Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 01:39 AM EDT

PDB ID	:	6WYB
Title	:	RTX (Reverse Transcription Xenopolymerase) in complex with an RNA/DNA hybrid
Authors	:	Choi, W.S.; He, P.; Pothukuchy, A.; Gollihar, J.; Ellington, A.D.; Yang, W.
Deposited on	:	2020-05-12
Resolution	:	2.50 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:

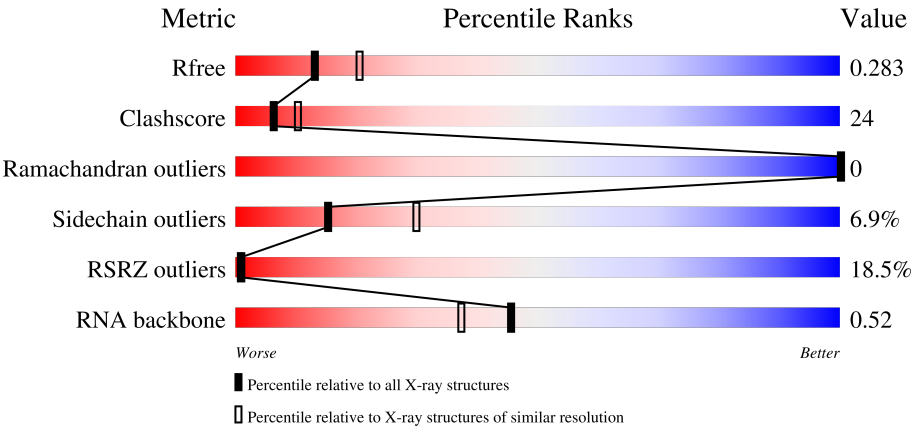
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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 <=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	774	18% 60% 33% • 5%
2	B	16	25% 31% 12% 31%
3	C	13	8% 54% 38% 8%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6527 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 DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	739	5870	3787	987	1080	16	0	2	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	LEU	PHE	conflict	UNP D0VWU9
A	97	MET	ARG	conflict	UNP D0VWU9
A	118	ILE	LYS	conflict	UNP D0VWU9
A	137	LEU	MET	conflict	UNP D0VWU9
A	147	HIS	GLU	conflict	UNP D0VWU9
A	210	ASP	ASN	conflict	UNP D0VWU9
A	381	HIS	ARG	conflict	UNP D0VWU9
A	384	HIS	TYR	conflict	UNP D0VWU9
A	389	ILE	VAL	conflict	UNP D0VWU9
A	466	ARG	LYS	conflict	UNP D0VWU9
A	493	LEU	TYR	conflict	UNP D0VWU9
A	514	ILE	THR	conflict	UNP D0VWU9
A	521	LEU	ILE	conflict	UNP D0VWU9
A	584	LYS	GLU	conflict	UNP D0VWU9
A	587	LEU	PHE	conflict	UNP D0VWU9
A	664	LYS	GLU	conflict	UNP D0VWU9
A	711	VAL	GLY	conflict	UNP D0VWU9
A	735	LYS	ASN	conflict	UNP D0VWU9
A	768	ARG	TRP	conflict	UNP D0VWU9

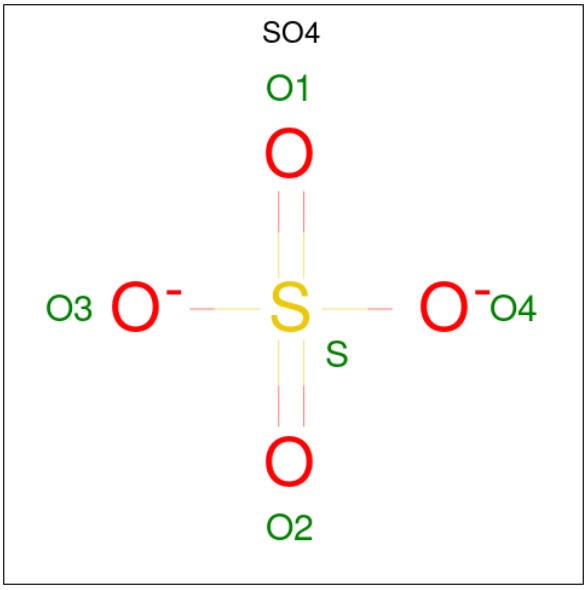
- Molecule 2 is a RNA chain called RNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	11	234	105	44	74	11	0	0	0

- Molecule 3 is a DNA chain called DNA strand.

