



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:03 AM UTC

PDB ID : 7B9Q / pdb_00007b9q
Title : The SERp optimized structure of Ribonucleotide reductase from Rhodobacter sphaeroides
Authors : Loderer, C.; Feiler, C.; Wilk, P.; Kabinger, F.
Deposited on : 2020-12-14
Resolution : 2.78 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

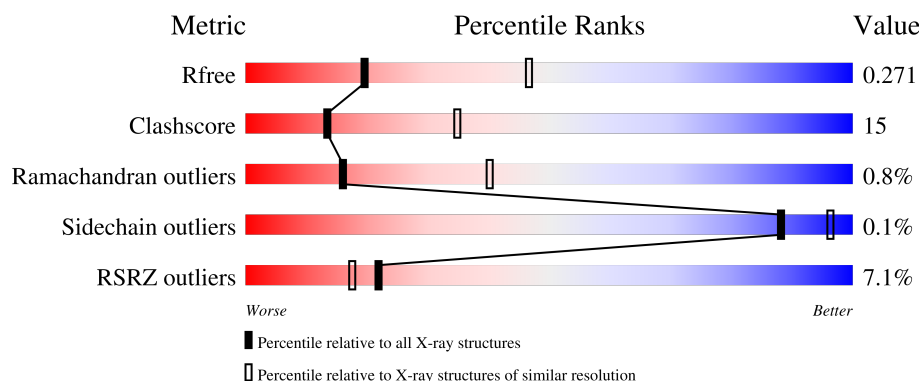
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	925	
1	B	925	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13460 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.

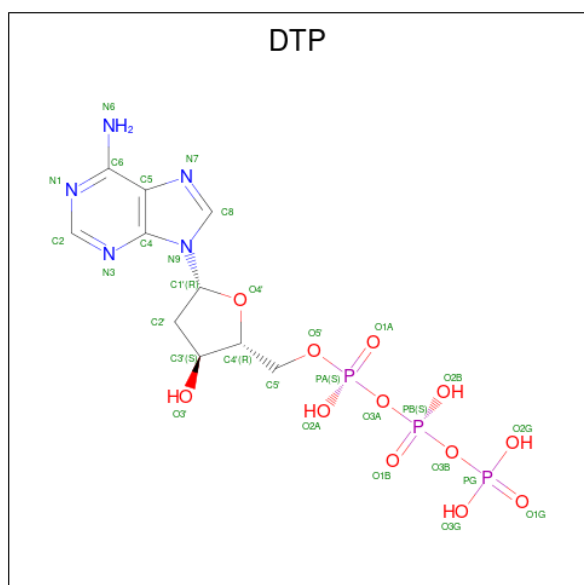
- Molecule 1 is a protein called Vitamin B12-dependent ribonucleotide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	868	Total	C	N	O	S	0	1	0
			6625	4167	1167	1255	36			
1	B	860	Total	C	N	O	S	0	0	0
			6564	4130	1160	1239	35			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	ALA	GLU	engineered mutation	UNP A0A6H2IRA4
A	97	ALA	GLU	engineered mutation	UNP A0A6H2IRA4
A	98	ALA	GLU	engineered mutation	UNP A0A6H2IRA4
B	96	ALA	GLU	engineered mutation	UNP A0A6H2IRA4
B	97	ALA	GLU	engineered mutation	UNP A0A6H2IRA4
B	98	ALA	GLU	engineered mutation	UNP A0A6H2IRA4

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$)



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	149	Total	O	0	0
			149	149		
4	B	60	Total	O	0	0
			60	60		

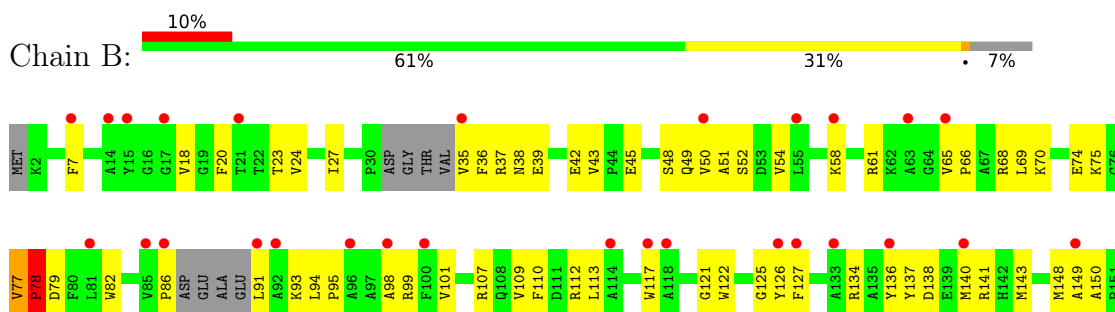
3 Residue-property plots

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: Vitamin B12-dependent ribonucleotide reductase



- Molecule 1: Vitamin B12-dependent ribonucleotide reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	161.59Å 161.59Å 97.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.59 – 2.78 46.59 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.59-2.78) 99.9 (46.59-2.78)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.220 , 0.271 0.224 , 0.271	Depositor DCC
R_{free} test set	2100 reflections (3.32%)	wwPDB-VP
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 79.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13460	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: DTP, MG

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	0.17	0/6778	0.37	1/9175 (0.0%)
1	B	0.23	1/6707 (0.0%)	0.48	4/9074 (0.0%)
All	All	0.20	1/13485 (0.0%)	0.43	5/18249 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	640	ASP	C-O	-6.73	1.20	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	VAL	C-N-CD	-8.73	89.21	125.00
1	B	78	PRO	N-CA-C	8.31	129.59	112.47
1	B	78	PRO	N-CD-CG	-8.02	91.17	103.20
1	B	78	PRO	CA-N-CD	7.46	122.44	112.00
1	A	334	GLY	N-CA-C	-5.89	108.00	115.31

