



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:51 pm GMT

PDB ID : 1PEU  
Title : Ribonucleotide Reductase Protein R1E from Salmonella typhimurium  
Authors : Uppsten, M.; Farnegardh, M.; Jordan, A.; Eliasson, R.; Eklund, H.; Uhlin, U.  
Deposited on : 2003-05-22  
Resolution : 3.20 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

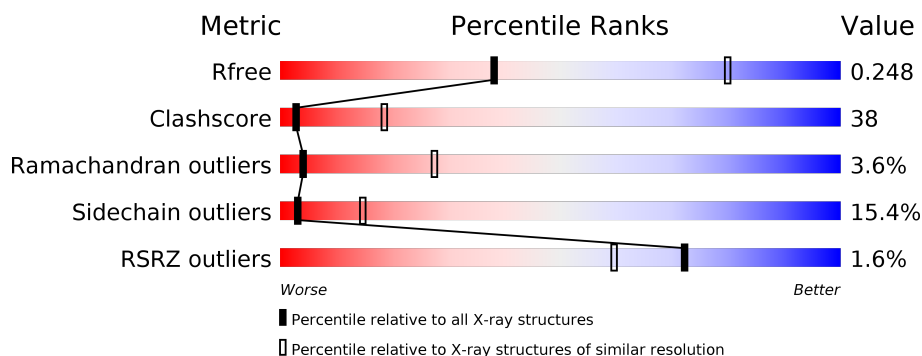
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	714	<div> <div>2%</div> <div>38%</div> <div>47%</div> <div>11%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5586 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.

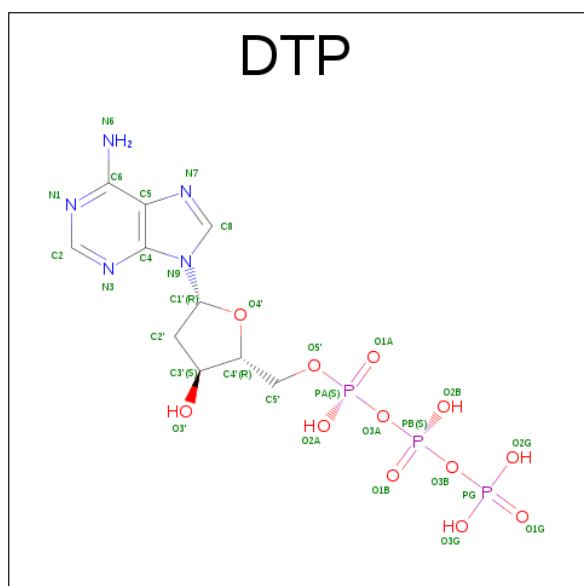
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase 2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	692	5528	3502	978	1025	23	0	0	0

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

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

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula:  $C_{10}H_{16}N_5O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	30	10	5	12	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total	O	0	0
			27	27		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.99Å 98.99Å 291.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.00 – 3.20 42.36 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.00-3.20) 99.7 (42.36-3.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.56 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.204 , 0.251 0.202 , 0.248	Depositor DCC
$R_{free}$ test set	1261 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.0	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5586	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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

### 5.1 Standard geometry

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

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	0.82	0/5654	1.04	25/7654 (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

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	PRO	N-CD-CG	-9.35	89.17	103.20
1	A	637	ASP	CB-CG-OD2	9.31	126.68	118.30
1	A	604	PRO	N-CD-CG	-8.61	90.29	103.20
1	A	185	ASP	CB-CG-OD2	7.23	124.81	118.30
1	A	42	ASP	CB-CG-OD2	6.72	124.35	118.30
1	A	363	TYR	N-CA-C	6.70	129.09	111.00
1	A	387	LEU	CA-CB-CG	6.66	130.61	115.30
1	A	633	ASP	CB-CG-OD2	6.65	124.28	118.30
1	A	349	ASP	CB-CG-OD2	6.47	124.13	118.30
1	A	215	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	A	402	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	81	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	215	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	A	162	PRO	N-CD-CG	-5.86	94.41	103.20
1	A	640	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	73	ASP	CB-CG-OD2	5.71	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	141	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	337	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	665	LEU	CA-CB-CG	-5.34	103.01	115.30
1	A	74	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	412	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	128	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	447	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	177	SER	N-CA-C	5.05	124.64	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	363	TYR	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	5528	0	5416	422	1
2	A	1	0	0	0	0
3	A	30	0	12	1	0
4	A	27	0	0	5	0
All	All	5586	0	5428	423	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 38.