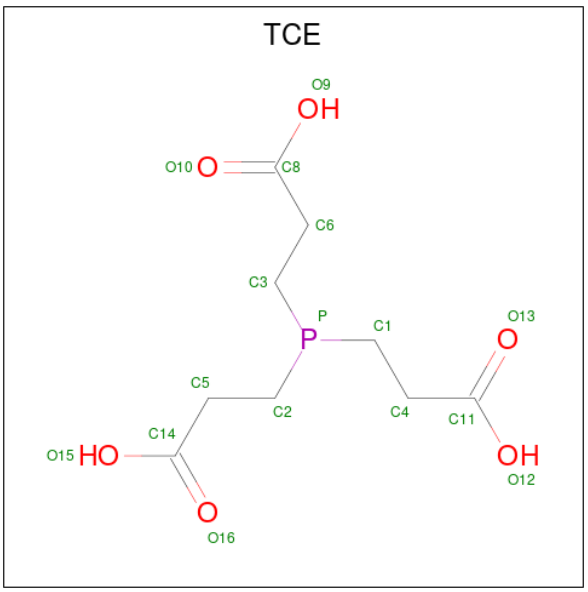
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			243	117	42	73	11			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



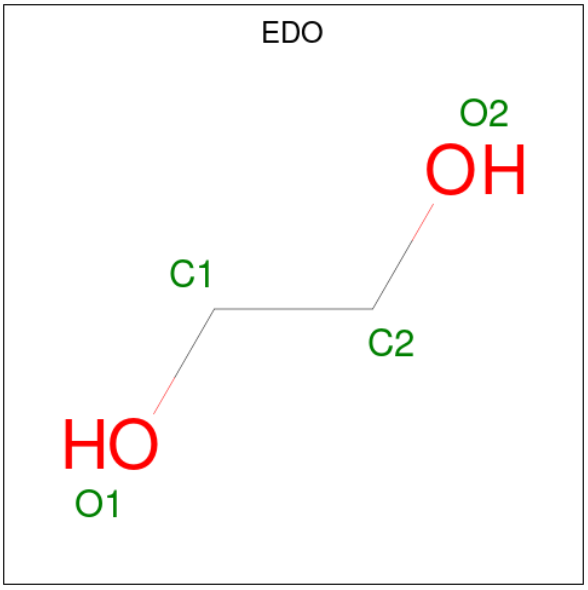
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 3,3',3''-phosphanetriyltripropanoic acid (three-letter code: TCE) (formula: $C_9H_{15}O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			16	9	6	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

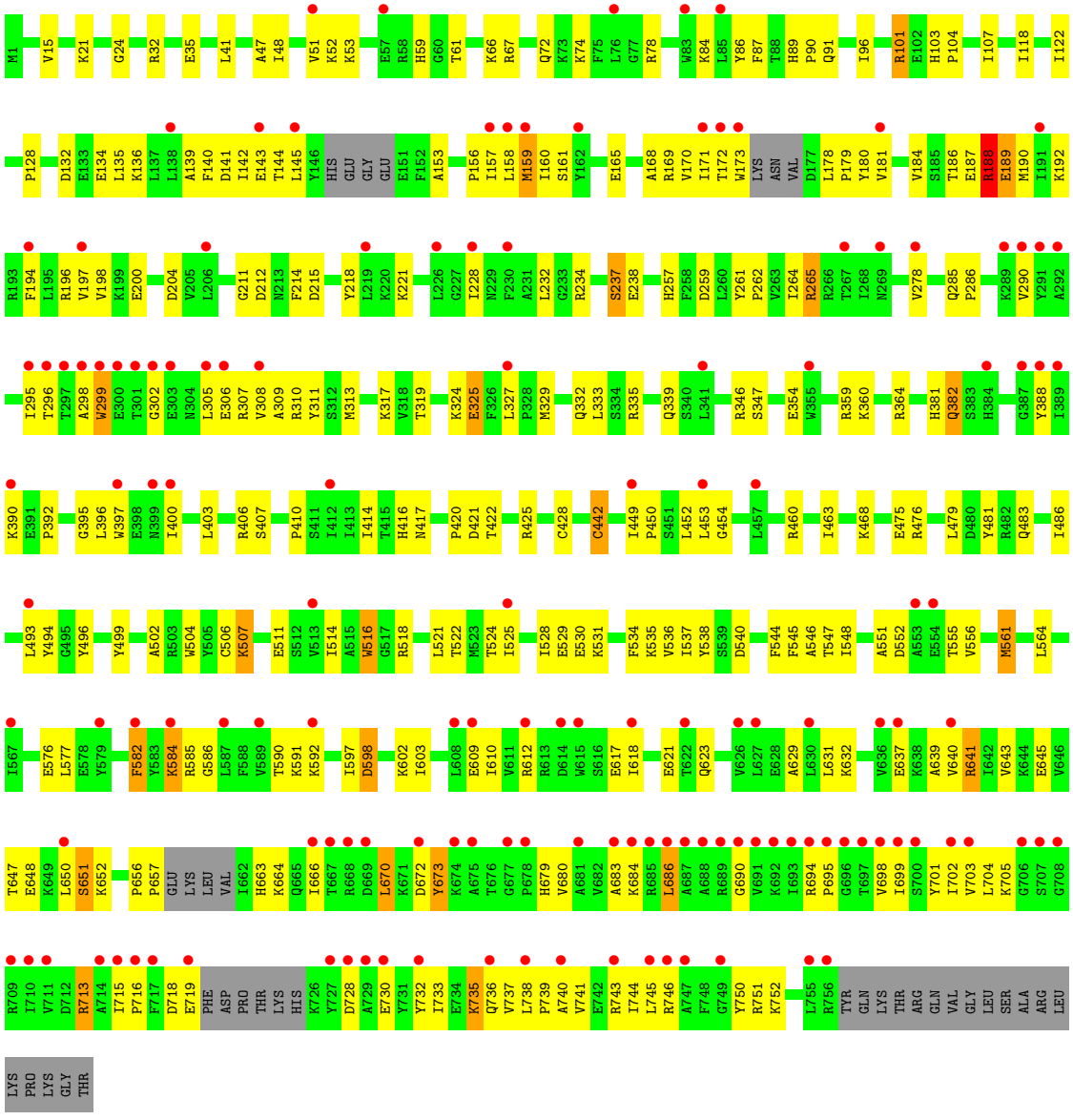
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	139	Total	O	0	0
			139	139		
7	B	3	Total	O	0	0
			3	3		
7	C	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

