



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:37 AM UTC

PDB ID : 1PEU / pdb_00001peu
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

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>.

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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

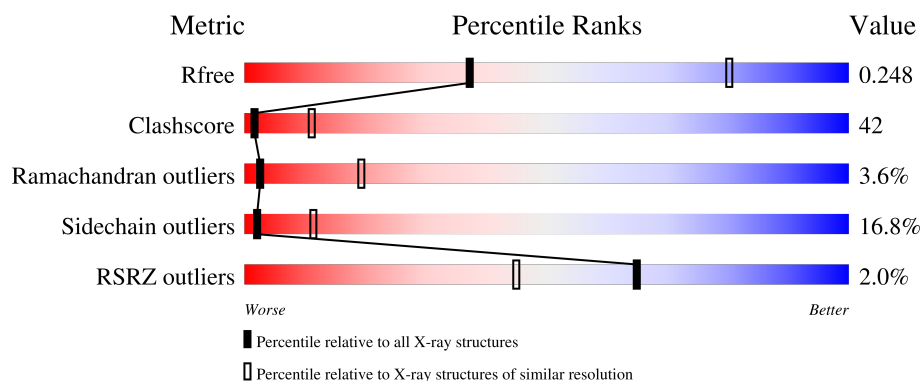
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	2% 34% 47% 14% ..

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.

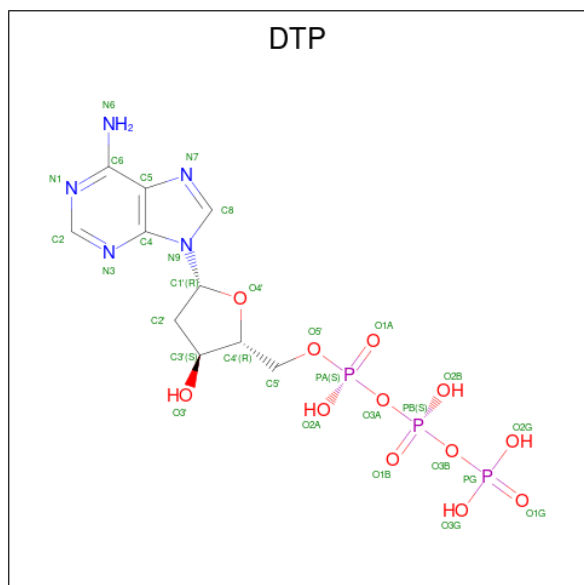
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase 2 alpha chain.

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

- Molecule 2 is MAGNESIUM ION (CCD ID: 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 (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃)



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

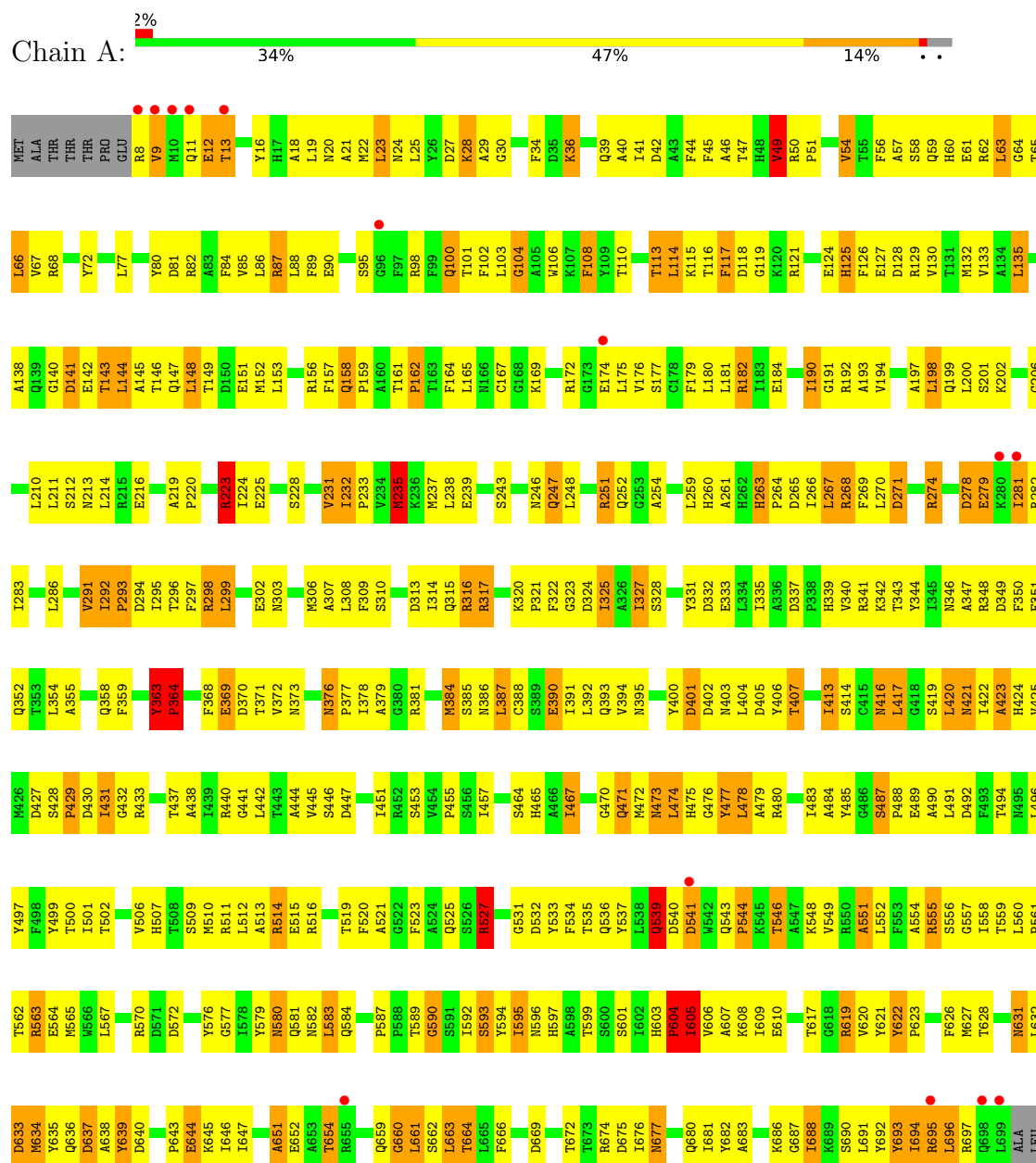
- Molecule 4 is water.

