Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 07:52 PM EDT

PDB ID	:	4OSZ
Title	:	Crystal structure of the S505P 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	:	2.61 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:

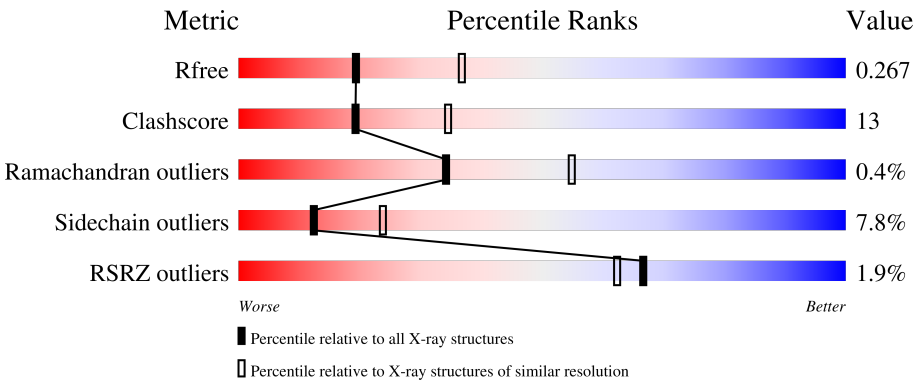
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.61 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	3%, 73%, 23%, • •
1	B	499	%, 65%, 30%, • •
2	G	17	29%, 41%, 29%
2	I	17	53%, 47%
3	H	17	47%, 47%, 6%

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Mol	Chain	Length	Quality of chain
3	J	17	65% 29% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8638 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	491	3599	2249	671	667	12	1	6	0
1	B	488	3544	2215	655	662	12	2	2	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	PRO	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	PRO	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
			Total	C	N	O	P			
2	G	17	333	163	46	108	16	0	0	0
			Total	C	N	O	P			
2	I	17	334	164	46	108	16	0	0	0

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

- Molecule 4 is water.

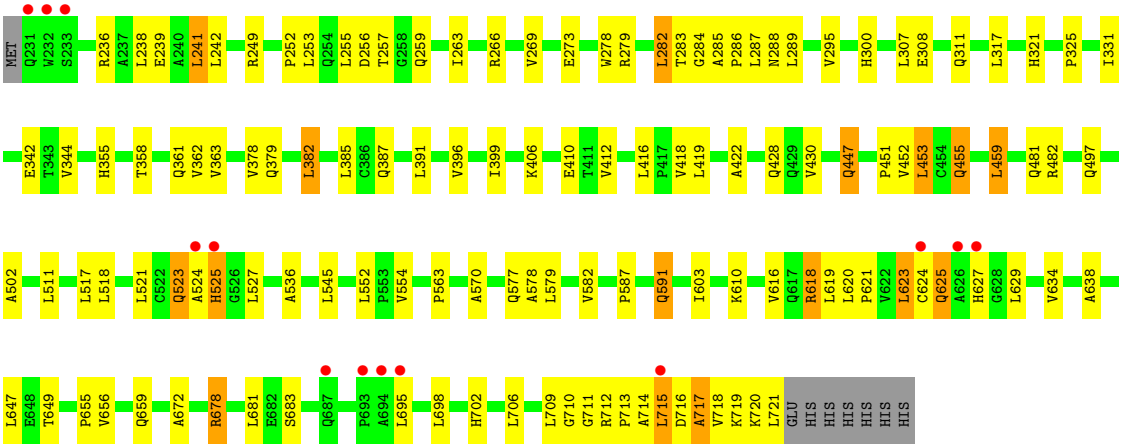
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	46	46	46	0	0
4	B	43	43	43	0	0
4	G	5	5	5	0	0
4	H	5	5	5	0	0
4	I	14	14	14	0	0
4	J	1	1	1	0	0

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.