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

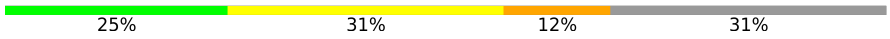
- Molecule 1: DNA polymerase

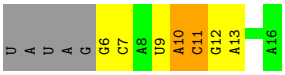
Chain A:



- Molecule 2: RNA strand

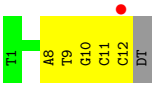
Chain B:





• Molecule 3: DNA strand

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.97Å 112.94Å 148.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 2.50 89.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.97-2.50) 88.6 (89.91-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.267 , 0.283 0.264 , 0.283	Depositor DCC
R_{free} test set	989 reflections (2.45%)	wwPDB-VP
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 58.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6527	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, TCE, SO4

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	0.46	0/5995	0.62	2/8118 (0.0%)
2	B	0.48	0/261	1.29	3/404 (0.7%)
3	C	0.63	0/271	0.99	0/417
All	All	0.47	0/6527	0.68	5/8939 (0.1%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	327	LEU	C-N-CD	5.78	140.54	128.40
1	A	584	LYS	CD-CE-NZ	-5.62	98.77	111.70
2	B	6	G	N9-C4-C5	-5.09	103.36	105.40
2	B	6	G	C6-C5-N7	-5.05	127.37	130.40
2	B	6	G	N3-C4-N9	5.01	129.01	126.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	ARG	Mainchain

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	5870	0	5775	295	2
2	B	234	0	121	4	0
3	C	243	0	138	5	0
4	A	5	0	0	0	0
5	A	16	0	12	1	0
6	A	16	0	24	3	0
7	A	139	0	0	37	1
7	B	3	0	0	0	1
7	C	1	0	0	0	0
All	All	6527	0	6070	302	3

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 24.

