W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2016 – 05:16 PM EST

PDB ID	:	4Y5U
Title	:	Transcription factor
Authors	:	Li, J.; Niu, F.; Ouyang, S.; Liu, Z.
Deposited on	:	2015-02-12
Resolution	:	2.71 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320
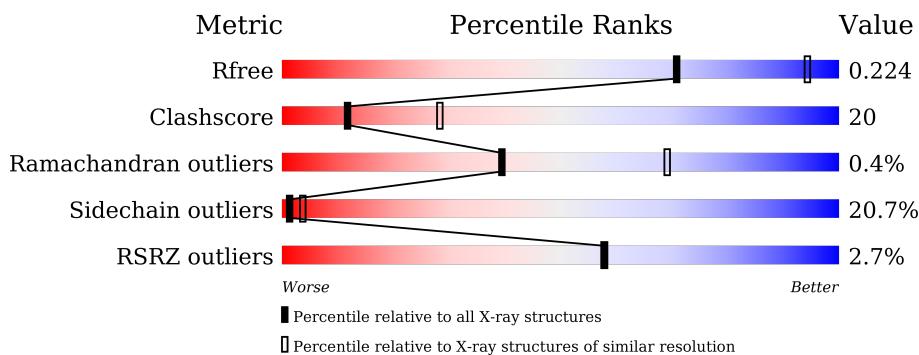
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*
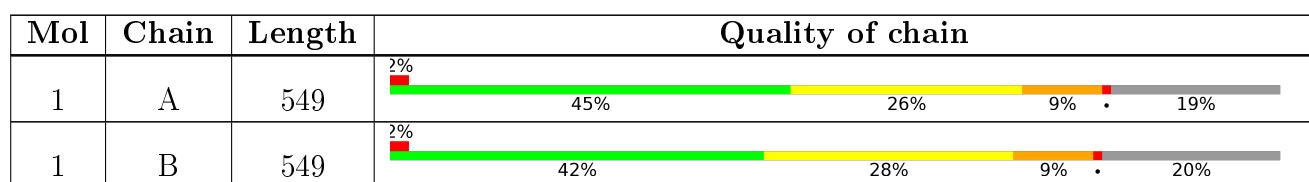
The reported resolution of this entry is 2.71 Å.

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	549	2% 45% 26% 9% • 19%
1	B	549	2% 42% 28% 9% • 20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7227 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 Signal transducer and activator of transcription 6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	P	S	0	0	0
			3550	2268	622	645	1	14			
1	B	438	Total	C	N	O	P	S	0	0	0
			3500	2240	611	634	1	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	SER	-	expression tag	UNP P42226
A	111	ASN	-	expression tag	UNP P42226
A	112	ALA	-	expression tag	UNP P42226
B	110	SER	-	expression tag	UNP P42226
B	111	ASN	-	expression tag	UNP P42226
B	112	ALA	-	expression tag	UNP P42226