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	ILE	Peptide
1	A	762	GLU	Peptide
1	B	333	GLU	Peptide
1	B	351	ALA	Peptide
1	B	408	LEU	Peptide
1	B	728	SER	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	6625	0	6435	122	2
1	B	6564	0	6387	266	2
2	A	30	0	12	1	0
2	B	30	0	12	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	149	0	0	6	0
4	B	60	0	0	9	0
All	All	13460	0	12846	384	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (384) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:VAL:CG2	1:B:78:PRO:HD2	1.52	1.37
1:B:77:VAL:HG22	1:B:78:PRO:CD	1.57	1.35
1:B:77:VAL:CG2	1:B:78:PRO:CD	2.18	1.15
1:B:408:LEU:HA	1:B:411:VAL:HG13	1.31	1.13
1:B:91:LEU:HB2	1:B:99:ARG:HD3	1.50	0.92
1:B:77:VAL:CG2	1:B:78:PRO:HD3	2.07	0.84
1:B:74:GLU:O	1:B:75:LYS:HD2	1.79	0.82
1:B:332:ILE:HG12	1:B:334:GLY:H	1.45	0.81
1:B:77:VAL:HG23	1:B:78:PRO:HD3	1.65	0.78
1:B:74:GLU:C	1:B:75:LYS:HD2	2.09	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:SER:HA	1:B:525:MET:HB3	1.65	0.78
1:B:175:PHE:HD2	1:B:531:LYS:HB3	1.46	0.77
1:B:242:GLY:HA2	1:B:250:LYS:HD3	1.68	0.75
1:A:723:ALA:H	1:A:726:GLN:HE21	1.33	0.74
1:B:610:ARG:NH1	1:B:614:THR:OG1	2.21	0.74
1:B:408:LEU:CA	1:B:411:VAL:HG13	2.16	0.73
1:B:726:GLN:HG2	1:B:729:GLN:NE2	2.03	0.73
1:B:522:SER:HB3	1:B:525:MET:HE3	1.69	0.72
1:B:352:LYS:O	1:B:353:LYS:HB3	1.89	0.71
1:B:841:LEU:HD12	1:B:844:PHE:HD2	1.54	0.71
1:B:122:TRP:CE3	1:B:127:PHE:HB2	2.25	0.71
1:B:37:ARG:NH2	1:B:39:GLU:OE2	2.24	0.70
1:B:478:GLU:OE1	1:B:673:PRO:HD3	1.92	0.69
1:B:635:GLN:NE2	4:B:1204:HOH:O	2.24	0.69
1:B:497:PHE:HB2	1:B:503:PHE:CE1	2.28	0.69
1:A:239:ARG:HH11	1:A:423:THR:HG22	1.56	0.69
1:A:332:ILE:HA	1:A:335:ALA:HB3	1.73	0.69
1:B:523:VAL:HG11	1:B:541:ARG:HA	1.75	0.68
1:A:194:PRO:HG2	1:A:525:MET:HE2	1.75	0.68
1:B:95:PRO:O	1:B:99:ARG:NE	2.27	0.68
1:A:760:GLU:HA	1:A:763:LYS:HE3	1.76	0.68
1:B:727:ILE:C	1:B:729:GLN:HB2	2.19	0.68
1:B:77:VAL:HG22	1:B:78:PRO:HD2	0.73	0.68
1:B:816:GLN:C	1:B:818:GLU:OE2	2.37	0.68
1:B:557:MET:HB3	1:B:559:LEU:CD2	2.23	0.67
1:B:140:MET:HE1	1:B:514:LEU:HB3	1.76	0.67
1:A:370:GLN:HE22	1:B:890:ILE:H	1.42	0.67
1:B:43:VAL:HG21	1:B:52:SER:HB3	1.77	0.67
1:B:557:MET:HB3	1:B:559:LEU:HD23	1.76	0.67
1:A:280:MET:HB2	1:A:475:PRO:HA	1.75	0.66
1:B:495:LEU:HB2	1:B:553:LEU:HB3	1.77	0.66
1:B:610:ARG:NH2	1:B:622:GLY:O	2.28	0.66
1:B:478:GLU:OE1	1:B:673:PRO:CD	2.43	0.66
1:A:70:LYS:HD2	1:A:87:ASP:HA	1.77	0.66
2:B:1102:DTP:O5'	4:B:1201:HOH:O	2.15	0.65
1:B:717:LEU:HD23	1:B:720:LEU:HD13	1.77	0.65
1:A:4:GLU:OE2	4:A:1101:HOH:O	2.15	0.65
1:B:610:ARG:NH1	4:B:1209:HOH:O	2.28	0.64
1:A:827:THR:HG23	1:A:829:THR:H	1.62	0.64
1:B:50:VAL:H	1:B:698:LYS:HZ3	1.44	0.64
1:B:23:THR:HG22	1:B:24:VAL:H	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:PHE:HZ	1:A:605:MET:HE1	1.62	0.63
1:B:560:GLY:HA2	1:B:843:VAL:HA	1.81	0.63
1:B:728:SER:HA	1:B:731:VAL:HG12	1.79	0.63
1:B:630:PRO:HB2	1:B:872:SER:HB3	1.80	0.63
1:B:24:VAL:HG13	1:B:39:GLU:HA	1.80	0.63
1:A:739:THR:HG23	1:A:764:ILE:O	1.99	0.63
1:B:607:ARG:HH21	1:B:610:ARG:HD3	1.64	0.63
1:A:763:LYS:NZ	1:A:764:ILE:HB	2.13	0.63
1:B:613:ARG:HB3	1:B:651:TRP:HB3	1.80	0.63
1:B:411:VAL:HG23	1:B:412:LYS:CG	2.28	0.62
1:B:77:VAL:HG23	1:B:78:PRO:CD	2.18	0.62
1:A:221:GLU:HG2	1:A:231:THR:HG21	1.80	0.62
1:B:420:VAL:O	1:B:422:ARG:NH1	2.33	0.62
1:A:323:ALA:O	1:A:327:SER:OG	2.17	0.62
1:B:411:VAL:HG23	1:B:412:LYS:HG3	1.80	0.62
1:B:341:ASN:OD1	1:B:342:ALA:N	2.33	0.61
1:B:641:PRO:HD2	1:B:643:LEU:HD12	1.83	0.61
1:B:814:ARG:O	1:B:816:GLN:N	2.33	0.61
1:B:273:THR:HG22	1:B:274:THR:H	1.66	0.61
1:B:699:LYS:HA	1:B:705:TYR:H	1.64	0.61
1:B:138:ASP:OD1	1:B:141:ARG:NH2	2.34	0.61
1:A:739:THR:N	1:A:824:VAL:HG23	2.16	0.61
1:B:79:ASP:HA	1:B:82:TRP:CE2	2.35	0.61
1:B:421:ARG:HG3	1:B:428:ALA:HB2	1.82	0.61
1:A:488:ASN:HD22	1:A:522:SER:HB2	1.67	0.60
1:B:354:ALA:O	4:B:1202:HOH:O	2.16	0.60
1:B:816:GLN:HA	1:B:818:GLU:OE2	2.01	0.60
1:A:421:ARG:HG3	1:A:428:ALA:HB2	1.83	0.60
1:B:196:PRO:HG3	1:B:522:SER:HB2	1.83	0.60
1:A:333:GLU:HA	1:A:336:THR:HG23	1.83	0.60
1:B:65:VAL:HG13	1:B:101:VAL:HG13	1.84	0.59
1:B:402:ARG:NH1	1:B:470:ILE:O	2.35	0.59
1:B:49:GLN:NE2	1:B:700:LEU:HD12	2.17	0.59
1:B:317:LYS:HD2	1:B:350:ALA:O	2.01	0.59
1:A:363:ARG:NH2	1:B:915:SER:O	2.31	0.59
1:B:143:MET:HE1	1:B:511:ALA:HA	1.84	0.59
1:B:497:PHE:HB3	1:B:504:ASP:HB3	1.85	0.59
1:A:27:ILE:HG22	1:A:36:PHE:HD1	1.68	0.59
1:B:20:PHE:HE1	1:B:42:GLU:HB3	1.68	0.58
1:B:171:SER:HB2	1:B:190:ALA:HB2	1.84	0.58
1:A:402:ARG:NH2	4:A:1106:HOH:O	2.29	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:818:GLU:OE2	1:B:818:GLU:N	2.37	0.58
1:A:221:GLU:OE2	4:A:1102:HOH:O	2.17	0.58
1:B:150:ALA:HB1	1:B:156:TRP:HE1	1.68	0.58
1:A:742:ASN:HB2	1:A:823:HIS:NE2	2.19	0.58
1:B:280:MET:HB2	1:B:475:PRO:HA	1.84	0.58
1:B:79:ASP:HA	1:B:82:TRP:CD2	2.39	0.58
1:B:613:ARG:HA	1:B:616:ALA:HB3	1.86	0.58
1:A:489:LEU:HD22	1:A:670:VAL:HG11	1.86	0.58
1:B:700:LEU:HG	1:B:701:ALA:H	1.68	0.58
1:B:27:ILE:C	1:B:27:ILE:HD12	2.29	0.57
1:B:698:LYS:HD2	1:B:699:LYS:H	1.69	0.57
1:B:50:VAL:N	1:B:698:LYS:HZ3	2.01	0.57
1:A:273:THR:HG22	1:A:274:THR:H	1.69	0.57
1:A:768:LEU:N	1:A:769:PRO:HD2	2.20	0.57
1:A:239:ARG:HH21	2:A:1001:DTP:H5'1	1.69	0.57
1:A:733:TYR:CE2	1:A:827:THR:HG21	2.39	0.57
1:A:71:ARG:NH1	1:A:82:TRP:O	2.37	0.57
2:B:1102:DTP:H2'2	4:B:1201:HOH:O	2.04	0.57
1:A:668:VAL:HG13	1:A:669:THR:HG23	1.86	0.57
1:B:201:ILE:O	1:B:484:ASP:N	2.36	0.56
1:B:61:ARG:HB2	1:B:157:PHE:HE1	1.70	0.56
1:A:28:ARG:HG3	1:A:35:VAL:HG23	1.88	0.56
1:A:4:GLU:H	1:A:4:GLU:CD	2.13	0.55
1:B:722:TYR:HB3	1:B:727:ILE:HD11	1.87	0.55
1:A:738:GLY:O	1:A:739:THR:OG1	2.20	0.55
1:B:156:TRP:NE1	1:B:677:ILE:HD11	2.20	0.55
1:A:304:VAL:O	1:A:308:VAL:HG23	2.06	0.55
1:B:152:ASN:HD22	1:B:154:PRO:HG2	1.72	0.55
1:B:707:LYS:NZ	1:B:768:LEU:HB3	2.21	0.55
1:B:841:LEU:HD12	1:B:844:PHE:CD2	2.39	0.55