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

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: Ribonucleoside-diphosphate reductase 2 alpha chain



GLU
GLY
THR
GLU
ILE
GLU
GLY
CYS
VAL
SER
CYS
ALA
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.99Å 98.99Å 291.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.00 – 3.20 43.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.00-3.20) 99.7 (43.00-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.56 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.204 , 0.251 0.202 , 0.248	Depositor DCC
R_{free} test set	1261 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	64.0	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.09	11/5654 (0.2%)	1.36	42/7654 (0.5%)

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	ILE	CA-CB	-9.38	1.47	1.54
1	A	378	ILE	CA-CB	-6.52	1.46	1.54
1	A	292	ILE	CA-C	-6.39	1.47	1.52
1	A	651	ALA	CA-CB	-6.29	1.43	1.53
1	A	654	THR	CA-C	5.80	1.60	1.52
1	A	467	ILE	CA-CB	-5.75	1.45	1.54
1	A	46	ALA	CA-CB	-5.56	1.44	1.53
1	A	519	THR	CA-CB	-5.48	1.46	1.53
1	A	692	TYR	C-O	-5.37	1.19	1.23
1	A	692	TYR	CA-C	-5.21	1.48	1.53
1	A	104	GLY	CA-C	5.13	1.59	1.51

All (42) 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	363	TYR	N-CA-C	8.72	129.09	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	604	PRO	N-CD-CG	-8.61	90.29	103.20
1	A	177	SER	N-CA-C	7.85	124.64	114.75
1	A	125	HIS	N-CA-C	-7.14	98.50	109.14
1	A	268	ARG	N-CA-C	-6.89	103.79	111.71
1	A	142	GLU	N-CA-C	6.61	118.48	111.28
1	A	148	LEU	N-CA-C	-6.57	103.22	111.11
1	A	693	TYR	CA-C-N	-6.41	114.58	123.10
1	A	693	TYR	C-N-CA	-6.41	114.58	123.10
1	A	407	THR	N-CA-C	-6.35	105.85	113.97
1	A	660	GLY	N-CA-C	6.20	120.22	111.42
1	A	506	VAL	CB-CA-C	-6.02	104.26	111.97
1	A	453	SER	N-CA-C	6.02	120.48	113.20
1	A	162	PRO	N-CD-CG	-5.86	94.41	103.20
1	A	527	ARG	N-CA-C	-5.75	106.25	113.20
1	A	414	SER	N-CA-C	-5.74	101.03	109.81
1	A	601	SER	CB-CA-C	-5.65	108.43	115.89
1	A	622	TYR	N-CA-C	5.65	120.97	108.27
1	A	605	ILE	N-CA-C	5.59	116.22	108.84
1	A	233	PRO	N-CA-C	-5.53	106.95	113.86
1	A	291	VAL	CA-C-N	-5.46	118.10	122.85
1	A	291	VAL	C-N-CA	-5.46	118.10	122.85
1	A	608	LYS	N-CA-C	-5.35	104.34	111.24
1	A	235	MET	N-CA-C	-5.31	105.39	111.07
1	A	686	LYS	N-CA-C	5.29	119.37	113.02
1	A	251	ARG	N-CA-C	-5.26	101.59	109.95
1	A	638	ALA	N-CA-C	-5.21	105.77	111.82
1	A	223	ARG	CA-C-N	-5.19	116.05	123.11
1	A	223	ARG	C-N-CA	-5.19	116.05	123.11
1	A	626	PHE	CA-C-N	-5.18	114.88	122.19
1	A	626	PHE	C-N-CA	-5.18	114.88	122.19
1	A	66	LEU	CA-C-N	-5.17	113.94	120.56
1	A	66	LEU	C-N-CA	-5.17	113.94	120.56
1	A	471	GLN	N-CA-C	5.14	117.49	109.52
1	A	557	GLY	N-CA-C	-5.14	108.13	115.64
1	A	433	ARG	N-CA-C	-5.12	105.62	111.14
1	A	384	MET	CA-C-N	-5.09	114.01	122.11
1	A	384	MET	C-N-CA	-5.09	114.01	122.11
1	A	135	LEU	N-CA-C	-5.04	105.47	110.97
1	A	639	TYR	N-CA-C	-5.04	105.67	111.07
1	A	293	PRO	CA-C-O	-5.03	115.78	121.96

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5528	0	5416	456	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	457	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 42.

