



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:45 AM GMT

PDB ID : 2O1X  
Title : 1-deoxy-D-xylulose 5-phosphate synthase (DXS) from *Deinococcus radiodurans*  
Authors : Xiang, S.; Usunow, G.; Lange, G.; Busch, M.; Tong, L.  
Deposited on : 2006-11-29  
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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

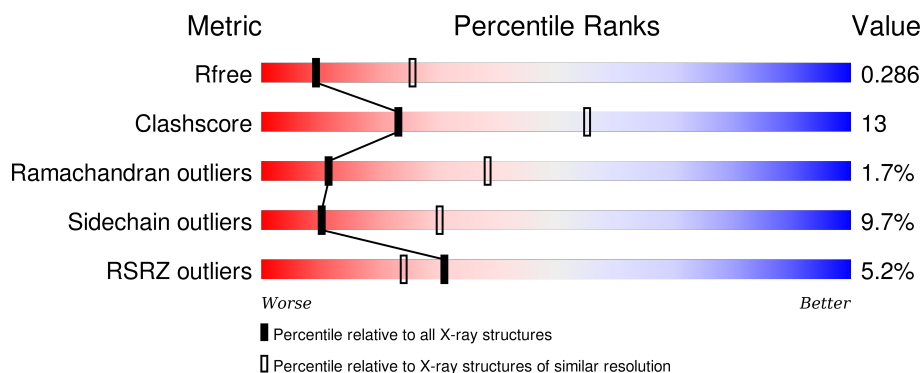
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	629	<div> <div>8%</div> <div>65% 23% 8%</div> </div>
1	B	629	<div> <div>8%</div> <div>64% 22% 5% 8%</div> </div>
1	C	629	<div> <div>8%</div> <div>58% 23% 14%</div> </div>
1	D	629	<div> <div>8%</div> <div>58% 24% 16%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	2001	-	-	-	X
2	MG	B	2002	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16910 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 1-deoxy-D-xylulose-5-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4362	2753	771	821	17			
1	B	579	Total	C	N	O	S	0	0	0
			4376	2761	775	823	17			
1	C	538	Total	C	N	O	S	0	0	0
			4063	2558	724	766	15			
1	D	530	Total	C	N	O	S	0	0	0
			4001	2521	715	750	15			

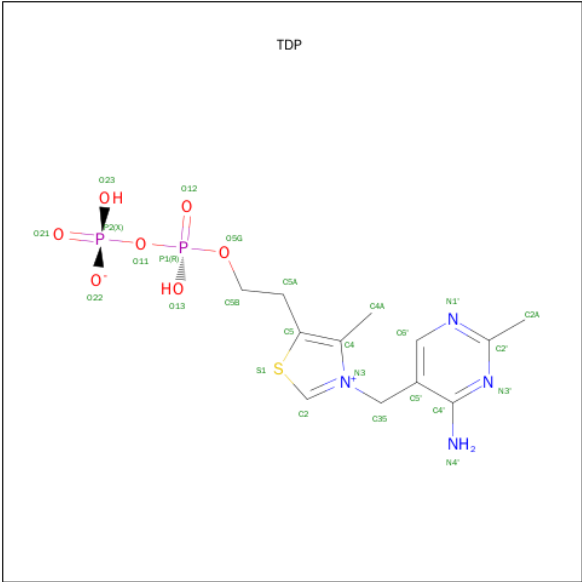
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	THR	ALA	ENGINEERED	UNP Q9RUB5
B	130	THR	ALA	ENGINEERED	UNP Q9RUB5
C	130	THR	ALA	ENGINEERED	UNP Q9RUB5
D	130	THR	ALA	ENGINEERED	UNP Q9RUB5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

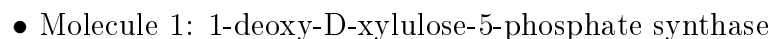
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

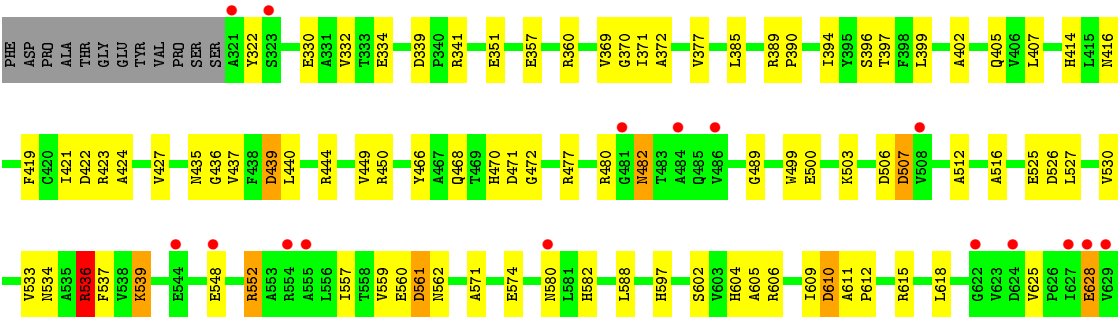
- Molecule 3 is THIAMIN DIPHOSPHATE (three-letter code: TDP) (formula: C<sub>12</sub>H<sub>18</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.26Å 154.06Å 124.88Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.25 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-2.90) 97.4 (29.25-2.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.44 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.209 , 0.272 0.242 , 0.286	Depositor DCC
$R_{free}$ test set	3206 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.7	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 33.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 62969 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	16910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.83% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.53	0/4452	0.85	19/6049 (0.3%)
1	B	0.53	0/4465	0.87	16/6066 (0.3%)
1	C	0.43	0/4139	0.80	18/5621 (0.3%)
1	D	0.83	6/4076 (0.1%)	0.80	15/5534 (0.3%)
All	All	0.60	6/17132 (0.0%)	0.83	68/23270 (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	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	36	GLU	CD-OE2	28.08	1.56	1.25
1	D	628	GLU	CD-OE1	23.04	1.50	1.25
1	D	628	GLU	CD-OE2	18.05	1.45	1.25
1	D	36	GLU	CD-OE1	16.34	1.43	1.25
1	D	28	GLU	CD-OE2	9.40	1.35	1.25
1	D	28	GLU	CD-OE1	7.49	1.33	1.25

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	ASP	CB-CG-OD2	7.46	125.02	118.30
1	D	561	ASP	CB-CG-OD2	7.41	124.97	118.30
1	B	310	ASP	CB-CG-OD2	7.27	124.84	118.30
1	A	154	ASP	CB-CG-OD2	7.21	124.79	118.30
1	C	422	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	182	ASP	CB-CG-OD2	7.19	124.77	118.30
1	A	439	ASP	CB-CG-OD2	6.92	124.52	118.30
1	C	518	ASP	CB-CG-OD2	6.81	124.43	118.30
1	D	422	ASP	CB-CG-OD2	6.81	124.43	118.30
1	B	422	ASP	CB-CG-OD2	6.64	124.28	118.30
1	B	154	ASP	CB-CG-OD2	6.53	124.18	118.30
1	B	278	ASP	CB-CG-OD2	6.49	124.14	118.30
1	B	561	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	493	ASP	CB-CG-OD2	6.25	123.92	118.30
1	D	182	ASP	CB-CG-OD2	6.22	123.90	118.30
1	C	409	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	21	ASP	CB-CG-OD2	6.08	123.77	118.30
1	B	540	PRO	N-CD-CG	-6.07	94.09	103.20
1	A	276	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	145	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	278	ASP	CB-CG-OD2	6.07	123.76	118.30
1	D	339	ASP	CB-CG-OD2	5.97	123.68	118.30
1	A	278	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	79	ASP	CB-CG-OD2	5.95	123.66	118.30
1	C	404	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	339	ASP	CB-CG-OD2	5.90	123.61	118.30
1	D	154	ASP	CB-CG-OD2	5.87	123.59	118.30
1	A	624	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	9	ASP	CB-CG-OD2	5.75	123.48	118.30
1	A	140	ASP	CB-CG-OD2	5.72	123.45	118.30
1	C	507	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	145	ASP	CB-CG-OD2	5.72	123.44	118.30
1	C	506	ASP	CB-CG-OD2	5.71	123.44	118.30
1	D	60	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	422	ASP	CB-CG-OD2	5.61	123.35	118.30
1	D	36	GLU	CG-CD-OE2	-5.61	107.08	118.30
1	D	276	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	99	ASP	CB-CG-OD2	5.58	123.33	118.30
1	B	21	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	506	ASP	CB-CG-OD2	5.54	123.28	118.30
1	C	74	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	561	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	95	ASP	CB-CG-OD2	5.45	123.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	561	ASP	CB-CG-OD2	5.45	123.21	118.30
1	C	339	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	70	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	592	ASP	CB-CG-OD2	5.38	123.15	118.30
1	C	624	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	21	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	339	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	260	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	526	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	610	ASP	CB-CG-OD2	5.27	123.05	118.30
1	D	36	GLU	OE1-CD-OE2	5.26	129.62	123.30
1	C	171	ASP	CB-CG-OD2	5.23	123.00	118.30
1	C	9	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	518	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	456	ASP	CB-CG-OD2	5.18	122.97	118.30
1	C	276	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	70	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	276	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	506	ASP	CB-CG-OD2	5.11	122.90	118.30
1	D	507	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	70	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	526	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	74	ASP	CB-CG-OD2	5.05	122.85	118.30
1	D	99	ASP	CB-CG-OD2	5.05	122.85	118.30
1	D	506	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	VAL	Peptide
1	B	539	LYS	Peptide
1	C	438	PHE	Peptide