1:A:184:LEU:HD21	1:A:531:LYS:HB3	1.88	0.55
1:B:18:VAL:HG13	1:B:45:GLU:HG2	1.87	0.54
1:B:584:THR:HG22	1:B:588:MET:HE2	1.88	0.54
1:A:745:THR:HG22	1:A:746:ILE:HG12	1.89	0.54
1:B:325:ILE:HG23	1:B:344:LEU:HD13	1.88	0.54
1:A:321:ILE:O	1:A:325:ILE:HG13	2.07	0.54
1:B:321:ILE:HG12	1:B:347:ALA:HB1	1.88	0.54
1:B:585:SER:HA	1:B:588:MET:HE3	1.89	0.54
1:B:117:TRP:HD1	1:B:525:MET:HE1	1.72	0.54
1:B:7:PHE:HZ	1:B:507:GLY:HA3	1.73	0.54
1:B:834:PRO:HB2	1:B:835:HIS:ND1	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:729:GLN:HB3	1:B:730:ILE:HG13	1.90	0.53
1:A:520:GLU:OE2	1:A:541:ARG:NH1	2.41	0.53
1:A:417:TRP:N	1:A:431:ILE:O	2.40	0.53
1:A:613:ARG:NH1	1:A:652:ASP:OD1	2.42	0.53
1:B:136:TYR:OH	1:B:518:THR:HB	2.08	0.53
1:B:325:ILE:HA	1:B:341:ASN:HD21	1.74	0.53
1:B:820:ALA:O	1:B:824:VAL:HG12	2.08	0.53
1:A:414:ASP:HB2	1:A:434:ARG:HH21	1.73	0.53
1:B:39:GLU:CD	1:B:39:GLU:H	2.16	0.53
1:A:383:ASP:HB2	1:A:386:SER:OG	2.08	0.52
1:B:77:VAL:CB	1:B:78:PRO:HD2	2.21	0.52
1:A:607:ARG:HG3	1:A:624:GLU:HB2	1.91	0.52
1:B:161:LEU:H	1:B:161:LEU:HD12	1.74	0.52
1:B:513:ARG:NH1	1:B:587:GLU:OE1	2.38	0.52
1:B:515:TRP:HA	1:B:518:THR:HG22	1.91	0.52
1:B:698:LYS:HD2	1:B:699:LYS:N	2.25	0.52
1:A:359:THR:HB	1:B:917:LEU:HD23	1.92	0.52
1:A:485:THR:HG22	1:A:536:LEU:HB3	1.92	0.52
1:B:48:SER:O	1:B:52:SER:OG	2.25	0.52
1:B:203:SER:HB3	1:B:483:ASP:HB3	1.92	0.52
1:B:54:VAL:O	1:B:58:LYS:HB2	2.10	0.51
1:B:374:SER:OG	1:B:375:ILE:N	2.41	0.51
1:B:519:LEU:HB3	1:B:543:LEU:HD22	1.93	0.51
1:B:134:ARG:HA	1:B:137:TYR:HB3	1.92	0.51
1:B:193:HIS:HB3	1:B:527:GLN:HB2	1.93	0.51
1:B:467:ASP:OD2	1:B:600:ARG:NH1	2.42	0.51
1:B:152:ASN:ND2	1:B:154:PRO:HG2	2.26	0.51
1:B:896:ALA:O	1:B:900:SER:OG	2.26	0.51
1:A:263:ARG:NH1	1:A:390:THR:O	2.37	0.51
1:B:332:ILE:HG12	1:B:334:GLY:N	2.21	0.51
1:A:710:ASN:HB3	1:A:713:VAL:HG23	1.93	0.51
1:B:50:VAL:HG22	1:B:698:LYS:HE2	1.93	0.51
1:B:613:ARG:HB3	1:B:651:TRP:CB	2.41	0.51
1:A:476:CYS:HB2	1:A:478:GLU:OE1	2.11	0.51
1:B:49:GLN:NE2	1:B:700:LEU:HA	2.26	0.51
1:B:49:GLN:HB3	1:B:698:LYS:NZ	2.26	0.50
1:B:66:PRO:HG2	1:B:69:LEU:HD11	1.93	0.50
1:A:24:VAL:HG22	1:A:39:GLU:HA	1.93	0.50
1:A:595:PHE:CZ	1:A:605:MET:HE1	2.45	0.50
1:B:66:PRO:HB2	1:B:69:LEU:HD11	1.93	0.50
1:A:203:SER:HB3	1:A:483:ASP:HB3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ALA:HB2	1:A:911:TYR:HD1	1.76	0.50
1:B:727:ILE:CA	1:B:729:GLN:HB2	2.42	0.50
1:A:140:MET:HE3	1:A:514:LEU:HB3	1.94	0.50
1:B:168:ASP:OD1	1:B:169:GLY:N	2.45	0.50
1:B:454:PHE:CE1	1:B:901:HIS:HB2	2.47	0.50
1:A:763:LYS:HZ2	1:A:764:ILE:HB	1.76	0.50
1:B:478:GLU:OE1	1:B:673:PRO:HD2	2.11	0.50
1:A:66:PRO:HG2	1:A:69:LEU:HD21	1.94	0.50
1:A:463:THR:HB	1:A:605:MET:HE2	1.93	0.50
1:A:129:THR:HG23	1:A:132:ASP:H	1.77	0.49
1:A:739:THR:CG2	1:A:764:ILE:HG12	2.42	0.49
1:A:770:SER:HB3	1:A:825:CYS:HB3	1.93	0.49
1:A:402:ARG:NH1	1:A:470:ILE:O	2.44	0.49
1:B:208:LEU:N	4:B:1201:HOH:O	2.45	0.49
1:A:437:TRP:CE2	1:A:894:LEU:HD22	2.47	0.49
1:B:713:VAL:HA	1:B:716:ALA:HB3	1.93	0.49
1:B:122:TRP:HE3	1:B:127:PHE:HD2	1.59	0.49
1:B:437:TRP:CE2	1:B:894:LEU:HD22	2.47	0.49
1:B:637:ASN:OD1	4:B:1203:HOH:O	2.19	0.49
1:B:109:VAL:O	1:B:113:LEU:HG	2.13	0.49
1:B:68:ARG:C	1:B:69:LEU:HD22	2.38	0.49
1:B:112:ARG:NH1	1:B:157:PHE:O	2.44	0.49
1:A:698:LYS:HE3	1:A:699:LYS:O	2.12	0.49
1:B:816:GLN:CA	1:B:818:GLU:OE2	2.61	0.49
1:B:824:VAL:HG13	1:B:825:CYS:SG	2.53	0.49
1:A:488:ASN:ND2	1:A:522:SER:HB2	2.27	0.48
1:B:335:ALA:O	1:B:344:LEU:HD22	2.12	0.48
1:A:739:THR:HG23	1:A:764:ILE:CG1	2.43	0.48
1:A:739:THR:OG1	1:A:768:LEU:HD12	2.13	0.48
1:A:36:PHE:CE1	1:A:57:GLN:HG2	2.48	0.48
1:B:323:ALA:HA	1:B:326:ARG:NH2	2.29	0.48
1:B:833:ALA:HB3	1:B:836:LEU:HD22	1.94	0.48
1:B:843:VAL:HG23	1:B:844:PHE:CE1	2.49	0.48
1:A:235:PHE:HB3	1:A:254:LEU:HD11	1.95	0.48
1:B:109:VAL:HA	1:B:112:ARG:HG2	1.95	0.48
1:A:698:LYS:HA	1:A:698:LYS:HD2	1.76	0.47
1:A:723:ALA:O	1:A:727:ILE:HG12	2.14	0.47
1:B:156:TRP:CD1	1:B:677:ILE:HD11	2.49	0.47
1:B:336:THR:HG21	1:B:369:ARG:HG3	1.96	0.47
1:A:162:HIS:HD2	4:A:1234:HOH:O	1.97	0.47
1:A:1:MET:HE3	1:A:1:MET:HB2	1.70	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:871:GLN:NE2	1:B:878:ILE:HG13	2.30	0.47
1:B:202:GLN:O	1:B:233:THR:HG23	2.15	0.47
1:B:398:ASN:ND2	4:B:1214:HOH:O	2.37	0.47
1:B:739:THR:N	1:B:824:VAL:HG23	2.29	0.47
1:B:122:TRP:C	1:B:125:GLY:H	2.23	0.47
1:B:154:PRO:HG3	1:B:198:ALA:HB2	1.96	0.47
1:B:667:GLN:NE2	1:B:875:SER:HB3	2.31	0.46
1:A:75[B]:LYS:HA	1:A:75[B]:LYS:HD3	1.54	0.46
1:A:328:PHE:CD2	1:A:335:ALA:HB2	2.51	0.46
1:B:402:ARG:HH22	1:B:470:ILE:HG22	1.79	0.46
1:B:730:ILE:HG21	1:B:830:LEU:HG	1.96	0.46
1:A:761:ILE:HG13	1:A:762:GLU:N	2.31	0.46
1:B:94:LEU:HD22	1:B:98:ALA:HB1	1.97	0.46
1:A:40:SER:HB3	1:A:104:THR:OG1	2.14	0.46
1:B:122:TRP:HB2	1:B:127:PHE:CD2	2.51	0.46
1:B:27:ILE:HD12	1:B:35:VAL:N	2.30	0.46
1:B:27:ILE:CG1	1:B:36:PHE:HB3	2.45	0.46
1:B:841:LEU:CD1	1:B:844:PHE:HD2	2.27	0.46
1:B:351:ALA:C	1:B:352:LYS:O	2.58	0.46
1:B:517:VAL:O	1:B:521:ILE:HG13	2.16	0.46
1:B:713:VAL:HG12	1:B:714:PRO:HD3	1.98	0.46
1:B:867:MET:HE3	1:B:905:ILE:HD13	1.97	0.46
1:A:859:SER:O	1:A:862:SER:OG	2.28	0.46
1:B:27:ILE:CD1	1:B:35:VAL:N	2.79	0.46
1:B:613:ARG:NH1	1:B:652:ASP:OD1	2.49	0.46
1:B:695:VAL:C	1:B:696:LYS:HG3	2.41	0.46
1:A:88:GLU:CD	1:A:88:GLU:H	2.24	0.45
1:B:252:SER:OG	2:B:1102:DTP:H2	2.16	0.45
1:B:559:LEU:HB2	1:B:565:GLU:OE2	2.16	0.45
1:B:93:LYS:HA	1:B:93:LYS:HD3	1.75	0.45
1:B:411:VAL:HG23	1:B:412:LYS:HG2	1.99	0.45
1:B:875:SER:O	1:B:906:LYS:NZ	2.50	0.45
1:B:77:VAL:HG11	1:B:122:TRP:HB3	1.98	0.45
1:B:107:ARG:HA	1:B:110:PHE:HB2	1.97	0.45
1:A:44:PRO:HB2	1:A:47:TRP:CD1	2.52	0.45
1:A:225:PHE:O	1:A:270:SER:HA	2.17	0.45
1:B:328:PHE:HE2	1:B:340:GLY:O	1.99	0.45
1:B:322:PHE:O	1:B:326:ARG:HG2	2.17	0.45
1:B:709:ILE:HB	1:B:735:VAL:HG11	1.99	0.45
1:B:257:PHE:HA	1:B:260:ILE:HD12	1.99	0.45