All (423) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ARG:HH21	1:A:316:ARG:NH2	1.29	1.30
1:A:63:LEU:N	1:A:63:LEU:HD23	1.44	1.17
1:A:695:ARG:HH11	1:A:695:ARG:HG2	1.19	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:HD23	1:A:63:LEU:H	1.20	1.01
1:A:695:ARG:HH11	1:A:695:ARG:CG	1.75	0.99
1:A:485:TYR:CZ	1:A:604:PRO:HD3	1.97	0.98
1:A:102:PHE:O	1:A:102:PHE:CD2	2.16	0.98
1:A:223:ARG:NH2	1:A:316:ARG:NH2	2.12	0.98
1:A:148:LEU:HD23	1:A:437:THR:HG22	1.48	0.95
1:A:63:LEU:N	1:A:63:LEU:CD2	2.27	0.95
1:A:627:MET:HG3	1:A:635:TYR:CE1	2.03	0.94
1:A:130:VAL:HG13	1:A:152:MET:HE2	1.49	0.94
1:A:628:THR:H	1:A:631:ASN:HD21	1.15	0.92
1:A:23:LEU:CD1	1:A:623:PRO:HD3	2.00	0.92
1:A:27:ASP:O	1:A:29:ALA:N	2.03	0.91
1:A:80:TYR:CE2	1:A:140:GLY:HA2	2.05	0.91
1:A:485:TYR:CE2	1:A:604:PRO:HD3	2.05	0.91
1:A:87:ARG:HH11	1:A:87:ARG:HG3	1.33	0.90
1:A:644:GLU:HG3	1:A:682:TYR:CE2	2.06	0.90
1:A:80:TYR:CE1	1:A:135:LEU:HD22	2.08	0.88
1:A:19:LEU:HD13	1:A:39:GLN:HB3	1.55	0.87
1:A:592:ILE:HG13	1:A:593:SER:H	1.40	0.86
1:A:72:TYR:CD1	1:A:132:MET:HE1	2.10	0.85
1:A:56:PHE:CD1	1:A:62:ARG:HG3	2.12	0.85
1:A:72:TYR:CD1	1:A:132:MET:CE	2.60	0.85
1:A:115:LYS:NZ	4:A:734:HOH:O	2.10	0.84
1:A:475:HIS:ND1	1:A:605:ILE:HG22	1.91	0.84
1:A:56:PHE:CE1	1:A:62:ARG:HG3	2.13	0.82
1:A:628:THR:H	1:A:631:ASN:ND2	1.77	0.82
1:A:151:GLU:OE1	1:A:156:ARG:NE	2.12	0.81
1:A:295:ILE:HG23	1:A:296:THR:N	1.94	0.81
1:A:663:LEU:C	1:A:663:LEU:HD12	1.99	0.81
1:A:554:ALA:C	1:A:556:SER:H	1.85	0.80
1:A:127:GLU:N	1:A:127:GLU:OE1	2.12	0.80
1:A:274:ARG:HH11	1:A:274:ARG:HG2	1.45	0.80
1:A:393:GLN:HB2	1:A:413:ILE:HD13	1.61	0.80
1:A:592:ILE:O	1:A:593:SER:C	2.19	0.80
1:A:514:ARG:HD2	1:A:576:TYR:CD1	2.16	0.80
1:A:546:THR:HG22	1:A:549:VAL:H	1.44	0.79
1:A:386:ASN:HD21	1:A:388:CYS:HB2	1.47	0.79
1:A:663:LEU:HD12	1:A:664:THR:N	1.98	0.79
1:A:103:LEU:HD21	1:A:594:TYR:CD1	2.18	0.78
1:A:496:LEU:O	1:A:499:TYR:HB3	1.84	0.78
1:A:627:MET:HG3	1:A:635:TYR:CD1	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:VAL:O	1:A:342:LYS:HD2	1.85	0.76
1:A:103:LEU:HD23	1:A:594:TYR:HB3	1.65	0.76
1:A:210:LEU:HB2	1:A:384:MET:CE	2.16	0.76
1:A:386:ASN:ND2	1:A:388:CYS:H	1.84	0.76
1:A:554:ALA:O	1:A:556:SER:N	2.19	0.75
1:A:63:LEU:CD2	1:A:63:LEU:H	1.94	0.75
1:A:527:ARG:HG3	1:A:527:ARG:NH1	2.01	0.74
1:A:592:ILE:O	1:A:595:ILE:N	2.19	0.74
1:A:23:LEU:HD12	1:A:623:PRO:HD3	1.67	0.74
1:A:644:GLU:HG3	1:A:682:TYR:HE2	1.52	0.74
1:A:45:PHE:HA	1:A:49:VAL:CG2	2.17	0.73
1:A:672:THR:O	1:A:675:ASP:HB2	1.89	0.72
1:A:581:GLN:HG2	1:A:582:ASN:ND2	2.04	0.71
1:A:335:ILE:HA	1:A:342:LYS:HE2	1.72	0.71
1:A:34:PHE:CE2	1:A:628:THR:HA	2.26	0.71
1:A:639:TYR:CD2	1:A:666:PHE:HB3	2.24	0.71
1:A:130:VAL:HG21	1:A:153:LEU:HD21	1.71	0.71
1:A:45:PHE:HA	1:A:49:VAL:HG23	1.72	0.70
1:A:447:ASP:OD2	1:A:516:ARG:NH1	2.19	0.70
1:A:102:PHE:O	1:A:102:PHE:CG	2.44	0.70
1:A:87:ARG:NH1	1:A:87:ARG:HG3	2.01	0.70
1:A:603:HIS:ND1	1:A:603:HIS:O	2.24	0.70
1:A:148:LEU:CD2	1:A:437:THR:HG22	2.21	0.69
1:A:695:ARG:NH1	1:A:695:ARG:CG	2.40	0.69
1:A:210:LEU:HB2	1:A:384:MET:HE2	1.73	0.69