All (457) 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:HD23	1:A:63:LEU:N	1.44	1.17
1:A:72:TYR:CD1	1:A:132:MET:HE2	1.83	1.13
1:A:695:ARG:HG2	1:A:695:ARG:HH11	1.19	1.07
1:A:210:LEU:HB2	1:A:384:MET:HE2	1.41	1.03
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:TYR:CE2	1:A:604:PRO:HD3	2.05	0.91
1:A:87:ARG:HG3	1:A:87:ARG:HH11	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:130:VAL:HG13	1:A:152:MET:HE2	1.56	0.86
1:A:663:LEU:HD12	1:A:663:LEU:C	1.99	0.86
1:A:592:ILE:HG13	1:A:593:SER:H	1.40	0.86
1:A:554:ALA:C	1:A:556:SER:H	1.85	0.85
1:A:56:PHE:CD1	1:A:62:ARG:HG3	2.12	0.85
1:A:72:TYR:CE1	1:A:132:MET:HE2	2.11	0.85
1:A:592:ILE:O	1:A:593:SER:C	2.19	0.85
1:A:72:TYR:CD1	1:A:132:MET:CE	2.60	0.84
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:127:GLU:OE1	1:A:127:GLU:N	2.12	0.80
1:A:274:ARG:HG2	1:A:274:ARG:HH11	1.45	0.80
1:A:393:GLN:HB2	1:A:413:ILE:HD13	1.61	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
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:H	1:A:63:LEU:CD2	1.94	0.75
1:A:527:ARG:NH1	1:A:527:ARG:HG3	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:18:ALA:O	1:A:19:LEU:C	2.27	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:34:PHE:CE2	1:A:628:THR:HA	2.26	0.71
1:A:335:ILE:HA	1:A:342:LYS:HE2	1.72	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:87:ARG:HG3	1:A:87:ARG:NH1	2.01	0.70
1:A:102:PHE:O	1:A:102:PHE:CG	2.44	0.70
1:A:603:HIS:O	1:A:603:HIS:ND1	2.24	0.70
1:A:148:LEU:CD2	1:A:437:THR:HG22	2.21	0.69
1:A:695:ARG:CG	1:A:695:ARG:NH1	2.40	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:554:ALA:C	1:A:556:SER:N	2.46	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:88:LEU:O	1:A:89:PHE:C	2.36	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:274:ARG:HG2	1:A:274:ARG:NH1	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:108:PHE:C	1:A:108:PHE:CD1	2.72	0.67
1:A:485:TYR:CZ	1:A:604:PRO:CD	2.78	0.67
1:A:23:LEU:HD11	1:A:623:PRO:HD3	1.76	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:477:TYR:O	1:A:478:LEU:C	2.37	0.67
1:A:108:PHE:HB2	1:A:595:ILE:HD11	1.76	0.66
1:A:534:PHE:O	1:A:535:THR:C	2.39	0.66
1:A:72:TYR:CG	1:A:132:MET:HE2	2.31	0.66
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:27:ASP:C	1:A:29:ALA:H	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:HD12	1:A:620:VAL:HG11	1.80	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:421:ASN:C	1:A:421:ASN:OD1	2.39	0.64
1:A:555:ARG:O	1:A:555:ARG:HG2	1.96	0.64
1:A:102:PHE:CD2	1:A:102:PHE:C	2.75	0.63
1:A:485:TYR:CE2	1:A:604:PRO:CD	2.81	0.63
1:A:532:ASP:O	1:A:533:TYR:C	2.39	0.63
1:A:562:THR:OG1	1:A:565:MET:HG3	1.98	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:210:LEU:CB	1:A:384:MET:HE2	2.26	0.62
1:A:483:ILE:HG22	1:A:484:ALA:N	2.12	0.62
1:A:148:LEU:HD23	1:A:437:THR:CG2	2.26	0.62
1:A:403:ASN:OD1	1:A:405:ASP:HB2	1.99	0.62
1:A:80:TYR:CD1	1:A:135:LEU:HD22	2.34	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:416:ASN:C	1:A:417:LEU:HD13	2.23	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: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:370:ASP:O	1:A:371:THR:C	2.42	0.60
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:605:ILE:CG1	1:A:607:ALA:O	2.50	0.59
1:A:351:PHE:HB3	1:A:677:ASN:HD21	1.67	0.59
1:A:108:PHE:CE1	1:A:113:THR:HB	2.37	0.59
1:A:223:ARG:HH21	1:A:316:ARG:CZ	2.08	0.59
1:A:146:THR:O	1:A:149:THR:HB	2.03	0.58
1:A:294:ASP:O	1:A:295:ILE:C	2.45	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:PHE:O	1:A:369:GLU:C	2.46	0.58