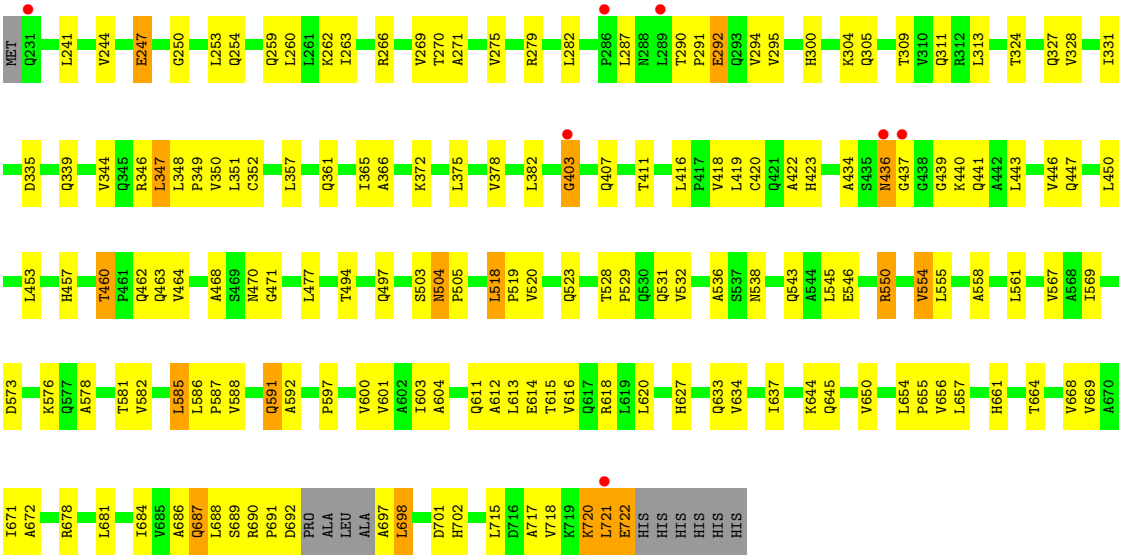
- Molecule 1: Hax3

Chain A:



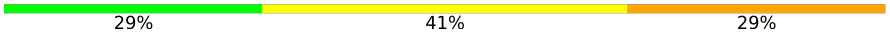
- Molecule 1: Hax3

Chain B:



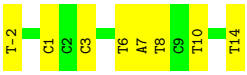
• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*TP*AP*TP*CP*TP*CP*TP*CP*T)-3')

Chain G:



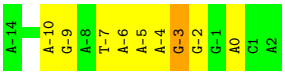
• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*TP*AP*TP*CP*TP*CP*TP*CP*T)-3')

Chain I:



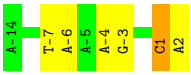
• Molecule 3: DNA (5'-D(*AP*GP*AP*GP*AP*GP*AP*TP*AP*AP*AP*GP*GP*GP*AP*CP*A)-3')

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	81.31Å 86.28Å 86.21Å 90.00° 102.42° 90.00°	Depositor
Resolution (Å)	42.10 – 2.61 44.80 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.10-2.61) 99.4 (44.80-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.217 , 0.275 0.209 , 0.267	Depositor DCC
R_{free} test set	1760 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 32.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8638	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 5.75% 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	0.41	0/3651	0.58	0/4987
1	B	0.42	0/3594	0.64	4/4908 (0.1%)
2	G	0.91	0/368	1.91	13/564 (2.3%)
2	I	0.83	0/369	1.60	8/566 (1.4%)
3	H	0.81	1/405 (0.2%)	1.66	12/625 (1.9%)
3	J	0.79	0/405	1.49	4/625 (0.6%)
All	All	0.52	1/8792 (0.0%)	0.92	41/12275 (0.3%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	-4	DA	C3'-O3'	5.10	1.50	1.44