1:A:554:ALA:C	1:A:556:SER:N	2.46	0.69
1:A:232:ILE:HA	1:A:235:MET:HG3	1.75	0.69
1:A:261:ALA:HA	1:A:266:ILE:HD13	1.74	0.68
1:A:388:CYS:O	1:A:662:SER:OG	2.11	0.68
1:A:251:ARG:O	1:A:252:GLN:HB2	1.92	0.68
1:A:617:THR:HG22	4:A:735:HOH:O	1.94	0.68
1:A:80:TYR:CZ	1:A:140:GLY:HA2	2.29	0.68
1:A:18:ALA:O	1:A:19:LEU:C	2.27	0.67
1:A:274:ARG:NH1	1:A:274:ARG:HG2	2.08	0.67
1:A:291:VAL:CG1	1:A:369:GLU:HB2	2.23	0.67
1:A:406:TYR:CE1	1:A:455:PRO:HG2	2.30	0.67
1:A:485:TYR:CZ	1:A:604:PRO:CD	2.78	0.67
1:A:377:PRO:HA	1:A:527:ARG:HG3	1.77	0.67
1:A:422:ILE:HG23	1:A:497:TYR:CE1	2.30	0.67
1:A:23:LEU:HD11	1:A:623:PRO:HD3	1.76	0.67
1:A:108:PHE:HB2	1:A:595:ILE:HD11	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ILE:CG2	1:A:296:THR:N	2.58	0.66
1:A:527:ARG:HG3	1:A:527:ARG:HH11	1.60	0.65
1:A:126:PHE:O	1:A:130:VAL:HG23	1.95	0.65
1:A:592:ILE:HG13	1:A:593:SER:N	2.10	0.65
1:A:103:LEU:HD12	1:A:620:VAL:CG1	2.26	0.65
1:A:19:LEU:HD13	1:A:39:GLN:CB	2.26	0.65
1:A:510:MET:SD	1:A:572:ASP:HB3	2.37	0.64
1:A:103:LEU:HD12	1:A:620:VAL:HG11	1.80	0.64
1:A:555:ARG:O	1:A:555:ARG:HG2	1.96	0.64
1:A:584:GLN:HG3	4:A:719:HOH:O	1.96	0.64
1:A:80:TYR:CE2	1:A:140:GLY:CA	2.80	0.64
1:A:485:TYR:CE2	1:A:604:PRO:CD	2.81	0.63
1:A:562:THR:OG1	1:A:565:MET:HG3	1.98	0.63
1:A:88:LEU:O	1:A:89:PHE:C	2.36	0.63
1:A:527:ARG:HH11	1:A:527:ARG:CG	2.11	0.63
1:A:540:ASP:O	1:A:541:ASP:HB2	1.98	0.63
1:A:664:THR:HG22	1:A:666:PHE:CE1	2.33	0.63
1:A:643:PRO:O	1:A:647:ILE:HD12	1.98	0.63
1:A:223:ARG:HH21	1:A:316:ARG:HH22	1.37	0.63
1:A:335:ILE:HA	1:A:342:LYS:CE	2.29	0.63
1:A:59:GLN:O	1:A:62:ARG:HB3	2.00	0.62
1:A:483:ILE:HG22	1:A:484:ALA:N	2.12	0.62
1:A:108:PHE:CD1	1:A:108:PHE:C	2.72	0.62
1:A:148:LEU:HD23	1:A:437:THR:CG2	2.26	0.62
1:A:477:TYR:O	1:A:478:LEU:C	2.37	0.62
1:A:403:ASN:OD1	1:A:405:ASP:HB2	1.99	0.62
1:A:130:VAL:HG21	1:A:153:LEU:CD2	2.29	0.62
1:A:500:THR:HG22	1:A:561:PRO:HD2	1.82	0.62
1:A:80:TYR:CD1	1:A:135:LEU:HD22	2.34	0.62
1:A:617:THR:HG23	1:A:619:ARG:H	1.64	0.62
1:A:572:ASP:O	1:A:576:TYR:N	2.33	0.62
1:A:534:PHE:O	1:A:535:THR:C	2.39	0.61
1:A:266:ILE:HG23	1:A:267:LEU:HD23	1.81	0.61
1:A:500:THR:HG22	1:A:561:PRO:CD	2.31	0.61
1:A:103:LEU:CD2	1:A:594:TYR:HB3	2.32	0.60
1:A:639:TYR:CE2	1:A:666:PHE:HB3	2.36	0.60
1:A:80:TYR:CE1	1:A:135:LEU:CD2	2.83	0.60
1:A:359:PHE:CD1	1:A:696:LEU:HD21	2.37	0.60
1:A:595:ILE:HG22	1:A:596:ASN:N	2.15	0.60
1:A:467:ILE:HD11	1:A:583:LEU:HD12	1.83	0.60
1:A:72:TYR:CE1	1:A:132:MET:CE	2.85	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:ILE:CG1	1:A:607:ALA:O	2.50	0.59
1:A:72:TYR:CD1	1:A:132:MET:HE2	2.37	0.59
1:A:27:ASP:C	1:A:29:ALA:H	2.05	0.59
1:A:351:PHE:HB3	1:A:677:ASN:HD21	1.67	0.59
1:A:421:ASN:OD1	1:A:421:ASN:C	2.39	0.59
1:A:108:PHE:CE1	1:A:113:THR:HB	2.37	0.59
1:A:102:PHE:C	1:A:102:PHE:CD2	2.75	0.59
1:A:223:ARG:HH21	1:A:316:ARG:CZ	2.08	0.59
1:A:532:ASP:O	1:A:533:TYR:C	2.39	0.59
1:A:146:THR:O	1:A:149:THR:HB	2.03	0.58
1:A:190:ILE:HG22	1:A:191:GLY:N	2.18	0.58
1:A:310:SER:O	1:A:314:ILE:HG12	2.02	0.58
1:A:116:THR:O	1:A:119:GLY:N	2.31	0.58