1:A:27:ASP:C	1:A:29:ALA:N	2.57	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:421:ASN:O	1:A:422:ILE:C	2.45	0.58
1:A:632:LEU:O	1:A:634:MET:N	2.37	0.58
1:A:640:ASP:C	1:A:640:ASP:OD1	2.45	0.58
1:A:695:ARG:NH1	1:A:695:ARG:HG3	2.17	0.58
1:A:440:ARG:O	1:A:441:GLY:C	2.46	0.58
1:A:63:LEU:O	1:A:64:GLY:C	2.46	0.58
1:A:133:VAL:HG22	1:A:167:CYS:HB2	1.86	0.57
1:A:158:GLN:OE1	1:A:158:GLN:CA	2.51	0.57
1:A:603:HIS:O	1:A:604:PRO:O	2.21	0.57
1:A:88:LEU:C	1:A:90:GLU:N	2.61	0.57
1:A:534:PHE:O	1:A:537:TYR:N	2.32	0.56
1:A:8:ARG:O	1:A:9:VAL:C	2.48	0.56
1:A:444:ALA:O	1:A:445:VAL:C	2.46	0.56
1:A:379:ALA:O	1:A:394:VAL:HG11	2.05	0.56
1:A:88:LEU:O	1:A:90:GLU:N	2.39	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:HG2	1:A:695:ARG:NH1	2.01	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:72:TYR:CE1	1:A:132:MET:CE	2.85	0.55
1:A:54:VAL:HG22	1:A:121:ARG:NH2	2.22	0.55
1:A:539:GLN:N	1:A:539:GLN:OE1	2.39	0.55
1:A:19:LEU:CD1	1:A:39:GLN:HB3	2.31	0.55
1:A:303:ASN:OD1	1:A:303:ASN:O	2.24	0.55
1:A:158:GLN:OE1	1:A:158:GLN:C	2.50	0.55
1:A:309:PHE:N	1:A:309:PHE:CD1	2.74	0.54
1:A:295:ILE:CG2	1:A:296:THR:H	2.19	0.54
1:A:422:ILE:O	1:A:423:ALA:C	2.50	0.54
1:A:114:LEU:HB2	1:A:124:GLU:OE2	2.07	0.54
1:A:147:GLN:O	1:A:148:LEU:C	2.47	0.54
1:A:393:GLN:HB2	1:A:413:ILE:CD1	2.32	0.54
1:A:161:THR:O	1:A:162:PRO:C	2.50	0.54
1:A:192:ARG:NH1	1:A:406:TYR:HE1	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ASN:HB2	1:A:348:ARG:NH2	2.23	0.54
1:A:355:ALA:HA	1:A:358:GLN:HG3	1.88	0.54
1:A:141:ASP:C	1:A:141:ASP:OD2	2.51	0.54
1:A:237:MET:O	1:A:238:LEU:C	2.49	0.54
1:A:477:TYR:O	1:A:480:ARG:N	2.41	0.54
1:A:295:ILE:O	1:A:296:THR:C	2.51	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:174:GLU:HG3	1:A:175:LEU:H	1.73	0.53
1:A:213:ASN:OD1	1:A:323:GLY:HA3	2.08	0.53
1:A:216:GLU:OE1	1:A:310:SER:HB2	2.08	0.53
1:A:643:PRO:O	1:A:644:GLU:C	2.51	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:HG3	1:A:316:ARG:NH1	2.23	0.53
1:A:631:ASN:O	1:A:632:LEU:C	2.52	0.53
1:A:59:GLN:CG	1:A:86:LEU:CD2	2.87	0.52
1:A:603:HIS:O	1:A:604:PRO:C	2.52	0.52
1:A:313:ASP:O	1:A:314:ILE:C	2.53	0.52
1:A:632:LEU:C	1:A:634:MET:H	2.17	0.52
1:A:358:GLN:OE1	1:A:680:GLN:NE2	2.43	0.52
1:A:475:HIS:O	1:A:476:GLY:C	2.52	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:223:ARG:NH2	1:A:316:ARG:HH22	2.01	0.51
1:A:283:ILE:O	1:A:283:ILE:HG22	2.09	0.51
1:A:327:ILE:O	1:A:328:SER:C	2.52	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:197:ALA:O	1:A:198:LEU:C	2.49	0.51
1:A:16:TYR:HD2	1:A:102:PHE:CZ	2.28	0.51
1:A:555:ARG:O	1:A:555:ARG:CG	2.58	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:34:PHE:HE2	1:A:628:THR:HA	1.72	0.51
1:A:274:ARG:HH11	1:A:274:ARG:CG	2.21	0.51
1:A:562:THR:O	1:A:565:MET:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ILE:O	1:A:42:ASP:C	2.54	0.50
1:A:343:THR:HG22	1:A:344:TYR:N	2.27	0.50
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:322:PHE:CD1	1:A:322:PHE:C	2.90	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:509:SER:OG	1:A:580:ASN:ND2	2.28	0.49
1:A:316:ARG:HH11	1:A:316:ARG:CG	2.25	0.49
1:A:332:ASP:O	1:A:333:GLU:C	2.54	0.49
1:A:694:ILE:O	1:A:694:ILE:CG1	2.60	0.49
1:A:511:ARG:HD2	4:A:723:HOH:O	2.13	0.49
1:A:212:SER:OG	1:A:260:HIS:N	2.41	0.49
1:A:278:ASP:N	1:A:278:ASP:OD1	2.46	0.49
1:A:346:ASN:HD22	1:A:349:ASP:CG	2.20	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:100:GLN:C	1:A:101:THR:HG23	2.38	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