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		
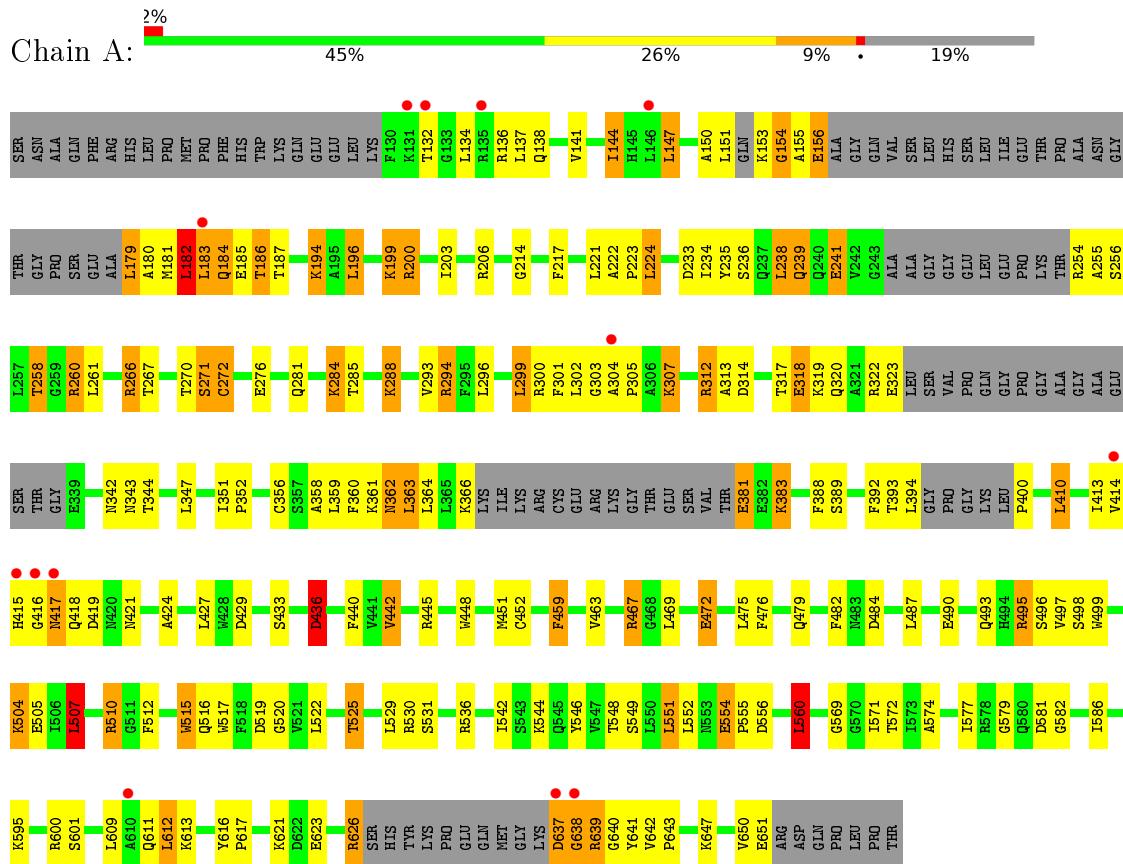
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	98	Total	O	0	0
			98	98		
3	B	78	Total	O	0	0
			78	78		
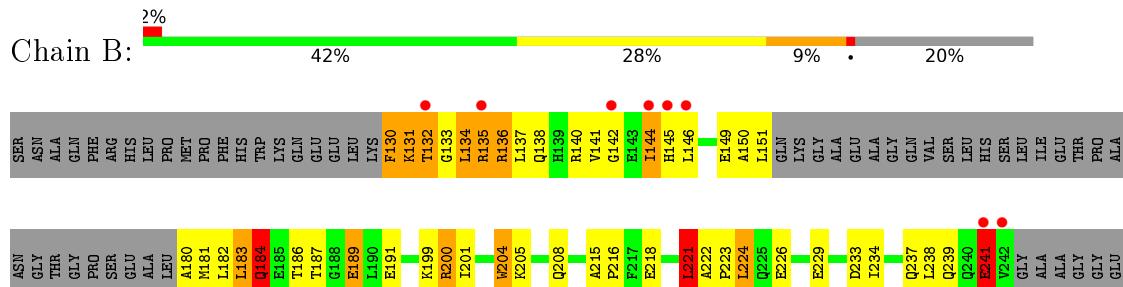
3 Residue-property plots ⓘ
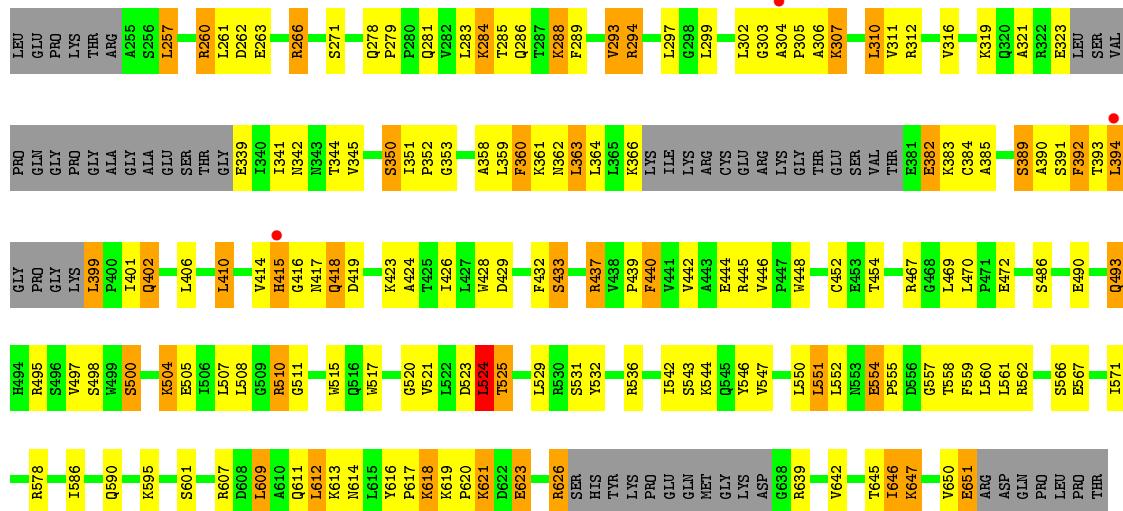
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Signal transducer and activator of transcription 6

• Molecule 1: Signal transducer and activator of transcription 6

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.15Å 94.32Å 179.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.36 – 2.71 46.36 – 2.71	Depositor EDS
% Data completeness (in resolution range)	90.8 (46.36-2.71) 89.1 (46.36-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	5.10 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.185 , 0.253 0.196 , 0.224	Depositor DCC
R_{free} test set	1951 reflections (6.99%)	DCC
Wilson B-factor (Å^2)	23.2	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.5	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.43, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7227	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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)

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

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	1.77	18/3594 (0.5%)	1.07	9/4843 (0.2%)
1	B	1.72	18/3545 (0.5%)	1.06	6/4782 (0.1%)
All	All	1.74	36/7139 (0.5%)	1.06	15/9625 (0.2%)

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	A	0	2
1	B	0	2
All	All	0	4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	554	GLU	CD-OE1	-6.66	1.18	1.25
1	A	517	TRP	CE3-CZ3	-6.52	1.27	1.38
1	B	498	SER	CB-OG	-6.14	1.34	1.42
1	B	505	GLU	CD-OE1	-6.10	1.19	1.25
1	A	520	GLY	C-O	-6.05	1.14	1.23
1	A	569	GLY	C-O	-6.00	1.14	1.23
1	B	517	TRP	CE3-CZ3	-5.91	1.28	1.38
1	A	318	GLU	CD-OE2	-5.76	1.19	1.25
1	B	428	TRP	CG-CD1	-5.68	1.28	1.36
1	A	235	TYR	CE1-CZ	-5.67	1.31	1.38
1	B	554	GLU	CD-OE1	-5.56	1.19	1.25
1	B	601	SER	CB-OG	-5.53	1.35	1.42
1	A	381	GLU	CD-OE2	-5.53	1.19	1.25
1	B	532	TYR	CE1-CZ	-5.51	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	505	GLU	CD-OE1	-5.50	1.19	1.25
1	B	452	CYS	CB-SG	-5.44	1.73	1.81
1	B	204	TRP	CG-CD1	-5.42	1.29	1.36
1	B	221	LEU	C-O	-5.35	1.13	1.23
1	B	448	TRP	CE3-CZ3	-5.35	1.29	1.38
1	A	294	ARG	CZ-NH2	-5.32	1.26	1.33
1	A	517	TRP	C-O	-5.31	1.13	1.23
1	A	499	TRP	CE3-CZ3	-5.27	1.29	1.38
1	A	459	PHE	CG-CD2	-5.24	1.30	1.38
1	B	511	GLY	C-O	-5.24	1.15	1.23
1	B	504	LYS	C-O	-5.23	1.13	1.23
1	B	204	TRP	CE3-CZ3	-5.23	1.29	1.38
1	B	520	GLY	C-O	-5.21	1.15	1.23
1	B	294	ARG	CZ-NH2	-5.20	1.26	1.33
1	A	381	GLU	CD-OE1	-5.20	1.20	1.25
1	A	515	TRP	CG-CD1	-5.18	1.29	1.36
1	A	448	TRP	CE3-CZ3	-5.16	1.29	1.38
1	A	601	SER	CB-OG	-5.16	1.35	1.42
1	A	517	TRP	CD2-CE2	-5.15	1.35	1.41
1	B	525	THR	C-O	-5.12	1.13	1.23
1	B	428	TRP	CD2-CE2	-5.11	1.35	1.41
1	A	452	CYS	CB-SG	-5.06	1.73	1.81