1:A:632:LEU:O	1:A:634:MET:N	2.37	0.58
1:A:695:ARG:HG3	1:A:695:ARG:NH1	2.17	0.58
1:A:133:VAL:HG22	1:A:167:CYS:HB2	1.86	0.57
1:A:158:GLN:CA	1:A:158:GLN:OE1	2.51	0.57
1:A:603:HIS:O	1:A:604:PRO:O	2.21	0.57
1:A:416:ASN:C	1:A:417:LEU:HD13	2.23	0.57
1:A:534:PHE:O	1:A:537:TYR:N	2.32	0.56
1:A:379:ALA:O	1:A:394:VAL:HG11	2.05	0.56
1:A:295:ILE:HG23	1:A:296:THR:H	1.68	0.56
1:A:347:ALA:O	1:A:350:PHE:HB3	2.06	0.56
1:A:695:ARG:NH1	1:A:695:ARG:HG2	2.01	0.56
1:A:88:LEU:O	1:A:90:GLU:N	2.39	0.56
1:A:370:ASP:O	1:A:371:THR:C	2.42	0.56
1:A:666:PHE:CD1	1:A:666:PHE:N	2.74	0.56
1:A:180:LEU:N	1:A:180:LEU:HD12	2.21	0.55
1:A:385:SER:OG	1:A:386:ASN:N	2.40	0.55
1:A:628:THR:N	1:A:631:ASN:HD21	1.96	0.55
1:A:539:GLN:N	1:A:539:GLN:OE1	2.39	0.55
1:A:54:VAL:HG22	1:A:121:ARG:NH2	2.22	0.55
1:A:303:ASN:O	1:A:303:ASN:OD1	2.24	0.55
1:A:19:LEU:CD1	1:A:39:GLN:HB3	2.31	0.55
1:A:309:PHE:CD1	1:A:309:PHE:N	2.74	0.54
1:A:295:ILE:CG2	1:A:296:THR:H	2.19	0.54
1:A:114:LEU:HB2	1:A:124:GLU:OE2	2.07	0.54
1:A:393:GLN:HB2	1:A:413:ILE:CD1	2.32	0.54
1:A:294:ASP:O	1:A:295:ILE:C	2.45	0.54
1:A:192:ARG:NH1	1:A:406:TYR:HE1	2.05	0.54
1:A:303:ASN:HB2	1:A:348:ARG:NH2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ALA:HA	1:A:358:GLN:HG3	1.88	0.54
1:A:368:PHE:O	1:A:369:GLU:C	2.46	0.54
1:A:477:TYR:O	1:A:480:ARG:N	2.41	0.54
1:A:27:ASP:C	1:A:29:ALA:N	2.57	0.53
1:A:473:ASN:ND2	1:A:476:GLY:HA3	2.23	0.53
1:A:11:GLN:HG2	1:A:12:GLU:H	1.73	0.53
1:A:421:ASN:O	1:A:422:ILE:C	2.45	0.53
1:A:174:GLU:HG3	1:A:175:LEU:H	1.73	0.53
1:A:440:ARG:O	1:A:441:GLY:C	2.46	0.53
1:A:640:ASP:C	1:A:640:ASP:OD1	2.45	0.53
1:A:216:GLU:OE1	1:A:310:SER:HB2	2.08	0.53
1:A:213:ASN:OD1	1:A:323:GLY:HA3	2.08	0.53
1:A:63:LEU:O	1:A:64:GLY:C	2.46	0.53
1:A:50:ARG:HB2	1:A:51:PRO:HD3	1.91	0.53
1:A:59:GLN:HG2	1:A:86:LEU:CD2	2.39	0.53
1:A:316:ARG:NH1	1:A:316:ARG:HG3	2.23	0.53
1:A:59:GLN:CG	1:A:86:LEU:CD2	2.87	0.52
1:A:88:LEU:C	1:A:90:GLU:N	2.61	0.52
1:A:358:GLN:OE1	1:A:680:GLN:NE2	2.43	0.52
1:A:114:LEU:HD22	1:A:115:LYS:O	2.09	0.52
1:A:219:ALA:HB1	1:A:220:PRO:CD	2.40	0.52
1:A:13:THR:HG23	1:A:13:THR:O	2.10	0.52
1:A:428:SER:O	1:A:430:ASP:N	2.43	0.52
1:A:16:TYR:HB2	1:A:102:PHE:CE1	2.45	0.51
1:A:548:LYS:O	1:A:551:ALA:HB3	2.09	0.51
1:A:8:ARG:O	1:A:9:VAL:C	2.48	0.51
1:A:444:ALA:O	1:A:445:VAL:C	2.46	0.51
1:A:223:ARG:NH2	1:A:316:ARG:HH22	2.01	0.51
1:A:283:ILE:HG22	1:A:283:ILE:O	2.09	0.51
1:A:496:LEU:HD13	1:A:560:LEU:HD21	1.92	0.51
1:A:669:ASP:OD2	1:A:697:ARG:NH1	2.44	0.51
1:A:16:TYR:HD2	1:A:102:PHE:CZ	2.28	0.51
1:A:555:ARG:CG	1:A:555:ARG:O	2.58	0.51
1:A:210:LEU:HB2	1:A:384:MET:HE1	1.93	0.51
1:A:562:THR:H	1:A:565:MET:HG3	1.75	0.51
1:A:605:ILE:HG12	1:A:607:ALA:H	1.76	0.51
1:A:274:ARG:HH11	1:A:274:ARG:CG	2.21	0.51
1:A:34:PHE:HE2	1:A:628:THR:HA	1.72	0.51
1:A:562:THR:O	1:A:565:MET:N	2.44	0.50
1:A:343:THR:HG22	1:A:344:TYR:N	2.27	0.50
1:A:158:GLN:C	1:A:158:GLN:OE1	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:TYR:OH	1:A:138:ALA:HB3	2.11	0.50
1:A:605:ILE:HG13	1:A:607:ALA:O	2.11	0.50
1:A:307:ALA:O	1:A:309:PHE:CE1	2.65	0.50