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: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:551:ALA:O	1:A:552:LEU:C	2.56	0.48
1:A:391:ILE:HA	1:A:659:GLN:OE1	2.13	0.48
1:A:321:PRO:O	1:A:322:PHE:C	2.53	0.48
1:A:40:ALA:HB1	1:A:102:PHE:CD1	2.49	0.48
1:A:72:TYR:CE1	1:A:132:MET:SD	3.07	0.48
1:A:192:ARG:HG3	1:A:400:TYR:CE1	2.49	0.48
1:A:347:ALA:O	1:A:348:ARG:C	2.55	0.48
1:A:419:SER:HA	1:A:470:GLY:O	2.14	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
1:A:531:GLY:O	1:A:532:ASP:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASP:O	1:A:28:LYS:C	2.55	0.48
1:A:16:TYR:CD2	1:A:102:PHE:CE1	3.02	0.47
1:A:77:LEU:HD22	1:A:85:VAL:HG11	1.96	0.47
1:A:349:ASP:O	1:A:352:GLN:HB3	2.14	0.47
1:A:643:PRO:C	1:A:647:ILE:HD12	2.39	0.47
1:A:127:GLU:O	1:A:128:ASP:C	2.57	0.47
1:A:144:LEU:O	1:A:145:ALA:C	2.57	0.47
1:A:562:THR:O	1:A:564:GLU:N	2.47	0.47
1:A:646:ILE:O	1:A:647:ILE:C	2.54	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:116:THR:O	1:A:117:PHE:C	2.54	0.47
1:A:157:PHE:CD2	1:A:159:PRO:HD3	2.48	0.47
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.67	0.47
1:A:41:ILE:O	1:A:44:PHE:N	2.46	0.47
1:A:86:LEU:HD23	1:A:86:LEU:HA	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:490:ALA:O	1:A:491:LEU:C	2.57	0.47
1:A:580:ASN:ND2	1:A:580:ASN:N	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:143:THR:O	1:A:144:LEU:C	2.58	0.47
1:A:231:VAL:CG2	1:A:232:ILE:N	2.77	0.46
1:A:65:THR:O	1:A:66:LEU:C	2.58	0.46
1:A:157:PHE:CE2	1:A:159:PRO:HD3	2.51	0.46
1:A:158:GLN:OE1	1:A:158:GLN:HA	2.13	0.46
1:A:428:SER:HA	1:A:429:PRO:HD2	1.66	0.46
1:A:562:THR:C	1:A:564:GLU:N	2.73	0.46
1:A:59:GLN:OE1	1:A:62:ARG:HD3	2.16	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:132:MET:O	1:A:133:VAL:C	2.58	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:148:LEU:O	1:A:149:THR:C	2.57	0.46
1:A:199:GLN:HA	1:A:199:GLN:NE2	2.31	0.46
1:A:238:LEU:O	1:A:239:GLU:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:193:ALA:O	1:A:194:VAL:C	2.59	0.46
1:A:316:ARG:HG3	1:A:316:ARG:HH11	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
1:A:308:LEU:HD23	1:A:308:LEU:N	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:510:MET:HE3	1:A:511:ARG:HG2	1.98	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:644:GLU:O	1:A:645:LYS:C	2.59	0.45
1:A:22:MET:C	1:A:24:ASN:H	2.24	0.45
1:A:24:ASN:CG	1:A:24:ASN:O	2.60	0.45
1:A:676:ILE:O	1:A:677:ASN:C	2.58	0.45
1:A:386:ASN:CG	1:A:388:CYS:H	2.24	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:44:PHE:O	1:A:45:PHE:C	2.56	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:266:ILE:O	1:A:266:ILE:HG13	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: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:560:LEU:O	1:A:561:PRO:C	2.59	0.45
1:A:669:ASP:OD1	1:A:669:ASP:N	2.48	0.45
1:A:485:TYR:CD1	1:A:485:TYR:C	2.94	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:151:GLU:CD	1:A:156:ARG:HH21	2.25	0.45
1:A:294:ASP:O	1:A:297:PHE:N	2.34	0.45
1:A:592:ILE:O	1:A:594:TYR:N	2.51	0.44
1:A:21:ALA:O	1:A:22:MET:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ASN:ND2	1:A:416:ASN:N	2.66	0.44
1:A:632:LEU:C	1:A:634:MET:N	2.74	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:512:LEU:O	1:A:513:ALA:C	2.57	0.44
1:A:138:ALA:CB	1:A:145:ALA:HB2	2.47	0.44
1:A:211:LEU:HA	1:A:211:LEU:HD23	1.40	0.44
1:A:520:PHE:CD2	1:A:581:GLN:HA	2.53	0.44
1:A:562:THR:O	1:A:563:ARG:C	2.60	0.44