## 5.2 Too-close contacts ⓘ

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	4362	0	4337	101	0
1	B	4376	0	4352	140	0
1	C	4063	0	4054	115	0
1	D	4001	0	3997	106	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	26	0	16	2	0
3	B	26	0	16	4	0
3	C	26	0	16	1	0
3	D	26	0	16	2	0
All	All	16910	0	16804	451	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (451) 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:C:1003:TDP:H2	3:C:1003:TDP:C2	0.97	1.49
3:B:1002:TDP:H2	3:B:1002:TDP:C2	0.97	1.47
3:D:1004:TDP:H2	3:D:1004:TDP:C2	0.97	1.47
3:A:1001:TDP:H2	3:A:1001:TDP:C2	0.97	1.46
1:D:439:ASP:OD2	1:D:477:ARG:HD2	1.47	1.11
1:C:75:ARG:HH11	1:C:75:ARG:HG3	0.93	1.09
1:B:440:LEU:HD21	1:B:477:ARG:HD3	1.34	1.08
1:B:365:ARG:HG3	1:B:365:ARG:HH11	1.19	1.02
1:C:423:ARG:HD2	1:C:480:ARG:HG3	1.44	0.99
1:C:552:ARG:HG3	1:C:552:ARG:HH11	1.24	0.99
1:B:486:VAL:HG12	1:B:487:PRO:HD2	1.45	0.97
1:C:402:ALA:HA	1:C:405:GLN:NE2	1.78	0.97
1:D:552:ARG:HH11	1:D:552:ARG:HG2	1.30	0.96
1:C:75:ARG:NH1	1:C:75:ARG:HG3	1.73	0.95
1:B:198:MET:HG2	1:B:198:MET:O	1.66	0.95
1:B:139:ARG:HD3	1:B:145:ASP:HA	1.47	0.94
1:C:486:VAL:HG12	1:C:487:PRO:HD2	1.49	0.94
1:A:110:THR:HG22	1:A:120:ILE:O	1.68	0.93
1:C:250:ALA:H	1:D:247:PRO:HG2	1.30	0.93
1:B:71:SER:OG	1:B:117:HIS:HD2	1.50	0.92
1:A:187:ILE:HD12	1:A:349:MET:HE1	1.55	0.88
1:A:61:ILE:CD1	1:A:179:VAL:HG11	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:THR:HG22	1:C:38:ARG:HH12	1.41	0.84
1:A:138:ALA:O	1:A:142:GLN:HG3	1.79	0.83
1:B:21:ASP:HA	1:B:24:ARG:NH1	1.94	0.82
1:A:61:ILE:HD12	1:A:179:VAL:HG11	1.63	0.81
1:B:26:SER:H	1:B:29:GLN:NE2	1.80	0.80
1:C:602:SER:HB2	1:C:606:ARG:HH12	1.46	0.80
1:A:93:ARG:HA	1:A:96:GLN:HE21	1.47	0.79
1:A:427:VAL:H	1:A:435:ASN:HD22	1.29	0.79
1:D:499:TRP:HB2	1:D:534:ASN:O	1.83	0.79
1:B:38:ARG:O	1:B:42:VAL:HG23	1.83	0.78
1:A:416:ASN:HD21	1:A:471:ASP:HA	1.45	0.77
1:B:439:ASP:OD1	1:B:477:ARG:HD2	1.84	0.77
1:B:427:VAL:H	1:B:435:ASN:ND2	1.83	0.77
1:B:440:LEU:CD2	1:B:477:ARG:HD3	2.14	0.77
1:B:402:ALA:HA	1:B:405:GLN:NE2	1.99	0.77
1:B:427:VAL:H	1:B:435:ASN:HD22	1.34	0.75
1:B:402:ALA:HA	1:B:405:GLN:HE21	1.50	0.75
1:C:423:ARG:HD2	1:C:480:ARG:CG	2.17	0.75
1:A:139:ARG:HB2	1:A:146:PHE:CZ	2.21	0.75
1:A:26:SER:H	1:A:29:GLN:NE2	1.84	0.74
1:A:335:TRP:CZ3	1:A:468:GLN:HG2	2.23	0.73
1:B:611:ALA:HB3	1:B:612:PRO:HD3	1.69	0.73
1:D:440:LEU:HD21	1:D:477:ARG:HD3	1.71	0.73
1:C:552:ARG:HG3	1:C:552:ARG:NH1	1.98	0.73
1:C:75:ARG:HH11	1:C:75:ARG:CG	1.85	0.73
1:C:402:ALA:HA	1:C:405:GLN:HE22	1.52	0.72
1:B:323:SER:HA	1:B:482:ASN:HA	1.70	0.72
1:B:26:SER:H	1:B:29:GLN:HE21	1.36	0.72
1:B:139:ARG:NH1	1:B:140:ASP:OD1	2.23	0.71
1:A:485:GLN:HG3	1:A:486:VAL:H	1.54	0.71
1:C:486:VAL:CG1	1:C:487:PRO:HD2	2.20	0.70
1:D:402:ALA:HA	1:D:405:GLN:HE21	1.56	0.70
1:A:21:ASP:HA	1:A:24:ARG:HH11	1.55	0.70
1:B:498:GLU:O	1:B:536:ARG:NH1	2.24	0.70
1:B:365:ARG:HG3	1:B:365:ARG:NH1	1.93	0.70
1:A:440:LEU:HD21	1:A:477:ARG:HD3	1.72	0.69
1:B:486:VAL:HG12	1:B:487:PRO:CD	2.21	0.69
1:D:439:ASP:HB3	1:D:477:ARG:NH1	2.08	0.69
1:B:105:GLY:O	1:B:597:HIS:HE1	1.75	0.69
1:C:96:GLN:HG3	1:C:106:ILE:HD11	1.72	0.69
1:D:186:SER:OG	1:D:189:GLU:O	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:THR:CG2	1:A:120:ILE:O	2.40	0.68
1:C:437:VAL:HG22	1:C:562:ASN:HA	1.76	0.68
1:A:69:LEU:HD21	1:A:275:VAL:HG21	1.76	0.67
1:B:426:ILE:CD1	1:B:590:ILE:HG12	2.25	0.67
1:B:499:TRP:HB2	1:B:534:ASN:O	1.93	0.67
1:D:322:TYR:O	1:D:482:ASN:HB3	1.94	0.67
1:C:274:LEU:HD22	1:C:281:THR:HG21	1.77	0.66
1:C:174:ARG:HE	1:C:174:ARG:N	1.92	0.66
1:C:535:ALA:O	1:C:537:PHE:N	2.25	0.66
1:C:590:ILE:HD12	1:C:590:ILE:N	2.11	0.66
1:C:402:ALA:CA	1:C:405:GLN:NE2	2.56	0.66
1:D:31:PRO:O	1:D:34:THR:HG22	1.96	0.66
1:B:71:SER:OG	1:B:117:HIS:CD2	2.42	0.65
1:A:594:PHE:CE2	1:B:447:PRO:HG2	2.32	0.65
1:D:246:ASN:O	1:D:248:PHE:N	2.30	0.64
1:D:402:ALA:HA	1:D:405:GLN:NE2	2.12	0.64
1:A:26:SER:H	1:A:29:GLN:HE21	1.42	0.64
1:C:457:ALA:HB3	1:C:486:VAL:HG23	1.78	0.64
1:A:93:ARG:HA	1:A:96:GLN:NE2	2.12	0.64
1:A:21:ASP:HA	1:A:24:ARG:NH1	2.13	0.64
1:A:439:ASP:OD2	1:A:477:ARG:NH1	2.30	0.63
1:C:427:VAL:H	1:C:435:ASN:HD22	1.45	0.63
1:B:339:ASP:O	1:B:365:ARG:NH2	2.32	0.63
1:B:597:HIS:CD2	1:B:597:HIS:H	2.14	0.63
1:D:44:VAL:HG12	1:D:44:VAL:O	1.99	0.63
1:C:466:TYR:O	1:C:470:HIS:HD2	1.82	0.63
1:D:602:SER:HB2	1:D:606:ARG:HH12	1.64	0.62
1:D:449:VAL:O	1:D:539:LYS:HG2	1.99	0.62
1:D:503:LYS:HD3	1:D:530:VAL:O	1.99	0.62
1:C:586:ARG:HH22	1:D:580:ASN:HD21	1.46	0.62
1:D:93:ARG:NH1	1:D:114:GLU:OE2	2.32	0.62
1:A:586:ARG:NH2	1:A:620:GLU:OE1	2.33	0.62
1:D:466:TYR:O	1:D:470:HIS:HD2	1.83	0.62
1:A:611:ALA:HB3	1:A:612:PRO:HD3	1.81	0.61
1:A:394:ILE:O	1:A:421:ILE:HA	2.00	0.61
1:A:246:ASN:ND2	1:A:248:PHE:H	1.98	0.61
1:C:602:SER:HB2	1:C:606:ARG:NH1	2.16	0.61
1:D:75:ARG:HH11	1:D:75:ARG:HG2	1.66	0.60
1:D:450:ARG:HH22	1:D:472:GLY:HA3	1.65	0.60
1:A:187:ILE:HD12	1:A:349:MET:CE	2.29	0.60
1:C:611:ALA:HB3	1:C:612:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:LEU:HD12	1:B:494:LEU:O	2.01	0.60
1:A:615:ARG:HH12	1:A:626:PRO:HD2	1.66	0.60
1:B:194:MET:O	1:B:196:LYS:N	2.34	0.60