All (302) 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:145:LEU:HD21	1:A:156:PRO:HD2	1.24	1.17
1:A:670:LEU:CD2	1:A:684:LYS:HA	1.76	1.16
1:A:738:LEU:HD21	1:A:752:LYS:HD3	1.35	1.08
1:A:650:LEU:HD13	1:A:733:ILE:HG21	1.31	1.07
1:A:670:LEU:HD23	1:A:684:LYS:HA	1.10	1.06
1:A:395:GLY:O	7:A:902:HOH:O	1.75	1.02
1:A:178:LEU:HB2	1:A:306:GLU:OE1	1.59	1.01
1:A:172:THR:OG1	1:A:299:TRP:HZ2	1.43	1.01
1:A:623:GLN:NE2	7:A:904:HOH:O	1.90	1.01
1:A:145:LEU:O	1:A:145:LEU:HD12	1.64	0.96
1:A:172:THR:OG1	1:A:299:TRP:CZ2	2.20	0.94
1:A:156:PRO:HB3	1:A:187:GLU:OE2	1.68	0.93
1:A:156:PRO:CB	1:A:187:GLU:OE2	2.18	0.92
1:A:157:ILE:N	1:A:187:GLU:OE1	2.02	0.92
1:A:629:ALA:O	7:A:903:HOH:O	1.89	0.89
1:A:141:ASP:HB3	7:A:907:HOH:O	1.72	0.88
1:A:686:LEU:O	1:A:690:GLY:N	2.07	0.87
1:A:101:ARG:HH21	1:A:101:ARG:HG2	1.37	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:HD21	1:A:156:PRO:CD	2.04	0.86
1:A:212:ASP:N	7:A:908:HOH:O	2.07	0.86
1:A:670:LEU:HD23	1:A:684:LYS:CA	2.03	0.85
5:A:802:TCE:O16	7:A:905:HOH:O	1.94	0.85
1:A:416:HIS:CD2	1:A:516:TRP:CE2	2.65	0.85
1:A:673:TYR:OH	3:C:8:DA:OP2	1.93	0.85
1:A:597:ILE:HB	1:A:603:ILE:HG22	1.59	0.85
1:A:743:ARG:HH12	1:A:746:ARG:NH1	1.74	0.84
1:A:651:SER:O	1:A:652:LYS:HG3	1.75	0.84
1:A:158:LEU:HG	1:A:299:TRP:CD1	2.12	0.83
1:A:666:ILE:HG13	1:A:699:ILE:HD11	1.59	0.83
1:A:178:LEU:CB	1:A:306:GLU:OE1	2.27	0.82
1:A:299:TRP:HA	1:A:299:TRP:CE3	2.13	0.81
6:A:804:EDO:H12	7:A:906:HOH:O	1.79	0.81
1:A:66:LYS:HG2	1:A:67:ARG:HG2	1.63	0.81
1:A:738:LEU:HD21	1:A:752:LYS:CD	2.11	0.80
1:A:178:LEU:HD22	1:A:179:PRO:HD2	1.64	0.78
1:A:145:LEU:CD2	1:A:156:PRO:HD2	2.12	0.77
1:A:142:ILE:HG22	1:A:160:ILE:HG12	1.67	0.76
1:A:738:LEU:CD2	1:A:752:LYS:HD3	2.13	0.75
1:A:159:MET:CE	1:A:308:VAL:HG12	2.16	0.75
1:A:170:VAL:HB	1:A:181:VAL:HG22	1.69	0.75
1:A:618:ILE:HG21	1:A:657:PRO:HB2	1.69	0.74
1:A:388:TYR:HD2	1:A:521:LEU:HD23	1.50	0.74
1:A:325:GLU:OE2	7:A:906:HOH:O	2.03	0.74
1:A:157:ILE:O	1:A:190:MET:CE	2.36	0.74
1:A:132:ASP:HB3	6:A:806:EDO:O1	1.87	0.73
1:A:145:LEU:HB3	1:A:158:LEU:HD11	1.69	0.73
1:A:159:MET:HB3	1:A:172:THR:HB	1.69	0.73
1:A:143:GLU:OE2	7:A:907:HOH:O	2.05	0.73
1:A:172:THR:HG1	1:A:299:TRP:HZ2	1.20	0.73
1:A:597:ILE:HG21	1:A:631:LEU:HB3	1.71	0.73
6:A:804:EDO:C1	7:A:906:HOH:O	2.35	0.73
1:A:397:TRP:O	1:A:585:ARG:HG3	1.89	0.72
1:A:703:VAL:HG13	1:A:713:ARG:HG3	1.71	0.72
1:A:744:ILE:HG13	7:A:988:HOH:O	1.89	0.71
1:A:299:TRP:HA	1:A:299:TRP:HE3	1.51	0.71
1:A:189[A]:GLU:OE2	1:A:189[A]:GLU:HA	1.91	0.70
1:A:290:VAL:HB	1:A:311:TYR:CB	2.21	0.70
1:A:663:HIS:HB3	1:A:698:VAL:HG22	1.72	0.70
1:A:640:VAL:HG21	1:A:750:TYR:CG	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:HIS:ND1	1:A:90:PRO:HD2	2.07	0.70
1:A:157:ILE:O	1:A:190:MET:HE1	1.91	0.70
1:A:178:LEU:HG	1:A:306:GLU:OE1	1.91	0.69
1:A:673:TYR:OH	3:C:8:DA:P	2.51	0.69
1:A:180:TYR:CE1	1:A:181:VAL:HG23	2.28	0.69
1:A:552:ASP:O	1:A:556:VAL:HG23	1.92	0.68
1:A:670:LEU:CD2	1:A:684:LYS:CA	2.64	0.68
1:A:178:LEU:CG	1:A:306:GLU:OE1	2.43	0.67
1:A:582:PHE:CE1	7:A:1005:HOH:O	2.47	0.67
1:A:78:ARG:NH2	7:A:909:HOH:O	2.23	0.67
1:A:158:LEU:HD21	1:A:296:THR:HA	1.75	0.67
1:A:738:LEU:HD11	1:A:752:LYS:HB3	1.76	0.66
1:A:305:LEU:C	1:A:305:LEU:HD23	2.15	0.66
1:A:650:LEU:HD13	1:A:733:ILE:CG2	2.18	0.66
1:A:101:ARG:HG2	1:A:101:ARG:NH2	2.10	0.65