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	LEU	CA-CB-CG	7.26	132.00	115.30
1	A	560	LEU	CA-CB-CG	6.82	130.98	115.30
1	A	507	LEU	CA-CB-CG	6.74	130.79	115.30
1	A	294	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	B	609	LEU	CB-CG-CD2	-5.98	100.84	111.00
1	A	467	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	241	GLU	N-CA-C	-5.78	95.40	111.00
1	A	206	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	560	LEU	CB-CG-CD2	5.46	120.28	111.00
1	B	524	LEU	CA-CB-CG	5.36	127.62	115.30
1	B	550	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	A	206	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	560	LEU	CB-CG-CD2	-5.20	102.15	111.00
1	B	524	LEU	CB-CG-CD2	5.08	119.64	111.00
1	A	363	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	GLY	Peptide
1	A	436	ASP	Peptide
1	B	184	GLN	Peptide
1	B	418	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	3550	0	3614	145	1
1	B	3500	0	3568	147	0
2	A	1	0	0	0	0
3	A	98	0	0	8	0
3	B	78	0	0	12	0
All	All	7227	0	7182	288	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 20.

All (288) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LEU:O	1:B:186:THR:OG1	1.56	1.23
1:B:144:ILE:CG2	1:B:183:LEU:HD12	1.73	1.17
1:A:153:LYS:O	1:A:155:ALA:N	1.86	1.09
1:A:233:ASP:OD1	1:A:300:ARG:NH1	1.85	1.08
1:A:153:LYS:C	1:A:155:ALA:H	1.50	1.02
1:B:415:HIS:O	1:B:418:GLN:HB3	1.59	1.02
1:B:144:ILE:HG22	1:B:183:LEU:HD12	1.46	0.97
1:B:391:SER:HB3	1:B:402:GLN:HG2	1.48	0.95
1:A:184:GLN:HA	1:A:186:THR:H	1.33	0.93
1:A:184:GLN:N	1:A:184:GLN:OE1	2.02	0.92
1:A:554:GLU:HB3	1:A:555:PRO:HD2	1.54	0.88
1:A:233:ASP:CG	1:A:300:ARG:HH12	1.78	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:C	1:A:155:ALA:N	2.25	0.85
1:A:184:GLN:CB	1:A:187:THR:HG23	2.07	0.85
1:B:215:ALA:O	3:B:754:HOH:O	1.94	0.85
1:A:132:THR:HG23	3:A:867:HOH:O	1.76	0.83
1:A:183:LEU:C	1:A:184:GLN:OE1	2.15	0.83
1:B:359:LEU:CD2	1:B:361:LYS:HE3	2.10	0.81
1:B:184:GLN:N	1:B:184:GLN:OE1	2.14	0.80
1:B:495:ARG:NH1	3:B:762:HOH:O	2.12	0.80
1:B:144:ILE:HG22	1:B:183:LEU:CD1	2.11	0.79
1:A:184:GLN:HA	1:A:186:THR:N	1.98	0.79
1:A:429:ASP:O	1:A:433:SER:OG	2.00	0.79
1:A:639:ARG:HH11	1:A:639:ARG:HG3	1.46	0.79
1:A:266:ARG:O	1:A:270:THR:HG23	1.82	0.78
1:B:180:ALA:O	3:B:752:HOH:O	2.02	0.77
1:B:281:GLN:HA	1:B:410:LEU:HD12	1.64	0.77
1:B:429:ASP:OD1	1:B:437:ARG:NH2	2.18	0.77
1:B:399:LEU:O	1:B:399:LEU:HD22	1.85	0.76
1:B:239:GLN:OE1	1:B:261:LEU:HD12	1.85	0.76
1:A:184:GLN:HB3	1:A:187:THR:HG23	1.65	0.76
1:B:359:LEU:HD23	1:B:361:LYS:HE3	1.68	0.75
1:A:132:THR:CG2	3:A:867:HOH:O	2.33	0.75
1:A:351:ILE:HB	1:A:352:PRO:HD3	1.68	0.74
1:B:208:GLN:OE1	3:B:712:HOH:O	2.04	0.74
1:A:281:GLN:HA	1:A:410:LEU:HD12	1.70	0.74
1:B:310:LEU:HD21	1:B:344:THR:HB	1.67	0.74
1:A:307:LYS:C	1:A:307:LYS:HD2	2.08	0.73
1:B:651:GLU:O	3:B:769:HOH:O	2.05	0.73
1:B:140:ARG:NH1	1:B:189:GLU:OE1	2.22	0.73
1:A:134:LEU:O	1:A:138:GLN:HG3	1.89	0.72
1:B:262:ASP:OD2	3:B:772:HOH:O	2.07	0.72
1:A:643:PRO:HG2	1:B:651:GLU:HG2	1.72	0.72
1:A:137:LEU:O	1:A:141:VAL:HG23	1.90	0.71
1:B:284:LYS:HE3	1:B:285:THR:O	1.90	0.71
1:A:288:LYS:HG3	1:A:362:ASN:HB3	1.72	0.71
1:B:507:LEU:HB2	1:B:510:ARG:HG3	1.73	0.71
1:A:623:GLU:O	1:A:626:ARG:HD2	1.90	0.71
1:A:272:CYS:SG	1:A:296:LEU:HB2	2.31	0.70
1:A:317:THR:OG1	1:A:320:GLN:HG3	1.90	0.70
1:A:417:ASN:CB	1:A:418:GLN:HA	2.20	0.70
1:B:432:PHE:O	3:B:750:HOH:O	2.08	0.70
