



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:06 AM UTC

PDB ID : 1BF5 / pdb\_00001bf5  
Title : TYROSINE PHOSPHORYLATED STAT-1/DNA COMPLEX  
Authors : Kuriyan, J.; Zhao, Y.; Chen, X.; Vinkemeier, U.; Jeruzalmi, D.; Darnell Jr., J.E.  
Deposited on : 1998-05-27  
Resolution : 2.90 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
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

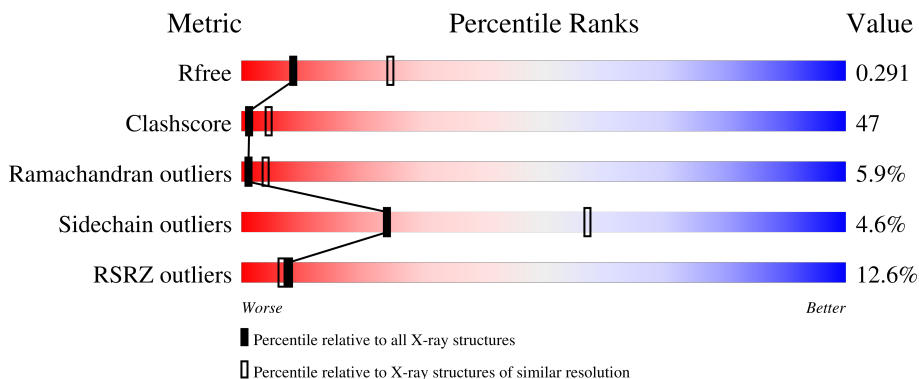
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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  $\geq 3$ , 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	B	18	
2	C	18	
3	A	575	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 5117 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 DNA chain called DNA (5'-D(\*AP\*CP\*AP\*GP\*TP\*TP\*TP\*CP\*CP\*CP\*GP\*TP\*AP\*AP\*AP\*TP\*G P\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	18	363	175	65	106	17	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(\*TP\*GP\*CP\*AP\*TP\*TP\*TP\*AP\*CP\*GP\*GP\*GP\*AP\*AP\*AP\*CP\*T P\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	18	369	177	69	106	17	0	0	0

- Molecule 3 is a protein called SIGNAL TRANSDUCER AND ACTIVATOR OF TRANSCRIPTION 1-ALPHA/BETA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
3	A	545	4385	2808	751	807	1	18	0	0	0

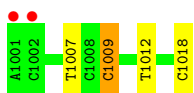
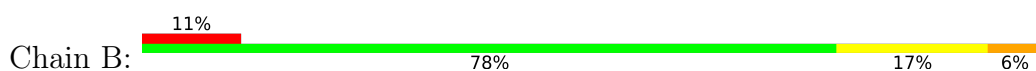
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	701	PTR	TYR	modified residue	UNP P42224

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

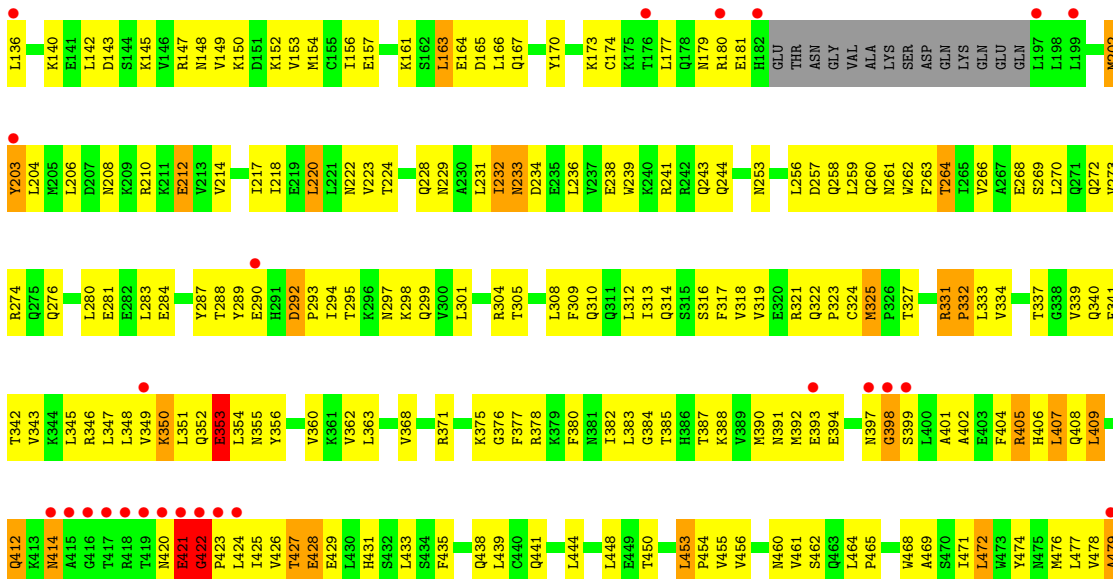
- Molecule 1: DNA (5'-D(\*AP\*CP\*AP\*GP\*TP\*TP\*TP\*CP\*CP\*CP\*GP\*TP\*AP\*AP\*AP\*TP\*G P\*C)-3')

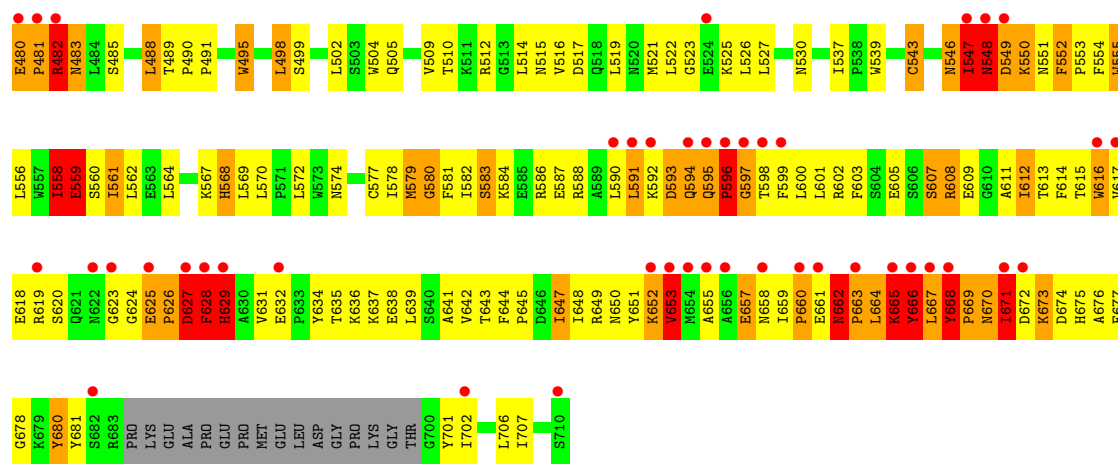


- Molecule 2: DNA (5'-D(\*TP\*GP\*CP\*AP\*TP\*TP\*TP\*AP\*CP\*GP\*GP\*GP\*AP\*AP\*AP\*CP\*T P\*G)-3')



- Molecule 3: SIGNAL TRANSDUCER AND ACTIVATOR OF TRANSCRIPTION 1-ALPHA/BETA





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.60Å 148.20Å 181.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.8 (30.00-2.90) 88.5 (30.00-2.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.32 (at 2.80Å)	Xtrriage
Refinement program	CNS 3.0	Depositor
R, $R_{free}$	0.227 , 0.293 0.226 , 0.291	Depositor DCC
$R_{free}$ test set	2177 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.5	Xtrriage
Anisotropy	0.152	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	5117	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	B	0.43	0/405	0.86	0/620
2	C	3.13	1/414 (0.2%)	0.96	4/638 (0.6%)
3	A	1.20	21/4460 (0.5%)	1.57	86/6035 (1.4%)
All	All	1.42	22/5279 (0.4%)	1.47	90/7293 (1.2%)