1:A:360:LYS:HD2	1:A:364:ARG:HH11	1.60	0.65
1:A:159:MET:HE3	1:A:308:VAL:HG12	1.78	0.65
1:A:496:TYR:HE2	1:A:504:TRP:HB2	1.61	0.65
1:A:158:LEU:HB3	1:A:299:TRP:HE1	1.62	0.65
2:B:11:C:H2'	2:B:12:G:C8	2.32	0.64
1:A:702:ILE:HG13	1:A:715:ILE:HB	1.78	0.64
1:A:743:ARG:NH1	1:A:746:ARG:HG3	2.12	0.64
1:A:89:HIS:CG	1:A:90:PRO:HD2	2.33	0.63
1:A:663:HIS:CB	1:A:698:VAL:HG22	2.28	0.63
1:A:159:MET:HE1	1:A:308:VAL:HG12	1.78	0.63
1:A:169:ARG:HG2	1:A:180:TYR:O	1.98	0.63
1:A:158:LEU:CB	1:A:299:TRP:HE1	2.11	0.63
1:A:592:LYS:NZ	2:B:7:C:O2	2.31	0.63
1:A:738:LEU:HB3	1:A:739:PRO:HD3	1.80	0.63
1:A:670:LEU:HD21	1:A:684:LYS:HA	1.78	0.62
1:A:265:ARG:HH21	1:A:265:ARG:CG	2.11	0.62
1:A:332:GLN:NE2	7:A:911:HOH:O	2.26	0.62
1:A:400:ILE:HA	1:A:547:THR:HB	1.81	0.62
1:A:548:ILE:HG22	7:A:901:HOH:O	1.99	0.61
1:A:156:PRO:HB2	1:A:187:GLU:OE2	1.99	0.61
1:A:212:ASP:OD2	1:A:346:ARG:NE	2.29	0.61
1:A:257:HIS:CE1	7:A:908:HOH:O	2.53	0.60
1:A:382:GLN:HA	1:A:382:GLN:NE2	2.14	0.60
1:A:87:PHE:HB3	7:A:959:HOH:O	2.01	0.60
1:A:382:GLN:HA	1:A:382:GLN:HE21	1.67	0.60
1:A:582:PHE:HE1	7:A:1005:HOH:O	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:ASP:HA	1:A:732:TYR:HB3	1.84	0.60
1:A:89:HIS:CE1	1:A:90:PRO:HD2	2.37	0.60
1:A:156:PRO:HB2	1:A:187:GLU:CD	2.22	0.60
1:A:551:ALA:HB1	1:A:555:THR:OG1	2.02	0.59
1:A:144:THR:HG22	1:A:157:ILE:HG12	1.84	0.59
1:A:157:ILE:O	1:A:190:MET:HE3	2.03	0.59
1:A:547:THR:OG1	1:A:548:ILE:N	2.35	0.58
1:A:666:ILE:CG1	1:A:699:ILE:HD11	2.32	0.58
1:A:265:ARG:HH21	1:A:265:ARG:HG2	1.68	0.58
1:A:679:HIS:CD2	1:A:699:ILE:HD13	2.38	0.58
1:A:158:LEU:HG	1:A:299:TRP:HD1	1.65	0.58
1:A:396:LEU:HA	1:A:586:GLY:O	2.04	0.58
1:A:705:LYS:HD3	1:A:705:LYS:N	2.19	0.58
1:A:158:LEU:HA	1:A:173:TRP:HE1	1.69	0.58
1:A:159:MET:HA	1:A:190:MET:SD	2.44	0.58
1:A:144:THR:HA	1:A:157:ILE:HA	1.86	0.57
1:A:392:PRO:HG3	1:A:590:THR:C	2.25	0.57
1:A:453:LEU:HG	1:A:493:LEU:HD13	1.87	0.57
1:A:186:THR:HG23	1:A:189[B]:GLU:H	1.69	0.56
1:A:298:ALA:O	1:A:302:GLY:N	2.31	0.56
1:A:53:LYS:HA	7:A:967:HOH:O	2.05	0.56
1:A:518:ARG:O	1:A:522:THR:HG23	2.05	0.56
1:A:743:ARG:HH12	1:A:746:ARG:HH11	1.52	0.56
1:A:186:THR:HG22	1:A:189[A]:GLU:HG2	1.86	0.56
1:A:158:LEU:CG	1:A:299:TRP:CD1	2.87	0.56
1:A:186:THR:HG23	1:A:189[A]:GLU:H	1.70	0.56
1:A:597:ILE:CB	1:A:603:ILE:HG22	2.35	0.56
1:A:428:CYS:SG	7:A:948:HOH:O	2.58	0.56
1:A:740:ALA:HB1	7:A:904:HOH:O	2.06	0.56
1:A:718:ASP:OD1	1:A:719:GLU:N	2.39	0.56
1:A:261:TYR:N	1:A:262:PRO:HD2	2.21	0.55
1:A:156:PRO:CB	1:A:187:GLU:CD	2.75	0.55
1:A:159:MET:CE	1:A:308:VAL:CG1	2.84	0.55
1:A:410:PRO:O	1:A:414:ILE:HG13	2.07	0.55
1:A:499:TYR:HB3	1:A:502:ALA:HB2	1.88	0.55
1:A:536:VAL:HG12	1:A:546:ALA:HB2	1.88	0.55
1:A:640:VAL:HG11	1:A:750:TYR:CD2	2.42	0.55
1:A:136:LYS:HD3	7:A:916:HOH:O	2.07	0.54
1:A:673:TYR:CE2	1:A:680:VAL:HG21	2.42	0.54
1:A:648:GLU:O	1:A:651:SER:HB3	2.07	0.54
1:A:666:ILE:HD11	1:A:683:ALA:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:LYS:HD2	7:A:910:HOH:O	2.06	0.54
1:A:264:ILE:HG21	1:A:278:VAL:HG11	1.90	0.54
3:C:10:DG:H2"	3:C:11:DC:H5"	1.88	0.54
1:A:476:ARG:HH11	1:A:476:ARG:HG2	1.73	0.54
1:A:178:LEU:HD13	1:A:179:PRO:N	2.23	0.53
1:A:259:ASP:N	7:A:915:HOH:O	2.40	0.53
1:A:360:LYS:HG3	1:A:452:LEU:HD22	1.90	0.53
1:A:67:ARG:HB2	7:A:977:HOH:O	2.07	0.53