1:A:478:GLU:HB2	1:A:670:VAL:HG22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:SER:OG	1:B:49:GLN:N	2.50	0.45
1:A:70:LYS:NZ	1:A:88:GLU:OE2	2.45	0.45
1:A:206:ASP:OD2	1:A:239:ARG:HG3	2.17	0.45
1:B:408:LEU:HA	1:B:411:VAL:CG1	2.23	0.45
1:B:820:ALA:O	1:B:824:VAL:N	2.43	0.45
1:B:194:PRO:HD2	1:B:525:MET:HG3	1.99	0.44
1:B:224:LEU:HD23	1:B:231:THR:HB	1.98	0.44
1:B:325:ILE:HA	1:B:335:ALA:HB1	1.98	0.44
1:A:742:ASN:OD1	1:A:742:ASN:N	2.51	0.44
1:B:286:ASP:CG	1:B:422:ARG:HH22	2.26	0.44
1:B:323:ALA:HA	1:B:326:ARG:CZ	2.48	0.44
1:B:370:GLN:HB2	1:B:372:PHE:HD2	1.82	0.44
1:B:560:GLY:CA	1:B:843:VAL:HA	2.46	0.44
1:B:95:PRO:C	1:B:99:ARG:HE	2.25	0.44
1:B:280:MET:CG	1:B:282:ILE:HD11	2.48	0.44
1:A:66:PRO:HD2	1:A:165:TYR:HB3	1.99	0.44
1:A:454:PHE:CZ	1:A:901:HIS:HB2	2.53	0.44
1:A:578:THR:OG1	1:A:873:PHE:O	2.32	0.44
1:B:122:TRP:O	1:B:125:GLY:N	2.50	0.44
1:B:489:LEU:CD2	1:B:670:VAL:HG21	2.48	0.44
1:B:658:GLY:HA3	1:B:663:TYR:CZ	2.52	0.44
1:B:707:LYS:HZ3	1:B:768:LEU:HB3	1.83	0.44
1:A:315:GLU:HG2	1:A:319:ASN:HD21	1.83	0.44
1:B:48:SER:OG	1:B:698:LYS:CE	2.66	0.44
1:B:143:MET:HB3	1:B:148:MET:HB3	2.00	0.44
1:B:573:LEU:HD21	1:B:643:LEU:HD13	1.99	0.44
1:A:871:GLN:HE22	1:A:877:ALA:HA	1.83	0.44
1:B:831:GLU:HA	1:B:841:LEU:HD21	1.99	0.44
1:A:488:ASN:OD1	1:A:488:ASN:N	2.41	0.44
1:B:161:LEU:HB3	1:B:167:ILE:HD12	1.99	0.44
1:A:341:ASN:HB3	1:A:344:LEU:HB3	2.00	0.43
1:A:528:PHE:HB2	1:A:534:ALA:HB2	1.99	0.43
1:A:733:TYR:O	1:A:827:THR:HG22	2.18	0.43
1:A:738:GLY:C	1:A:739:THR:HG1	2.21	0.43
1:B:700:LEU:HG	1:B:701:ALA:N	2.31	0.43
1:B:813:THR:O	1:B:814:ARG:HG3	2.18	0.43
1:A:889:THR:O	1:A:893:THR:HG23	2.19	0.43
1:B:320:ASP:O	1:B:323:ALA:HB3	2.19	0.43
1:A:58:LYS:HA	1:A:58:LYS:HD3	1.86	0.43
1:A:232:GLY:HA3	1:A:473:SER:O	2.18	0.43
1:A:682:ASP:OD1	4:A:1103:HOH:O	2.21	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:GLY:O	1:B:332:ILE:HD12	2.19	0.43
1:B:411:VAL:HG23	1:B:412:LYS:N	2.32	0.43
1:B:434:ARG:O	1:B:438:ASP:N	2.50	0.43
1:A:370:GLN:NE2	1:B:890:ILE:H	2.12	0.43
1:A:740:LEU:O	1:A:764:ILE:HD11	2.19	0.43
1:A:561:TYR:CD1	1:A:690:PRO:HB3	2.54	0.43
1:A:739:THR:HA	1:A:767:ALA:HB3	2.01	0.43
1:B:575:ALA:HA	1:B:873:PHE:HB3	2.01	0.43
1:B:208:LEU:HB2	4:B:1201:HOH:O	2.18	0.43
1:B:559:LEU:HD12	1:B:565:GLU:HB2	2.00	0.43
1:B:122:TRP:O	1:B:122:TRP:CD1	2.72	0.43
1:B:350:ALA:HA	1:B:353:LYS:HD3	2.00	0.43
1:B:384:TRP:HA	1:B:389:TYR:CD2	2.53	0.43
1:B:621:THR:HG22	1:B:622:GLY:H	1.83	0.43
1:A:713:VAL:HB	1:A:714:PRO:HD3	2.00	0.42
1:A:860:VAL:HG13	1:A:882:ILE:HG21	2.00	0.42
1:B:39:GLU:OE2	1:B:39:GLU:N	2.52	0.42
1:B:48:SER:HG	1:B:50:VAL:HG22	1.84	0.42
1:B:833:ALA:HB3	1:B:836:LEU:CD2	2.48	0.42
1:B:48:SER:OG	1:B:50:VAL:HG22	2.20	0.42
1:B:126:TYR:CE1	1:B:592:LEU:HD12	2.53	0.42
1:B:196:PRO:HG2	1:B:197:HIS:CE1	2.54	0.42
1:B:325:ILE:HD12	1:B:326:ARG:N	2.34	0.42
1:B:403:VAL:HG11	1:B:452:ILE:HD11	2.01	0.42
1:A:454:PHE:CE1	1:A:901:HIS:HB2	2.54	0.42
1:B:77:VAL:HG21	1:B:122:TRP:CD2	2.54	0.42
1:B:183:LYS:HG3	1:B:185:GLN:HG2	2.01	0.42
1:B:255:MET:HG3	1:B:292:GLN:HB3	2.00	0.42
1:B:460:ALA:HB1	1:B:626:VAL:HA	2.00	0.42
1:B:494:LEU:HD23	1:B:494:LEU:HA	1.81	0.42
1:B:554:LEU:C	1:B:557:MET:HB2	2.44	0.42
1:A:366:GLN:HE21	1:A:366:GLN:HB2	1.59	0.42
1:B:239:ARG:HA	1:B:422:ARG:HB2	2.00	0.42
1:B:557:MET:HB3	1:B:559:LEU:HD21	2.00	0.42
1:A:423:THR:OG1	1:A:424:ASP:N	2.53	0.42
1:B:121:GLY:HA2	1:B:521:ILE:HD13	2.01	0.42
1:B:489:LEU:HD22	1:B:670:VAL:HG21	2.02	0.42
1:A:308:VAL:HG12	1:A:312:LYS:HE3	2.01	0.42
1:A:416:ASP:OD1	1:A:432:LYS:NZ	2.35	0.42
1:B:86:PRO:HD3	1:B:166:GLY:HA3	2.02	0.42
1:B:375:ILE:HD12	1:B:375:ILE:HA	1.89	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:HIS:HB3	1:B:527:GLN:HG2	2.02	0.42
1:A:1:MET:HE2	1:A:587:GLU:HG2	2.02	0.42
1:A:120:TRP:CD1	1:A:525:MET:HE3	2.55	0.42
1:B:522:SER:O	1:B:526:ALA:HB2	2.20	0.42
1:A:739:THR:HG23	1:A:764:ILE:C	2.45	0.41
1:B:384:TRP:HB3	1:B:918:SER:OG	2.20	0.41
1:B:877:ALA:HB2	1:B:906:LYS:HB2	2.02	0.41
1:A:420:VAL:O	1:A:422:ARG:NH2	2.35	0.41
1:A:437:TRP:NE1	1:A:894:LEU:HD22	2.34	0.41
1:A:824:VAL:HG13	1:A:825:CYS:SG	2.60	0.41
1:B:27:ILE:HG12	1:B:36:PHE:HB3	2.02	0.41
1:B:70:LYS:HA	1:B:70:LYS:HD3	1.81	0.41
1:B:810:LEU:C	1:B:812:PHE:H	2.27	0.41
1:B:322:PHE:HE2	1:B:375:ILE:HB	1.85	0.41
1:B:677:ILE:O	1:B:681:MET:HG3	2.20	0.41
1:B:716:ALA:O	1:B:720:LEU:HD12	2.20	0.41
1:A:378:PRO:HD2	1:B:302:GLN:OE1	2.20	0.41
1:A:442:HIS:NE2	1:B:367:TYR:OH	2.42	0.41
1:B:136:TYR:CZ	1:B:140:MET:HE2	2.56	0.41
1:B:49:GLN:HE22	1:B:700:LEU:HD12	1.84	0.41
1:B:695:VAL:HG21	1:B:828:MET:HE3	2.03	0.41
1:B:817:ILE:N	1:B:818:GLU:OE2	2.53	0.41
1:B:51:ALA:HA	1:B:680:VAL:HA	2.03	0.41
1:A:734:ALA:HA	1:A:827:THR:HG22	2.03	0.41
1:B:389:TYR:OH	1:B:917:LEU:HB2	2.19	0.41
1:B:463:THR:HG21	1:B:666:ALA:O	2.21	0.41
1:B:193:HIS:O	1:B:527:GLN:NE2	2.54	0.41
1:B:233:THR:HB	1:B:235:PHE:CE1	2.56	0.41
1:B:667:GLN:CD	1:B:875:SER:HB3	2.46	0.41
1:B:77:VAL:HG21	1:B:122:TRP:CG	2.56	0.41
1:B:710:ASN:C	1:B:712:SER:H	2.29	0.41
1:A:4:GLU:OE1	1:A:4:GLU:N	2.52	0.41
1:B:561:TYR:CD2	1:B:690:PRO:HB3	2.56	0.41
1:B:643:LEU:HD23	1:B:643:LEU:HA	1.91	0.41
1:A:860:VAL:O	1:A:864:ILE:HG13	2.22	0.40
1:B:157:PHE:O	1:B:161:LEU:HD11	2.21	0.40
1:B:730:ILE:HA	1:B:733:TYR:HB3	2.03	0.40
1:B:65:VAL:HG23	1:B:165:TYR:HB3	2.03	0.40
1:A:600:ARG:NH2	4:A:1120:HOH:O	2.44	0.40
1:B:94:LEU:HD22	1:B:98:ALA:CB	2.51	0.40
1:B:175:PHE:CD2	1:B:531:LYS:HB3	2.39	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:THR:HB	1:B:677:ILE:HG22	2.03	0.40
1:B:810:LEU:HD23	1:B:810:LEU:HA	1.88	0.40
1:A:760:GLU:HG3	1:A:763:LYS:NZ	2.36	0.40
1:B:149:ALA:HA	1:B:492:MET:HA	2.03	0.40
1:B:726:GLN:HA	1:B:729:GLN:HG3	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:TYR:O	1:B:813:THR:OG1[2_545]	1.80	0.40
1:A:742:ASN:ND2	1:B:424:ASP:O[3_554]	2.03	0.17