1:A:485:GLN:HG3	1:A:486:VAL:N	2.16	0.60
1:B:563:THR:HG23	1:B:565:VAL:H	1.67	0.59
1:C:427:VAL:H	1:C:435:ASN:ND2	2.00	0.59
1:A:27:ARG:NH2	1:A:272:GLU:OE1	2.35	0.59
1:D:444:ARG:HH22	1:D:574:GLU:CD	2.06	0.59
1:D:423:ARG:HD2	1:D:480:ARG:HB2	1.83	0.59
1:C:172:MET:HB2	1:C:174:ARG:CZ	2.32	0.59
1:D:611:ALA:HB3	1:D:612:PRO:CD	2.33	0.59
1:B:322:TYR:O	1:B:323:SER:HB3	2.01	0.58
1:A:335:TRP:CZ3	1:A:468:GLN:CG	2.86	0.58
1:B:322:TYR:O	1:B:323:SER:CB	2.52	0.58
1:B:502:LEU:HD22	1:B:534:ASN:HB2	1.85	0.58
1:B:548:GLU:HG2	1:B:552:ARG:NH1	2.18	0.58
1:A:105:GLY:O	1:A:597:HIS:HE1	1.85	0.58
1:D:552:ARG:HG2	1:D:552:ARG:NH1	2.07	0.58
1:B:170:GLY:HA3	1:B:251:MET:O	2.03	0.58
1:D:512:ALA:HB2	1:D:559:VAL:HB	1.84	0.58
1:B:426:ILE:HG12	1:B:603:VAL:HG11	1.86	0.58
1:B:554:ARG:NH2	1:B:621:LEU:O	2.36	0.58
1:C:605:ALA:HA	1:C:610:ASP:HB2	1.86	0.58
1:C:106:ILE:HG23	1:C:114:GLU:OE2	2.03	0.58
1:C:440:LEU:O	1:C:444:ARG:HB2	2.04	0.58
1:C:45:CYS:SG	1:C:52:LEU:HA	2.44	0.58
1:C:55:SER:HB3	1:C:85:TYR:HB2	1.84	0.58
1:B:335:TRP:HD1	1:B:342:THR:HG1	1.52	0.57
1:C:432:ALA:HB1	1:C:594:PHE:HB3	1.86	0.57
1:B:563:THR:CG2	1:B:565:VAL:H	2.17	0.57
1:D:560:GLU:OE2	1:D:562:ASN:HB3	2.04	0.57
1:B:506:ASP:O	1:B:507:ASP:CB	2.53	0.57
1:B:486:VAL:CG1	1:B:487:PRO:HD2	2.27	0.57
1:C:426:ILE:HD11	1:C:590:ILE:HG12	1.88	0.56
1:D:396:SER:HB3	1:D:436:GLY:HA3	1.87	0.56
1:D:61:ILE:HD13	1:D:285:ILE:HD13	1.87	0.56
1:B:365:ARG:CG	1:B:365:ARG:NH1	2.67	0.56
1:D:394:ILE:O	1:D:421:ILE:HA	2.05	0.56
1:B:350:ARG:HD2	1:B:359:SER:OG	2.05	0.56
1:A:94:ARG:HH11	1:A:94:ARG:CG	2.18	0.56
1:A:322:TYR:O	1:A:482:ASN:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:PRO:HA	1:C:284:HIS:HB3	1.86	0.56
1:B:416:ASN:HD21	1:B:471:ASP:HA	1.71	0.56
1:D:552:ARG:CG	1:D:552:ARG:HH11	2.13	0.56
1:D:158:THR:HG21	1:D:191:VAL:HG21	1.87	0.56
1:D:75:ARG:HH11	1:D:75:ARG:CG	2.18	0.56
1:C:256:VAL:HG21	1:C:274:LEU:HD21	1.88	0.55
1:A:71:SER:OG	1:A:117:HIS:HD2	1.89	0.55
1:C:328:PHE:O	1:C:331:ALA:N	2.38	0.55
1:D:548:GLU:HG2	1:D:552:ARG:HH12	1.72	0.55
1:C:439:ASP:OD1	1:C:477:ARG:HD2	2.07	0.55
1:D:527:LEU:HD11	1:D:625:VAL:HG22	1.88	0.55
1:C:424:ALA:HB1	1:C:477:ARG:NE	2.22	0.55
1:B:590:ILE:N	1:B:590:ILE:HD12	2.20	0.55
1:B:26:SER:N	1:B:29:GLN:HE21	2.02	0.55
1:D:588:LEU:HB3	1:D:609:ILE:HG22	1.89	0.55
1:C:590:ILE:HD12	1:C:590:ILE:H	1.70	0.55
1:B:477:ARG:NH2	1:B:561:ASP:O	2.39	0.54
1:B:439:ASP:CG	1:B:477:ARG:HH11	2.10	0.54
1:B:21:ASP:OD1	1:B:24:ARG:NH1	2.37	0.54
1:B:140:ASP:OD2	1:B:174:ARG:HD2	2.08	0.54
1:B:197:PHE:O	1:B:198:MET:HB3	2.07	0.54
1:A:416:ASN:ND2	1:A:471:ASP:HA	2.21	0.54
1:A:27:ARG:HH22	1:A:272:GLU:CD	2.11	0.54
1:A:440:LEU:CD2	1:A:477:ARG:HD3	2.38	0.53
1:D:414:HIS:CE1	1:D:450:ARG:NH2	2.77	0.53
1:C:437:VAL:HG22	1:C:562:ASN:CA	2.39	0.53
1:A:506:ASP:O	1:A:507:ASP:HB2	2.08	0.53
1:A:450:ARG:HH22	1:A:472:GLY:HA3	1.73	0.53
1:D:377:VAL:HG22	1:D:419:PHE:HE2	1.74	0.53
1:D:516:ALA:HB1	1:D:559:VAL:HG12	1.90	0.53
1:C:440:LEU:HD12	1:C:562:ASN:HB2	1.91	0.53
1:A:193:ALA:HB3	1:B:167:ASN:OD1	2.08	0.53
1:C:177:LEU:HD21	1:C:271:LEU:HD22	1.90	0.53
1:C:77:LEU:HD22	1:C:132:ALA:HB2	1.91	0.53
1:A:250:ALA:HB3	1:B:196:LYS:HG2	1.89	0.52
1:D:439:ASP:HB3	1:D:477:ARG:HH11	1.73	0.52
1:C:440:LEU:HD22	1:C:538:VAL:HG21	1.91	0.52
1:C:31:PRO:O	1:C:34:THR:HB	2.09	0.52
1:D:499:TRP:CD1	1:D:533:VAL:CG1	2.92	0.52
1:D:424:ALA:HB1	1:D:477:ARG:CZ	2.39	0.52
1:C:133:LEU:HD13	1:C:174:ARG:HH22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ASN:ND2	1:A:185:MET:H	2.06	0.52
1:C:457:ALA:HB3	1:C:486:VAL:CG2	2.40	0.52
1:D:246:ASN:C	1:D:248:PHE:H	2.13	0.52
1:D:499:TRP:CD1	1:D:533:VAL:HG11	2.44	0.52
1:B:506:ASP:O	1:B:507:ASP:HB3	2.09	0.52
1:A:506:ASP:O	1:A:507:ASP:CB	2.57	0.52
1:D:53:ALA:HB1	1:D:289:LYS:HG2	1.92	0.52
1:C:536:ARG:HD3	1:C:537:PHE:CE1	2.45	0.52
1:D:394:ILE:HG21	1:D:399:LEU:HD13	1.90	0.52
1:B:465:LYS:HE2	1:B:493:ASP:OD2	2.09	0.52
1:B:394:ILE:O	1:B:421:ILE:HA	2.10	0.51
1:B:194:MET:HB2	1:B:198:MET:HB3	1.92	0.51
1:A:427:VAL:H	1:A:435:ASN:ND2	2.05	0.51
1:C:274:LEU:HD23	1:C:277:LEU:HD12	1.93	0.51
1:B:457:ALA:HB3	1:B:486:VAL:HG23	1.92	0.51
1:D:246:ASN:C	1:D:248:PHE:N	2.64	0.51
1:D:500:GLU:CD	1:D:536:ARG:HH21	2.13	0.51
1:D:526:ASP:HB2	1:D:615:ARG:HH22	1.74	0.51
1:A:341:ARG:HD2	1:A:387:GLY:O	2.09	0.51
1:D:88:LYS:HD2	1:D:106:ILE:HD11	1.93	0.51
1:C:335:TRP:CZ3	1:C:465:LYS:HG3	2.45	0.51
1:B:192:GLY:O	1:B:193:ALA:HB3	2.10	0.51
1:D:557:ILE:HG23	1:D:588:LEU:HD23	1.92	0.51
1:A:402:ALA:HA	1:A:405:GLN:NE2	2.25	0.51
1:C:402:ALA:CA	1:C:405:GLN:HE21	2.23	0.51
1:B:154:ASP:HB2	1:B:197:PHE:CZ	2.46	0.51
1:C:627:ILE:O	1:C:628:GLU:HG2	2.11	0.50
1:A:395:TYR:CE2	1:A:423:ARG:HG2	2.46	0.50
1:A:405:GLN:NE2	1:A:405:GLN:H	2.09	0.50
1:D:444:ARG:NH2	1:D:571:ALA:HA	2.27	0.50
1:B:21:ASP:HA	1:B:24:ARG:HH12	1.74	0.50
1:C:416:ASN:ND2	1:C:472:GLY:H	2.10	0.50
1:D:105:GLY:O	1:D:597:HIS:HE1	1.94	0.50
1:A:50:LEU:O	1:A:305:GLY:HA2	2.11	0.50
1:C:351:GLU:HA	1:C:356:VAL:HG23	1.94	0.50
1:C:432:ALA:CB	1:C:594:PHE:HB3	2.41	0.50
1:C:75:ARG:NH1	1:C:75:ARG:CG	2.56	0.50
1:C:399:LEU:HD22	1:C:421:ILE:HD13	1.93	0.50