1:A:705:LYS:HD3	1:A:705:LYS:H	1.74	0.53
1:A:652:LYS:HE3	1:A:730:GLU:OE1	2.09	0.53
1:A:651:SER:O	1:A:652:LYS:CG	2.54	0.53
1:A:428:CYS:HG	1:A:442:CYS:HG	1.56	0.52
1:A:142:ILE:HB	1:A:157:ILE:HG21	1.91	0.52
1:A:158:LEU:HA	1:A:173:TRP:NE1	2.25	0.52
1:A:171:ILE:HD11	1:A:197:VAL:HG21	1.90	0.52
1:A:670:LEU:N	1:A:670:LEU:CD1	2.73	0.52
1:A:145:LEU:O	1:A:145:LEU:CD1	2.49	0.52
1:A:396:LEU:HD13	1:A:585:ARG:HE	1.74	0.52
1:A:701:TYR:HA	1:A:715:ILE:O	2.10	0.52
1:A:160:ILE:HG21	1:A:194:PHE:CD2	2.45	0.52
1:A:738:LEU:HD21	1:A:752:LYS:CG	2.40	0.52
1:A:153:ALA:HA	1:A:218:TYR:CZ	2.45	0.52
1:A:59:HIS:H	1:A:61:THR:HG22	1.75	0.52
1:A:158:LEU:HG	1:A:299:TRP:NE1	2.25	0.52
1:A:198:VAL:HG11	1:A:232:LEU:HD22	1.92	0.51
1:A:420:PRO:HG3	1:A:506:CYS:HB2	1.92	0.51
1:A:612:ARG:HH12	3:C:9:DT:H1'	1.75	0.51
1:A:475:GLU:O	1:A:479:LEU:HG	2.10	0.51
1:A:41:LEU:O	1:A:107:ILE:N	2.43	0.51
1:A:525:ILE:O	1:A:528:ILE:HG22	2.10	0.51
1:A:610:ILE:HD12	1:A:610:ILE:H	1.74	0.51
1:A:643:VAL:O	1:A:647:THR:HG23	2.10	0.51
1:A:290:VAL:HG21	1:A:308:VAL:HG22	1.93	0.51
1:A:400:ILE:HG22	1:A:547:THR:HB	1.93	0.51
1:A:460:ARG:HB2	1:A:486:ILE:HG21	1.93	0.51
1:A:305:LEU:HD23	1:A:305:LEU:O	2.09	0.51
1:A:382:GLN:NE2	1:A:382:GLN:CA	2.73	0.51
1:A:730:GLU:O	1:A:733:ILE:CG1	2.59	0.51
1:A:165:GLU:OE1	1:A:165:GLU:N	2.36	0.51
1:A:142:ILE:HD11	1:A:214:PHE:CE2	2.45	0.51
1:A:666:ILE:O	1:A:695:PRO:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ILE:O	1:A:122:ILE:HG13	2.11	0.50
1:A:259:ASP:HB2	7:A:908:HOH:O	2.10	0.50
1:A:396:LEU:HD13	1:A:585:ARG:CD	2.40	0.50
1:A:664:LYS:O	1:A:699:ILE:HD12	2.11	0.50
1:A:139:ALA:HB1	1:A:319:THR:HG22	1.93	0.50
1:A:89:HIS:CG	1:A:90:PRO:CD	2.94	0.50
1:A:406:ARG:NH1	1:A:576:GLU:OE2	2.45	0.49
1:A:265:ARG:CG	1:A:265:ARG:NH2	2.73	0.49
1:A:641:ARG:O	1:A:645:GLU:HB3	2.12	0.49
1:A:396:LEU:HD13	1:A:585:ARG:NE	2.28	0.49
1:A:540:ASP:OD1	3:C:12:DC:H4'	2.13	0.49
1:A:666:ILE:HD11	1:A:683:ALA:HB2	1.94	0.48
1:A:751:ARG:HG2	1:A:752:LYS:N	2.28	0.48
1:A:128:PRO:HG2	1:A:339:GLN:C	2.33	0.48
1:A:204:ASP:OD1	1:A:234:ARG:NH1	2.45	0.48
1:A:449:ILE:HB	1:A:450:PRO:HD3	1.94	0.48
1:A:257:HIS:HE1	7:A:908:HOH:O	1.93	0.48
1:A:145:LEU:HD12	1:A:145:LEU:C	2.30	0.48
1:A:188:ARG:HG3	1:A:228:ILE:HD11	1.95	0.48
1:A:597:ILE:CG2	1:A:631:LEU:HB3	2.43	0.48
1:A:35:GLU:HG3	1:A:86:TYR:CD1	2.48	0.48
1:A:204:ASP:OD1	1:A:234:ARG:NH2	2.45	0.48
1:A:159:MET:HE1	1:A:308:VAL:CG1	2.44	0.48
1:A:740:ALA:CB	7:A:904:HOH:O	2.62	0.47
1:A:21:LYS:NZ	1:A:24:GLY:HA2	2.29	0.47
1:A:507:LYS:O	1:A:511:GLU:HG3	2.15	0.47
1:A:584:LYS:HD2	1:A:597:ILE:HG23	1.97	0.47
1:A:639:ALA:O	1:A:643:VAL:HG23	2.14	0.47
1:A:416:HIS:CD2	1:A:516:TRP:CZ2	3.02	0.47
2:B:12:G:H2'	2:B:13:A:C8	2.50	0.47
1:A:192:LYS:O	1:A:196:ARG:HG3	2.14	0.47
1:A:590:THR:OG1	1:A:591:LYS:N	2.48	0.46
1:A:158:LEU:HB3	1:A:299:TRP:NE1	2.29	0.46
1:A:561:MET:SD	1:A:561:MET:N	2.88	0.46
1:A:407:SER:HA	7:A:964:HOH:O	2.16	0.46
1:A:738:LEU:HD11	1:A:752:LYS:CB	2.44	0.46
1:A:528:ILE:HG12	1:A:534:PHE:HB2	1.97	0.46
1:A:640:VAL:HG22	1:A:745:LEU:HD13	1.97	0.46
1:A:656:PRO:HA	1:A:657:PRO:HD3	1.78	0.46
1:A:192:LYS:NZ	7:A:912:HOH:O	2.27	0.46
1:A:663:HIS:HA	1:A:699:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:ILE:HG12	1:A:657:PRO:CB	2.46	0.45
1:A:476:ARG:HG2	1:A:476:ARG:NH1	2.32	0.45