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	861/925 (93%)	825 (96%)	32 (4%)	4 (0%)	24	52
1	B	844/925 (91%)	777 (92%)	58 (7%)	9 (1%)	11	32
All	All	1705/1850 (92%)	1602 (94%)	90 (5%)	13 (1%)	16	40

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	740	LEU
1	B	38	ASN
1	B	78	PRO
1	B	701	ALA
1	B	729	GLN
1	B	815	ALA
1	A	332	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	333	GLU
1	A	330	GLY
1	B	352	LYS
1	A	333	GLU
1	B	769	PRO
1	B	721	GLY

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	674/718 (94%)	674 (100%)	0	100	100
1	B	669/718 (93%)	668 (100%)	1 (0%)	88	96
All	All	1343/1436 (94%)	1342 (100%)	1 (0%)	88	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	353	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	A	319	ASN
1	A	362	ASN
1	A	370	GLN
1	A	395	GLN
1	A	398	ASN
1	A	399	ASN
1	A	409	GLN
1	A	453	GLN
1	A	726	GLN
1	A	748	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	835	HIS
1	A	871	GLN
1	A	883	ASN
1	B	49	GLN
1	B	147	GLN
1	B	185	GLN
1	B	193	HIS
1	B	195	GLN
1	B	210	ASN
1	B	292	GLN
1	B	395	GLN
1	B	604	HIS
1	B	635	GLN
1	B	886	ASN