1:A:321:PRO:HD2	1:A:324:ASP:HB2	1.92	0.50
1:A:477:TYR:O	1:A:479:ALA:N	2.45	0.50
1:A:510:MET:HE3	1:A:511:ARG:HG2	1.94	0.50
1:A:509:SER:OG	1:A:580:ASN:ND2	2.28	0.49
1:A:316:ARG:CG	1:A:316:ARG:HH11	2.25	0.49
1:A:422:ILE:O	1:A:423:ALA:C	2.50	0.49
1:A:694:ILE:CG1	1:A:694:ILE:O	2.60	0.49
1:A:147:GLN:O	1:A:148:LEU:C	2.47	0.49
1:A:511:ARG:HD2	4:A:723:HOH:O	2.13	0.49
1:A:161:THR:O	1:A:162:PRO:C	2.50	0.49
1:A:212:SER:OG	1:A:260:HIS:N	2.41	0.49
1:A:278:ASP:OD1	1:A:278:ASP:N	2.46	0.49
1:A:401:ASP:OD1	1:A:402:ASP:N	2.45	0.49
1:A:484:ALA:O	1:A:487:SER:HB3	2.11	0.49
1:A:259:LEU:HD23	1:A:269:PHE:CG	2.48	0.49
1:A:372:VAL:HG13	1:A:392:LEU:HD13	1.94	0.49
1:A:141:ASP:OD2	1:A:141:ASP:C	2.51	0.49
1:A:237:MET:O	1:A:238:LEU:C	2.49	0.49
3:A:716:DTP:O5'	3:A:716:DTP:H8	2.12	0.49
1:A:114:LEU:HD22	1:A:115:LYS:N	2.28	0.49
1:A:295:ILE:O	1:A:296:THR:C	2.51	0.49
1:A:472:MET:HB3	1:A:589:THR:HG21	1.93	0.49
1:A:431:ILE:CG2	1:A:432:GLY:N	2.76	0.49
1:A:651:ALA:O	1:A:654:THR:N	2.46	0.49
1:A:271:ASP:OD1	1:A:274:ARG:HD2	2.12	0.48
1:A:617:THR:CG2	1:A:619:ARG:O	2.61	0.48
1:A:172:ARG:NH1	1:A:175:LEU:HD13	2.29	0.48
1:A:643:PRO:O	1:A:644:GLU:C	2.51	0.48
1:A:391:ILE:HA	1:A:659:GLN:OE1	2.13	0.48
1:A:192:ARG:HG3	1:A:400:TYR:CE1	2.49	0.48
1:A:201:SER:OG	1:A:245:ALA:O	2.23	0.48
1:A:40:ALA:HB1	1:A:102:PHE:CD1	2.49	0.48
1:A:419:SER:HA	1:A:470:GLY:O	2.14	0.48
1:A:631:ASN:O	1:A:632:LEU:C	2.52	0.48
1:A:72:TYR:CE1	1:A:132:MET:SD	3.07	0.48
1:A:359:PHE:CE1	1:A:696:LEU:HD21	2.48	0.48
1:A:421:ASN:OD1	1:A:421:ASN:O	2.32	0.48
1:A:520:PHE:CE2	1:A:581:GLN:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:TYR:CD2	1:A:102:PHE:CE1	3.02	0.47
1:A:349:ASP:O	1:A:352:GLN:HB3	2.14	0.47
1:A:603:HIS:O	1:A:604:PRO:C	2.52	0.47
1:A:77:LEU:HD22	1:A:85:VAL:HG11	1.96	0.47
1:A:313:ASP:O	1:A:314:ILE:C	2.53	0.47
1:A:562:THR:O	1:A:564:GLU:N	2.47	0.47
1:A:158:GLN:HA	1:A:158:GLN:OE1	2.13	0.47
1:A:622:TYR:O	1:A:622:TYR:CG	2.66	0.47
1:A:661:LEU:HD12	1:A:661:LEU:N	2.28	0.47
1:A:157:PHE:CD2	1:A:159:PRO:HD3	2.48	0.47
1:A:475:HIS:O	1:A:476:GLY:C	2.52	0.47
1:A:632:LEU:C	1:A:634:MET:H	2.17	0.47
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.67	0.47
1:A:210:LEU:CB	1:A:384:MET:HE1	2.44	0.47
1:A:41:ILE:O	1:A:44:PHE:N	2.46	0.47
1:A:86:LEU:HA	1:A:86:LEU:HD23	1.47	0.47
1:A:363:TYR:HD1	1:A:364:PRO:CD	2.28	0.47
1:A:386:ASN:OD1	1:A:390:GLU:N	2.43	0.47
1:A:390:GLU:HG2	1:A:587:PRO:HA	1.96	0.47
1:A:580:ASN:N	1:A:580:ASN:ND2	2.63	0.47
1:A:129:ARG:NH1	1:A:164:PHE:O	2.48	0.47
1:A:165:LEU:O	1:A:169:LYS:HE3	2.15	0.47
1:A:116:THR:O	1:A:118:ASP:N	2.48	0.47
1:A:327:ILE:O	1:A:328:SER:C	2.52	0.47
1:A:197:ALA:O	1:A:198:LEU:C	2.49	0.46
1:A:231:VAL:CG2	1:A:232:ILE:N	2.77	0.46
1:A:157:PHE:CE2	1:A:159:PRO:HD3	2.51	0.46
1:A:428:SER:HA	1:A:429:PRO:HD2	1.66	0.46
1:A:59:GLN:OE1	1:A:62:ARG:HD3	2.16	0.46
1:A:72:TYR:CE1	1:A:132:MET:HE2	2.51	0.46
1:A:371:THR:HG21	1:A:687:GLY:O	2.16	0.46
1:A:584:GLN:O	1:A:659:GLN:HB2	2.16	0.46
1:A:20:ASN:O	1:A:23:LEU:HB2	2.15	0.46
1:A:299:LEU:HD23	1:A:306:MET:HA	1.97	0.46