1:A:45:PHE:HA	1:A:49:VAL:CB	2.48	0.44
1:A:192:ARG:HE	1:A:404:LEU:HG	1.82	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
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:84:PHE:C	1:A:86:LEU:N	2.76	0.43
1:A:417:LEU:HD13	1:A:417:LEU:N	2.33	0.43
1:A:157:PHE:CE1	1:A:438:ALA:HB1	2.53	0.43
1:A:401:ASP:HB2	1:A:407:THR:HG23	2.01	0.43
1:A:487:SER:O	1:A:488:PRO:C	2.60	0.43
1:A:156:ARG:O	1:A:420:LEU:HA	2.18	0.43
1:A:279:GLU:C	1:A:281:ILE:H	2.26	0.43
1:A:386:ASN:ND2	1:A:388:CYS:N	2.60	0.43
1:A:489:GLU:O	1:A:490:ALA:C	2.60	0.43
1:A:543:GLN:O	1:A:544:PRO:C	2.60	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:464:SER:O	1:A:465:HIS:C	2.62	0.43
1:A:677:ASN:O	1:A:681:ILE:HG13	2.17	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:103:LEU:O	1:A:104:GLY:C	2.61	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: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:299:LEU:HD12	1:A:299:LEU:HA	1.72	0.43
1:A:306:MET:HB3	1:A:306:MET:HE2	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ASN:O	1:A:347:ALA:C	2.61	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: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:603:HIS:ND1	1:A:603:HIS:C	2.76	0.42
1:A:81:ASP:O	1:A:82:ARG:C	2.62	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:395:ASN:OD1	1:A:395:ASN:C	2.62	0.42
1:A:651:ALA:O	1:A:652:GLU:C	2.62	0.42
1:A:60:HIS:O	1:A:61:GLU:C	2.61	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:428:SER:O	1:A:429:PRO:C	2.63	0.42
1:A:19:LEU:HD12	1:A:40:ALA:HA	2.01	0.42
1:A:40:ALA:O	1:A:41:ILE:C	2.60	0.42
1:A:85:VAL:O	1:A:85:VAL:HG12	2.19	0.42
1:A:118:ASP:OD1	1:A:118:ASP:C	2.62	0.42
1:A:223:ARG:HE	1:A:316:ARG:HH21	1.66	0.42
1:A:696:LEU:O	1:A:697:ARG:C	2.58	0.42
1:A:484:ALA:O	1:A:485:TYR:C	2.59	0.42
1:A:247:GLN:HG3	1:A:248:LEU:N	2.35	0.42
1:A:67:VAL:O	1:A:68:ARG:C	2.62	0.42
1:A:95:SER:OG	1:A:153:LEU:HD13	2.20	0.42
1:A:501:ILE:O	1:A:502:THR:C	2.59	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:302:GLU:O	1:A:303:ASN:C	2.63	0.42
1:A:475:HIS:CE1	1:A:605:ILE:HG22	2.54	0.42
1:A:660:GLY:C	1:A:661:LEU:HD12	2.45	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:425:VAL:C	1:A:427:ASP:N	2.77	0.41
1:A:346:ASN:ND2	1:A:349:ASP:CG	2.79	0.41
1:A:337:ASP:OD1	1:A:339:HIS:HB2	2.21	0.41
1:A:479:ALA:O	1:A:480:ARG:C	2.63	0.41
1:A:520:PHE:CD1	1:A:520:PHE:C	2.99	0.41
1:A:589:THR:O	1:A:590:GLY:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:LEU:HD23	1:A:632:LEU:HA	1.66	0.41
1:A:36:LYS:HD2	1:A:36:LYS:HA	1.76	0.41
1:A:283:ILE:HG21	1:A:286:LEU:HB2	2.03	0.41
1:A:492:ASP:HB3	1:A:549:VAL:HG21	2.02	0.41
1:A:688:ILE:N	1:A:688:ILE:HD13	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:496:LEU:HA	1:A:496:LEU:HD23	1.57	0.41
1:A:507:HIS:O	1:A:510:MET:HB3	2.21	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:CD2	1:A:400:TYR:N	2.89	0.41
1:A:514:ARG:HD2	1:A:576:TYR:CG	2.53	0.41
1:A:681:ILE:O	1:A:682:TYR:C	2.63	0.41
1:A:201:SER:O	1:A:202:LYS:C	2.64	0.40
1:A:307:ALA:HB2	1:A:344:TYR:CE1	2.56	0.40
1:A:675:ASP:O	1:A:676:ILE:C	2.64	0.40
1:A:680:GLN:O	1:A:683:ALA:HB3	2.22	0.40
1:A:84:PHE:O	1:A:85:VAL:C	2.64	0.40
1:A:49:VAL:O	1:A:50:ARG:C	2.64	0.40
1:A:125:HIS:O	1:A:126:PHE:C	2.63	0.40
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: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:68:ARG:CB	1:A:68:ARG:NH1	2.85	0.40
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.77	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%)	2	19