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
2	DTP	B	1102	3	31,32,32	0.64	0	46,50,50	0.62	0
2	DTP	A	1001	3	31,32,32	0.57	0	46,50,50	0.63	0

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
2	DTP	B	1102	3	-	3/22/34/34	0/3/3/3
2	DTP	A	1001	3	-	2/22/34/34	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1102	DTP	C5'-O5'-PA-O1A
2	B	1102	DTP	C5'-O5'-PA-O3A
2	A	1001	DTP	C5'-O5'-PA-O1A
2	B	1102	DTP	C5'-O5'-PA-O2A
2	A	1001	DTP	PA-O3A-PB-O2B

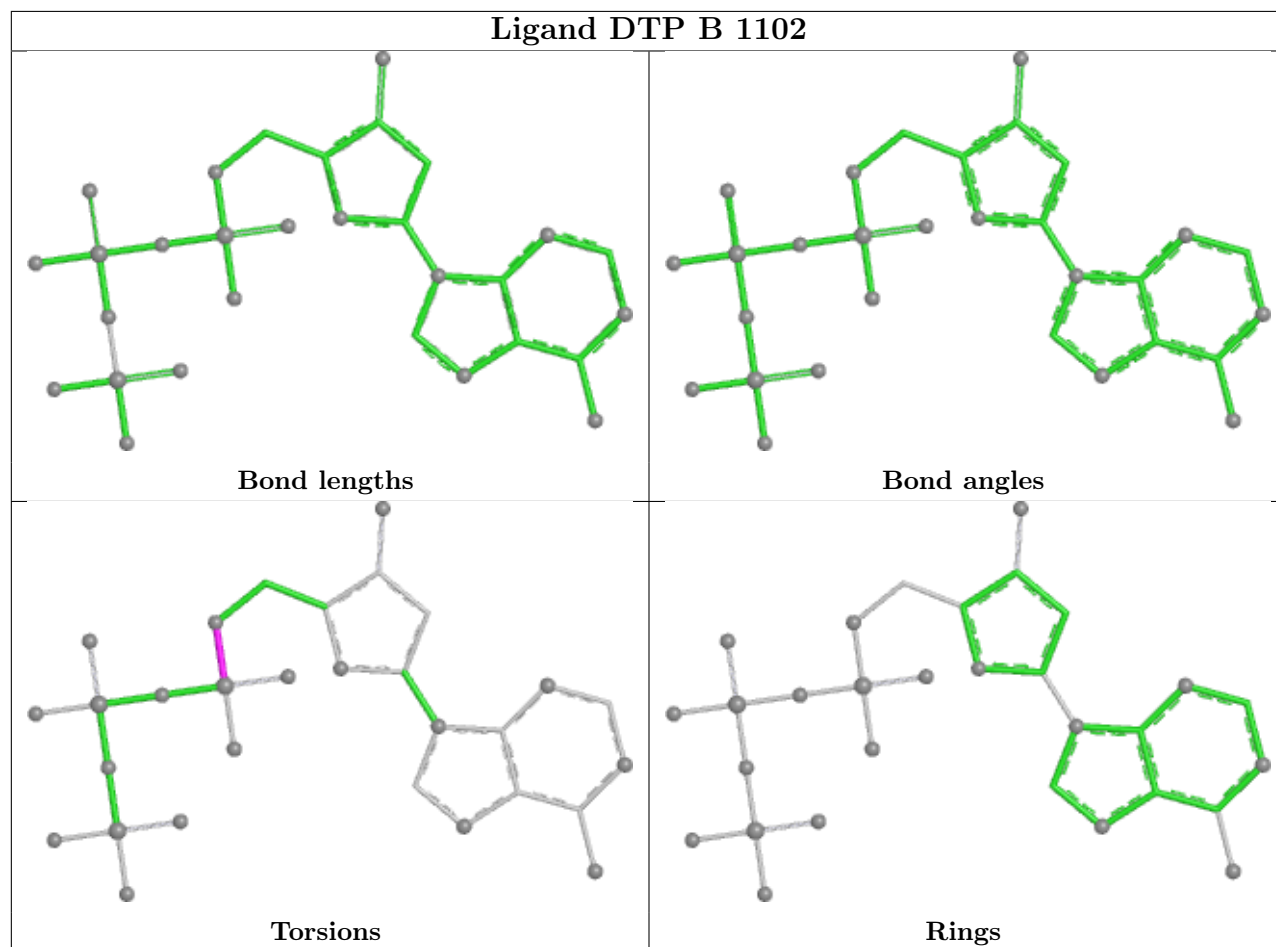
There are no ring outliers.