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	B	0	2
2	C	0	2
3	A	1	7
All	All	1	11

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2010	DG	O3'-P	-63.10	0.66	1.61
3	A	480	GLU	N-CA	30.42	1.89	1.46
3	A	623	GLY	C-N	-29.18	0.90	1.33
3	A	422	GLY	N-CA	17.26	1.68	1.44
3	A	607	SER	C-N	13.83	1.52	1.33
3	A	579	MET	SD-CE	12.62	2.11	1.79
3	A	666	TYR	CA-CB	11.65	1.73	1.53
3	A	608	ARG	C-N	-11.59	1.12	1.33
3	A	629	HIS	N-CA	11.36	1.60	1.46
3	A	626	PRO	C-N	-8.26	1.22	1.33
3	A	543	CYS	CB-SG	8.11	2.08	1.81
3	A	628	PHE	C-O	-7.93	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	407	LEU	N-CA	7.43	1.55	1.45
3	A	548	ASN	CA-C	7.25	1.62	1.52
3	A	608	ARG	CA-C	-7.24	1.42	1.52
3	A	667	LEU	N-CA	-6.94	1.38	1.46
3	A	550	LYS	N-CA	6.26	1.52	1.46
3	A	550	LYS	CA-C	5.97	1.60	1.53
3	A	559	GLU	CA-C	-5.85	1.44	1.52
3	A	548	ASN	N-CA	5.43	1.53	1.46
3	A	558	ILE	N-CA	-5.28	1.40	1.46
3	A	547	ILE	CA-C	5.25	1.59	1.52

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	671	ILE	N-CA-C	-17.00	84.38	108.17
3	A	628	PHE	N-CA-CB	15.88	136.05	111.91
3	A	407	LEU	N-CA-C	-15.63	85.46	110.32
3	A	480	GLU	N-CA-C	-15.20	76.22	109.81
3	A	629	HIS	N-CA-C	14.30	141.26	110.80
3	A	668	TYR	CA-C-N	-13.68	102.74	119.84
3	A	668	TYR	C-N-CA	-13.68	102.74	119.84
3	A	550	LYS	N-CA-C	12.96	127.72	109.31
3	A	595	GLN	N-CA-C	-12.93	82.36	108.21
3	A	593	ASP	N-CA-C	-11.86	95.83	113.61
3	A	482	ARG	N-CA-C	11.61	128.80	109.76
3	A	421	GLU	CA-C-N	-10.86	104.82	121.87
3	A	421	GLU	C-N-CA	-10.86	104.82	121.87
3	A	662	ASN	CA-C-N	10.50	152.21	127.00
3	A	662	ASN	C-N-CA	10.50	152.21	127.00
3	A	422	GLY	N-CA-C	-9.89	92.17	112.34
3	A	665	LYS	N-CA-C	9.74	131.55	110.80
3	A	546	ASN	N-CA-C	-9.52	95.19	110.32
3	A	331	ARG	CA-C-N	9.43	129.65	119.28
3	A	331	ARG	C-N-CA	9.43	129.65	119.28
3	A	662	ASN	C-N-CD	-9.24	100.27	120.60
3	A	332	PRO	CA-C-N	-8.92	108.69	122.60
3	A	332	PRO	C-N-CA	-8.92	108.69	122.60
3	A	481	PRO	N-CA-C	-8.81	97.39	111.14
3	A	627	ASP	CA-C-N	-8.71	110.23	122.34
3	A	627	ASP	C-N-CA	-8.71	110.23	122.34
2	C	2010	DG	P-O3'-C3'	8.57	133.06	120.20
3	A	667	LEU	N-CA-C	8.53	120.19	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	592	LYS	N-CA-C	-8.40	93.94	108.56
3	A	332	PRO	N-CA-C	8.28	124.83	113.65
3	A	233	ASN	N-CA-C	8.27	121.41	111.82
3	A	392	MET	N-CA-C	-7.83	103.03	114.39
3	A	595	GLN	CA-C-N	7.82	129.61	119.84
3	A	595	GLN	C-N-CA	7.82	129.61	119.84
3	A	583	SER	N-CA-C	-7.81	99.42	110.35
3	A	626	PRO	CA-C-N	7.78	136.41	121.54
3	A	626	PRO	C-N-CA	7.78	136.41	121.54
3	A	680	TYR	N-CA-C	7.55	121.75	112.54
3	A	561	ILE	N-CA-C	-7.51	102.81	111.00
3	A	552	PHE	CA-C-N	7.39	127.55	120.31
3	A	552	PHE	C-N-CA	7.39	127.55	120.31
3	A	405	ARG	N-CA-C	-7.38	98.10	109.24
3	A	597	GLY	N-CA-C	-7.33	95.80	113.18
3	A	660	PRO	N-CA-CB	7.22	110.83	103.25
3	A	429	GLU	N-CA-C	-7.07	99.18	110.14
3	A	668	TYR	N-CA-C	-7.02	94.29	109.81
3	A	670	ASN	N-CA-C	6.95	120.66	111.28
3	A	161	LYS	N-CA-C	-6.93	103.73	111.28
3	A	653	VAL	N-CA-C	6.90	123.69	109.34
3	A	555	TRP	N-CA-C	6.66	118.53	111.28
3	A	626	PRO	O-C-N	6.61	131.03	123.10
3	A	664	LEU	N-CA-C	-6.49	99.97	109.18
3	A	591	LEU	N-CA-C	6.48	120.89	112.92
3	A	547	ILE	CB-CA-C	6.46	121.89	111.29
3	A	539	TRP	N-CA-C	-6.33	103.52	111.11
3	A	472	LEU	N-CA-C	-6.28	104.36	111.14
3	A	425	ILE	N-CA-C	6.15	117.21	108.42
3	A	625	GLU	CA-C-N	6.10	125.86	119.76
3	A	625	GLU	C-N-CA	6.10	125.86	119.76
3	A	579	MET	N-CA-C	-6.09	105.16	112.59
3	A	577	CYS	N-CA-C	-6.02	105.58	113.17
3	A	414	ASN	N-CA-C	6.00	116.48	108.38
3	A	232	ILE	N-CA-C	5.99	116.45	110.23
2	C	2010	DG	OP1-P-O3'	5.98	125.93	108.00
3	A	292	ASP	CA-C-N	5.83	125.52	119.05
3	A	292	ASP	C-N-CA	5.83	125.52	119.05
3	A	657	GLU	N-CA-C	5.78	123.11	110.80
3	A	623	GLY	O-C-N	5.77	130.19	122.70
2	C	2010	DG	OP2-P-O3'	-5.73	90.80	108.00
3	A	480	GLU	N-CA-CB	5.70	120.51	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	670	ASN	CA-C-N	-5.67	116.16	123.19
3	A	670	ASN	C-N-CA	-5.67	116.16	123.19
3	A	516	VAL	N-CA-C	5.64	116.37	110.62
3	A	668	TYR	C-N-CD	5.62	148.04	125.00
3	A	483	ASN	N-CA-C	5.55	117.52	108.63
3	A	217	ILE	N-CA-C	-5.49	105.37	110.53
3	A	495	TRP	N-CA-C	5.42	118.11	111.82
3	A	412	GLN	N-CA-C	-5.35	103.91	110.65
3	A	453	LEU	N-CA-C	-5.35	102.50	110.20
3	A	401	ALA	N-CA-C	5.23	115.04	108.45
2	C	2011	DG	N9-C1'-C2'	5.18	121.27	113.50
3	A	382	ILE	N-CA-C	-5.16	98.60	109.34
3	A	668	TYR	CA-CB-CG	-5.13	104.67	113.90
3	A	488	LEU	N-CA-C	-5.07	106.35	112.54
3	A	299	GLN	N-CA-C	5.04	116.47	111.07
3	A	477	LEU	N-CA-C	5.04	118.97	112.41
3	A	325	MET	CA-C-N	5.03	124.69	119.56
3	A	325	MET	C-N-CA	5.03	124.69	119.56
3	A	530	ASN	N-CA-C	-5.03	107.64	112.97
3	A	671	ILE	CB-CA-C	5.02	118.31	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	628	PHE	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	421	GLU	Peptide
3	A	479	ALA	Peptide
3	A	607	SER	Mainchain
3	A	608	ARG	Mainchain
3	A	628	PHE	Peptide,Mainchain
3	A	668	TYR	Sidechain
1	B	1007	DT	Sidechain
1	B	1009	DC	Sidechain
2	C	2007	DT	Sidechain
2	C	2016	DC	Sidechain

## 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	B	363	0	206	4	0
2	C	369	0	206	1	0
3	A	4385	0	4357	467	2
All	All	5117	0	4769	467	2

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 47.