1:A:431:ILE:HG22	1:A:432:GLY:N	2.31	0.46
1:A:199:GLN:HA	1:A:199:GLN:NE2	2.31	0.46
1:A:442:LEU:HA	1:A:442:LEU:HD23	1.54	0.46
1:A:23:LEU:HD23	1:A:23:LEU:HA	1.71	0.46
1:A:316:ARG:HH11	1:A:316:ARG:HG3	1.81	0.46
1:A:520:PHE:HD1	1:A:521:ALA:O	1.98	0.46
1:A:263:HIS:HA	1:A:264:PRO:HD3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:N	1:A:308:LEU:HD23	2.31	0.46
1:A:247:GLN:CG	1:A:248:LEU:N	2.78	0.46
1:A:440:ARG:NH2	1:A:515:GLU:OE2	2.47	0.46
1:A:633:ASP:OD1	1:A:633:ASP:N	2.48	0.46
1:A:473:ASN:HA	1:A:599:THR:OG1	2.15	0.45
1:A:41:ILE:O	1:A:42:ASP:C	2.54	0.45
1:A:540:ASP:O	1:A:541:ASP:CB	2.63	0.45
1:A:23:LEU:HD11	1:A:623:PRO:CD	2.45	0.45
1:A:266:ILE:HG13	1:A:266:ILE:O	2.14	0.45
1:A:354:LEU:HD12	1:A:354:LEU:HA	1.74	0.45
1:A:421:ASN:OD1	1:A:423:ALA:HB3	2.16	0.45
1:A:56:PHE:CD1	1:A:62:ARG:CG	2.94	0.45
1:A:59:GLN:HB3	1:A:86:LEU:HD22	1.98	0.45
1:A:483:ILE:HG22	1:A:484:ALA:H	1.81	0.45
1:A:483:ILE:CG2	1:A:484:ALA:N	2.79	0.45
1:A:502:THR:OG1	1:A:584:GLN:NE2	2.50	0.45
1:A:114:LEU:CD2	1:A:115:LYS:N	2.80	0.45
1:A:376:ASN:HA	1:A:377:PRO:HD3	1.73	0.45
1:A:669:ASP:OD1	1:A:669:ASP:N	2.48	0.45
1:A:322:PHE:CD1	1:A:322:PHE:C	2.90	0.45
1:A:509:SER:HG	1:A:579:TYR:H	1.64	0.45
1:A:422:ILE:HD12	1:A:474:LEU:N	2.32	0.45
1:A:294:ASP:O	1:A:297:PHE:N	2.34	0.45
1:A:332:ASP:O	1:A:333:GLU:C	2.54	0.45
1:A:346:ASN:HD22	1:A:349:ASP:CG	2.20	0.44
1:A:592:ILE:O	1:A:594:TYR:N	2.51	0.44
1:A:100:GLN:C	1:A:101:THR:HG23	2.38	0.44
1:A:181:LEU:HD21	1:A:457:ILE:HD11	2.00	0.44
1:A:317:ARG:HH11	1:A:317:ARG:HB3	1.83	0.44
1:A:416:ASN:ND2	1:A:416:ASN:N	2.66	0.44
1:A:500:THR:HG22	1:A:561:PRO:HD3	1.98	0.44
1:A:594:TYR:OH	1:A:610:GLU:OE2	2.34	0.44
1:A:161:THR:N	1:A:162:PRO:HD2	2.32	0.44
1:A:416:ASN:ND2	1:A:416:ASN:H	2.15	0.44
1:A:138:ALA:CB	1:A:145:ALA:HB2	2.47	0.44
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.40	0.44
1:A:520:PHE:CD2	1:A:581:GLN:HA	2.53	0.44
1:A:192:ARG:HE	1:A:404:LEU:HG	1.82	0.44
1:A:45:PHE:HA	1:A:49:VAL:CB	2.48	0.44
1:A:593:SER:O	1:A:597:HIS:N	2.51	0.44
1:A:691:LEU:HD23	1:A:691:LEU:HA	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:TRP:O	1:A:110:THR:HG23	2.18	0.43
1:A:216:GLU:HB2	1:A:264:PRO:HB2	2.00	0.43
1:A:567:LEU:HD12	1:A:570:ARG:HH11	1.83	0.43
1:A:417:LEU:N	1:A:417:LEU:HD13	2.33	0.43
1:A:551:ALA:O	1:A:552:LEU:C	2.56	0.43
1:A:401:ASP:HB2	1:A:407:THR:HG23	2.01	0.43
1:A:157:PHE:CE1	1:A:438:ALA:HB1	2.53	0.43
1:A:321:PRO:O	1:A:322:PHE:C	2.53	0.43
1:A:386:ASN:ND2	1:A:388:CYS:N	2.60	0.43
1:A:156:ARG:O	1:A:420:LEU:HA	2.18	0.43
1:A:347:ALA:O	1:A:348:ARG:C	2.55	0.43
1:A:20:ASN:HD21	1:A:621:TYR:H	1.66	0.43
1:A:254:ALA:HB1	1:A:387:LEU:HD21	2.01	0.43
1:A:531:GLY:O	1:A:532:ASP:C	2.55	0.43
1:A:677:ASN:O	1:A:681:ILE:HG13	2.17	0.43
1:A:27:ASP:O	1:A:28:LYS:C	2.55	0.43
1:A:567:LEU:CD1	1:A:570:ARG:HH11	2.31	0.43
1:A:27:ASP:O	1:A:30:GLY:N	2.44	0.43
1:A:315:GLN:HA	1:A:320:LYS:O	2.19	0.43
1:A:543:GLN:HA	1:A:544:PRO:HD2	1.80	0.43
1:A:643:PRO:C	1:A:647:ILE:HD12	2.39	0.43
1:A:103:LEU:CD2	1:A:594:TYR:CB	2.97	0.43
1:A:103:LEU:CD2	1:A:594:TYR:CG	3.01	0.43