1:A:598:ASP:OD1	1:A:602:LYS:N	2.48	0.45
1:A:200:GLU:HG3	7:A:925:HOH:O	2.16	0.45
1:A:295:ILE:CB	1:A:308:VAL:HG11	2.47	0.45
1:A:159:MET:HE3	1:A:308:VAL:CG1	2.44	0.45
1:A:679:HIS:HD2	1:A:699:ILE:HD13	1.78	0.45
1:A:48:ILE:O	1:A:52:LYS:HG2	2.17	0.45
1:A:295:ILE:HA	1:A:308:VAL:HG21	1.98	0.45
1:A:101:ARG:NH2	1:A:101:ARG:CG	2.74	0.45
1:A:650:LEU:CD1	1:A:733:ILE:HG21	2.23	0.45
1:A:730:GLU:O	1:A:733:ILE:HG13	2.16	0.45
1:A:178:LEU:HD11	1:A:180:TYR:CE2	2.51	0.45
1:A:153:ALA:HB3	1:A:221:LYS:HD3	1.98	0.44
1:A:417:ASN:ND2	1:A:422:THR:HG21	2.32	0.44
1:A:704:LEU:HD13	1:A:705:LYS:N	2.31	0.44
1:A:305:LEU:C	1:A:305:LEU:CD2	2.85	0.44
1:A:403:LEU:HD12	1:A:544:PHE:CZ	2.53	0.44
1:A:463:ILE:HG23	1:A:479:LEU:HB3	1.99	0.44
1:A:425:ARG:HG2	1:A:428:CYS:SG	2.57	0.44
1:A:733:ILE:O	1:A:737:VAL:CG2	2.66	0.44
1:A:733:ILE:O	1:A:737:VAL:HG21	2.17	0.44
1:A:145:LEU:HD21	1:A:156:PRO:CG	2.46	0.44
1:A:416:HIS:CD2	1:A:516:TRP:CD2	3.06	0.44
1:A:564:LEU:HD23	1:A:564:LEU:HA	1.76	0.44
1:A:285:GLN:HG3	1:A:286:PRO:HD2	1.99	0.43
2:B:9:U:H2'	2:B:10:A:C8	2.53	0.43
1:A:673:TYR:CD2	1:A:680:VAL:HG21	2.54	0.43
1:A:494:TYR:OH	1:A:514:ILE:HD11	2.18	0.43
1:A:145:LEU:HB3	1:A:158:LEU:CD1	2.44	0.43
1:A:158:LEU:CG	1:A:299:TRP:NE1	2.82	0.43
1:A:360:LYS:HD2	1:A:364:ARG:NH1	2.28	0.43
1:A:650:LEU:HD23	1:A:650:LEU:HA	1.81	0.43
1:A:211:GLY:CA	7:A:908:HOH:O	2.66	0.43
1:A:354:GLU:OE1	1:A:496:TYR:OH	2.31	0.43
1:A:168:ALA:HB2	1:A:317:LYS:HG3	2.00	0.43
1:A:333:LEU:HD12	1:A:333:LEU:HA	1.92	0.43
1:A:715:ILE:HG22	1:A:716:PRO:O	2.19	0.43
1:A:537:ILE:N	1:A:545:PHE:O	2.46	0.43
1:A:170:VAL:HG21	1:A:309:ALA:O	2.19	0.42
1:A:730:GLU:O	1:A:733:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:LEU:HD13	1:A:670:LEU:H	1.84	0.42
1:A:290:VAL:O	1:A:290:VAL:HG13	2.18	0.42
1:A:335:ARG:NH2	7:A:911:HOH:O	2.39	0.42
1:A:414:ILE:HD13	1:A:454:GLY:HA2	2.02	0.42
1:A:172:THR:O	1:A:184:VAL:HG22	2.20	0.42
1:A:524:THR:HG21	1:A:577:LEU:HD22	2.01	0.42
1:A:728:ASP:HA	1:A:732:TYR:CB	2.48	0.42
1:A:143:GLU:O	1:A:158:LEU:N	2.52	0.42
1:A:180:TYR:CD1	1:A:181:VAL:HG23	2.55	0.42
1:A:525:ILE:HG23	1:A:536:VAL:HG11	2.02	0.42
1:A:529:GLU:HA	1:A:534:PHE:H	1.85	0.42
1:A:15:VAL:HG22	1:A:32:ARG:HG2	2.00	0.41
1:A:47:ALA:O	1:A:51:VAL:HG23	2.20	0.41
1:A:72:GLN:CG	7:A:990:HOH:O	2.67	0.41
1:A:87:PHE:CE1	1:A:96:ILE:HG21	2.54	0.41
1:A:122:ILE:HG23	1:A:359:ARG:HA	2.03	0.41
1:A:237:SER:OG	1:A:238:GLU:O	2.38	0.41
1:A:21:LYS:HD2	1:A:135:LEU:CD2	2.51	0.41
1:A:84:LYS:HD3	1:A:86:TYR:OH	2.20	0.41
1:A:103:HIS:HA	1:A:104:PRO:HD3	1.95	0.41
1:A:735:LYS:HD2	1:A:735:LYS:HA	1.71	0.41
1:A:72:GLN:HG3	7:A:990:HOH:O	2.19	0.41
1:A:140:PHE:HA	1:A:161[B]:SER:O	2.21	0.41
1:A:637:GLU:O	1:A:637:GLU:HG2	2.20	0.41
1:A:157:ILE:HD11	1:A:218:TYR:HD1	1.85	0.41
1:A:329:MET:HG2	1:A:481:TYR:HD1	1.85	0.41
1:A:392:PRO:HB3	1:A:538:TYR:CD1	2.56	0.41
1:A:400:ILE:HD13	1:A:400:ILE:HG21	1.79	0.41
1:A:584:LYS:NZ	1:A:632:LYS:HA	2.36	0.41
1:A:142:ILE:HD11	1:A:214:PHE:HE2	1.84	0.41
1:A:313:MET:HE3	1:A:313:MET:HB3	1.97	0.40
1:A:618:ILE:HG12	1:A:657:PRO:HB2	2.03	0.40
1:A:751:ARG:HG3	1:A:751:ARG:HH11	1.86	0.40
1:A:160:ILE:HG21	1:A:194:PHE:CG	2.55	0.40
1:A:713:ARG:H	1:A:713:ARG:HG2	1.79	0.40
1:A:536:VAL:HG22	7:A:910:HOH:O	2.21	0.40
1:A:609:GLU:CB	7:A:922:HOH:O	2.69	0.40
1:A:21:LYS:HD2	1:A:204:ASP:OD2	2.22	0.40