All (467) 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)
3:A:617:VAL:HG22	3:A:628:PHE:CD1	1.07	1.57
3:A:422:GLY:N	3:A:422:GLY:CA	1.68	1.53
3:A:617:VAL:CG2	3:A:628:PHE:CD1	1.89	1.52
3:A:422:GLY:H	3:A:423:PRO:CD	1.21	1.51
3:A:543:CYS:CB	3:A:543:CYS:SG	2.08	1.41
3:A:579:MET:CE	3:A:579:MET:SD	2.11	1.38
3:A:480:GLU:CA	3:A:480:GLU:N	1.89	1.34
3:A:620:SER:CB	3:A:624:GLY:O	1.76	1.33
3:A:422:GLY:N	3:A:423:PRO:HD2	1.39	1.31
3:A:617:VAL:CG2	3:A:628:PHE:CE1	2.15	1.28
3:A:620:SER:HB2	3:A:624:GLY:O	1.27	1.23
3:A:617:VAL:CG1	3:A:628:PHE:HE1	1.50	1.21
3:A:617:VAL:CG2	3:A:628:PHE:HD1	1.34	1.21
3:A:422:GLY:N	3:A:423:PRO:CD	1.98	1.17
3:A:617:VAL:CG1	3:A:628:PHE:CE1	2.28	1.16
3:A:617:VAL:HG22	3:A:628:PHE:CE1	1.78	1.14
3:A:667:LEU:HD22	3:A:676:ALA:HB1	1.24	1.12
3:A:643:THR:HG22	3:A:645:PRO:HD2	1.16	1.10
3:A:480:GLU:N	3:A:480:GLU:O	1.85	1.08
3:A:525:LYS:HG3	3:A:548:ASN:HD21	1.07	1.08
3:A:525:LYS:HE3	3:A:548:ASN:ND2	1.68	1.08
3:A:333:LEU:HB2	3:A:471:ILE:HD13	1.35	1.07
3:A:609:GLU:HB3	3:A:636:LYS:NZ	1.70	1.06
3:A:480:GLU:N	3:A:480:GLU:C	2.12	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:564:LEU:HD21	3:A:612:ILE:HD11	1.37	1.03
3:A:591:LEU:HD22	3:A:598:THR:HG23	1.36	1.02
3:A:629:HIS:H	3:A:629:HIS:CD2	1.63	1.01
3:A:593:ASP:O	3:A:595:GLN:HG3	1.58	1.01
3:A:617:VAL:HG11	3:A:628:PHE:HE1	1.23	1.00
3:A:594:GLN:HG2	3:A:594:GLN:O	1.60	1.00
3:A:620:SER:HB3	3:A:624:GLY:O	1.59	1.00
3:A:617:VAL:HG13	3:A:628:PHE:CE1	1.94	1.00
3:A:617:VAL:HG21	3:A:628:PHE:CE1	1.97	0.99
3:A:609:GLU:HB3	3:A:636:LYS:HZ1	1.30	0.96
3:A:649:ARG:HB2	3:A:681:TYR:CE1	2.00	0.96
3:A:616:TRP:HB3	3:A:629:HIS:HB2	1.47	0.95
3:A:643:THR:CG2	3:A:645:PRO:HD2	1.95	0.95
3:A:483:ASN:ND2	3:A:485:SER:H	1.64	0.95
3:A:390:MET:HG2	3:A:402:ALA:HB2	1.48	0.95
3:A:288:THR:HG22	3:A:289:TYR:H	1.31	0.94
3:A:421:GLU:C	3:A:422:GLY:CA	2.39	0.94
3:A:590:LEU:HD21	3:A:668:TYR:OH	1.66	0.94
3:A:525:LYS:CG	3:A:548:ASN:HD21	1.81	0.92
3:A:629:HIS:CD2	3:A:629:HIS:N	2.36	0.92
3:A:590:LEU:HD12	3:A:590:LEU:O	1.70	0.92
3:A:634:TYR:CZ	3:A:647:ILE:HD11	2.05	0.91
3:A:474:TYR:OH	3:A:482:ARG:HB2	1.70	0.91
3:A:643:THR:HG22	3:A:645:PRO:CD	2.00	0.91
3:A:667:LEU:HD13	3:A:677:PHE:CE1	2.06	0.90
3:A:153:VAL:HG22	3:A:220:LEU:HD11	1.54	0.90
3:A:629:HIS:H	3:A:629:HIS:HD2	1.18	0.89
3:A:665:LYS:HA	3:A:673:LYS:HB2	1.55	0.89
3:A:422:GLY:N	3:A:422:GLY:C	2.30	0.89
3:A:156:ILE:HD12	3:A:220:LEU:HD12	1.56	0.87
3:A:474:TYR:OH	3:A:482:ARG:CB	2.23	0.87
3:A:525:LYS:HG3	3:A:548:ASN:ND2	1.89	0.87
3:A:553:PRO:HD2	3:A:556:LEU:HD12	1.55	0.87
3:A:564:LEU:HD21	3:A:612:ILE:CD1	2.06	0.86
3:A:578:ILE:HG22	3:A:580:GLY:H	1.38	0.85
3:A:572:LEU:HD21	3:A:645:PRO:HG3	1.59	0.84
3:A:616:TRP:CE2	3:A:663:PRO:HG3	2.13	0.84
3:A:550:LYS:HD3	3:A:552:PHE:CZ	2.13	0.84
3:A:153:VAL:HG21	3:A:269:SER:HB3	1.59	0.84
3:A:617:VAL:HG21	3:A:628:PHE:CD1	2.07	0.83
3:A:422:GLY:N	3:A:423:PRO:N	2.26	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:616:TRP:CB	3:A:629:HIS:HB2	2.09	0.82
3:A:618:GLU:O	3:A:626:PRO:CG	2.28	0.82
3:A:349:VAL:HG12	3:A:351:LEU:HG	1.62	0.82
3:A:591:LEU:HD22	3:A:598:THR:CG2	2.09	0.82
3:A:546:ASN:HD21	3:A:550:LYS:C	1.88	0.81
3:A:590:LEU:HD21	3:A:668:TYR:CZ	2.14	0.81
3:A:636:LYS:H	3:A:636:LYS:HD2	1.43	0.81
3:A:170:TYR:HD2	3:A:202:MET:HA	1.44	0.81
3:A:616:TRP:CZ2	3:A:663:PRO:HG3	2.15	0.81
3:A:422:GLY:H	3:A:423:PRO:N	1.80	0.79
3:A:667:LEU:HD11	3:A:677:PHE:CZ	2.18	0.79
3:A:422:GLY:H	3:A:423:PRO:HD2	0.62	0.78
3:A:667:LEU:CD2	3:A:676:ALA:HB1	2.10	0.78
3:A:218:ILE:HG12	3:A:301:LEU:HD21	1.66	0.78
3:A:618:GLU:C	3:A:626:PRO:HG3	2.08	0.77
3:A:550:LYS:HD3	3:A:552:PHE:CE2	2.20	0.77
3:A:170:TYR:CD2	3:A:202:MET:HA	2.19	0.77
3:A:522:LEU:HD21	3:A:581:PHE:CD2	2.20	0.77
3:A:260:GLN:O	3:A:264:THR:HG23	1.85	0.76
3:A:288:THR:HG22	3:A:289:TYR:N	2.00	0.76
3:A:617:VAL:HG11	3:A:628:PHE:CE1	2.10	0.76
3:A:166:LEU:HD23	3:A:166:LEU:O	1.86	0.75
3:A:224:THR:HG21	3:A:270:LEU:HD11	1.68	0.75
3:A:643:THR:O	3:A:647:ILE:HG22	1.86	0.75
3:A:609:GLU:HB3	3:A:636:LYS:HZ2	1.50	0.75
3:A:376:GLY:HA3	3:A:423:PRO:HG3	1.70	0.74
3:A:649:ARG:HB2	3:A:681:TYR:HE1	1.51	0.74