1:A:250:ALA:CB	1:B:196:LYS:HG2	2.42	0.49
1:B:426:ILE:HD12	1:B:437:VAL:HG21	1.94	0.49
1:D:615:ARG:HA	1:D:618:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:THR:CG2	1:B:469:THR:O	2.60	0.49
1:C:140:ASP:OD2	1:C:174:ARG:HG2	2.12	0.49
1:D:183:ASN:ND2	3:D:1004:TDP:O21	2.42	0.49
1:C:93:ARG:HB3	1:C:106:ILE:HD11	1.94	0.49
1:B:263:ASN:C	1:B:263:ASN:HD22	2.14	0.49
1:C:525:GLU:HB2	1:C:615:ARG:HH21	1.77	0.49
1:B:402:ALA:CA	1:B:405:GLN:HE21	2.21	0.49
1:C:440:LEU:HD21	1:C:477:ARG:HD3	1.95	0.49
1:B:499:TRP:CD1	1:B:545:MET:SD	3.05	0.49
1:B:295:TYR:CD2	1:B:314:GLY:HA3	2.47	0.49
1:B:440:LEU:O	1:B:444:ARG:HB2	2.12	0.49
1:C:440:LEU:HD12	1:C:562:ASN:CB	2.42	0.49
1:A:395:TYR:CD2	1:A:423:ARG:HG2	2.47	0.49
1:B:53:ALA:HB1	1:B:289:LYS:HD3	1.94	0.49
1:A:289:LYS:HE3	3:A:1001:TDP:O21	2.12	0.49
1:C:590:ILE:H	1:C:590:ILE:CD1	2.25	0.49
1:D:37:LEU:O	1:D:41:ILE:HD12	2.11	0.49
1:B:561:ASP:OD2	1:B:604:HIS:HE1	1.96	0.49
1:D:611:ALA:HB3	1:D:612:PRO:HD2	1.94	0.49
1:B:469:THR:O	1:B:469:THR:HG22	2.12	0.49
1:A:263:ASN:HD21	1:A:265:GLN:HB2	1.77	0.49
1:B:444:ARG:NH1	1:B:566:GLY:O	2.45	0.48
1:D:133:LEU:O	1:D:137:LEU:HB2	2.13	0.48
1:B:149:ALA:HA	1:B:177:LEU:O	2.13	0.48
1:B:51:HIS:HA	1:B:304:HIS:O	2.13	0.48
1:D:183:ASN:HD22	1:D:289:LYS:HB2	1.78	0.48
1:B:154:ASP:O	1:B:195:ASN:ND2	2.47	0.48
1:C:499:TRP:CD1	1:C:535:ALA:O	2.66	0.48
1:C:407:LEU:O	1:C:411:ALA:HB3	2.13	0.48
1:D:42:VAL:HA	1:D:52:LEU:HD21	1.95	0.48
1:B:501:ARG:NH2	1:B:505:GLY:O	2.46	0.48
1:D:416:ASN:HD21	1:D:471:ASP:HA	1.78	0.48
1:C:186:SER:O	1:C:187:ILE:C	2.51	0.48
1:C:486:VAL:HG11	1:C:490:THR:HG21	1.96	0.48
1:C:426:ILE:HG12	1:C:603:VAL:HG11	1.94	0.48
1:C:28:GLU:CD	1:C:28:GLU:H	2.16	0.48
1:A:149:ALA:HA	1:A:177:LEU:O	2.14	0.48
1:D:605:ALA:HA	1:D:610:ASP:HB2	1.96	0.48
1:A:175:LYS:O	1:A:176:MET:HG3	2.14	0.48
1:A:407:LEU:O	1:A:411:ALA:HB3	2.14	0.48
1:A:263:ASN:C	1:A:263:ASN:HD22	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ALA:O	1:A:142:GLN:CG	2.59	0.47
1:C:69:LEU:HD22	1:C:74:ASP:OD2	2.14	0.47
1:A:449:VAL:O	1:A:539:LYS:HG2	2.14	0.47
1:B:183:ASN:ND2	3:B:1002:TDP:O22	2.48	0.47
1:B:193:ALA:O	1:B:194:MET:C	2.53	0.47
1:D:499:TRP:HZ3	1:D:537:PHE:O	1.98	0.47
1:D:477:ARG:NH2	1:D:561:ASP:O	2.47	0.47
1:A:373:GLU:HG2	1:A:398:PHE:O	2.14	0.47
1:B:69:LEU:HD21	1:B:275:VAL:HG21	1.97	0.47
1:B:579:MET:HE3	1:B:581:LEU:HD12	1.97	0.47
1:B:499:TRP:HD1	1:B:545:MET:SD	2.37	0.47
1:D:110:THR:HG22	1:D:120:ILE:O	2.15	0.47
1:D:80:VAL:HG22	1:D:125:ALA:HA	1.97	0.47
1:D:253:VAL:HG13	1:D:280:PRO:HB2	1.96	0.47
1:D:341:ARG:NE	1:D:389:ARG:HE	2.12	0.47
1:B:439:ASP:CB	1:B:477:ARG:HH11	2.28	0.47
1:B:195:ASN:O	1:B:196:LYS:HG3	2.14	0.47
1:A:61:ILE:HD12	1:A:285:ILE:HD13	1.96	0.47
1:A:26:SER:N	1:A:29:GLN:HE21	2.10	0.47
1:A:539:LYS:HA	1:A:540:PRO:HA	1.81	0.47
1:C:34:THR:CG2	1:C:38:ARG:HH12	2.20	0.47
1:C:106:ILE:HG22	1:C:107:SER:O	2.15	0.47
1:A:170:GLY:HA3	1:A:251:MET:O	2.15	0.47
1:C:270:LEU:O	1:C:274:LEU:N	2.48	0.47
1:C:612:PRO:HA	1:C:615:ARG:HB2	1.97	0.47
1:D:582:HIS:N	1:D:582:HIS:ND1	2.62	0.47
1:D:341:ARG:HE	1:D:389:ARG:HE	1.63	0.46
1:C:386:GLN:HG2	1:D:135:MET:HG3	1.97	0.46
1:D:561:ASP:OD2	1:D:604:HIS:HE1	1.97	0.46
1:D:44:VAL:CG1	1:D:44:VAL:O	2.63	0.46
1:D:75:ARG:CG	1:D:75:ARG:NH1	2.78	0.46
1:C:123:GLY:HA3	1:C:433:THR:OG1	2.15	0.46
1:B:50:LEU:HD23	1:B:101:LYS:HD3	1.98	0.46
1:A:427:VAL:HG21	1:A:434:HIS:HB3	1.97	0.46
1:A:130:THR:HG21	1:A:161:MET:HE2	1.98	0.46
1:D:552:ARG:CG	1:D:552:ARG:NH1	2.77	0.46
1:D:444:ARG:NE	1:D:571:ALA:HB2	2.30	0.46
1:A:291:LYS:HA	1:A:297:GLU:OE2	2.15	0.46
1:A:601:GLU:CD	1:A:601:GLU:H	2.19	0.46
1:C:395:TYR:HB2	1:C:398:PHE:CD2	2.51	0.46
3:B:1002:TDP:H2	3:B:1002:TDP:H4'2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:GLY:O	1:B:597:HIS:CE1	2.63	0.46
1:B:341:ARG:HD2	1:B:387:GLY:O	2.15	0.46
1:B:93:ARG:O	1:B:96:GLN:HG2	2.16	0.46
1:D:466:TYR:O	1:D:470:HIS:CD2	2.68	0.46
1:B:188:SER:HB3	1:B:351:GLU:OE1	2.16	0.46
1:A:498:GLU:O	1:A:536:ARG:NH1	2.35	0.46
1:B:20:LYS:HE2	1:B:20:LYS:HB2	1.77	0.46
1:B:486:VAL:HG11	1:B:490:THR:HG21	1.97	0.46
1:B:196:LYS:HD3	1:B:247:PRO:O	2.15	0.46
1:B:437:VAL:O	1:B:437:VAL:HG13	2.15	0.46
1:B:26:SER:N	1:B:29:GLN:NE2	2.58	0.45
1:D:189:GLU:HB3	1:D:190:ASN:H	1.50	0.45
1:B:449:VAL:O	1:B:539:LYS:HD3	2.16	0.45
1:D:147:HIS:ND1	1:D:275:VAL:O	2.50	0.45
1:C:511:LEU:HD23	1:C:511:LEU:N	2.31	0.45
1:A:594:PHE:CZ	1:B:447:PRO:HG2	2.51	0.45
1:B:437:VAL:O	1:B:437:VAL:CG1	2.63	0.45
1:D:173:GLY:HA2	1:D:280:PRO:HD3	1.99	0.45
1:B:590:ILE:HA	1:B:591:PRO:HD2	1.81	0.45
1:C:133:LEU:CD1	1:C:174:ARG:HH12	2.28	0.45
1:C:398:PHE:O	1:C:401:ARG:HB2	2.15	0.45
1:B:378:THR:HG23	1:B:409:ASP:HB3	1.98	0.45
1:B:124:HIS:NE2	1:B:397:THR:HB	2.32	0.45
1:C:438:PHE:CD2	1:D:407:LEU:HD11	2.51	0.45
1:B:324:TRP:HB3	1:B:478:TYR:CD1	2.51	0.45
1:A:291:LYS:HD2	1:A:297:GLU:OE2	2.16	0.45
1:A:46:SER:HA	1:A:309:PHE:CE2	2.51	0.45
1:D:477:ARG:HG3	1:D:477:ARG:O	2.15	0.45
1:C:439:ASP:HB3	1:C:440:LEU:H	1.48	0.45
1:B:120:ILE:HG13	1:B:122:VAL:HG13	1.99	0.45
1:B:194:MET:HB2	1:B:197:PHE:O	2.17	0.45
1:B:45:CYS:HA	1:B:50:LEU:HD12	1.99	0.45