1:B:187:THR:O	1:B:191:GLU:HG3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:THR:HA	1:B:529:LEU:HB2	1.74	0.69
1:A:650:VAL:HG12	1:A:651:GLU:H	1.55	0.69
1:A:184:GLN:HB2	1:A:187:THR:HG23	1.76	0.68
1:A:650:VAL:HG12	1:A:651:GLU:N	2.08	0.68
1:A:132:THR:O	1:A:136:ARG:HG3	1.94	0.67
1:A:626:ARG:O	1:A:626:ARG:HG2	1.93	0.67
1:A:284:LYS:HE3	1:A:415:HIS:HB2	1.77	0.67
1:A:322:ARG:C	1:A:323:GLU:HG2	2.16	0.65
1:B:383:LYS:HE3	3:B:727:HOH:O	1.96	0.65
1:A:187:THR:OG1	1:A:260:ARG:NH1	2.29	0.65
1:B:341:ILE:O	1:B:342:ASN:HB2	1.97	0.65
1:A:637:ASP:N	1:A:640:GLY:HA2	2.12	0.64
1:A:415:HIS:CD2	1:A:416:GLY:H	2.15	0.64
1:B:609:LEU:O	1:B:621:LYS:NZ	2.30	0.64
1:B:467:ARG:HD2	1:B:536:ARG:HG2	1.80	0.64
1:B:222:ALA:HB3	1:B:223:PRO:HD3	1.79	0.64
1:A:312:ARG:HD2	1:A:314:ASP:OD2	1.99	0.63
1:B:607:ARG:HH11	1:B:626:ARG:NH1	1.96	0.63
1:A:307:LYS:O	1:A:307:LYS:HD2	1.98	0.63
1:A:267:THR:O	1:A:271:SER:OG	2.17	0.62
1:B:137:LEU:O	1:B:141:VAL:HG23	1.98	0.62
1:B:201:ILE:O	1:B:205:LYS:HG3	1.99	0.62
1:B:310:LEU:CD2	1:B:344:THR:HB	2.30	0.62
1:B:351:ILE:HB	1:B:352:PRO:HD3	1.82	0.62
1:A:554:GLU:HB3	1:A:555:PRO:CD	2.28	0.62
1:B:345:VAL:HG12	1:B:358:ALA:HB1	1.81	0.62
1:B:144:ILE:HG22	1:B:183:LEU:CG	2.30	0.61
1:B:607:ARG:NH1	1:B:626:ARG:NH1	2.49	0.60
1:B:144:ILE:CG2	1:B:183:LEU:CD1	2.62	0.60
1:B:359:LEU:HD21	1:B:361:LYS:HE3	1.83	0.60
1:A:239:GLN:OE1	1:A:261:LEU:HD12	2.01	0.60
1:B:389:SER:HB2	3:B:734:HOH:O	2.00	0.60
1:A:200:ARG:HB3	1:A:224:LEU:HD11	1.83	0.60
1:B:304:ALA:HB3	1:B:305:PRO:HD3	1.84	0.59
1:A:542:ILE:HD11	1:A:546:TYR:HD2	1.66	0.59
1:B:140:ARG:O	1:B:144:ILE:HG23	2.03	0.59
1:B:307:LYS:HG3	1:B:307:LYS:O	2.02	0.59
1:B:429:ASP:O	1:B:433:SER:HB2	2.03	0.59
1:B:260:ARG:NH2	3:B:702:HOH:O	2.34	0.59
1:B:394:LEU:HD12	1:B:394:LEU:C	2.23	0.59
1:B:284:LYS:HD2	1:B:415:HIS:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LYS:HD2	1:A:285:THR:H	1.67	0.58
1:B:142:GLY:O	1:B:145:HIS:HB3	2.02	0.58
1:B:562:ARG:O	1:B:571:ILE:HG13	2.04	0.58
1:B:311:VAL:HG22	1:B:390:ALA:HB2	1.84	0.58
1:B:144:ILE:HG23	1:B:183:LEU:HD12	1.79	0.58
1:B:524:LEU:HD13	1:B:529:LEU:HD12	1.86	0.58
1:A:222:ALA:HB3	1:A:223:PRO:HD3	1.85	0.57
1:A:144:ILE:HG22	1:A:183:LEU:HD13	1.85	0.57
1:A:199:LYS:O	1:A:203:ILE:HG12	2.05	0.56
1:A:301:PHE:CD1	1:A:394:LEU:HD11	2.41	0.56
1:A:284:LYS:HD3	1:A:415:HIS:H	1.71	0.56
1:B:567:GLU:HG3	3:B:733:HOH:O	2.06	0.56
1:A:301:PHE:O	1:A:302:LEU:HD23	2.07	0.55
1:A:284:LYS:HD2	1:A:285:THR:N	2.21	0.55
1:A:179:LEU:N	1:A:182:LEU:CD1	2.69	0.55
1:A:421:ASN:OD1	3:A:801:HOH:O	2.18	0.55
1:B:144:ILE:HG21	1:B:183:LEU:HD12	1.77	0.54
1:B:524:LEU:HD13	1:B:529:LEU:CD1	2.37	0.54
1:A:417:ASN:CG	1:A:418:GLN:HA	2.28	0.54
1:B:417:ASN:CG	1:B:418:GLN:H	2.10	0.54
1:A:637:ASP:N	1:A:637:ASP:OD1	2.40	0.54
1:B:415:HIS:CG	1:B:416:GLY:H	2.26	0.54
1:A:184:GLN:HB2	1:A:187:THR:CG2	2.38	0.54
1:A:415:HIS:CD2	1:A:416:GLY:N	2.75	0.53
1:B:440:PHE:N	1:B:440:PHE:CD1	2.74	0.53
1:A:150:ALA:N	1:A:151:LEU:CA	2.72	0.53
1:A:525:THR:HG23	1:A:529:LEU:HB2	1.89	0.53
1:B:360:PHE:CD1	1:B:360:PHE:N	2.76	0.53
1:A:507:LEU:HB3	1:A:510:ARG:HG3	1.90	0.53
1:B:360:PHE:HB3	1:B:363:LEU:HD13	1.89	0.52
1:B:392:PHE:O	1:B:401:ILE:HG22	2.08	0.52
1:B:399:LEU:HD22	1:B:399:LEU:C	2.30	0.52
1:B:200:ARG:HB3	1:B:224:LEU:HD11	1.91	0.52
1:A:560:LEU:HD22	1:A:574:ALA:HB3	1.91	0.51
1:A:611:GLN:O	1:A:613:LYS:HE3	2.09	0.51
1:A:179:LEU:N	1:A:182:LEU:HD12	2.26	0.51
1:A:475:LEU:HD21	1:A:487:LEU:HD23	1.92	0.51
1:A:551:LEU:HB3	1:A:586:ILE:CD1	2.40	0.51