3:A:590:LEU:HD11	3:A:668:TYR:OH	1.87	0.74
3:A:673:LYS:O	3:A:676:ALA:HB3	1.89	0.73
3:A:214:VAL:HG11	3:A:297:ASN:ND2	2.04	0.73
3:A:617:VAL:CB	3:A:628:PHE:CE1	2.72	0.73
3:A:173:LYS:O	3:A:177:LEU:HD13	1.89	0.72
3:A:587:GLU:HG3	3:A:600:LEU:HD23	1.71	0.72
3:A:635:THR:HG22	3:A:638:GLU:OE1	1.89	0.72
3:A:645:PRO:HG2	3:A:680:TYR:HB3	1.70	0.72
3:A:525:LYS:HE3	3:A:548:ASN:HD22	1.54	0.72
3:A:553:PRO:CD	3:A:556:LEU:HD12	2.20	0.72
3:A:323:PRO:HG2	3:A:433:LEU:HD12	1.72	0.72
3:A:453:LEU:HD23	3:A:482:ARG:HH21	1.56	0.71
3:A:599:PHE:HD2	3:A:667:LEU:HD12	1.55	0.71
3:A:609:GLU:CB	3:A:636:LYS:HZ1	2.01	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:241:ARG:HE	3:A:479:ALA:HB1	1.55	0.71
3:A:485:SER:HB3	3:A:488:LEU:HD12	1.72	0.71
3:A:241:ARG:NE	3:A:479:ALA:HB1	2.05	0.71
3:A:243:GLN:HA	3:A:253:ASN:ND2	2.06	0.71
3:A:152:LYS:O	3:A:156:ILE:HG13	1.92	0.70
3:A:167:GLN:HE22	3:A:210:ARG:HH21	1.38	0.70
3:A:667:LEU:CD1	3:A:677:PHE:CE1	2.74	0.70
3:A:672:ASP:O	3:A:673:LYS:C	2.35	0.70
3:A:510:THR:HG22	3:A:570:LEU:HD21	1.74	0.69
3:A:617:VAL:CB	3:A:628:PHE:HE1	2.04	0.69
3:A:618:GLU:O	3:A:626:PRO:CD	2.41	0.69
3:A:333:LEU:CB	3:A:471:ILE:HD13	2.20	0.69
3:A:525:LYS:HE3	3:A:548:ASN:HD21	1.56	0.69
1:B:1018:DC:O2	3:A:421:GLU:OE2	2.10	0.69
3:A:331:ARG:NH2	3:A:559:GLU:OE2	2.21	0.69
3:A:667:LEU:HD13	3:A:677:PHE:HE1	1.53	0.69
3:A:550:LYS:HE2	3:A:605:GLU:O	1.92	0.69
3:A:546:ASN:ND2	3:A:550:LYS:O	2.26	0.68
3:A:568:HIS:O	3:A:569:LEU:HD23	1.92	0.68
3:A:651:TYR:O	3:A:653:VAL:N	2.27	0.68
3:A:412:GLN:HG2	3:A:414:ASN:ND2	2.09	0.68
3:A:391:ASN:HD22	3:A:394:GLU:HG3	1.59	0.67
3:A:243:GLN:HA	3:A:253:ASN:HD21	1.59	0.67
3:A:599:PHE:HB2	3:A:666:TYR:O	1.94	0.67
3:A:590:LEU:CD2	3:A:668:TYR:OH	2.42	0.67
3:A:613:THR:HG22	3:A:614:PHE:N	2.10	0.67
3:A:667:LEU:HD22	3:A:676:ALA:CB	2.14	0.67
3:A:616:TRP:HB2	3:A:629:HIS:O	1.94	0.67
3:A:244:GLN:HE22	3:A:479:ALA:HA	1.60	0.66
3:A:391:ASN:HB3	3:A:393:GLU:HG2	1.78	0.66
3:A:218:ILE:CG1	3:A:301:LEU:HD21	2.25	0.66
3:A:474:TYR:OH	3:A:482:ARG:HB3	1.95	0.66
3:A:594:GLN:O	3:A:594:GLN:CG	2.40	0.65
3:A:667:LEU:CD1	3:A:677:PHE:CZ	2.79	0.65
3:A:260:GLN:OE1	3:A:350:LYS:HE3	1.96	0.65
3:A:651:TYR:O	3:A:651:TYR:CG	2.50	0.65
3:A:629:HIS:N	3:A:629:HIS:HD2	1.81	0.65
3:A:260:GLN:CD	3:A:350:LYS:HE3	2.21	0.65
3:A:256:LEU:HD13	3:A:348:LEU:HD21	1.77	0.65
3:A:420:ASN:CB	3:A:423:PRO:HD3	2.26	0.65
3:A:547:ILE:HD13	3:A:554:PHE:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:664:LEU:HB3	3:A:673:LYS:HD2	1.80	0.64
3:A:671:ILE:HG22	3:A:676:ALA:HB2	1.78	0.64
3:A:143:ASP:O	3:A:147:ARG:HD3	1.98	0.64
3:A:616:TRP:HE1	3:A:663:PRO:HB3	1.63	0.64
3:A:136:LEU:CB	3:A:140:LYS:HE3	2.28	0.63
3:A:170:TYR:HB3	3:A:202:MET:SD	2.38	0.63
3:A:378:ARG:NH2	3:A:427:THR:HB	2.13	0.63
3:A:264:THR:O	3:A:268:GLU:HG3	1.99	0.63
3:A:599:PHE:HD2	3:A:667:LEU:CD1	2.12	0.63
3:A:619:ARG:HA	3:A:626:PRO:HD3	1.80	0.62
1:B:1018:DC:C2	3:A:421:GLU:OE2	2.52	0.62
3:A:304:ARG:O	3:A:308:LEU:HD23	1.98	0.62
3:A:525:LYS:CE	3:A:548:ASN:ND2	2.54	0.62
3:A:350:LYS:HE2	3:A:398:GLY:O	1.99	0.62
3:A:355:ASN:HD21	3:A:356:TYR:HE1	1.47	0.62
3:A:136:LEU:HB2	3:A:140:LYS:HE3	1.82	0.62
3:A:587:GLU:HG3	3:A:600:LEU:CD2	2.29	0.62
3:A:616:TRP:NE1	3:A:663:PRO:CB	2.62	0.62
3:A:264:THR:HG21	3:A:350:LYS:HB2	1.82	0.62
3:A:150:LYS:HG2	3:A:154:MET:HE2	1.81	0.61
3:A:644:PHE:O	3:A:647:ILE:HG23	2.00	0.61
3:A:468:TRP:HE1	3:A:505:GLN:NE2	1.97	0.61
3:A:609:GLU:CB	3:A:636:LYS:NZ	2.55	0.61
3:A:164:GLU:HG2	3:A:283:LEU:HD21	1.82	0.61
3:A:325:MET:HE3	3:A:339:VAL:HG11	1.83	0.61
3:A:153:VAL:HG21	3:A:269:SER:CB	2.29	0.61
3:A:594:GLN:O	3:A:596:PRO:HD3	2.01	0.61
3:A:616:TRP:HE1	3:A:663:PRO:CB	2.14	0.61
3:A:149:VAL:O	3:A:153:VAL:HG23	2.01	0.61
3:A:274:ARG:NH2	3:A:444:LEU:HG	2.16	0.60
3:A:391:ASN:CB	3:A:393:GLU:HG2	2.31	0.60
3:A:550:LYS:CE	3:A:605:GLU:O	2.49	0.60
3:A:479:ALA:C	3:A:480:GLU:CA	2.71	0.60
3:A:208:ASN:O	3:A:212:GLU:HB2	2.00	0.60
3:A:668:TYR:CD2	3:A:669:PRO:HD3	2.37	0.60
3:A:582:ILE:HG22	3:A:583:SER:O	2.01	0.60
3:A:668:TYR:CG	3:A:669:PRO:CD	2.85	0.60
3:A:362:VAL:C	3:A:363:LEU:HD12	2.27	0.59