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
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%)	482 (83%)	97 (17%)	2 11

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	23	LEU
1	A	25	LEU
1	A	36	LYS
1	A	47	THR
1	A	49	VAL
1	A	54	VAL
1	A	58	SER
1	A	63	LEU
1	A	87	ARG
1	A	98	ARG
1	A	100	GLN
1	A	108	PHE
1	A	113	THR
1	A	114	LEU
1	A	141	ASP
1	A	143	THR
1	A	144	LEU
1	A	158	GLN
1	A	176	VAL
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

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Mol	Chain	Res	Type
1	A	235	MET
1	A	243	SER
1	A	246	ASN
1	A	247	GLN
1	A	263	HIS
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	279	GLU
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	325	ILE
1	A	327	ILE
1	A	341	ARG
1	A	376	ASN
1	A	387	LEU
1	A	390	GLU
1	A	401	ASP
1	A	413	ILE
1	A	416	ASN
1	A	417	LEU
1	A	420	LEU
1	A	421	ASN
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

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Mol	Chain	Res	Type
1	A	546	THR
1	A	558	ILE
1	A	559	THR
1	A	563	ARG
1	A	580	ASN
1	A	583	LEU
1	A	595	ILE
1	A	605	ILE
1	A	606	VAL
1	A	609	ILE
1	A	619	ARG
1	A	631	ASN
1	A	634	MET
1	A	636	GLN
1	A	637	ASP
1	A	661	LEU
1	A	663	LEU
1	A	664	THR
1	A	674	ARG
1	A	677	ASN
1	A	688	ILE
1	A	693	TYR
1	A	694	ILE
1	A	695	ARG
1	A	696	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) 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	315	GLN
1	A	346	ASN
1	A	352	GLN
1	A	358	GLN
1	A	386	ASN

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Mol	Chain	Res	Type
1	A	411	HIS
1	A	416	ASN
1	A	424	HIS
1	A	525	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 oligosaccharides 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	31,32,32	2.88	9 (29%)	46,50,50	2.52	10 (21%)

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	-	1/22/34/34	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	716	DTP	PB-O3B	-9.28	1.49	1.59
3	A	716	DTP	PB-O3A	-6.92	1.52	1.59
3	A	716	DTP	PA-O3A	-5.63	1.53	1.59
3	A	716	DTP	C5-N7	-5.17	1.29	1.39
3	A	716	DTP	C5-C4	3.96	1.46	1.39
3	A	716	DTP	C2-N1	3.36	1.39	1.33
3	A	716	DTP	C6-N6	-3.25	1.25	1.34
3	A	716	DTP	C8-N7	2.37	1.36	1.31
3	A	716	DTP	PA-O5'	-2.11	1.51	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	716	DTP	C5-C4-N3	-7.85	115.91	126.72
3	A	716	DTP	N3-C4-N9	7.58	140.05	127.17
3	A	716	DTP	N3-C2-N1	-6.90	118.13	128.58
3	A	716	DTP	C2-N3-C4	5.01	124.06	111.83
3	A	716	DTP	O4'-C1'-N9	-4.32	100.20	107.96
3	A	716	DTP	C2-N1-C6	3.00	123.65	118.73
3	A	716	DTP	C4'-O4'-C1'	2.88	116.36	109.51
3	A	716	DTP	C6-C5-C4	2.74	120.92	117.18
3	A	716	DTP	C4-N9-C8	2.32	108.18	105.74
3	A	716	DTP	C1'-N9-C8	-2.25	119.09	126.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

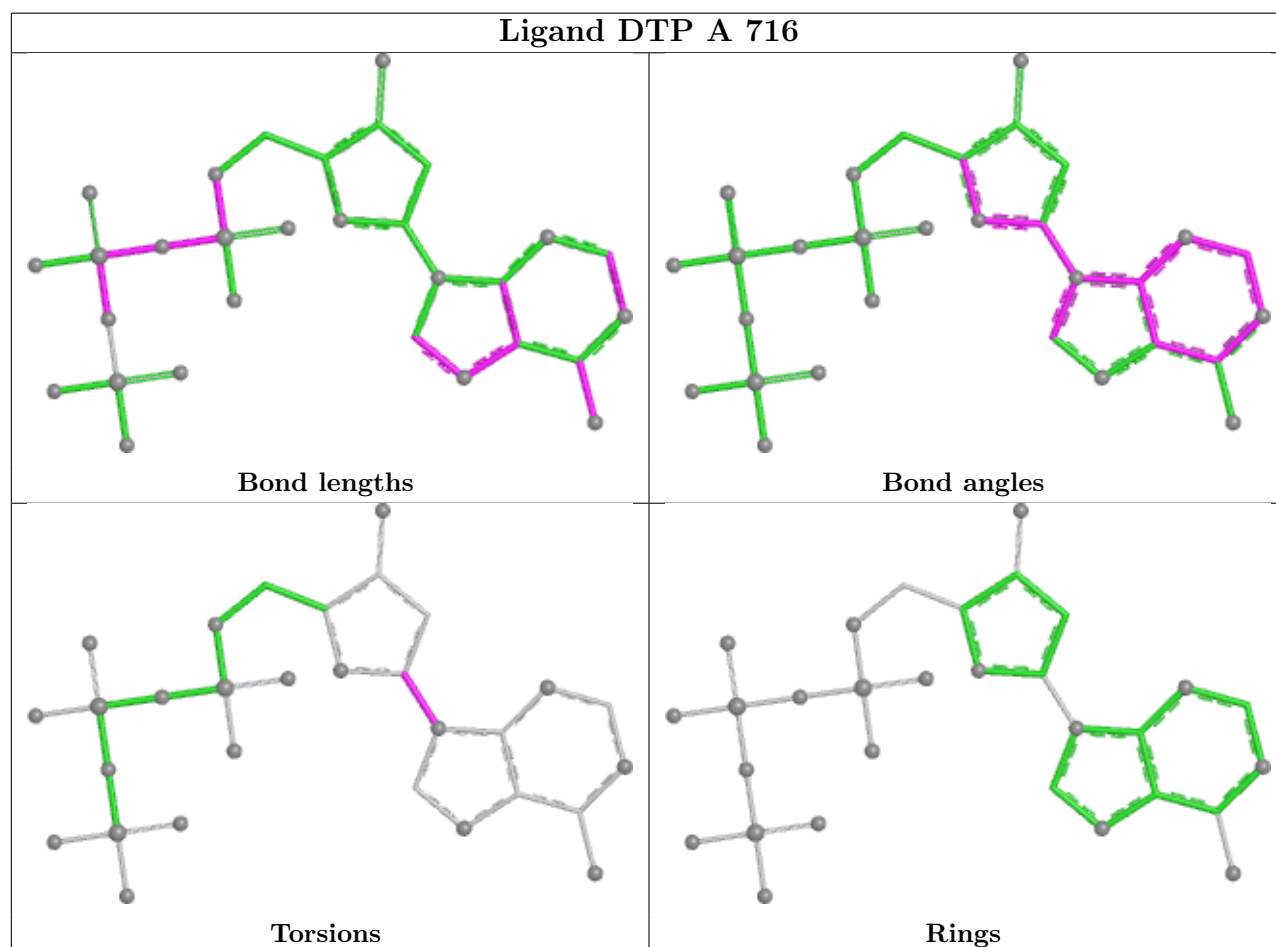
Mol	Chain	Res	Type	Atoms
3	A	716	DTP	C2'-C1'-N9-C4