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	9	DC	O4'-C1'-N1	-14.19	98.07	108.00
3	J	-3	DG	O4'-C1'-N9	10.20	115.14	108.00
1	B	720	LYS	CB-CA-C	-9.96	90.48	110.40
1	B	403	GLY	N-CA-C	8.98	135.54	113.10
3	H	-3	DG	O4'-C1'-N9	8.69	114.08	108.00
1	B	720	LYS	N-CA-C	8.39	133.66	111.00
3	H	-2	DG	O4'-C1'-N9	7.91	113.53	108.00
2	G	7	DA	O4'-C1'-N9	6.99	112.89	108.00
3	J	-4	DA	O4'-C1'-N9	6.94	112.86	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	-7	DT	C5-C4-O4	-6.77	120.16	124.90
2	G	12	DT	N3-C4-O4	6.56	123.84	119.90
2	I	-2	DT	O4'-C4'-C3'	-6.51	101.90	104.50
2	G	-1	DG	O4'-C1'-N9	-6.38	103.53	108.00
2	I	8	DT	O4'-C1'-N1	-6.30	103.59	108.00
2	I	10	DT	N3-C4-O4	6.23	123.64	119.90
3	H	-4	DA	O4'-C4'-C3'	-6.00	102.10	104.50
2	I	3	DC	O4'-C1'-C2'	-5.82	101.24	105.90
3	H	-10	DA	P-O5'-C5'	-5.79	111.64	120.90
2	G	8	DT	N3-C4-O4	5.76	123.35	119.90
3	H	0	DA	C1'-O4'-C4'	-5.76	104.34	110.10
2	G	12	DT	P-O5'-C5'	-5.58	111.97	120.90
3	H	-7	DT	N3-C4-O4	5.50	123.20	119.90
3	J	-7	DT	O4'-C1'-N1	-5.43	104.20	108.00
2	G	-2	DT	N3-C4-O4	5.40	123.14	119.90
2	I	8	DT	N3-C4-O4	5.35	123.11	119.90
2	I	-2	DT	C3'-C2'-C1'	-5.33	96.10	102.50
3	H	-9	DG	P-O5'-C5'	-5.30	112.42	120.90
2	G	2	DC	O4'-C1'-C2'	-5.28	101.68	105.90
2	G	-2	DT	C5-C4-O4	-5.27	121.21	124.90
2	I	8	DT	C5-C4-O4	-5.26	121.22	124.90
1	B	436	ASN	N-CA-C	5.25	125.18	111.00
2	G	12	DT	C5-C4-O4	-5.24	121.23	124.90
3	H	0	DA	O4'-C1'-N9	-5.12	104.41	108.00
2	G	8	DT	C5-C4-O4	-5.08	121.34	124.90
2	I	6	DT	C5-C4-O4	-5.07	121.35	124.90
2	G	2	DC	C1'-O4'-C4'	-5.06	105.04	110.10
3	H	-6	DA	O4'-C1'-N9	-5.04	104.47	108.00
3	H	-3	DG	P-O5'-C5'	-5.04	112.83	120.90
3	H	-7	DT	O4'-C1'-N1	5.03	111.52	108.00
2	G	4	DT	N3-C4-O4	5.01	122.91	119.90
3	J	1	DC	O4'-C1'-C2'	-5.00	101.90	105.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	437	GLY	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	3599	0	3748	79	3
1	B	3544	0	3676	124	0
2	G	333	0	195	10	0
2	I	334	0	198	6	0
3	H	357	0	190	2	0
3	J	357	0	190	2	0
4	A	46	0	0	3	0
4	B	43	0	0	9	0
4	G	5	0	0	3	0
4	H	5	0	0	0	0
4	I	14	0	0	1	0
4	J	1	0	0	0	0
All	All	8638	0	8197	212	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 13.