3:A:489:THR:HG22	3:A:489:THR:O	1.99	0.59
3:A:618:GLU:O	3:A:626:PRO:HG3	1.98	0.59
3:A:202:MET:HE3	3:A:203:TYR:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:288:THR:CG2	3:A:289:TYR:H	2.11	0.59
3:A:355:ASN:ND2	3:A:356:TYR:CE1	2.71	0.59
3:A:292:ASP:OD2	3:A:294:ILE:HG22	2.02	0.59
3:A:385:THR:HG22	3:A:387:THR:O	2.04	0.58
3:A:514:LEU:HD12	3:A:519:LEU:HD21	1.85	0.58
3:A:483:ASN:ND2	3:A:483:ASN:C	2.61	0.58
3:A:243:GLN:CA	3:A:253:ASN:HD21	2.16	0.58
3:A:612:ILE:N	3:A:612:ILE:HD12	2.18	0.58
3:A:284:GLU:HA	3:A:287:TYR:O	2.04	0.58
3:A:341:PHE:CZ	3:A:407:LEU:HB3	2.39	0.58
3:A:453:LEU:CD2	3:A:482:ARG:HH21	2.16	0.58
3:A:472:LEU:O	3:A:476:MET:HB2	2.03	0.58
3:A:594:GLN:C	3:A:596:PRO:HD3	2.29	0.57
3:A:318:VAL:HG22	3:A:319:VAL:N	2.19	0.57
3:A:611:ALA:HA	3:A:634:TYR:O	2.04	0.57
2:C:2002:DG:N2	3:A:421:GLU:OE1	2.37	0.57
3:A:512:ARG:HD2	3:A:574:ASN:O	2.04	0.57
3:A:547:ILE:CD1	3:A:554:PHE:HB2	2.33	0.57
3:A:591:LEU:HB3	3:A:617:VAL:HG21	1.85	0.57
3:A:340:GLN:CD	3:A:406:HIS:HA	2.30	0.57
3:A:483:ASN:C	3:A:483:ASN:HD22	2.12	0.56
3:A:334:VAL:HG23	3:A:471:ILE:HD12	1.87	0.56
3:A:631:VAL:HG12	3:A:632:GLU:O	2.06	0.56
3:A:662:ASN:CB	3:A:664:LEU:HG	2.36	0.56
3:A:590:LEU:CD1	3:A:668:TYR:OH	2.53	0.56
3:A:590:LEU:O	3:A:590:LEU:CD1	2.50	0.56
3:A:264:THR:HB	3:A:349:VAL:O	2.06	0.56
3:A:309:PHE:O	3:A:313:ILE:HG22	2.06	0.56
3:A:388:LYS:NZ	3:A:394:GLU:OE2	2.39	0.56
3:A:483:ASN:HD22	3:A:485:SER:H	1.49	0.55
3:A:555:TRP:CZ2	3:A:559:GLU:HG2	2.41	0.55
3:A:668:TYR:CE2	3:A:669:PRO:HD3	2.42	0.55
3:A:598:THR:O	3:A:615:THR:O	2.25	0.55
3:A:546:ASN:OD1	3:A:552:PHE:N	2.39	0.55
3:A:668:TYR:CD2	3:A:669:PRO:CD	2.90	0.55
3:A:260:GLN:CD	3:A:346:ARG:HH21	2.15	0.55
3:A:280:LEU:HD22	3:A:294:ILE:HD11	1.87	0.55
3:A:351:LEU:HB3	3:A:353:GLU:OE2	2.07	0.55
3:A:371:ARG:HA	3:A:377:PHE:CD2	2.40	0.55
3:A:148:ASN:HD22	3:A:223:VAL:HG11	1.71	0.55
3:A:280:LEU:HB3	3:A:294:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:483:ASN:HD21	3:A:485:SER:HB2	1.71	0.55
3:A:522:LEU:HD21	3:A:581:PHE:CE2	2.41	0.55
3:A:375:LYS:O	3:A:423:PRO:HB2	2.07	0.54
3:A:478:VAL:HG12	3:A:479:ALA:N	2.22	0.54
3:A:667:LEU:HD11	3:A:677:PHE:HZ	1.69	0.54
3:A:341:PHE:CE2	3:A:407:LEU:HD13	2.42	0.54
3:A:273:VAL:HA	3:A:276:GLN:OE1	2.08	0.54
3:A:527:LEU:HD21	3:A:537:ILE:HG12	1.88	0.54
3:A:627:ASP:O	3:A:628:PHE:C	2.48	0.54
3:A:483:ASN:ND2	3:A:485:SER:N	2.46	0.54
3:A:523:GLY:C	3:A:525:LYS:H	2.15	0.54
3:A:345:LEU:HD11	3:A:435:PHE:CD1	2.43	0.53
3:A:341:PHE:HE1	3:A:409:LEU:HD13	1.73	0.53
3:A:243:GLN:CB	3:A:253:ASN:HD21	2.20	0.53
3:A:554:PHE:CZ	3:A:558:ILE:HD12	2.43	0.53
3:A:591:LEU:HD13	3:A:598:THR:CG2	2.38	0.53
3:A:441:GLN:O	3:A:444:LEU:O	2.26	0.53
3:A:177:LEU:HD12	3:A:180:ARG:HH21	1.73	0.53
3:A:292:ASP:CG	3:A:294:ILE:HG22	2.34	0.53
3:A:525:LYS:CE	3:A:548:ASN:HD21	2.21	0.52
3:A:547:ILE:O	3:A:549:ASP:N	2.42	0.52
3:A:582:ILE:O	3:A:583:SER:C	2.52	0.52
3:A:597:GLY:O	3:A:666:TYR:O	2.27	0.52
3:A:616:TRP:N	3:A:629:HIS:O	2.33	0.52
3:A:313:ILE:HG12	3:A:448:LEU:HD21	1.91	0.52
3:A:649:ARG:HD2	3:A:681:TYR:CD1	2.44	0.52
3:A:526:LEU:HD23	3:A:547:ILE:HD11	1.92	0.52
1:B:1012:DT:O4	3:A:460:ASN:ND2	2.35	0.52
3:A:567:LYS:O	3:A:568:HIS:CG	2.63	0.52
3:A:655:ALA:HB1	3:A:661:GLU:CB	2.40	0.52
3:A:595:GLN:CD	3:A:670:ASN:OD1	2.53	0.52
3:A:598:THR:CB	3:A:617:VAL:HB	2.39	0.52
3:A:288:THR:O	3:A:289:TYR:HB3	2.10	0.52
3:A:229:ASN:ND2	3:A:233:ASN:HD22	2.07	0.52
3:A:167:GLN:HE22	3:A:210:ARG:NH2	2.08	0.52
3:A:316:SER:CB	3:A:349:VAL:HG23	2.40	0.51
3:A:325:MET:CE	3:A:339:VAL:HG11	2.40	0.51
3:A:526:LEU:HD21	3:A:554:PHE:CG	2.46	0.51
3:A:602:ARG:HH11	3:A:602:ARG:HB3	1.75	0.51
3:A:360:VAL:O	3:A:387:THR:HG23	2.11	0.51
3:A:167:GLN:NE2	3:A:210:ARG:HH21	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:586:ARG:O	3:A:586:ARG:HG2	2.08	0.51
3:A:266:VAL:HG13	3:A:312:LEU:HD21	1.91	0.51
3:A:593:ASP:O	3:A:595:GLN:N	2.44	0.51
3:A:645:PRO:O	3:A:648:ILE:HB	2.11	0.51
3:A:321:ARG:HD2	3:A:322:GLN:N	2.25	0.51
3:A:147:ARG:HH22	3:A:261:ASN:ND2	2.09	0.51
3:A:480:GLU:O	3:A:481:PRO:C	2.54	0.51
3:A:599:PHE:CD2	3:A:667:LEU:HD12	2.41	0.51
