2"	3:J:2:DA:C8	2.45	0.52
1:B:569:ILE:HD11	1:B:601:VAL:HG22	1.90	0.52
1:A:257:THR:CA	4:A:834:HOH:O	2.56	0.52
1:B:266:ARG:HG2	1:B:300:HIS:HA	1.92	0.52
1:A:241:LEU:HD21	1:A:272:VAL:HG21	1.92	0.52
1:B:306:ALA:O	1:B:310:VAL:HG13	2.11	0.51
1:A:238:LEU:O	1:A:242:LEU:HG	2.10	0.51
1:A:266:ARG:HG3	1:A:300:HIS:HA	1.92	0.51
1:B:578:ALA:O	1:B:582:VAL:HG23	2.11	0.51
1:A:702:HIS:CE1	4:B:829:HOH:O	2.23	0.49
1:B:315:PRO:O	1:B:319:GLN:HB2	2.12	0.49
1:B:620:LEU:HD23	1:B:634:VAL:HG11	1.94	0.49
1:A:720:LYS:C	1:A:722:GLU:N	2.66	0.49
1:A:717:ALA:O	1:A:721:LEU:HD23	2.13	0.48
1:A:582:VAL:O	1:A:586:LEU:HB2	2.12	0.48
1:A:565:GLN:O	1:A:569:ILE:HG13	2.12	0.48
1:A:710:GLY:HA3	1:B:721:LEU:HD12	1.95	0.48
1:B:448:ARG:NH2	1:B:478:GLU:OE1	2.39	0.48
1:A:285:ALA:HA	1:A:286:PRO:HA	1.56	0.47
1:B:348:LEU:HB3	1:B:349:PRO:HD3	1.96	0.47
1:B:344:VAL:O	1:B:348:LEU:HB2	2.14	0.47
1:B:348:LEU:HD23	1:B:362:VAL:HG11	1.97	0.47
1:B:440:LYS:NZ	1:B:444:GLU:OE2	2.43	0.47
1:B:262:LYS:HE3	3:H:-5:DA:OP1	2.16	0.46
2:G:-2:DT:H2"	2:G:-1:DG:C8	2.50	0.46
1:B:543:GLN:HB3	1:B:576:LYS:HD2	1.98	0.46
1:A:672:ALA:HB2	1:A:681:LEU:HD11	1.97	0.46
1:A:416:LEU:HD13	1:A:430:VAL:HG11	1.97	0.46
1:B:423[B]:HIS:HB3	1:B:450:LEU:HD23	1.97	0.46
1:B:244:VAL:HG13	1:B:276:HIS:HB2	1.98	0.45
1:A:517:LEU:HD12	1:A:517:LEU:HA	1.77	0.45
1:A:302:GLY:O	1:A:305:GLN:N	2.48	0.45
1:B:291:PRO:O	1:B:295:VAL:HG23	2.17	0.45
1:A:475:GLN:HB3	1:A:508:LYS:HD2	1.99	0.45
1:A:720:LYS:O	1:A:721:LEU:C	2.54	0.45
1:B:253:LEU:HD11	1:B:291:PRO:HA	1.98	0.45
1:B:650:VAL:O	1:B:654:LEU:HB2	2.16	0.45
1:A:259:GLN:O	1:A:263:ILE:HG13	2.17	0.44
1:A:695:LEU:HD11	1:A:719:LYS:HG3	1.99	0.44
2:I:-2:DT:H2"	2:I:-1:DG:C8	2.53	0.44
1:B:314:LEU:HB3	1:B:315:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:-2:DT:C6	2:G:-2:DT:H5'	2.53	0.44
1:A:287:LEU:O	1:A:288:ASN:HB2	2.17	0.44
1:A:535:ILE:HD13	1:A:548:VAL:HG21	2.00	0.44
1:B:378:VAL:O	1:B:382:LEU:HB2	2.18	0.44
1:B:253:LEU:HD12	1:B:253:LEU:HA	1.77	0.43
1:B:347:LEU:HD12	1:B:347:LEU:HA	1.80	0.43
1:A:722:GLU:OE1	1:A:722:GLU:O	2.36	0.43
1:A:450:LEU:HB3	1:A:451:PRO:HD3	2.00	0.43
1:A:633:GLN:O	1:A:637:ILE:HG13	2.18	0.43
1:B:310:VAL:HG12	1:B:341:LEU:HD11	2.00	0.43
1:B:400:ALA:HB2	1:B:409:LEU:HD11	2.00	0.43
1:A:278[A]:TRP:O	1:A:282:LEU:HG	2.19	0.42
1:A:457:HIS:HB3	1:A:484:LEU:CD2	2.48	0.42
1:A:581:THR:OG1	1:A:610:LYS:HG3	2.19	0.42
1:A:252:PRO:HB2	1:A:283:THR:HG21	2.00	0.42
1:A:257:THR:HB	4:A:834:HOH:O	2.19	0.42
1:A:687:GLN:NE2	1:A:695:LEU:HB2	2.34	0.42
1:A:287:LEU:HD11	1:A:311:GLN:HA	2.02	0.42
1:A:620:LEU:HD13	1:A:634:VAL:HG11	2.01	0.42
1:B:266:ARG:CG	1:B:300:HIS:HA	2.50	0.41
3:H:-12:DA:C8	3:H:-12:DA:H5'	2.55	0.41
1:B:249:ARG:O	1:B:254:GLN:HG3	2.21	0.41
1:B:231:GLN:HB2	1:B:232:TRP:H	1.52	0.41
2:G:-2:DT:H6	2:G:-2:DT:H2'	1.65	0.41
1:B:279:ARG:H	1:B:279:ARG:HG3	1.74	0.41
1:B:339:GLN:HB3	1:B:372:LYS:HD3	2.03	0.41
1:B:365:ILE:HD13	1:B:378:VAL:HG21	2.03	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	496/499 (99%)	479 (97%)	16 (3%)	1 (0%)	47	62
1	B	491/499 (98%)	475 (97%)	15 (3%)	1 (0%)	47	62
All	All	987/998 (99%)	954 (97%)	31 (3%)	2 (0%)	47	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	721	LEU
1	B	492	GLY