All (212) 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:12:DT:OP2	4:G:105:HOH:O	1.63	1.15
1:A:523:GLN:HG3	1:A:524:ALA:N	1.48	1.12
1:B:689:SER:O	1:B:691:PRO:HD3	1.53	1.08
1:A:716:ASP:O	1:A:719:LYS:N	1.86	1.06
1:A:284:GLY:O	1:A:288:ASN:OD1	1.70	1.06
1:B:721:LEU:HD22	1:B:721:LEU:N	1.72	1.02
1:B:721:LEU:HD22	1:B:721:LEU:H	0.88	1.01
1:B:689:SER:C	1:B:691:PRO:HD3	1.80	1.01
1:A:523:GLN:HG3	1:A:524:ALA:H	1.28	0.96
1:B:721:LEU:H	1:B:721:LEU:CD2	1.69	0.96
1:B:503:SER:O	1:B:504:ASN:CG	2.04	0.95
1:B:717:ALA:O	1:B:721:LEU:HD21	1.67	0.93
1:B:720:LYS:O	2:I:14:DT:H2'	1.71	0.88
1:A:523:GLN:CG	1:A:524:ALA:N	2.35	0.87
1:B:411:THR:OG1	1:B:440:LYS:HG3	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:VAL:O	1:B:592:ALA:HB3	1.77	0.85
1:A:524:ALA:O	1:A:525:HIS:CG	2.30	0.84
1:B:403:GLY:O	4:B:802:HOH:O	1.94	0.84
1:B:352:CYS:HA	4:B:808:HOH:O	1.79	0.82
1:B:721:LEU:HA	2:I:14:DT:H72	1.63	0.81
1:B:689:SER:O	1:B:691:PRO:CD	2.30	0.79
1:B:266:ARG:NH1	3:H:-3:DG:O6	2.16	0.79
1:A:711:GLY:O	1:A:715:LEU:HD12	1.83	0.78
1:B:503:SER:O	1:B:504:ASN:ND2	2.17	0.77
1:B:718:VAL:HA	1:B:721:LEU:HD21	1.65	0.77
1:A:623:LEU:O	1:A:627:HIS:HB2	1.85	0.77
1:A:621:PRO:O	1:A:625:GLN:HB2	1.85	0.76
1:B:721:LEU:O	1:B:722:GLU:C	2.25	0.75
1:B:357:LEU:O	4:B:808:HOH:O	2.04	0.75
1:B:633:GLN:HE21	1:B:669:VAL:HG21	1.52	0.75
2:G:9:DC:OP2	4:G:103:HOH:O	2.05	0.74
1:B:722:GLU:C	1:B:722:GLU:CD	2.45	0.74
1:A:523:GLN:CG	1:A:524:ALA:H	1.98	0.73
1:A:683:SER:HB3	1:A:715:LEU:HD22	1.71	0.72
1:A:279:ARG:O	1:A:283:THR:OG1	2.07	0.72
1:B:450:LEU:HD13	1:B:464:VAL:HG11	1.72	0.72
1:A:282:LEU:HB2	1:A:289:LEU:HD12	1.71	0.72
1:B:718:VAL:HA	1:B:721:LEU:CD2	2.19	0.72
1:A:714:ALA:O	1:A:718:VAL:HG23	1.89	0.72
1:A:252:PRO:HB2	1:A:283:THR:HG21	1.72	0.71
1:A:284:GLY:C	1:A:288:ASN:OD1	2.29	0.70
1:B:671:ILE:O	4:B:840:HOH:O	2.10	0.69
1:A:570:ALA:O	4:A:843:HOH:O	2.09	0.69
1:B:645:GLN:HB3	1:B:678:ARG:HD2	1.75	0.69
1:B:717:ALA:O	1:B:721:LEU:CD2	2.40	0.69
1:B:692:ASP:C	4:B:836:HOH:O	2.33	0.67
1:B:721:LEU:HA	2:I:14:DT:C7	2.24	0.67
1:B:504:ASN:HB3	1:B:505:PRO:HD2	1.77	0.67
1:B:536:ALA:HB2	1:B:545:LEU:HD11	1.77	0.66
1:A:342:GLU:O	4:A:803:HOH:O	2.13	0.66
1:B:569:ILE:HD13	1:B:582:VAL:HG21	1.78	0.66
1:A:253:LEU:HB3	1:A:255:LEU:HD21	1.77	0.65
1:A:638:ALA:HB2	1:A:647:LEU:HD11	1.77	0.65
1:B:470:ASN:OD1	4:B:813:HOH:O	2.14	0.64