3:A:706:LEU:C	3:A:707:ILE:HG13	2.35	0.51
3:A:325:MET:HE3	3:A:339:VAL:CG1	2.40	0.51
3:A:582:ILE:C	3:A:583:SER:O	2.49	0.50
3:A:668:TYR:O	3:A:670:ASN:N	2.45	0.50
3:A:174:CYS:SG	3:A:202:MET:HE2	2.51	0.50
3:A:142:LEU:HD23	3:A:262:TRP:CZ3	2.47	0.50
3:A:546:ASN:ND2	3:A:550:LYS:C	2.65	0.50
3:A:579:MET:CE	3:A:579:MET:CG	2.89	0.50
3:A:522:LEU:O	3:A:525:LYS:HB3	2.12	0.50
3:A:602:ARG:HB3	3:A:602:ARG:NH1	2.27	0.50
3:A:387:THR:HG22	3:A:388:LYS:N	2.26	0.50
3:A:498:LEU:CD2	3:A:502:LEU:HG	2.42	0.50
3:A:293:PRO:C	3:A:295:THR:H	2.19	0.49
3:A:510:THR:HG22	3:A:570:LEU:CD2	2.40	0.49
3:A:420:ASN:C	3:A:423:PRO:HD3	2.37	0.49
3:A:136:LEU:O	3:A:140:LYS:HG3	2.12	0.49
3:A:495:TRP:CE2	3:A:499:SER:HB3	2.47	0.49
3:A:618:GLU:C	3:A:626:PRO:CG	2.77	0.49
3:A:136:LEU:HB3	3:A:140:LYS:HE3	1.94	0.49
3:A:352:GLN:C	3:A:354:LEU:H	2.20	0.49
3:A:546:ASN:OD1	3:A:551:ASN:CA	2.59	0.49
3:A:145:LYS:O	3:A:149:VAL:HG23	2.13	0.49
3:A:214:VAL:HG11	3:A:297:ASN:HD22	1.76	0.49
3:A:378:ARG:HD2	3:A:380:PHE:CZ	2.47	0.49
3:A:421:GLU:O	3:A:422:GLY:CA	2.59	0.49
3:A:454:PRO:HG3	3:A:474:TYR:CE2	2.48	0.49
3:A:170:TYR:HB3	3:A:202:MET:HG2	1.95	0.49
3:A:664:LEU:O	3:A:665:LYS:HB2	2.12	0.49
3:A:264:THR:CG2	3:A:350:LYS:HB2	2.41	0.48
3:A:599:PHE:HB2	3:A:667:LEU:HA	1.93	0.48
3:A:147:ARG:HH22	3:A:261:ASN:HD21	1.60	0.48
3:A:634:TYR:HB3	3:A:639:LEU:CD1	2.43	0.48
3:A:702:ILE:HG22	3:A:702:ILE:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:706:LEU:O	3:A:707:ILE:HG13	2.14	0.48
3:A:270:LEU:HD21	3:A:308:LEU:HB3	1.96	0.48
3:A:170:TYR:CD2	3:A:202:MET:HG2	2.48	0.48
3:A:305:THR:O	3:A:305:THR:HG22	2.13	0.48
3:A:600:LEU:O	3:A:614:PHE:HA	2.14	0.48
3:A:515:ASN:C	3:A:515:ASN:OD1	2.56	0.48
3:A:668:TYR:CG	3:A:669:PRO:HD3	2.49	0.48
3:A:281:GLU:O	3:A:284:GLU:HG2	2.13	0.48
3:A:634:TYR:CZ	3:A:647:ILE:CD1	2.90	0.47
3:A:324:CYS:SG	3:A:332:PRO:HA	2.54	0.47
3:A:355:ASN:ND2	3:A:356:TYR:HE1	2.07	0.47
3:A:376:GLY:HA3	3:A:423:PRO:CG	2.40	0.47
3:A:378:ARG:HD2	3:A:380:PHE:HZ	1.78	0.47
3:A:170:TYR:HD2	3:A:202:MET:HG2	1.79	0.47
3:A:626:PRO:O	3:A:628:PHE:N	2.44	0.47
3:A:222:ASN:HA	3:A:304:ARG:NH2	2.29	0.47
3:A:521:MET:HG3	3:A:581:PHE:C	2.39	0.47
3:A:274:ARG:CZ	3:A:444:LEU:HG	2.45	0.47
3:A:351:LEU:O	3:A:354:LEU:HB3	2.15	0.47
3:A:636:LYS:HD2	3:A:636:LYS:N	2.21	0.47
3:A:672:ASP:HB2	3:A:675:HIS:HB3	1.97	0.47
3:A:148:ASN:ND2	3:A:223:VAL:HG11	2.29	0.47
3:A:390:MET:HG2	3:A:402:ALA:CB	2.33	0.47
3:A:397:ASN:O	3:A:399:SER:N	2.47	0.47
3:A:327:THR:HG22	3:A:327:THR:O	2.15	0.47
3:A:617:VAL:CG2	3:A:628:PHE:HE1	1.89	0.47
3:A:525:LYS:CD	3:A:548:ASN:HD21	2.27	0.46
3:A:460:ASN:C	3:A:462:SER:N	2.73	0.46
3:A:593:ASP:O	3:A:594:GLN:C	2.57	0.46
3:A:598:THR:HG21	3:A:617:VAL:CG2	2.45	0.46
3:A:613:THR:HG23	3:A:631:VAL:O	2.15	0.46
3:A:231:LEU:HG	3:A:263:PHE:CE1	2.49	0.46
3:A:323:PRO:O	3:A:332:PRO:O	2.34	0.46
3:A:340:GLN:NE2	3:A:406:HIS:ND1	2.64	0.46
3:A:502:LEU:HD23	3:A:502:LEU:HA	1.78	0.46
3:A:224:THR:CG2	3:A:270:LEU:HD11	2.44	0.46
3:A:368:VAL:O	3:A:371:ARG:HG3	2.16	0.46
3:A:427:THR:C	3:A:428:GLU:OE1	2.58	0.46
3:A:613:THR:CG2	3:A:614:PHE:N	2.77	0.46
3:A:635:THR:CG2	3:A:638:GLU:OE1	2.62	0.46
3:A:293:PRO:C	3:A:295:THR:N	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:349:VAL:CG1	3:A:351:LEU:HG	2.39	0.46
3:A:405:ARG:O	3:A:406:HIS:CB	2.63	0.46
3:A:593:ASP:OD2	3:A:595:GLN:OE1	2.34	0.46
3:A:526:LEU:HD11	3:A:554:PHE:CE2	2.51	0.46
3:A:595:GLN:O	3:A:597:GLY:N	2.49	0.46
3:A:664:LEU:HB3	3:A:673:LYS:CD	2.46	0.45
3:A:266:VAL:O	3:A:270:LEU:HD13	2.16	0.45
3:A:569:LEU:HD11	3:A:612:ILE:HD11	1.99	0.45
3:A:383:LEU:HD23	3:A:408:GLN:NE2	2.32	0.45
3:A:504:TRP:O	3:A:505:GLN:C	2.58	0.45
3:A:634:TYR:HB3	3:A:639:LEU:HD13	1.98	0.45
3:A:651:TYR:O	3:A:652:LYS:C	2.58	0.45
3:A:613:THR:HG22	3:A:614:PHE:O	2.16	0.45
3:A:655:ALA:CB	3:A:661:GLU:CB	2.95	0.45
3:A:354:LEU:CD1	3:A:439:LEU:HD13	2.47	0.45
3:A:256:LEU:CD2	3:A:259:LEU:HD12	2.47	0.45
3:A:280:LEU:CB	3:A:294:ILE:HD11	2.46	0.45
3:A:641:ALA:C	3:A:642:VAL:HG23	2.42	0.45
3:A:405:ARG:C	3:A:406:HIS:CG	2.93	0.45
3:A:460:ASN:C	3:A:462:SER:H	2.25	0.45
3:A:468:TRP:HE1	3:A:505:GLN:HE21	1.62	0.44