1:C:257:GLY:HA2	1:C:259:VAL:HG22	1.99	0.45
1:C:450:ARG:HH22	1:C:472:GLY:HA3	1.82	0.45
1:A:358:PHE:C	1:A:358:PHE:CD2	2.90	0.44
1:B:358:PHE:C	1:B:358:PHE:CD2	2.91	0.44
1:A:80:VAL:HG22	1:A:125:ALA:HA	1.98	0.44
1:C:246:ASN:ND2	1:C:248:PHE:H	2.15	0.44
1:C:539:LYS:HA	1:C:540:PRO:HA	1.81	0.44
1:C:394:ILE:O	1:C:421:ILE:HA	2.18	0.44
1:D:341:ARG:HE	1:D:389:ARG:HH21	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:GLY:CA	1:B:131:ASN:HD22	2.29	0.44
1:B:190:ASN:ND2	1:B:191:VAL:H	2.15	0.44
1:D:110:THR:O	1:D:121:THR:HA	2.18	0.44
1:D:468:GLN:HA	1:D:468:GLN:OE1	2.16	0.44
1:B:486:VAL:CG1	1:B:487:PRO:CD	2.91	0.44
1:B:16:ILE:HA	1:B:21:ASP:CB	2.48	0.44
1:A:427:VAL:N	1:A:435:ASN:HD22	2.06	0.44
1:B:426:ILE:HD12	1:B:437:VAL:CG2	2.48	0.44
1:A:502:LEU:HA	1:A:502:LEU:HD12	1.77	0.44
1:B:60:ASP:OD2	1:B:262:HIS:HA	2.18	0.44
1:D:68:VAL:HG21	1:D:271:LEU:HB2	1.99	0.44
1:D:427:VAL:H	1:D:435:ASN:ND2	2.15	0.43
1:C:369:VAL:HG21	1:C:376:ALA:HB2	1.99	0.43
1:B:424:ALA:HB1	1:B:477:ARG:CZ	2.48	0.43
1:A:250:ALA:HB1	1:B:196:LYS:HA	2.00	0.43
1:C:590:ILE:HA	1:C:591:PRO:HD2	1.83	0.43
1:C:173:GLY:C	1:C:174:ARG:HE	2.20	0.43
1:C:99:ASP:HA	1:C:102:LYS:HD2	2.01	0.43
1:C:408:HIS:HA	1:C:412:ILE:HD12	2.00	0.43
1:A:192:GLY:HA2	1:A:195:ASN:HB3	2.01	0.43
1:A:394:ILE:HD13	1:A:399:LEU:HA	2.00	0.43
1:B:147:HIS:NE2	1:B:275:VAL:HG13	2.34	0.43
1:B:391:VAL:HG22	1:B:418:THR:HB	2.00	0.43
1:B:53:ALA:CB	1:B:289:LYS:HD3	2.49	0.43
1:A:439:ASP:OD1	1:A:477:ARG:HD2	2.17	0.43
1:A:536:ARG:HG2	1:A:537:PHE:CD1	2.54	0.43
1:D:246:ASN:O	1:D:247:PRO:C	2.56	0.43
1:C:424:ALA:HB1	1:C:477:ARG:CZ	2.49	0.43
1:B:185:MET:HA	1:B:189:GLU:HA	2.01	0.43
1:B:34:THR:HG23	1:B:38:ARG:NH1	2.33	0.43
1:A:333:THR:O	1:A:362:HIS:HE1	2.01	0.43
1:C:152:ILE:HG13	1:C:156:SER:HB2	2.01	0.43
1:C:168:THR:HG21	1:D:369:VAL:HA	2.01	0.43
1:A:335:TRP:HD1	1:A:491:TRP:CH2	2.37	0.42
1:B:394:ILE:HG21	1:B:399:LEU:HD13	2.01	0.42
1:A:402:ALA:HA	1:A:405:GLN:HE21	1.83	0.42
1:B:590:ILE:HD12	1:B:590:ILE:H	1.83	0.42
1:C:187:ILE:HD12	1:C:188:SER:N	2.35	0.42
1:C:379:THR:HA	1:D:130:THR:O	2.19	0.42
1:B:561:ASP:OD2	1:B:604:HIS:CE1	2.72	0.42
1:C:402:ALA:C	1:C:405:GLN:NE2	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:TRP:CD1	1:A:491:TRP:CH2	3.08	0.42
1:D:423:ARG:HB3	1:D:427:VAL:CG1	2.49	0.42
1:C:424:ALA:HB2	1:C:477:ARG:HB2	2.02	0.42
1:B:21:ASP:HA	1:B:24:ARG:HH11	1.78	0.42
1:D:500:GLU:HG3	1:D:534:ASN:HB3	2.02	0.42
1:D:611:ALA:CB	1:D:612:PRO:CD	2.97	0.42
1:C:559:VAL:HA	1:C:588:LEU:O	2.19	0.42
1:D:370:GLY:O	1:D:372:ALA:N	2.47	0.42
1:A:500:GLU:OE1	1:A:500:GLU:HA	2.20	0.42
1:C:405:GLN:H	1:C:405:GLN:NE2	2.17	0.42
1:A:335:TRP:HZ3	1:A:339:ASP:OD1	2.03	0.42
1:D:44:VAL:HG11	1:D:97:MET:HB3	2.01	0.42
1:C:519:TYR:HE1	1:C:604:HIS:CD2	2.37	0.42
1:B:450:ARG:HH22	1:B:472:GLY:HA3	1.85	0.42
1:C:440:LEU:HD21	1:C:453:LEU:HD11	2.01	0.42
1:D:89:ILE:HG12	1:D:97:MET:HG3	2.02	0.42
1:B:194:MET:HB3	1:B:197:PHE:CE1	2.55	0.41
1:C:174:ARG:NE	1:C:174:ARG:N	2.64	0.41
1:C:546:LEU:HD11	1:C:572:VAL:HG13	2.02	0.41
1:A:346:THR:HA	1:A:347:PRO:HD3	1.93	0.41
1:B:195:ASN:HD22	1:B:197:PHE:HE2	1.68	0.41
1:A:45:CYS:HA	1:A:50:LEU:HD12	2.02	0.41
1:B:502:LEU:HD12	1:B:502:LEU:HA	1.80	0.41
1:D:55:SER:HB3	1:D:85:TYR:HB2	2.02	0.41
1:A:348:ALA:O	1:A:349:MET:HE3	2.20	0.41
1:A:407:LEU:HD23	1:A:407:LEU:C	2.41	0.41
1:C:421:ILE:HD11	1:C:475:ALA:HB1	2.03	0.41
1:D:390:PRO:HD2	1:D:416:ASN:O	2.20	0.41
1:D:69:LEU:HD21	1:D:275:VAL:HG11	2.02	0.41
1:C:549:VAL:O	1:C:553:ALA:HB3	2.21	0.41
1:A:154:ASP:OD1	1:A:184:GLU:HA	2.21	0.41
1:B:77:LEU:HD23	1:B:120:ILE:HD13	2.01	0.41
1:B:263:ASN:ND2	1:B:263:ASN:C	2.74	0.41
1:A:293:LEU:O	1:A:294:SER:C	2.59	0.41
1:B:289:LYS:HE3	3:B:1002:TDP:O21	2.20	0.41
1:A:615:ARG:HA	1:A:618:LEU:HD12	2.02	0.41
1:A:94:ARG:HH11	1:A:94:ARG:HG2	1.85	0.41
1:D:147:HIS:CG	1:D:275:VAL:HG13	2.56	0.41
1:B:450:ARG:NH2	1:B:472:GLY:HA3	2.35	0.41
1:D:78:PHE:HE1	1:D:87:HIS:ND1	2.19	0.41
1:A:455:LYS:HG2	1:A:459:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:VAL:O	1:D:437:VAL:HG12	2.21	0.41
1:A:403:TYR:HH	1:B:442:PHE:HD2	1.66	0.41
1:C:263:ASN:OD1	1:C:266:GLU:HB2	2.21	0.41
1:A:99:ASP:O	1:A:102:LYS:HB2	2.21	0.41
1:B:16:ILE:HA	1:B:21:ASP:HB3	2.02	0.41
1:A:442:PHE:HD2	1:B:403:TYR:HH	1.66	0.41
1:C:188:SER:OG	1:C:350:ARG:NH1	2.50	0.40
1:C:388:MET:HG2	1:D:138:ALA:HB1	2.03	0.40
1:B:426:ILE:HD11	1:B:590:ILE:HG12	2.02	0.40
1:A:324:TRP:CH2	1:A:456:ASP:HA	2.56	0.40
1:B:93:ARG:NH1	1:B:114:GLU:OE2	2.46	0.40
1:B:299:ASP:O	1:B:303:TRP:HD1	2.05	0.40
1:C:181:ASN:HD22	1:C:181:ASN:C	2.25	0.40
1:B:307:ALA:O	1:B:317:VAL:HB	2.22	0.40
1:B:602:SER:HB2	1:B:606:ARG:NH1	2.35	0.40
1:C:552:ARG:CG	1:C:552:ARG:NH1	2.74	0.40
1:D:334:GLU:OE1	1:D:489:GLY:N	2.55	0.40
1:D:166:LEU:HA	1:D:169:ILE:HB	2.03	0.40
1:D:26:SER:H	1:D:29:GLN:HE21	1.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	574/629 (91%)	536 (93%)	34 (6%)	4 (1%)	26	63
1	B	575/629 (91%)	531 (92%)	32 (6%)	12 (2%)	9	32
1	C	532/629 (85%)	473 (89%)	48 (9%)	11 (2%)	9	32
1	D	524/629 (83%)	470 (90%)	44 (8%)	10 (2%)	10	35
All	All	2205/2516 (88%)	2010 (91%)	158 (7%)	37 (2%)	11	38