1:A:313:ALA:HB3	1:A:343:ASN:HB2	1.92	0.51
1:A:548:THR:O	1:A:552:LEU:HB2	2.10	0.51
1:B:149:GLU:HB3	1:B:151:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:GLY:CA	1:A:639:ARG:C	2.80	0.51
1:B:144:ILE:CD1	1:B:241:GLU:HG2	2.41	0.51
1:B:149:GLU:HA	1:B:150:ALA:HB3	1.93	0.51
1:B:263:GLU:OE1	1:B:266:ARG:HD2	2.11	0.51
1:A:238:LEU:HB3	1:A:261:LEU:HD11	1.93	0.50
1:B:204:TRP:CE2	1:B:221:LEU:HD13	2.46	0.50
1:A:304:ALA:HB3	1:A:305:PRO:HD3	1.92	0.50
1:B:316:VAL:O	1:B:384:CYS:HB2	2.11	0.50
1:B:432:PHE:CG	1:B:446:VAL:HG11	2.46	0.50
1:A:479:GLN:HG2	1:A:484:ASP:O	2.11	0.50
1:A:552:LEU:HD13	1:A:586:ILE:HG12	1.93	0.50
1:B:554:GLU:HB3	1:B:555:PRO:HD2	1.93	0.50
1:A:137:LEU:HD22	1:A:234:ILE:HG21	1.94	0.49
1:A:415:HIS:O	1:A:416:GLY:C	2.49	0.49
1:B:137:LEU:HD13	1:B:234:ILE:HG21	1.94	0.49
1:A:459:PHE:O	1:A:463:VAL:HB	2.13	0.49
1:A:600:ARG:HD3	1:B:646:ILE:HD11	1.94	0.49
1:A:393:THR:HA	1:A:400:PRO:HA	1.94	0.49
1:A:184:GLN:CB	1:A:187:THR:CG2	2.87	0.49
1:A:542:ILE:HD11	1:A:546:TYR:CD2	2.46	0.49
1:A:556:ASP:OD2	1:A:613:LYS:NZ	2.44	0.48
1:A:194:LYS:HB3	1:A:194:LYS:HE3	1.53	0.48
1:A:144:ILE:HD11	1:A:241:GLU:HG3	1.95	0.48
1:B:239:GLN:NE2	1:B:262:ASP:OD1	2.46	0.48
1:B:239:GLN:O	1:B:241:GLU:O	2.32	0.48
1:A:650:VAL:CG1	1:A:651:GLU:H	2.23	0.48
1:B:490:GLU:O	1:B:493:GLN:HG2	2.14	0.48
1:B:281:GLN:HB3	1:B:426:ILE:HG13	1.96	0.48
1:B:278:GLN:OE1	1:B:279:PRO:HD2	2.13	0.48
1:A:147:LEU:HD13	1:A:183:LEU:HD12	1.94	0.48
1:A:150:ALA:N	1:A:151:LEU:HA	2.29	0.48
1:B:144:ILE:HG13	1:B:145:HIS:N	2.29	0.48
1:A:151:LEU:HG	1:A:151:LEU:O	2.13	0.48
1:A:181:MET:C	1:A:183:LEU:H	2.16	0.47
1:A:445:ARG:HG2	1:A:498:SER:HB3	1.95	0.47
1:A:200:ARG:HA	1:A:200:ARG:HD2	1.63	0.47
1:A:472:GLU:O	1:A:476:PHE:HD2	1.96	0.47
1:A:233:ASP:OD1	1:A:300:ARG:CZ	2.58	0.47
1:B:547:VAL:O	1:B:551:LEU:HB2	2.14	0.47
1:B:429:ASP:CG	1:B:437:ARG:NH2	2.67	0.47
1:B:424:ALA:HB2	1:B:515:TRP:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ALA:H	1:A:151:LEU:HA	1.79	0.47
1:A:144:ILE:CG1	1:A:241:GLU:HG3	2.45	0.47
1:A:318:GLU:OE2	1:A:440:PHE:N	2.36	0.47
1:A:638:GLY:HA3	1:A:639:ARG:CB	2.44	0.46
1:B:239:GLN:HA	1:B:239:GLN:OE1	2.14	0.46
1:A:638:GLY:HA3	1:A:639:ARG:HB3	1.98	0.46
1:A:154:GLY:O	1:A:156:GLU:HG3	2.15	0.46
1:A:383:LYS:NZ	3:A:877:HOH:O	2.40	0.46
1:B:360:PHE:HB2	1:B:363:LEU:HD22	1.98	0.46
1:B:619:LYS:HA	1:B:620:PRO:HD2	1.83	0.46
1:B:607:ARG:HA	1:B:621:LYS:HE3	1.98	0.46
1:A:179:LEU:N	1:A:182:LEU:HD11	2.30	0.46
1:A:519:ASP:O	1:A:522:LEU:HB2	2.16	0.46
1:A:616:TYR:HA	1:A:617:PRO:HA	1.62	0.45
1:B:558:THR:HA	1:B:614:ASN:O	2.16	0.45
1:A:194:LYS:HD3	1:A:267:THR:OG1	2.16	0.45
1:A:638:GLY:HA3	1:A:639:ARG:O	2.16	0.45
1:A:638:GLY:N	1:A:639:ARG:O	2.49	0.45
1:B:339:GLU:N	1:B:339:GLU:OE1	2.50	0.45
1:B:132:THR:O	1:B:135:ARG:HB3	2.15	0.45
1:B:134:LEU:O	1:B:138:GLN:OE1	2.35	0.45
1:A:347:LEU:HG	1:A:356:CYS:SG	2.57	0.45
1:B:239:GLN:C	1:B:241:GLU:O	2.55	0.45
1:A:424:ALA:HB2	1:A:515:TRP:CD1	2.52	0.45
1:A:638:GLY:CA	1:A:639:ARG:O	2.64	0.45
1:B:135:ARG:HA	1:B:138:GLN:OE1	2.16	0.45
1:B:144:ILE:HD12	1:B:241:GLU:HG2	1.98	0.45
1:B:312:ARG:HH11	1:B:312:ARG:HG3	1.82	0.45
1:B:385:ALA:HA	1:B:410:LEU:HD22	1.98	0.45
1:B:647:LYS:HE2	1:B:647:LYS:HB2	1.82	0.45
1:A:183:LEU:O	1:A:186:THR:HB	2.17	0.45
1:B:149:GLU:CA	1:B:150:ALA:HB3	2.46	0.45
1:B:419:ASP:O	1:B:423:LYS:HG3	2.15	0.45
1:A:199:LYS:HB3	1:A:199:LYS:HE2	1.59	0.44
1:B:416:GLY:HA2	1:B:417:ASN:C	2.36	0.44