1:B:439:GLY:O	1:B:443:LEU:HD12	1.96	0.64
2:G:0:DT:OP2	4:G:101:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:ALA:HB2	1:B:443:LEU:HD11	1.78	0.64
1:A:497:GLN:OE1	4:A:812:HOH:O	2.15	0.64
1:B:407:GLN:HB3	1:B:440:LYS:HD2	1.79	0.63
1:A:620:LEU:HD12	1:A:624:CYS:SG	2.39	0.63
1:B:262:LYS:NZ	3:H:-5:DA:OP1	2.31	0.63
1:B:247:GLU:HB3	4:B:821:HOH:O	2.00	0.62
1:A:263:ILE:HD11	1:A:295:VAL:HG22	1.80	0.62
1:B:718:VAL:O	1:B:721:LEU:HD23	2.01	0.61
1:B:611:GLN:O	1:B:615:THR:OG1	2.18	0.61
1:A:524:ALA:O	1:A:525:HIS:CD2	2.54	0.61
1:B:603:ILE:HD13	1:B:616:VAL:HG21	1.83	0.61
1:B:687:GLN:NE2	1:B:692:ASP:OD2	2.33	0.60
1:B:721:LEU:O	1:B:722:GLU:O	2.20	0.60
1:A:570:ALA:HB2	1:A:579:LEU:HD11	1.84	0.59
1:A:308[A]:GLU:O	1:A:311:GLN:HG3	2.04	0.58
1:B:247:GLU:OE1	4:B:821:HOH:O	2.17	0.58
1:B:419:LEU:HD21	1:B:447:GLN:HB2	1.84	0.58
1:B:588:VAL:O	1:B:592:ALA:CB	2.51	0.58
1:B:721:LEU:CA	2:I:14:DT:H72	2.32	0.58
1:A:716:ASP:O	1:A:717:ALA:C	2.42	0.57
1:B:611:GLN:HB3	1:B:644:LYS:HD2	1.86	0.57
2:G:-1:DG:H1'	2:G:0:DT:H5'	1.84	0.57
1:B:661:HIS:HB3	1:B:688:LEU:HD23	1.86	0.57
1:A:287:LEU:HD21	1:A:311:GLN:HA	1.87	0.57
1:B:612:ALA:O	1:B:616:VAL:HG23	2.04	0.57
1:A:716:ASP:O	1:A:718:VAL:N	2.37	0.57
1:A:253:LEU:HB3	1:A:255:LEU:CD2	2.35	0.56
1:B:327:GLN:O	1:B:331:ILE:HG13	2.06	0.56
1:B:503:SER:O	1:B:504:ASN:CB	2.54	0.56
1:B:543:GLN:HB3	1:B:576:LYS:HD3	1.88	0.55
1:B:578:ALA:O	1:B:582:VAL:HG23	2.07	0.55
1:A:710:GLY:HA3	1:A:714:ALA:HB2	1.89	0.55
1:A:712:ARG:HB3	1:A:713:PRO:HD3	1.90	0.54
1:B:365:ILE:HD13	1:B:378:VAL:HG21	1.89	0.54
1:A:578:ALA:O	1:A:582:VAL:HG23	2.07	0.54
1:A:502:ALA:HB2	1:A:511:LEU:HD11	1.89	0.54
1:A:358:THR:O	1:A:362:VAL:HG23	2.08	0.54
1:B:423:HIS:HB3	1:B:450:LEU:HD23	1.89	0.53
1:B:587:PRO:O	1:B:591:GLN:HG3	2.09	0.53
1:A:521:LEU:O	1:A:525:HIS:HB2	2.08	0.53
1:A:406:LYS:O	1:A:410:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:ASP:O	1:A:719:LYS:HB2	2.08	0.53
1:B:446:VAL:O	1:B:450:LEU:HB2	2.09	0.53
1:B:672:ALA:HB2	1:B:681:LEU:HD11	1.91	0.53
1:B:620:LEU:HD23	1:B:634:VAL:HG11	1.91	0.52
1:B:650:VAL:O	1:B:654:LEU:HB2	2.09	0.52
1:B:697:ALA:HB1	1:B:698:LEU:HD12	1.91	0.52
1:A:536:ALA:HB2	1:A:545:LEU:HD11	1.92	0.52
1:B:324:THR:O	1:B:328:VAL:HG23	2.09	0.52
1:A:577:GLN:HB3	1:A:610:LYS:HD2	1.91	0.51
1:B:324:THR:OG1	1:B:327:GLN:HG3	2.11	0.51
1:B:633:GLN:NE2	1:B:669:VAL:HG21	2.24	0.51