All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	507	ASP
1	B	194	MET
1	B	195	ASN
1	B	244	SER
1	B	439	ASP
1	B	540	PRO
1	C	439	ASP
1	D	247	PRO
1	D	439	ASP
1	D	536	ARG
1	D	628	GLU
1	A	49	GLY
1	B	507	ASP
1	C	187	ILE
1	C	322	TYR
1	B	323	SER
1	C	175	LYS
1	C	506	ASP
1	D	189	GLU
1	D	371	ILE
1	D	525	GLU
1	B	189	GLU
1	B	196	LYS
1	B	525	GLU
1	C	123	GLY
1	C	173	GLY
1	D	188	SER
1	A	328	PHE
1	C	51	HIS
1	C	507	ASP
1	C	580	ASN
1	B	246	ASN
1	B	123	GLY
1	D	123	GLY
1	D	187	ILE
1	A	123	GLY
1	C	258	PRO

### 5.3.2 Protein sidechains ⓘ

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	452/493 (92%)	404 (89%)	48 (11%)	8	25
1	B	453/493 (92%)	404 (89%)	49 (11%)	8	24
1	C	422/493 (86%)	380 (90%)	42 (10%)	9	28
1	D	414/493 (84%)	384 (93%)	30 (7%)	18	46
All	All	1741/1972 (88%)	1572 (90%)	169 (10%)	10	30