1:A:510:ARG:HD3	1:A:512:PHE:CZ	2.52	0.44
1:A:510:ARG:HD2	3:A:865:HOH:O	2.17	0.44
1:B:399:LEU:CD2	1:B:399:LEU:C	2.85	0.44
1:B:542:ILE:HD11	1:B:546:TYR:HD2	1.82	0.44
1:A:186:THR:HG22	1:A:238:LEU:HD21	2.00	0.44
1:B:183:LEU:C	1:B:184:GLN:OE1	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:SER:HB3	1:B:353:GLY:HA3	1.99	0.44
1:A:360:PHE:N	1:A:360:PHE:CD1	2.85	0.44
1:A:451:MET:HE3	1:A:451:MET:O	2.18	0.44
1:A:551:LEU:HB3	1:A:586:ILE:HD12	1.99	0.44
1:B:133:GLY:O	1:B:136:ARG:HB3	2.17	0.44
1:B:490:GLU:HA	1:B:493:GLN:HG2	1.99	0.44
1:A:579:GLY:O	1:A:582:GLY:N	2.51	0.44
1:B:470:LEU:HB2	1:B:472:GLU:HG2	2.00	0.44
1:A:293:VAL:CG2	1:A:358:ALA:HB3	2.47	0.44
1:B:130:PHE:HB3	1:B:131:LYS:H	1.58	0.44
1:B:293:VAL:HG21	1:B:311:VAL:HG11	2.00	0.43
1:B:394:LEU:CD1	1:B:394:LEU:C	2.85	0.43
1:A:414:VAL:O	1:A:415:HIS:HB3	2.18	0.43
1:B:288:LYS:NZ	1:B:362:ASN:OD1	2.51	0.43
1:B:618:LYS:HG3	1:B:618:LYS:O	2.16	0.43
1:A:183:LEU:HA	1:A:183:LEU:HD23	1.83	0.43
1:A:482:PHE:CE2	1:A:495:ARG:HG2	2.54	0.43
1:B:341:ILE:CG2	1:B:366:LYS:HZ2	2.31	0.43
1:A:436:ASP:N	1:A:436:ASP:OD1	2.46	0.43
1:B:183:LEU:HD22	1:B:183:LEU:HA	1.78	0.43
1:B:639:ARG:HG2	3:B:738:HOH:O	2.18	0.43
1:A:153:LYS:N	3:A:863:HOH:O	2.51	0.43
1:A:312:ARG:O	1:A:388:PHE:HA	2.19	0.43
1:A:417:ASN:HB3	1:A:418:GLN:HA	1.97	0.43
1:A:504:LYS:HB3	1:A:504:LYS:HE3	1.78	0.43
1:B:149:GLU:HA	1:B:150:ALA:C	2.38	0.43
1:B:616:TYR:HA	1:B:617:PRO:HA	1.67	0.43
1:A:255:ALA:HA	1:A:258:THR:OG1	2.18	0.42
1:A:299:LEU:HB2	3:A:823:HOH:O	2.19	0.42
1:A:552:LEU:HD12	1:A:552:LEU:HA	1.79	0.42
1:A:642:VAL:CG1	1:B:650:VAL:HG13	2.49	0.42
1:B:500:SER:HA	1:B:504:LYS:HB2	2.01	0.42
1:A:415:HIS:CG	1:A:416:GLY:H	2.35	0.42
1:B:233:ASP:O	1:B:237:GLN:HG3	2.19	0.42
1:B:551:LEU:HB3	1:B:586:ILE:CD1	2.49	0.42
1:B:283:LEU:HD11	1:B:289:PHE:CD1	2.54	0.42
1:B:229:GLU:HG3	1:B:297:LEU:HD23	2.00	0.42
1:A:467:ARG:NH1	1:A:536:ARG:HA	2.34	0.42
1:B:312:ARG:NH1	1:B:312:ARG:HG3	2.34	0.42
1:B:507:LEU:CB	1:B:510:ARG:HG3	2.48	0.42
1:A:641:PTR:HB2	1:B:590:GLN:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:ARG:HH11	1:B:626:ARG:HH11	1.64	0.42
1:B:215:ALA:HA	1:B:216:PRO:HD3	1.75	0.42
1:A:221:LEU:HD12	1:A:276:GLU:HG3	2.02	0.42
1:B:613:LYS:O	1:B:621:LYS:HB3	2.20	0.42
1:B:543:SER:O	1:B:547:VAL:HG23	2.19	0.41
1:B:221:LEU:HD12	1:B:221:LEU:HA	1.92	0.41
1:B:303:GLY:O	1:B:306:ALA:O	2.39	0.41
1:B:620:PRO:HG2	1:B:623:GLU:OE1	2.20	0.41
1:B:626:ARG:HH11	1:B:626:ARG:HD3	1.72	0.41
1:A:490:GLU:HG2	1:A:493:GLN:OE1	2.20	0.41
1:B:302:LEU:HD23	1:B:302:LEU:HA	1.79	0.41
1:B:341:ILE:HG12	1:B:364:LEU:HB3	2.02	0.41
1:A:519:ASP:HA	1:A:522:LEU:HD12	2.03	0.41
1:A:214:GLY:O	3:A:802:HOH:O	2.20	0.41
1:B:559:PHE:CD1	1:B:612:LEU:HG	2.56	0.41
1:A:429:ASP:HA	1:A:442:VAL:HG11	2.03	0.41
1:B:321:ALA:HB1	1:B:406:LEU:HD21	2.02	0.41
1:B:345:VAL:CG1	1:B:358:ALA:HB1	2.48	0.41
1:B:382:GLU:H	1:B:382:GLU:HG2	1.68	0.41
1:B:415:HIS:CG	1:B:416:GLY:N	2.89	0.41
1:B:557:GLY:HA3	1:B:613:LYS:HD2	2.02	0.41
1:B:237:GLN:O	1:B:241:GLU:HB2	2.20	0.41
1:B:257:LEU:HA	1:B:257:LEU:HD12	1.92	0.40
1:A:392:PHE:CZ	1:A:394:LEU:HD22	2.56	0.40
1:A:413:ILE:CD1	1:A:419:ASP:HB3	2.52	0.40
1:A:179:LEU:HD22	1:A:179:LEU:HA	1.84	0.40
1:A:612:LEU:O	1:A:621:LYS:HD3	2.21	0.40
1:B:406:LEU:HD12	1:B:406:LEU:HA	1.87	0.40
1:A:196:LEU:HA	1:A:196:LEU:HD12	1.84	0.40
1:A:639:ARG:NH1	1:A:639:ARG:HG3	2.24	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:A:180:ALA:CB	1:A:344:THR:O[3_544]	1.90	0.30