1:A:127:GLU:O	1:A:128:ASP:C	2.57	0.43
1:A:144:LEU:O	1:A:145:ALA:C	2.57	0.43
1:A:299:LEU:HA	1:A:299:LEU:HD12	1.72	0.43
1:A:646:ILE:O	1:A:647:ILE:C	2.54	0.43
1:A:16:TYR:HD2	1:A:102:PHE:CE1	2.37	0.42
1:A:179:PHE:N	1:A:206:GLY:O	2.50	0.42
1:A:373:ASN:OD1	1:A:381:ARG:HA	2.19	0.42
1:A:116:THR:O	1:A:117:PHE:C	2.54	0.42
1:A:473:ASN:HD21	1:A:476:GLY:HA3	1.85	0.42
1:A:487:SER:OG	1:A:489:GLU:N	2.49	0.42
1:A:20:ASN:ND2	1:A:620:VAL:HG13	2.34	0.42
1:A:291:VAL:HG13	1:A:369:GLU:HB2	2.00	0.42
1:A:490:ALA:O	1:A:491:LEU:C	2.57	0.42
1:A:213:ASN:OD1	1:A:323:GLY:N	2.52	0.42
1:A:263:HIS:CE1	1:A:265:ASP:HB2	2.55	0.42
1:A:292:ILE:HA	1:A:293:PRO:HD3	1.83	0.42
1:A:19:LEU:HD12	1:A:40:ALA:HA	2.01	0.42
1:A:223:ARG:HE	1:A:316:ARG:HH21	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:VAL:HG12	1:A:85:VAL:O	2.19	0.42
1:A:143:THR:O	1:A:144:LEU:C	2.58	0.42
1:A:247:GLN:HG3	1:A:248:LEU:N	2.35	0.42
1:A:95:SER:OG	1:A:153:LEU:HD13	2.20	0.42
1:A:690:SER:O	1:A:691:LEU:HD23	2.19	0.42
1:A:22:MET:HB2	1:A:36:LYS:HB3	2.02	0.42
1:A:562:THR:C	1:A:564:GLU:N	2.73	0.42
1:A:475:HIS:CE1	1:A:605:ILE:HG22	2.54	0.42
1:A:65:THR:O	1:A:66:LEU:C	2.58	0.42
1:A:20:ASN:HD21	1:A:620:VAL:HG13	1.85	0.41
1:A:617:THR:CG2	1:A:619:ARG:H	2.30	0.41
1:A:644:GLU:O	1:A:645:LYS:C	2.59	0.41
1:A:132:MET:O	1:A:133:VAL:C	2.58	0.41
1:A:148:LEU:O	1:A:149:THR:C	2.57	0.41
1:A:238:LEU:O	1:A:239:GLU:C	2.58	0.41
1:A:337:ASP:OD1	1:A:339:HIS:HB2	2.21	0.41
1:A:589:THR:O	1:A:590:GLY:O	2.39	0.41
1:A:193:ALA:O	1:A:194:VAL:C	2.59	0.41
1:A:632:LEU:HD23	1:A:632:LEU:HA	1.66	0.41
1:A:501:ILE:O	1:A:502:THR:C	2.59	0.41
1:A:283:ILE:HG21	1:A:286:LEU:HB2	2.03	0.41
1:A:36:LYS:HD2	1:A:36:LYS:HA	1.76	0.41
1:A:492:ASP:HB3	1:A:549:VAL:HG21	2.02	0.41
1:A:688:ILE:HD13	1:A:688:ILE:N	2.36	0.41
1:A:182:ARG:HG3	1:A:182:ARG:HH11	1.85	0.41
1:A:184:GLU:HG2	4:A:722:HOH:O	2.19	0.41
1:A:325:ILE:HG13	1:A:327:ILE:HD13	2.01	0.41
1:A:507:HIS:O	1:A:510:MET:HB3	2.21	0.41
1:A:22:MET:C	1:A:24:ASN:H	2.24	0.41
1:A:24:ASN:O	1:A:24:ASN:CG	2.60	0.41
1:A:496:LEU:HA	1:A:496:LEU:HD23	1.57	0.41
1:A:514:ARG:HD2	1:A:576:TYR:CE1	2.53	0.41
1:A:523:PHE:CE2	1:A:577:GLY:HA2	2.56	0.41
1:A:103:LEU:HD23	1:A:594:TYR:CB	2.42	0.41
1:A:174:GLU:HG3	1:A:175:LEU:N	2.36	0.41
1:A:400:TYR:N	1:A:400:TYR:CD2	2.89	0.41
1:A:514:ARG:HD2	1:A:576:TYR:CG	2.53	0.41
1:A:676:ILE:O	1:A:677:ASN:C	2.58	0.41
1:A:307:ALA:HB2	1:A:344:TYR:CE1	2.56	0.40
1:A:44:PHE:O	1:A:45:PHE:C	2.56	0.40
1:A:680:GLN:O	1:A:683:ALA:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:PHE:HZ	1:A:331:TYR:CE1	2.40	0.40
1:A:437:THR:O	1:A:441:GLY:N	2.40	0.40
1:A:484:ALA:O	1:A:485:TYR:C	2.59	0.40
1:A:560:LEU:O	1:A:561:PRO:C	2.59	0.40
1:A:594:TYR:CD2	1:A:622:TYR:CE2	3.09	0.40
1:A:298:ARG:NH2	1:A:302:GLU:OE2	2.50	0.40
1:A:485:TYR:C	1:A:485:TYR:CD1	2.94	0.40
1:A:632:LEU:C	1:A:634:MET:N	2.74	0.40
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.77	0.40
1:A:68:ARG:NH1	1:A:68:ARG:CB	2.85	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:57:ALA:N	1:A:637:ASP:OD1[6_565]	2.14	0.06