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	27	ARG
1	A	34	THR
1	A	37	LEU
1	A	61	ILE
1	A	73	ARG
1	A	75	ARG
1	A	94	ARG
1	A	96	GLN
1	A	107	SER
1	A	110	THR
1	A	112	VAL
1	A	122	VAL
1	A	156	SER
1	A	183	ASN
1	A	186	SER
1	A	188	SER
1	A	190	ASN
1	A	191	VAL
1	A	194	MET
1	A	198	MET
1	A	246	ASN
1	A	263	ASN
1	A	266	GLU

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Mol	Chain	Res	Type
1	A	275	VAL
1	A	289	LYS
1	A	332	VAL
1	A	335	TRP
1	A	343	PHE
1	A	351	GLU
1	A	353	SER
1	A	357	GLU
1	A	385	LEU
1	A	423	ARG
1	A	445	SER
1	A	477	ARG
1	A	482	ASN
1	A	483	THR
1	A	501	ARG
1	A	506	ASP
1	A	515	LYS
1	A	522	LYS
1	A	536	ARG
1	A	539	LYS
1	A	547	ARG
1	A	554	ARG
1	A	564	VAL
1	A	627	ILE
1	B	9	ASP
1	B	13	LEU
1	B	20	LYS
1	B	27	ARG
1	B	28	GLU
1	B	34	THR
1	B	70	ASP
1	B	73	ARG
1	B	96	GLN
1	B	115	SER
1	B	131	ASN
1	B	145	ASP
1	B	184	GLU
1	B	189	GLU
1	B	190	ASN
1	B	191	VAL
1	B	195	ASN
1	B	198	MET

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Mol	Chain	Res	Type
1	B	199	ARG
1	B	245	VAL
1	B	263	ASN
1	B	266	GLU
1	B	276	ASP
1	B	289	LYS
1	B	323	SER
1	B	332	VAL
1	B	357	GLU
1	B	365	ARG
1	B	385	LEU
1	B	426	ILE
1	B	439	ASP
1	B	450	ARG
1	B	477	ARG
1	B	495	LYS
1	B	499	TRP
1	B	501	ARG
1	B	502	LEU
1	B	503	LYS
1	B	506	ASP
1	B	515	LYS
1	B	526	ASP
1	B	536	ARG
1	B	552	ARG
1	B	562	ASN
1	B	563	THR
1	B	580	ASN
1	B	593	GLU
1	B	627	ILE
1	B	629	VAL
1	C	13	LEU
1	C	20	LYS
1	C	74	ASP
1	C	75	ARG
1	C	83	GLN
1	C	122	VAL
1	C	130	THR
1	C	131	ASN
1	C	137	LEU
1	C	168	THR
1	C	174	ARG

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Mol	Chain	Res	Type
1	C	181	ASN
1	C	185	MET
1	C	251	MET
1	C	259	VAL
1	C	263	ASN
1	C	269	TRP
1	C	332	VAL
1	C	351	GLU
1	C	357	GLU
1	C	385	LEU
1	C	397	THR
1	C	405	GLN
1	C	421	ILE
1	C	426	ILE
1	C	433	THR
1	C	434	HIS
1	C	437	VAL
1	C	439	ASP
1	C	450	ARG
1	C	494	LEU
1	C	511	LEU
1	C	515	LYS
1	C	543	GLU
1	C	552	ARG
1	C	554	ARG
1	C	565	VAL
1	C	580	ASN
1	C	581	LEU
1	C	585	VAL
1	C	610	ASP
1	C	624	ASP
1	D	17	HIS
1	D	22	LEU
1	D	28	GLU
1	D	34	THR
1	D	71	SER
1	D	75	ARG
1	D	96	GLN
1	D	113	SER
1	D	122	VAL
1	D	144	LYS
1	D	146	PHE

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Mol	Chain	Res	Type
1	D	185	MET
1	D	186	SER
1	D	190	ASN
1	D	191	VAL
1	D	259	VAL
1	D	266	GLU
1	D	273	ARG
1	D	330	GLU
1	D	332	VAL
1	D	351	GLU
1	D	357	GLU
1	D	360	ARG
1	D	385	LEU
1	D	397	THR
1	D	482	ASN
1	D	507	ASP
1	D	536	ARG
1	D	539	LYS
1	D	552	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	96	GLN
1	A	117	HIS
1	A	131	ASN
1	A	167	ASN
1	A	183	ASN
1	A	190	ASN
1	A	246	ASN
1	A	263	ASN
1	A	304	HIS
1	A	362	HIS
1	A	405	GLN
1	A	416	ASN
1	A	435	ASN
1	A	577	ASN
1	A	597	HIS
1	A	604	HIS
1	B	15	GLN
1	B	29	GLN

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Mol	Chain	Res	Type
1	B	117	HIS
1	B	131	ASN
1	B	190	ASN
1	B	195	ASN
1	B	263	ASN
1	B	304	HIS
1	B	405	GLN
1	B	416	ASN
1	B	435	ASN
1	B	470	HIS
1	B	595	GLN
1	B	597	HIS
1	B	604	HIS
1	C	29	GLN
1	C	117	HIS
1	C	131	ASN
1	C	181	ASN
1	C	246	ASN
1	C	362	HIS
1	C	405	GLN
1	C	416	ASN
1	C	435	ASN
1	C	470	HIS
1	C	580	ASN
1	C	604	HIS
1	D	29	GLN
1	D	96	GLN
1	D	131	ASN
1	D	362	HIS
1	D	400	GLN
1	D	405	GLN
1	D	416	ASN
1	D	435	ASN
1	D	470	HIS
1	D	577	ASN
1	D	580	ASN
1	D	595	GLN
1	D	597	HIS
1	D	604	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	TDP	A	1001	2	21,27,27	1.97	5 (23%)	31,40,40	1.72	8 (25%)
3	TDP	B	1002	2	21,27,27	1.88	4 (19%)	31,40,40	1.68	8 (25%)
3	TDP	C	1003	2	21,27,27	1.87	7 (33%)	31,40,40	1.82	8 (25%)
3	TDP	D	1004	2	21,27,27	1.89	6 (28%)	31,40,40	1.69	8 (25%)

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	TDP	A	1001	2	-	0/16/17/17	0/2/2/2
3	TDP	B	1002	2	-	0/16/17/17	0/2/2/2
3	TDP	C	1003	2	-	0/16/17/17	0/2/2/2
3	TDP	D	1004	2	-	0/16/17/17	0/2/2/2