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	692/714 (96%)	-0.08	14 (2%) 65 45	19, 38, 67, 119	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	699	LEU	6.2
1	A	10	MET	3.9
1	A	9	VAL	3.7
1	A	11	GLN	3.7
1	A	541	ASP	3.5
1	A	280	LYS	3.0
1	A	695	ARG	2.4
1	A	13	THR	2.3
1	A	655	ARG	2.3
1	A	698	GLN	2.3
1	A	96	GLY	2.2
1	A	281	ILE	2.1
1	A	174	GLU	2.1
1	A	8	ARG	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](#)

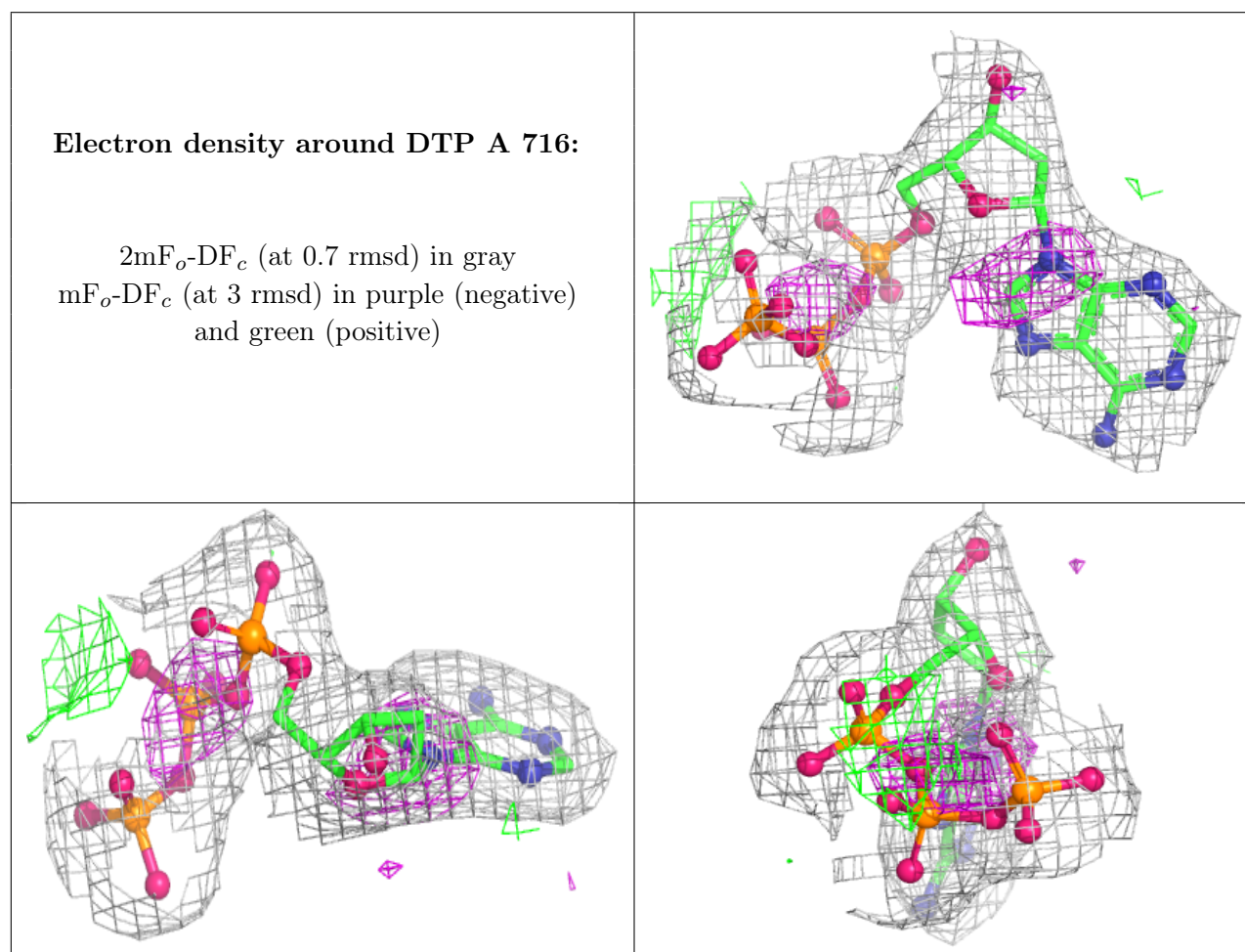
There are no oligosaccharides in this entry.

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	715	1/1	0.65	0.20	48,48,48,48	0
3	DTP	A	716	30/30	0.96	0.08	0,26,34,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.