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	428/549 (78%)	413 (96%)	13 (3%)	2 (0%)	34	63
1	B	423/549 (77%)	416 (98%)	6 (1%)	1 (0%)	52	80
All	All	851/1098 (78%)	829 (97%)	19 (2%)	3 (0%)	39	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	GLY
1	B	415	HIS
1	A	638	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	386/469 (82%)	311 (81%)	75 (19%)	2	4
1	B	382/469 (81%)	298 (78%)	84 (22%)	1	3
All	All	768/938 (82%)	609 (79%)	159 (21%)	1	4

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	ILE
1	A	147	LEU
1	A	156	GLU

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Mol	Chain	Res	Type
1	A	179	LEU
1	A	182	LEU
1	A	183	LEU
1	A	184	GLN
1	A	185	GLU
1	A	186	THR
1	A	194	LYS
1	A	196	LEU
1	A	199	LYS
1	A	200	ARG
1	A	217	PHE
1	A	224	LEU
1	A	236	SER
1	A	238	LEU
1	A	239	GLN
1	A	241	GLU
1	A	254	ARG
1	A	256	SER
1	A	258	THR
1	A	260	ARG
1	A	266	ARG
1	A	271	SER
1	A	272	CYS
1	A	284	LYS
1	A	288	LYS
1	A	294	ARG
1	A	299	LEU
1	A	307	LYS
1	A	312	ARG
1	A	319	LYS
1	A	342	ASN
1	A	359	LEU
1	A	361	LYS
1	A	362	ASN
1	A	363	LEU
1	A	364	LEU
1	A	366	LYS
1	A	381	GLU
1	A	383	LYS
1	A	389	SER
1	A	410	LEU
1	A	417	ASN