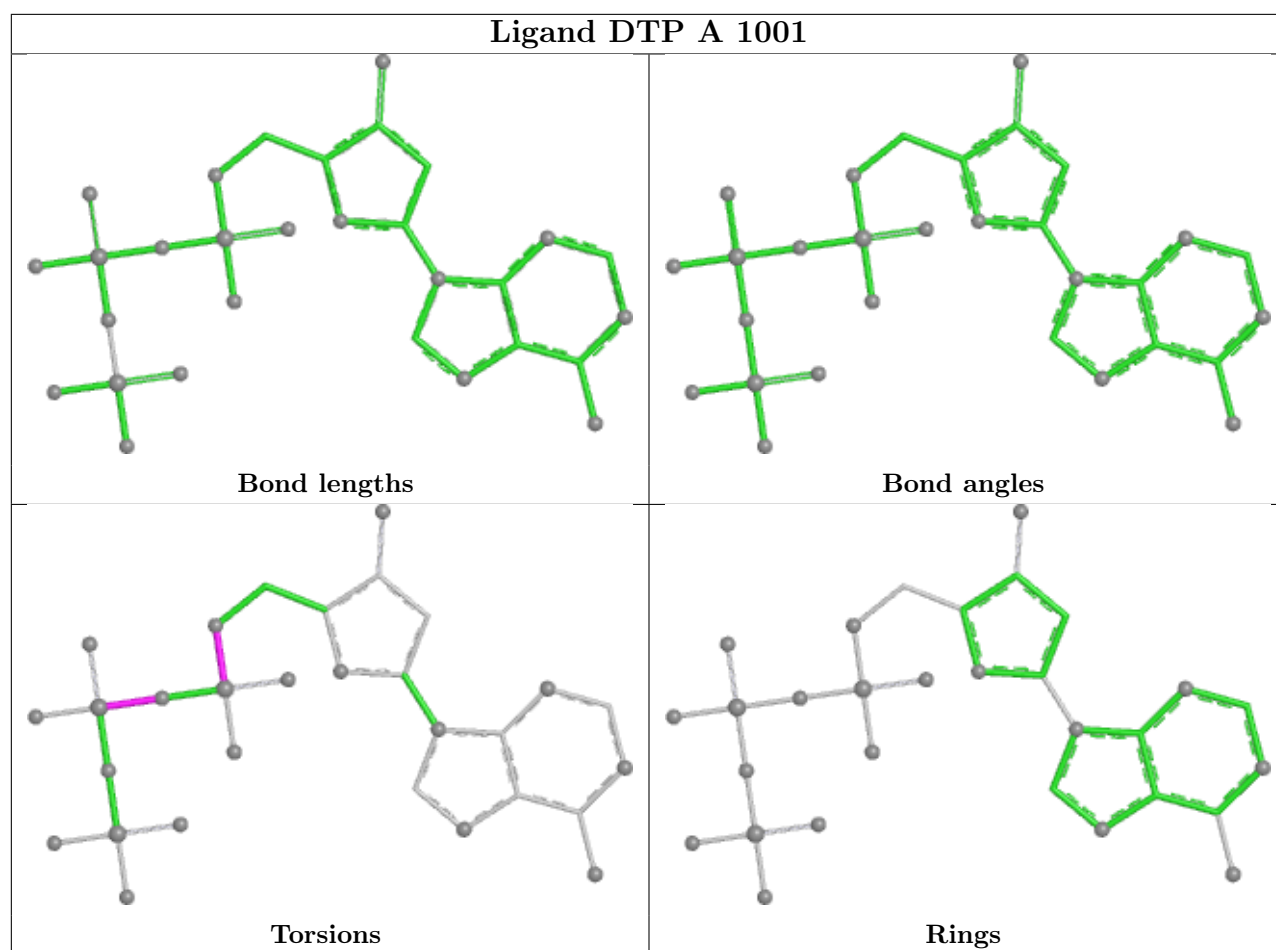
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1102	DTP	3	0
2	A	1001	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	868/925 (93%)	-0.03	32 (3%)	45	38	37, 65, 139, 214	1 (0%)
1	B	860/925 (92%)	0.77	90 (10%)	11	9	52, 115, 172, 216	0
All	All	1728/1850 (93%)	0.37	122 (7%)	22	17	37, 89, 163, 216	1 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	746	ILE	6.6
1	B	750	ALA	6.4
1	B	812	PHE	6.0
1	B	495	LEU	4.3
1	B	763	LYS	4.3
1	B	810	LEU	4.2
1	B	86	PRO	4.1
1	A	30	PRO	4.1
1	A	741	ALA	4.0
1	B	149	ALA	4.0
1	B	136	TYR	4.0
1	B	117	TRP	3.9
1	A	745	THR	3.5
1	B	140	MET	3.5
1	B	330	GLY	3.5
1	B	621	THR	3.5
1	B	873	PHE	3.5
1	B	411	VAL	3.4
1	B	336	THR	3.4
1	A	624	GLU	3.4
1	B	63	ALA	3.4
1	B	133	ALA	3.4
1	B	100	PHE	3.3
1	B	447	CYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	814	ARG	3.2
1	B	641	PRO	3.2
1	A	820	ALA	3.2
1	A	274	THR	3.2
1	A	756	PHE	3.2
1	B	503	PHE	3.1
1	B	118	ALA	3.1
1	A	622	GLY	3.1
1	B	114	ALA	3.1
1	B	81	LEU	3.0
1	A	277	ALA	3.0
1	B	14	ALA	3.0
1	B	672	ALA	3.0
1	A	772	PHE	3.0
1	B	493	ASN	3.0
1	B	342	ALA	3.0
1	B	21	THR	2.9
1	A	920	PRO	2.9
1	B	273	THR	2.9
1	B	91	LEU	2.9
1	B	768	LEU	2.9
1	A	273	THR	2.8
1	B	701	ALA	2.8
1	B	836	LEU	2.8
1	B	157	PHE	2.8
1	B	679	LEU	2.8
1	B	744	PRO	2.8
1	A	818	GLU	2.8
1	A	766	ALA	2.7
1	B	523	VAL	2.7
1	B	58	LYS	2.7
1	A	740	LEU	2.7
1	B	329	ASP	2.7
1	A	332	ILE	2.6
1	A	767	ALA	2.6
1	B	85	VAL	2.6
1	A	769	PRO	2.6
1	A	771	ALA	2.6
1	B	766	ALA	2.6
1	B	165	TYR	2.6
1	B	373	SER	2.5
1	B	17	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	50	VAL	2.5
1	B	774	ILE	2.5
1	A	404	THR	2.4
1	B	500	ALA	2.4
1	B	725	ALA	2.4
1	A	621	THR	2.4
1	B	274	THR	2.4
1	B	740	LEU	2.4
1	B	408	LEU	2.4
1	B	127	PHE	2.4
1	B	542	THR	2.4
1	A	1	MET	2.4
1	B	488	ASN	2.3
1	B	199	CYS	2.3
1	B	811	GLY	2.3
1	A	748	HIS	2.3
1	B	555	MET	2.3
1	A	819	ALA	2.3
1	B	96	ALA	2.3
1	B	681	MET	2.3
1	B	126	TYR	2.2
1	B	35	VAL	2.2
1	B	98	ALA	2.2
1	B	164	ALA	2.2
1	B	492	MET	2.2
1	B	526	ALA	2.2
1	A	199	CYS	2.2
1	B	813	THR	2.2
1	B	65	VAL	2.2
1	B	384	TRP	2.2
1	A	896	ALA	2.2
1	B	686	THR	2.2
1	B	497	PHE	2.2
1	B	15	TYR	2.2
1	A	823	HIS	2.2
1	B	7	PHE	2.2
1	B	919	GLN	2.1
1	B	175	PHE	2.1
1	B	769	PRO	2.1
1	A	325	ILE	2.1
1	A	744	PRO	2.1
1	B	700	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	92	ALA	2.1
1	A	623	TYR	2.1
1	B	325	ILE	2.1
1	B	412	LYS	2.0
1	B	152	ASN	2.0
1	A	591	GLU	2.0
1	B	741	ALA	2.0
1	B	773	ASP	2.0
1	B	909	ALA	2.0
1	B	55	LEU	2.0
1	B	910	LEU	2.0
1	B	174	HIS	2.0
1	B	817	ILE	2.0
1	B	547	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