3:A:626:PRO:C	3:A:628:PHE:H	2.22	0.44
3:A:650:ASN:O	3:A:707:ILE:HG23	2.17	0.44
3:A:464:LEU:N	3:A:465:PRO:HD2	2.31	0.44
3:A:616:TRP:NE1	3:A:663:PRO:HG3	2.31	0.44
3:A:674:ASP:O	3:A:678:GLY:N	2.49	0.44
3:A:631:VAL:HG12	3:A:632:GLU:N	2.33	0.44
3:A:464:LEU:C	3:A:464:LEU:HD23	2.43	0.44
3:A:222:ASN:HA	3:A:304:ARG:HH22	1.81	0.44
3:A:231:LEU:HD21	3:A:263:PHE:CD1	2.52	0.44
3:A:234:ASP:O	3:A:238:GLU:HB2	2.18	0.44
3:A:340:GLN:HA	3:A:407:LEU:O	2.17	0.44
3:A:243:GLN:HB2	3:A:253:ASN:HD21	1.83	0.44
3:A:292:ASP:HA	3:A:293:PRO:HD2	1.80	0.44
3:A:482:ARG:N	3:A:482:ARG:CD	2.81	0.44
3:A:469:ALA:HB2	3:A:555:TRP:CD1	2.53	0.43
3:A:547:ILE:O	3:A:548:ASN:C	2.58	0.43
3:A:584:LYS:O	3:A:588:ARG:HG3	2.18	0.43
3:A:323:PRO:HA	3:A:343:VAL:HG22	2.00	0.43
3:A:468:TRP:NE1	3:A:472:LEU:HD21	2.33	0.43
3:A:316:SER:OG	3:A:349:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:426:VAL:C	3:A:428:GLU:H	2.25	0.43
3:A:509:VAL:HG12	3:A:509:VAL:O	2.18	0.43
3:A:598:THR:HG21	3:A:617:VAL:HB	2.00	0.43
3:A:673:LYS:HG2	3:A:674:ASP:N	2.34	0.43
3:A:170:TYR:HD2	3:A:202:MET:CA	2.24	0.43
3:A:644:PHE:HA	3:A:647:ILE:CG2	2.49	0.43
3:A:157:GLU:CA	3:A:276:GLN:HE21	2.31	0.43
3:A:179:ASN:C	3:A:181:GLU:H	2.26	0.43
3:A:355:ASN:ND2	3:A:356:TYR:CD1	2.87	0.43
3:A:569:LEU:HD11	3:A:612:ILE:HG12	2.01	0.43
3:A:523:GLY:C	3:A:525:LYS:N	2.75	0.43
3:A:664:LEU:HD13	3:A:673:LYS:HZ1	1.83	0.43
3:A:153:VAL:HG12	3:A:272:GLN:NE2	2.34	0.43
3:A:292:ASP:OD1	3:A:294:ILE:HG22	2.19	0.43
3:A:310:GLN:O	3:A:314:GLN:HG3	2.18	0.43
3:A:455:VAL:CG1	3:A:456:VAL:N	2.81	0.43
3:A:627:ASP:HB2	3:A:629:HIS:NE2	2.34	0.43
3:A:314:GLN:HA	3:A:448:LEU:HD22	2.01	0.43
3:A:546:ASN:OD1	3:A:551:ASN:HA	2.18	0.43
3:A:561:ILE:HG21	3:A:603:PHE:CD2	2.54	0.42
3:A:591:LEU:HD13	3:A:598:THR:HG21	2.00	0.42
3:A:295:THR:O	3:A:298:LYS:HB3	2.19	0.42
3:A:314:GLN:HA	3:A:448:LEU:CD2	2.49	0.42
3:A:649:ARG:HD2	3:A:681:TYR:CE1	2.53	0.42
3:A:228:GLN:NE2	3:A:312:LEU:HB2	2.34	0.42
3:A:263:PHE:O	3:A:266:VAL:HG12	2.20	0.42
3:A:375:LYS:C	3:A:377:PHE:H	2.28	0.42
3:A:426:VAL:HG12	3:A:427:THR:N	2.34	0.42
3:A:454:PRO:HG3	3:A:474:TYR:CZ	2.55	0.42
3:A:478:VAL:CG1	3:A:479:ALA:N	2.82	0.42
3:A:163:LEU:HD22	3:A:283:LEU:CD1	2.49	0.42
3:A:334:VAL:CG2	3:A:471:ILE:HD12	2.48	0.42
3:A:166:LEU:HD22	3:A:206:LEU:HD23	2.02	0.42
3:A:482:ARG:H	3:A:482:ARG:HD3	1.85	0.42
3:A:232:ILE:HD11	3:A:312:LEU:HA	2.02	0.42
3:A:323:PRO:O	3:A:324:CYS:HB2	2.18	0.42
3:A:521:MET:C	3:A:521:MET:SD	3.03	0.42
3:A:288:THR:HG23	3:A:292:ASP:OD2	2.20	0.42
3:A:351:LEU:O	3:A:352:GLN:C	2.62	0.42
3:A:560:SER:HB2	3:A:609:GLU:O	2.20	0.42
3:A:601:LEU:HD23	3:A:614:PHE:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:347:LEU:HD12	3:A:347:LEU:HA	1.92	0.41
3:A:342:THR:HG23	3:A:404:PHE:O	2.19	0.41
3:A:393:GLU:HG3	3:A:394:GLU:N	2.35	0.41
3:A:643:THR:HG22	3:A:644:PHE:N	2.35	0.41
3:A:239:TRP:CD2	3:A:256:LEU:HD21	2.55	0.41
3:A:257:ASP:O	3:A:258:GLN:C	2.62	0.41
3:A:363:LEU:HD12	3:A:363:LEU:N	2.34	0.41
3:A:644:PHE:N	3:A:645:PRO:CD	2.84	0.41
1:B:1009:DC:P	3:A:339:VAL:HG13	2.60	0.41
3:A:317:PHE:CD2	3:A:450:THR:HG22	2.56	0.41
3:A:431:HIS:O	3:A:454:PRO:HA	2.21	0.41
3:A:490:PRO:HA	3:A:491:PRO:HD2	1.83	0.41
3:A:664:LEU:HD13	3:A:673:LYS:NZ	2.36	0.41
3:A:547:ILE:HG12	3:A:548:ASN:H	1.86	0.41
3:A:651:TYR:O	3:A:651:TYR:CD1	2.74	0.41
3:A:587:GLU:O	3:A:588:ARG:C	2.64	0.41
3:A:598:THR:O	3:A:598:THR:HG22	2.19	0.41
3:A:202:MET:O	3:A:204:LEU:N	2.54	0.41
3:A:270:LEU:HD23	3:A:309:PHE:HB2	2.02	0.41
3:A:345:LEU:HD12	3:A:360:VAL:HG11	2.01	0.41
3:A:387:THR:CG2	3:A:388:LYS:N	2.83	0.41
3:A:580:GLY:O	3:A:602:ARG:HG3	2.20	0.41
3:A:624:GLY:O	3:A:625:GLU:C	2.63	0.41
3:A:668:TYR:CZ	3:A:669:PRO:HD3	2.55	0.41
3:A:170:TYR:HB3	3:A:202:MET:CG	2.50	0.41
3:A:177:LEU:O	3:A:181:GLU:HG3	2.21	0.41
3:A:515:ASN:OD1	3:A:517:ASP:N	2.54	0.40
3:A:602:ARG:HH11	3:A:602:ARG:CB	2.34	0.40
3:A:461:VAL:O	3:A:461:VAL:HG12	2.20	0.40
3:A:582:ILE:HD13	3:A:582:ILE:HG21	1.81	0.40
3:A:568:HIS:HB3	3:A:639:LEU:HD23	2.02	0.40
3:A:618:GLU:O	3:A:626:PRO:HD2	2.21	0.40
3:A:341:PHE:CE1	3:A:409:LEU:HD13	2.54	0.40