1:A:399:ILE:HD13	1:A:412:VAL:HG21	1.93	0.51
1:B:722:GLU:C	1:B:722:GLU:OE2	2.48	0.51
1:A:451:PRO:O	1:A:455:GLN:HG2	2.11	0.51
2:G:-2:DT:H2'	2:G:-1:DG:C8	2.46	0.51
1:A:698:LEU:HD22	1:A:702:HIS:HB3	1.93	0.50
1:B:441:GLN:NE2	2:G:4:DT:OP1	2.31	0.50
1:A:385:LEU:HD22	1:A:391:LEU:HD12	1.94	0.49
1:B:627:HIS:HB3	1:B:654:LEU:HD23	1.94	0.49
1:B:698:LEU:HD23	1:B:702:HIS:CD2	2.48	0.49
1:B:453:LEU:HA	1:B:457:HIS:HB2	1.95	0.49
1:B:721:LEU:N	1:B:721:LEU:CD2	2.46	0.48
1:B:290:THR:OG1	1:B:292:GLU:HG2	2.13	0.48
1:A:720:LYS:O	1:A:721:LEU:HG	2.14	0.48
1:B:718:VAL:CA	1:B:721:LEU:HD21	2.38	0.47
1:A:256:ASP:O	1:A:257:THR:C	2.52	0.47
1:B:361:GLN:O	1:B:365:ILE:HG13	2.14	0.47
1:A:241:LEU:HD23	1:A:269[B]:VAL:HG12	1.95	0.47
1:B:304:LYS:HD3	2:G:0:DT:OP1	2.14	0.47
1:B:637:ILE:HD13	1:B:650:VAL:HG21	1.96	0.47
1:A:266:ARG:HG3	1:A:300:HIS:HA	1.96	0.47
2:G:11:DC:C6	2:G:12:DT:H72	2.50	0.47
1:A:382:LEU:HG	1:A:396:VAL:HG11	1.96	0.47
1:A:259:GLN:O	1:A:263:ILE:HG13	2.15	0.47
1:A:624:CYS:HB3	1:A:629:LEU:O	2.15	0.46
1:A:285:ALA:HA	1:A:286:PRO:HA	1.65	0.46
1:B:718:VAL:CA	1:B:721:LEU:CD2	2.91	0.46
1:B:357:LEU:HB3	1:B:361:GLN:OE1	2.15	0.46
1:B:528:THR:O	1:B:532:VAL:HG23	2.15	0.46
1:A:331:ILE:HD13	1:A:344:VAL:HG21	1.98	0.46
1:B:339:GLN:HB3	1:B:372:LYS:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:LEU:HD13	1:B:600:VAL:HG11	1.98	0.46
1:B:300:HIS:HB3	1:B:335:ASP:OD1	2.16	0.46
1:A:416:LEU:HD13	1:A:430:VAL:HG11	1.98	0.45
1:B:718:VAL:HA	1:B:721:LEU:HD23	1.98	0.45
3:J:1:DC:H2"	3:J:2:DA:C8	2.52	0.45
1:B:661:HIS:CB	1:B:688:LEU:HD23	2.46	0.45
1:A:331:ILE:HD11	1:A:363:VAL:HG22	1.97	0.45
1:B:241:LEU:HD23	1:B:269:VAL:HA	1.99	0.45
2:G:4:DT:H2"	2:G:5:DT:O5'	2.17	0.45
1:B:604:ALA:HB2	1:B:613:LEU:HD11	1.98	0.45
1:B:250:GLY:H	1:B:254:GLN:HA	1.82	0.45
1:A:317:LEU:HD23	1:A:321:HIS:CD2	2.53	0.44
1:B:346:ARG:HG2	1:B:347:LEU:HD13	1.99	0.44
1:B:282:LEU:HD21	1:B:311:GLN:HG2	1.98	0.44
1:B:654:LEU:HB3	1:B:655:PRO:HD3	1.98	0.44
1:A:452:VAL:HG11	1:A:481:GLN:HE21	1.82	0.44
1:B:347:LEU:HA	1:B:347:LEU:HD12	1.75	0.44
1:A:278:TRP:O	1:A:282:LEU:HG	2.18	0.44
1:B:253:LEU:HD21	1:B:294:VAL:HG11	1.99	0.44
1:A:238:LEU:O	1:A:242:LEU:HG	2.17	0.44
1:A:378:VAL:O	1:A:382:LEU:HB2	2.17	0.44
1:B:494:THR:OG1	1:B:497:GLN:HG3	2.17	0.44
1:B:538:ASN:HB3	1:B:573:ASP:OD1	2.18	0.44
1:B:569:ILE:O	4:B:801:HOH:O	2.21	0.44