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Mol	Chain	Res	Type
1	A	427	LEU
1	A	436	ASP
1	A	442	VAL
1	A	469	LEU
1	A	472	GLU
1	A	495	ARG
1	A	496	SER
1	A	497	VAL
1	A	504	LYS
1	A	507	LEU
1	A	510	ARG
1	A	516	GLN
1	A	525	THR
1	A	530	ARG
1	A	531	SER
1	A	544	LYS
1	A	549	SER
1	A	551	LEU
1	A	560	LEU
1	A	571	ILE
1	A	572	THR
1	A	577	ILE
1	A	581	ASP
1	A	595	LYS
1	A	609	LEU
1	A	612	LEU
1	A	626	ARG
1	A	637	ASP
1	A	639	ARG
1	A	647	LYS
1	B	130	PHE
1	B	131	LYS
1	B	132	THR
1	B	134	LEU
1	B	135	ARG
1	B	136	ARG
1	B	144	ILE
1	B	146	LEU
1	B	181	MET
1	B	182	LEU
1	B	183	LEU
1	B	184	GLN

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Mol	Chain	Res	Type
1	B	189	GLU
1	B	199	LYS
1	B	200	ARG
1	B	218	GLU
1	B	221	LEU
1	B	224	LEU
1	B	226	GLU
1	B	238	LEU
1	B	241	GLU
1	B	257	LEU
1	B	260	ARG
1	B	266	ARG
1	B	271	SER
1	B	284	LYS
1	B	286	GLN
1	B	288	LYS
1	B	293	VAL
1	B	294	ARG
1	B	299	LEU
1	B	307	LYS
1	B	310	LEU
1	B	319	LYS
1	B	323	GLU
1	B	350	SER
1	B	360	PHE
1	B	363	LEU
1	B	382	GLU
1	B	389	SER
1	B	392	PHE
1	B	393	THR
1	B	394	LEU
1	B	399	LEU
1	B	402	GLN
1	B	410	LEU
1	B	414	VAL
1	B	433	SER
1	B	437	ARG
1	B	439	PRO
1	B	440	PHE
1	B	442	VAL
1	B	444	GLU
1	B	445	ARG

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Mol	Chain	Res	Type
1	B	454	THR
1	B	469	LEU
1	B	486	SER
1	B	493	GLN
1	B	497	VAL
1	B	500	SER
1	B	508	LEU
1	B	510	ARG
1	B	521	VAL
1	B	523	ASP
1	B	524	LEU
1	B	531	SER
1	B	544	LYS
1	B	551	LEU
1	B	552	LEU
1	B	561	LEU
1	B	566	SER
1	B	578	ARG
1	B	595	LYS
1	B	611	GLN
1	B	612	LEU
1	B	618	LYS
1	B	621	LYS
1	B	623	GLU
1	B	626	ARG
1	B	642	VAL
1	B	645	THR
1	B	646	ILE
1	B	647	LYS
1	B	651	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	342	ASN
1	A	415	HIS
1	A	420	ASN
1	A	611	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
1	PTR	A	641	1	13,16,17	2.73	4 (30%)	19,22,24	1.38	3 (15%)
1	PTR	B	641	1	13,16,17	2.44	3 (23%)	19,22,24	2.03	7 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	A	641	1	-	0/9/11/13	0/1/1/1
1	PTR	B	641	1	-	0/9/11/13	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	641	PTR	P-O2P	-5.59	1.35	1.54
1	A	641	PTR	P-O3P	-5.47	1.35	1.54
1	B	641	PTR	P-O1P	-4.90	1.35	1.50
1	B	641	PTR	P-O2P	-4.87	1.38	1.54
1	B	641	PTR	P-O3P	-4.52	1.39	1.54
1	A	641	PTR	P-O1P	-4.04	1.38	1.50
1	A	641	PTR	OH-CZ	-2.43	1.34	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	641	PTR	O2P-P-OH	-3.74	93.56	105.47
1	B	641	PTR	O-C-CA	-3.06	117.51	125.72
1	A	641	PTR	O-C-CA	-2.37	119.37	125.72
1	B	641	PTR	CE1-CD1-CG	-2.15	118.00	121.02
1	B	641	PTR	P-OH-CZ	2.63	131.32	123.85
1	B	641	PTR	CD1-CE1-CZ	2.76	123.19	119.74
1	A	641	PTR	O2P-P-O1P	2.88	120.03	110.63
1	A	641	PTR	P-OH-CZ	3.04	132.48	123.85
1	B	641	PTR	O3P-P-O2P	3.36	119.79	107.44
1	B	641	PTR	O3P-P-OH	3.88	117.85	105.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	641	PTR	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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 (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(Å²)	Q<0.9
1	A	444/549 (80%)	-0.24	13 (2%)	55	55	1, 17, 50, 73	0
1	B	437/549 (79%)	-0.21	11 (2%)	61	61	2, 18, 58, 90	0
All	All	881/1098 (80%)	-0.22	24 (2%)	58	58	1, 18, 54, 90	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146	LEU	4.0
1	B	132	THR	3.9
1	B	304	ALA	3.9
1	B	415	HIS	3.4
1	B	144	ILE	3.2
1	B	146	LEU	3.1
1	A	637	ASP	2.9
1	B	142	GLY	2.9
1	B	145	HIS	2.9
1	A	183	LEU	2.9
1	A	415	HIS	2.9
1	A	416	GLY	2.4
1	A	638	GLY	2.4
1	A	417	ASN	2.4
1	A	135	ARG	2.3
1	A	414	VAL	2.3
1	A	304	ALA	2.2
1	A	610	ALA	2.2
1	B	135	ARG	2.2
1	B	394	LEU	2.2
1	B	241	GLU	2.1
1	A	131	LYS	2.1
1	A	132	THR	2.1
1	B	242	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
1	PTR	A	641	16/17	0.98	0.12	-	6,11,17,24	0
1	PTR	B	641	16/17	0.97	0.11	-	5,10,17,19	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	NI	A	701	1/1	1.00	0.11	-3.89	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.