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	381/383 (100%)	359 (94%)	22 (6%)	20	32
1	B	378/383 (99%)	361 (96%)	17 (4%)	27	44
All	All	759/766 (99%)	720 (95%)	39 (5%)	25	39

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	LEU
1	A	256	ASP
1	A	269[A]	VAL
1	A	269[B]	VAL
1	A	270[A]	THR
1	A	270[B]	THR
1	A	283	THR
1	A	288	ASN
1	A	292	GLU
1	A	307	LEU
1	A	353	GLN
1	A	453	LEU
1	A	455	GLN
1	A	459	LEU

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Mol	Chain	Res	Type
1	A	517	LEU
1	A	586	LEU
1	A	619	LEU
1	A	623	LEU
1	A	656	VAL
1	A	678	ARG
1	A	719	LYS
1	A	721	LEU
1	B	238	LEU
1	B	253	LEU
1	B	255	LEU
1	B	256	ASP
1	B	279	ARG
1	B	323	LEU
1	B	347	LEU
1	B	351	LEU
1	B	382	LEU
1	B	550	ARG
1	B	585	LEU
1	B	687	GLN
1	B	690	ARG
1	B	709	LEU
1	B	715	LEU
1	B	720	LYS
1	B	721	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	723	HIS
1	B	625	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	493/499 (98%)	0.30	18 (3%)	41	41	24, 43, 77, 113	13 (2%)
1	B	487/499 (97%)	0.26	19 (3%)	39	38	26, 42, 74, 101	11 (2%)
2	G	16/17 (94%)	-0.18	2 (12%)	3	3	30, 33, 70, 76	0
2	I	17/17 (100%)	0.17	1 (5%)	22	21	26, 31, 84, 121	0
3	H	16/17 (94%)	0.32	2 (12%)	3	3	41, 49, 100, 111	0
3	J	17/17 (100%)	0.81	2 (11%)	4	4	35, 58, 112, 114	0
All	All	1046/1066 (98%)	0.28	44 (4%)	36	35	24, 43, 78, 121	24 (2%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	721	LEU	5.1
1	A	525	HIS	4.9
2	I	14	DT	4.3
3	H	-13	DG	4.2
1	A	232	TRP	4.0
1	A	526	GLY	3.9
1	B	423[A]	HIS	3.7
1	B	255	LEU	3.7
3	H	2	DA	3.6
1	A	524	ALA	3.5
1	B	491	HIS	3.5
1	B	231	GLN	3.4
1	A	250	GLY	3.4
1	B	257	THR	3.1
1	A	709	LEU	3.1
1	A	721	LEU	3.0
3	J	2	DA	3.0
1	B	258	GLY	2.9
1	B	234	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	688	LEU	2.8
1	B	253	LEU	2.8
1	A	557	GLN	2.8
1	A	231	GLN	2.7
1	B	348	LEU	2.7
1	A	527	LEU	2.7
1	B	720	LYS	2.6
1	B	422[A]	ALA	2.6
1	A	456	ALA	2.5
1	B	354	ALA	2.5
1	A	255	LEU	2.5
2	G	13	DC	2.4
1	A	251	PRO	2.4
3	J	-14	DA	2.3
1	A	723	HIS	2.3
1	B	558	ALA	2.3
1	B	260	LEU	2.3
1	A	292	GLU	2.3
2	G	-2	DT	2.2
1	B	486	VAL	2.2
1	B	530	GLN	2.2
1	B	492	GLY	2.2
1	B	232	TRP	2.1
1	A	233	SER	2.1
1	A	717	ALA	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.