## 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
1	A	690/714 (97%)	556 (81%)	109 (16%)	25 (4%)	<b>4</b> <b>27</b>

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	28	LYS
1	A	225	GLU
1	A	363	TYR
1	A	364	PRO
1	A	555	ARG

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Mol	Chain	Res	Type
1	A	590	GLY
1	A	49	VAL
1	A	117	PHE
1	A	423	ALA
1	A	424	HIS
1	A	539	GLN
1	A	541	ASP
1	A	544	PRO
1	A	593	SER
1	A	633	ASP
1	A	644	GLU
1	A	13	THR
1	A	369	GLU
1	A	477	TYR
1	A	551	ALA
1	A	604	PRO
1	A	429	PRO
1	A	451	ILE
1	A	478	LEU

### 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	579/596 (97%)	490 (85%)	89 (15%)	<b>3</b> <b>15</b>

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	12	GLU
1	A	23	LEU
1	A	25	LEU
1	A	36	LYS
1	A	47	THR
1	A	58	SER

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Mol	Chain	Res	Type
1	A	63	LEU
1	A	82	ARG
1	A	98	ARG
1	A	100	GLN
1	A	108	PHE
1	A	114	LEU
1	A	143	THR
1	A	144	LEU
1	A	158	GLN
1	A	178	CYS
1	A	182	ARG
1	A	190	ILE
1	A	198	LEU
1	A	200	LEU
1	A	214	LEU
1	A	223	ARG
1	A	224	ILE
1	A	228	SER
1	A	231	VAL
1	A	232	ILE
1	A	243	SER
1	A	246	ASN
1	A	247	GLN
1	A	267	LEU
1	A	268	ARG
1	A	270	LEU
1	A	271	ASP
1	A	274	ARG
1	A	278	ASP
1	A	281	ILE
1	A	282	ARG
1	A	298	ARG
1	A	299	LEU
1	A	316	ARG
1	A	317	ARG
1	A	327	ILE
1	A	341	ARG
1	A	376	ASN
1	A	390	GLU
1	A	401	ASP
1	A	413	ILE
1	A	416	ASN

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Mol	Chain	Res	Type
1	A	417	LEU
1	A	420	LEU
1	A	421	ASN
1	A	429	PRO
1	A	431	ILE
1	A	446	SER
1	A	471	GLN
1	A	473	ASN
1	A	474	LEU
1	A	487	SER
1	A	494	THR
1	A	514	ARG
1	A	525	GLN
1	A	527	ARG
1	A	536	GLN
1	A	539	GLN
1	A	546	THR
1	A	555	ARG
1	A	559	THR
1	A	563	ARG
1	A	568	LYS
1	A	570	ARG
1	A	580	ASN
1	A	583	LEU
1	A	595	ILE
1	A	605	ILE
1	A	609	ILE
1	A	619	ARG
1	A	631	ASN
1	A	636	GLN
1	A	637	ASP
1	A	661	LEU
1	A	663	LEU
1	A	669	ASP
1	A	674	ARG
1	A	677	ASN
1	A	688	ILE
1	A	693	TYR
1	A	694	ILE
1	A	695	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	38	GLN
1	A	52	HIS
1	A	60	HIS
1	A	93	HIS
1	A	100	GLN
1	A	199	GLN
1	A	246	ASN
1	A	346	ASN
1	A	352	GLN
1	A	358	GLN
1	A	411	HIS
1	A	416	ASN
1	A	450	HIS
1	A	525	GLN
1	A	536	GLN
1	A	580	ASN
1	A	582	ASN
1	A	596	ASN
1	A	631	ASN
1	A	677	ASN
1	A	680	GLN
1	A	698	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	DTP	A	716	2	26,32,32	1.79	4 (15%)	26,50,50	2.81	4 (15%)

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	DTP	A	716	2	-	0/18/34/34	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	716	DTP	PG-O3B	-6.21	1.50	1.60
3	A	716	DTP	C5-N7	-2.88	1.29	1.39
3	A	716	DTP	C5-C4	2.51	1.46	1.40
3	A	716	DTP	C2-N1	3.20	1.39	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	716	DTP	N3-C2-N1	-12.32	118.13	128.86
3	A	716	DTP	O4'-C1'-N9	-4.50	100.20	107.78
3	A	716	DTP	C2-N1-C6	2.79	123.65	118.77
3	A	716	DTP	C4'-O4'-C1'	2.84	116.36	109.42

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
3	A	716	DTP	1	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 [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, 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	692/714 (96%)	-0.35	11 (1%) 72 59	19, 38, 67, 119	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	GLN	6.7
1	A	10	MET	3.4
1	A	276	ASN	3.1
1	A	8	ARG	3.0
1	A	279	GLU	2.9
1	A	9	VAL	2.6
1	A	617	THR	2.5
1	A	12	GLU	2.5
1	A	541	ASP	2.4
1	A	278	ASP	2.1
1	A	699	LEU	2.1

### 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( $\text{\AA}^2$ )	Q<0.9
3	DTP	A	716	30/30	0.96	0.12	-1.07	0,26,34,36	0
2	MG	A	715	1/1	0.74	0.25	-	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.