2:I:7:DA:C2	3:J:-6:DA:C2	3.06	0.44
1:A:418:VAL:O	1:A:422:ALA:HB3	2.18	0.44
1:B:253:LEU:HA	1:B:253:LEU:HD12	1.67	0.44
1:A:710:GLY:HA3	1:A:714:ALA:CB	2.48	0.43
1:A:387:GLN:O	1:B:420:CYS:HB3	2.19	0.43
1:A:716:ASP:C	1:A:718:VAL:N	2.71	0.43
1:B:531:GLN:HB3	1:B:567:VAL:HG11	2.00	0.43
1:B:657:LEU:HD23	1:B:657:LEU:HA	1.85	0.43
1:B:468:ALA:HB2	1:B:477:LEU:HD11	1.99	0.43
1:A:587:PRO:O	1:A:591:GLN:HB2	2.19	0.43
1:B:331:ILE:HD13	1:B:344:VAL:HG21	1.99	0.43
1:B:291:PRO:O	1:B:295:VAL:HG23	2.18	0.43
1:B:664:THR:O	1:B:668:VAL:HG23	2.19	0.43
1:A:624:CYS:SG	1:A:634:VAL:HG21	2.58	0.43
1:B:519:PRO:O	1:B:523:GLN:HG3	2.19	0.43
1:B:614:GLU:O	1:B:618:ARG:HG3	2.19	0.43
1:B:518:LEU:HB3	1:B:519:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LEU:HD21	1:A:447:GLN:HB2	2.01	0.42
1:A:453:LEU:HD11	1:A:481:GLN:HB2	2.01	0.42
1:B:555:LEU:HB3	1:B:561:LEU:HD22	2.00	0.42
1:B:597:PRO:O	1:B:601:VAL:HG23	2.20	0.42
1:B:418:VAL:O	1:B:422:ALA:HB3	2.20	0.42
1:A:249:ARG:HH22	1:A:257:THR:HG23	1.85	0.42
1:B:581:THR:O	1:B:585:LEU:HB2	2.19	0.42
1:A:649:THR:OG1	1:A:678:ARG:HD3	2.20	0.42
1:B:471:GLY:HA3	2:G:6:DT:H72	2.01	0.42
1:B:554:VAL:O	1:B:558:ALA:N	2.52	0.42
2:I:1:DC:H2"	4:I:114:HOH:O	2.19	0.42
1:B:244:VAL:O	1:B:247:GLU:HG2	2.19	0.41
1:B:292:GLU:CD	1:B:292:GLU:H	2.23	0.41
1:B:366:ALA:HB2	1:B:375:LEU:HD11	2.02	0.41
1:B:271:ALA:O	1:B:275:VAL:HG23	2.20	0.41
1:A:269[B]:VAL:O	1:A:273:GLU:HG3	2.20	0.41
1:B:287:LEU:HD11	1:B:311:GLN:HA	2.01	0.41
1:B:460:THR:HG23	1:B:463:GLN:OE1	2.21	0.41
1:A:358:THR:OG1	1:A:361:GLN:HG3	2.20	0.41
1:B:348:LEU:HB3	1:B:349:PRO:HD3	2.02	0.41
1:B:518:LEU:HD11	1:B:529:PRO:HA	2.02	0.41
1:A:603:ILE:HD13	1:A:616:VAL:HG21	2.02	0.41
1:B:309:THR:HG22	1:B:313:LEU:HD22	2.01	0.41
1:A:672:ALA:HB2	1:A:681:LEU:HD11	2.03	0.41
1:A:249:ARG:HH22	1:A:257:THR:CG2	2.33	0.41
1:B:305:GLN:O	1:B:309:THR:OG1	2.27	0.41
1:B:546:GLU:O	1:B:550:ARG:HG2	2.21	0.41
1:B:259:GLN:O	1:B:263:ILE:HG13	2.21	0.41
1:B:686:ALA:O	1:B:690:ARG:N	2.47	0.40
1:A:355:HIS:HB3	1:A:382:LEU:HD13	2.03	0.40
1:A:255:LEU:HD23	1:A:255:LEU:N	2.36	0.40
1:A:552:LEU:HD21	1:A:563:PRO:HB3	2.03	0.40
1:A:453:LEU:O	1:A:459:LEU:HB2	2.21	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:523:GLN:OE1	1:A:618:ARG:CZ[2_555]	1.83	0.37
1:A:523:GLN:OE1	1:A:618:ARG:NH1[2_555]	2.09	0.11
1:A:523:GLN:OE1	1:A:618:ARG:NH2[2_555]	2.13	0.07