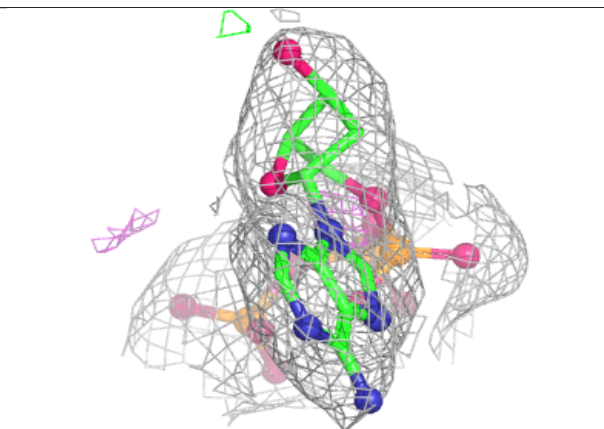
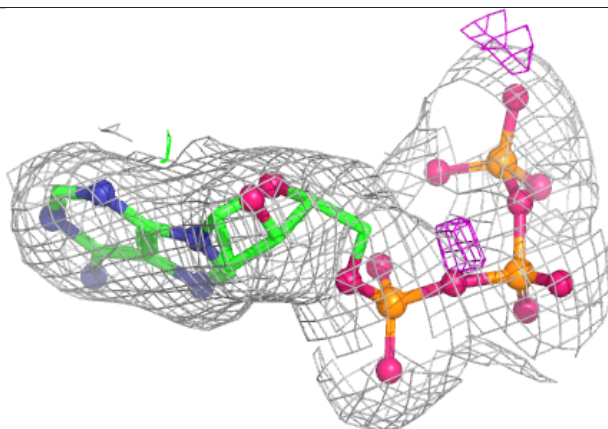
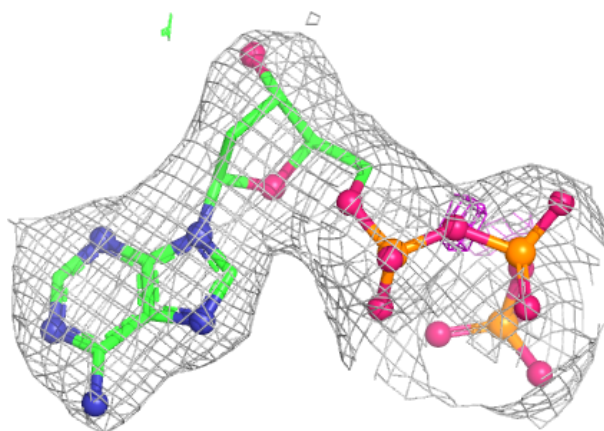
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DTP	B	1102	30/30	0.95	0.07	54,71,106,109	0
2	DTP	A	1001	30/30	0.96	0.08	49,74,101,106	0
3	MG	B	1101	1/1	0.98	0.06	49,49,49,49	0
3	MG	A	1002	1/1	0.99	0.04	39,39,39,39	0

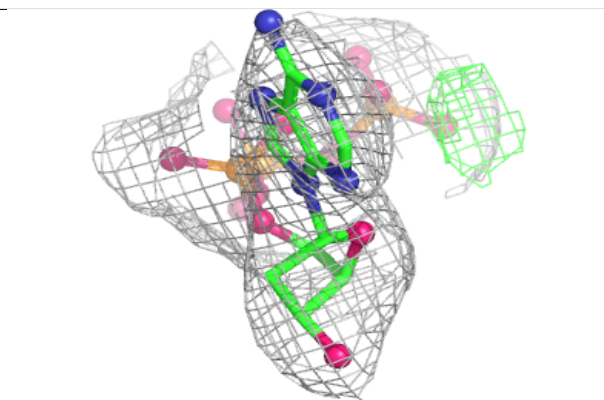
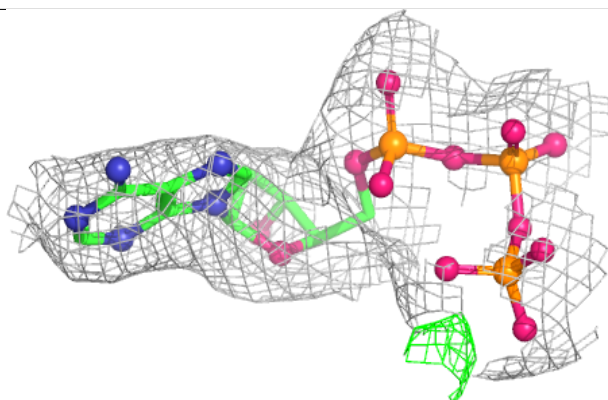
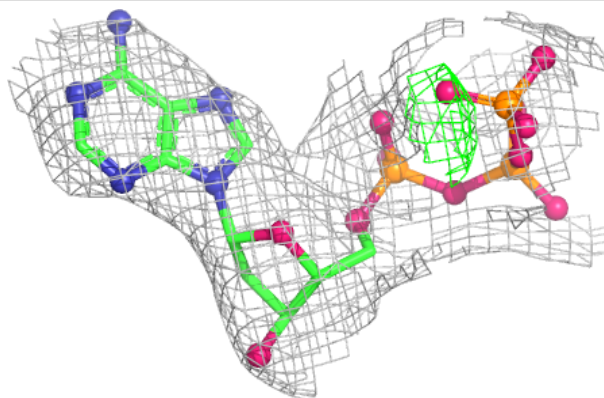
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DTP B 1102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around DTP A 1001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.