All (2) 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)
3:A:165:ASP:OD2	3:A:165:ASP:OD2[3_655]	1.82	0.38
3:A:438:GLN:OE1	3:A:670:ASN:ND2[1_455]	2.15	0.05

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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
3	A	538/575 (94%)	428 (80%)	78 (14%)	32 (6%)	<b>1</b> <b>4</b>

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	202	MET
3	A	548	ASN
3	A	580	GLY
3	A	594	GLN
3	A	596	PRO
3	A	627	ASP
3	A	637	LYS
3	A	652	LYS
3	A	658	ASN
3	A	659	ILE
3	A	662	ASN
3	A	663	PRO
3	A	665	LYS
3	A	668	TYR
3	A	203	TYR
3	A	384	GLY
3	A	398	GLY
3	A	427	THR
3	A	629	HIS
3	A	660	PRO
3	A	673	LYS
3	A	350	LYS
3	A	549	ASP
3	A	657	GLU
3	A	666	TYR
3	A	290	GLU
3	A	353	GLU
3	A	422	GLY

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Mol	Chain	Res	Type
3	A	424	LEU
3	A	568	HIS
3	A	653	VAL
3	A	547	ILE

### 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
3	A	480/528 (91%)	458 (95%)	22 (5%)	24 57

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	163	LEU
3	A	212	GLU
3	A	220	LEU
3	A	236	LEU
3	A	264	THR
3	A	337	THR
3	A	353	GLU
3	A	409	LEU
3	A	428	GLU
3	A	482	ARG
3	A	498	LEU
3	A	558	ILE
3	A	559	GLU
3	A	562	LEU
3	A	596	PRO
3	A	612	ILE
3	A	616	TRP
3	A	628	PHE
3	A	629	HIS
3	A	647	ILE
3	A	669	PRO
3	A	671	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	139	GLN
3	A	148	ASN
3	A	167	GLN
3	A	208	ASN
3	A	233	ASN
3	A	244	GLN
3	A	253	ASN
3	A	261	ASN
3	A	271	GLN
3	A	272	GLN
3	A	297	ASN
3	A	310	GLN
3	A	311	GLN
3	A	314	GLN
3	A	340	GLN
3	A	355	ASN
3	A	386	HIS
3	A	391	ASN
3	A	408	GLN
3	A	414	ASN
3	A	441	GLN
3	A	475	ASN
3	A	483	ASN
3	A	505	GLN
3	A	548	ASN
3	A	629	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
3	PTR	A	701	3	15,16,17	1.23	0	17,22,24	1.17	1 (5%)

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
3	PTR	A	701	3	-	0/10/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	PTR	CD2-CE2-CZ	-2.35	117.05	119.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	A	2
1	B	1
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1010:DC	O3'	1011:DG	P	3.61
1	A	608:ARG	C	609:GLU	N	1.12
1	A	623:GLY	C	624:GLY	N	0.90
1	C	2010:DG	O3'	2011:DG	P	0.66

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	18/18 (100%)	0.20	2 (11%) 10 9	7, 16, 28, 32	18 (100%)
2	C	18/18 (100%)	0.30	2 (11%) 10 9	7, 15, 29, 33	18 (100%)
3	A	544/575 (94%)	0.51	69 (12%) 8 6	5, 37, 103, 119	0
All	All	580/611 (94%)	0.49	73 (12%) 8 6	5, 36, 103, 119	36 (6%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	654	MET	8.4
3	A	416	GLY	8.2
3	A	665	LYS	8.0
3	A	415	ALA	6.4
3	A	628	PHE	5.9
3	A	627	ASP	5.6
3	A	597	GLY	5.0
3	A	625	GLU	5.0
3	A	547	ILE	4.8
3	A	655	ALA	4.8
3	A	592	LYS	4.6
3	A	548	ASN	4.6
3	A	419	THR	4.3
3	A	397	ASN	4.2
3	A	658	ASN	4.1
3	A	591	LEU	4.1
3	A	598	THR	4.0
3	A	482	ARG	4.0
3	A	656	ALA	3.9
3	A	672	ASP	3.9
3	A	668	TYR	3.8
3	A	666	TYR	3.7
2	C	2001	DT	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	A	667	LEU	3.6
3	A	180	ARG	3.6
3	A	481	PRO	3.5
1	B	1002	DC	3.4
3	A	596	PRO	3.3
3	A	417	THR	3.3
3	A	622	ASN	3.3
3	A	203	TYR	3.2
3	A	619	ARG	3.2
3	A	421	GLU	3.1
3	A	661	GLU	3.1
3	A	398	GLY	3.1
3	A	663	PRO	3.1
3	A	660	PRO	3.1
3	A	199	LEU	2.9
3	A	682	SER	2.9
3	A	616	TRP	2.9
3	A	524	GLU	2.9
2	C	2002	DG	2.8
3	A	197	LEU	2.8
3	A	671	ILE	2.8
3	A	422	GLY	2.8
3	A	599	PHE	2.7
3	A	480	GLU	2.7
3	A	702	ILE	2.7
3	A	653	VAL	2.7
3	A	424	LEU	2.6
3	A	652	LYS	2.6
3	A	393	GLU	2.6
1	B	1001	DA	2.6
3	A	182	HIS	2.6
3	A	710	SER	2.5
3	A	176	THR	2.5
3	A	423	PRO	2.4
3	A	414	ASN	2.4
3	A	617	VAL	2.3
3	A	629	HIS	2.3
3	A	420	ASN	2.3
3	A	594	GLN	2.3
3	A	418	ARG	2.3
3	A	623	GLY	2.3
3	A	479	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	136	LEU	2.2
3	A	290	GLU	2.2
3	A	590	LEU	2.2
3	A	595	GLN	2.1
3	A	399	SER	2.1
3	A	349	VAL	2.1
3	A	632	GLU	2.1
3	A	549	ASP	2.1

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PTR	A	701	16/17	0.95	0.11	20,30,54,57	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.