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	495/499 (99%)	456 (92%)	36 (7%)	3 (1%)	25	45
1	B	486/499 (97%)	441 (91%)	44 (9%)	1 (0%)	47	69
All	All	981/998 (98%)	897 (91%)	80 (8%)	4 (0%)	34	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	525	HIS
1	A	717	ALA
1	B	504	ASN
1	A	655	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	380/383 (99%)	349 (92%)	31 (8%)	11	21
1	B	374/383 (98%)	347 (93%)	27 (7%)	14	27
All	All	754/766 (98%)	696 (92%)	58 (8%)	12	24

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	ARG
1	A	239	GLU

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Mol	Chain	Res	Type
1	A	241	LEU
1	A	282	LEU
1	A	307	LEU
1	A	325	PRO
1	A	379	GLN
1	A	382	LEU
1	A	428	GLN
1	A	447	GLN
1	A	453	LEU
1	A	455	GLN
1	A	459	LEU
1	A	482	ARG
1	A	517	LEU
1	A	518	LEU
1	A	523	GLN
1	A	527	LEU
1	A	554	VAL
1	A	591	GLN
1	A	618	ARG
1	A	619	LEU
1	A	623	LEU
1	A	625	GLN
1	A	656	VAL
1	A	659	GLN
1	A	678	ARG
1	A	695	LEU
1	A	706	LEU
1	A	709	LEU
1	A	715	LEU
1	B	247	GLU
1	B	260	LEU
1	B	270	THR
1	B	279	ARG
1	B	292	GLU
1	B	347	LEU
1	B	350	VAL
1	B	351	LEU
1	B	382	LEU
1	B	416	LEU
1	B	436	ASN
1	B	460	THR
1	B	462	GLN

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Mol	Chain	Res	Type
1	B	518	LEU
1	B	520	VAL
1	B	550	ARG
1	B	554	VAL
1	B	585	LEU
1	B	591	GLN
1	B	656	VAL
1	B	684	ILE
1	B	687	GLN
1	B	698	LEU
1	B	701	ASP
1	B	715	LEU
1	B	721	LEU
1	B	722	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	436	ASN
1	B	470	ASN
1	B	633	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	491/499 (98%)	-0.22	13 (2%)	56	50	20, 40, 76, 127	6 (1%)
1	B	488/499 (97%)	-0.14	7 (1%)	75	71	23, 44, 84, 124	8 (1%)
2	G	17/17 (100%)	-0.58	0	100	100	29, 32, 67, 97	0
2	I	17/17 (100%)	-0.61	0	100	100	22, 29, 75, 80	0
3	H	17/17 (100%)	-0.14	0	100	100	39, 47, 95, 127	0
3	J	17/17 (100%)	-0.21	0	100	100	36, 47, 80, 87	0
All	All	1047/1066 (98%)	-0.19	20 (1%)	66	62	20, 42, 80, 127	14 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	715	LEU	5.1
1	B	289	LEU	3.9
1	A	231	GLN	3.5
1	B	231	GLN	3.3
1	A	695	LEU	3.3
1	A	525	HIS	3.1
1	A	626	ALA	3.0
1	A	624	CYS	2.9
1	B	721	LEU	2.9
1	A	232	TRP	2.8
1	A	694	ALA	2.7
1	B	403	GLY	2.5
1	A	524	ALA	2.5
1	A	627	HIS	2.3
1	B	286	PRO	2.3
1	B	436	ASN	2.3
1	A	233	SER	2.2
1	A	687	GLN	2.1
1	A	693	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	437	GLY	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.