All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	TDP	C4-N3	-4.18	1.36	1.39
3	A	1001	TDP	C4-N3	-3.11	1.37	1.39
3	D	1004	TDP	C4-N3	-3.06	1.37	1.39
3	C	1003	TDP	C4-N3	-2.30	1.37	1.39
3	A	1001	TDP	P2-O23	-2.07	1.46	1.55
3	C	1003	TDP	C35-C5'	2.14	1.55	1.51
3	C	1003	TDP	C4A-C4	2.15	1.54	1.49
3	D	1004	TDP	C35-C5'	2.22	1.56	1.51
3	D	1004	TDP	C4A-C4	2.25	1.54	1.49
3	C	1003	TDP	P2-O11	2.71	1.67	1.61
3	C	1003	TDP	P1-O12	2.79	1.61	1.51
3	B	1002	TDP	P1-O12	3.02	1.62	1.51
3	B	1002	TDP	P2-O21	3.14	1.60	1.50
3	D	1004	TDP	P2-O21	3.55	1.61	1.50
3	A	1001	TDP	P1-O12	3.66	1.64	1.51
3	D	1004	TDP	P1-O12	3.70	1.64	1.51
3	C	1003	TDP	P2-O22	3.84	1.63	1.50
3	C	1003	TDP	P2-O21	3.94	1.62	1.50
3	D	1004	TDP	P2-O22	4.12	1.64	1.50
3	A	1001	TDP	P2-O22	4.27	1.64	1.50
3	B	1002	TDP	P2-O22	4.61	1.65	1.50
3	A	1001	TDP	P2-O21	4.71	1.65	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	TDP	C4A-C4-C5	-4.03	119.83	128.90
3	C	1003	TDP	C4A-C4-C5	-3.61	120.78	128.90
3	D	1004	TDP	C4A-C4-C5	-3.18	121.75	128.90
3	B	1002	TDP	C4A-C4-C5	-3.13	121.86	128.90
3	B	1002	TDP	N1'-C2'-N3'	-3.09	119.88	125.60
3	A	1001	TDP	N1'-C2'-N3'	-3.00	120.05	125.60
3	D	1004	TDP	N1'-C2'-N3'	-2.90	120.24	125.60
3	C	1003	TDP	N1'-C2'-N3'	-2.74	120.53	125.60
3	A	1001	TDP	C35-C5'-C6'	-2.56	115.42	120.67
3	D	1004	TDP	O22-P2-O21	-2.52	102.63	114.72
3	B	1002	TDP	O22-P2-O21	-2.00	105.11	114.72
3	A	1001	TDP	C2A-C2'-N3'	2.02	120.64	117.20
3	C	1003	TDP	O23-P2-O11	2.08	114.23	104.65
3	B	1002	TDP	C5A-C5-C4	2.12	129.47	127.56
3	A	1001	TDP	C4A-C4-N3	2.21	125.54	122.59
3	B	1002	TDP	C5A-C5-S1	2.22	123.35	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	TDP	C5A-C5-C4	2.28	129.61	127.56
3	D	1004	TDP	C6'-N1'-C2'	2.42	120.00	115.77
3	D	1004	TDP	C5A-C5-S1	2.42	123.63	120.24
3	C	1003	TDP	C2A-C2'-N1'	2.54	120.07	117.03
3	D	1004	TDP	C5A-C5-C4	2.69	129.97	127.56
3	A	1001	TDP	C6'-N1'-C2'	2.71	120.50	115.77
3	C	1003	TDP	C5A-C5-S1	2.73	124.06	120.24
3	C	1003	TDP	C6'-N1'-C2'	2.80	120.67	115.77
3	D	1004	TDP	C5-C4-N3	3.04	114.38	107.69
3	B	1002	TDP	C6'-N1'-C2'	3.11	121.20	115.77
3	A	1001	TDP	C5-C4-N3	3.15	114.63	107.69
3	B	1002	TDP	C5-C4-N3	3.24	114.83	107.69
3	D	1004	TDP	C2A-C2'-N1'	3.39	121.10	117.03
3	C	1003	TDP	C5-C4-N3	3.55	115.50	107.69
3	B	1002	TDP	C2A-C2'-N1'	3.63	121.38	117.03
3	C	1003	TDP	C5A-C5-C4	4.15	131.28	127.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	TDP	2	0
3	B	1002	TDP	4	0
3	C	1003	TDP	1	0
3	D	1004	TDP	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	578/629 (91%)	-0.47	6 (1%) 84 82	-5, 10, 34, 53	0
1	B	579/629 (92%)	-0.48	7 (1%) 81 78	-3, 11, 39, 75	0
1	C	538/629 (85%)	0.39	49 (9%) 11 7	6, 65, 139, 191	0
1	D	530/629 (84%)	0.36	53 (10%) 9 5	7, 60, 133, 175	0
All	All	2225/2516 (88%)	-0.07	115 (5%) 31 24	-5, 24, 121, 191	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	15	GLN	6.3
1	D	46	SER	6.1
1	D	49	GLY	5.7
1	C	628	GLU	5.6
1	C	8	SER	5.6
1	C	321	ALA	5.5
1	D	45	CYS	5.4
1	C	104	GLY	4.8
1	B	244	SER	4.8
1	D	147	HIS	4.7
1	B	629	VAL	4.7
1	D	42	VAL	4.4
1	C	627	ILE	4.4
1	C	544	GLU	4.3
1	C	7	THR	4.2
1	D	48	GLY	4.2
1	C	9	ASP	4.1
1	C	251	MET	4.1
1	D	185	MET	3.9
1	B	628	GLU	3.9
1	D	247	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	627	ILE	3.7
1	C	67	TYR	3.6
1	C	145	ASP	3.5
1	C	95	ASP	3.5
1	D	245	VAL	3.5
1	C	263	ASN	3.4
1	C	508	VAL	3.4
1	C	11	PRO	3.4
1	A	320	SER	3.4
1	C	360	ARG	3.3
1	C	47	ARG	3.3
1	C	17	HIS	3.3
1	B	243	ALA	3.3
1	D	24	ARG	3.3
1	A	319	SER	3.2
1	C	46	SER	3.2
1	D	47	ARG	3.2
1	B	196	LYS	3.2
1	A	244	SER	3.1
1	C	277	LEU	3.1
1	C	269	TRP	3.1
1	D	254	ARG	3.0
1	A	245	VAL	2.9
1	C	246	ASN	2.9
1	C	528	PRO	2.9
1	D	96	GLN	2.9
1	D	555	ALA	2.9
1	C	249	ALA	2.9
1	D	628	GLU	2.8
1	D	622	GLY	2.8
1	C	257	GLY	2.8
1	D	481	GLY	2.8
1	C	555	ALA	2.8
1	D	44	VAL	2.8
1	D	554	ARG	2.8
1	D	32	ALA	2.8
1	C	322	TYR	2.7
1	C	245	VAL	2.7
1	D	191	VAL	2.7
1	D	278	ASP	2.7
1	D	508	VAL	2.6
1	C	62	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	62	ILE	2.6
1	C	175	LYS	2.6
1	C	526	ASP	2.6
1	C	52	LEU	2.6
1	D	188	SER	2.6
1	B	199	ARG	2.6
1	D	255	TYR	2.5
1	C	286	VAL	2.5
1	D	258	PRO	2.5
1	D	580	ASN	2.5
1	D	76	ILE	2.5
1	D	95	ASP	2.5
1	D	544	GLU	2.5
1	D	252	GLY	2.5
1	C	20	LYS	2.4
1	D	145	ASP	2.4
1	D	52	LEU	2.4
1	C	76	ILE	2.4
1	D	190	ASN	2.4
1	C	287	THR	2.4
1	D	73	ARG	2.3
1	C	258	PRO	2.3
1	D	28	GLU	2.3
1	C	278	ASP	2.3
1	C	185	MET	2.3
1	D	289	LYS	2.3
1	C	77	LEU	2.3
1	C	96	GLN	2.3
1	D	321	ALA	2.3
1	D	251	MET	2.3
1	C	289	LYS	2.3
1	D	548	GLU	2.3
1	D	250	ALA	2.2
1	C	255	TYR	2.2
1	D	17	HIS	2.2
1	D	484	ALA	2.2
1	C	288	THR	2.2
1	B	8	SER	2.1
1	C	184	GLU	2.1
1	D	486	VAL	2.1
1	D	629	VAL	2.1
1	C	552	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	323	SER	2.1
1	C	623	VAL	2.1
1	A	198	MET	2.0
1	A	312	ALA	2.0
1	D	104	GLY	2.0
1	D	269	TRP	2.0
1	D	624	ASP	2.0
1	D	151	VAL	2.0
1	C	79	ASP	2.0
1	D	256	VAL	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 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	2002	1/1	0.93	0.21	3.02	8,8,8,8	0
2	MG	A	2001	1/1	0.97	0.21	2.41	9,9,9,9	0
3	TDP	B	1002	26/26	0.98	0.13	-0.00	2,3,4,6	0
3	TDP	D	1004	26/26	0.92	0.16	-0.48	40,44,48,48	0
3	TDP	C	1003	26/26	0.93	0.16	-0.66	50,50,52,53	0
3	TDP	A	1001	26/26	0.98	0.11	-0.83	2,2,4,5	0
2	MG	D	2004	1/1	0.93	0.12	-0.96	35,35,35,35	0
2	MG	C	2003	1/1	0.93	0.12	-1.67	33,33,33,33	0

## 6.5 Other polymers

There are no such residues in this entry.