All (3) 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:530:GLU:O	1:A:746:ARG:NH2[2_555]	1.98	0.22
7:A:957:HOH:O	7:B:101:HOH:O[4_655]	2.11	0.09
1:A:531:LYS:CA	1:A:746:ARG:NH2[2_555]	2.18	0.02

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	731/774 (94%)	716 (98%)	15 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	598/675 (89%)	556 (93%)	42 (7%)	15 29

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LYS
1	A	91	GLN
1	A	101	ARG
1	A	134	GLU
1	A	159	MET
1	A	188	ARG

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Mol	Chain	Res	Type
1	A	189[A]	GLU
1	A	189[B]	GLU
1	A	215	ASP
1	A	237	SER
1	A	265	ARG
1	A	299	TRP
1	A	307	ARG
1	A	310	ARG
1	A	324	LYS
1	A	325	GLU
1	A	347	SER
1	A	381	HIS
1	A	382	GLN
1	A	390	LYS
1	A	421	ASP
1	A	442	CYS
1	A	468	LYS
1	A	483	GLN
1	A	507	LYS
1	A	516	TRP
1	A	561	MET
1	A	582	PHE
1	A	598	ASP
1	A	617	GLU
1	A	621	GLU
1	A	641	ARG
1	A	651	SER
1	A	670	LEU
1	A	672	ASP
1	A	673	TYR
1	A	686	LEU
1	A	694	ARG
1	A	713	ARG
1	A	735	LYS
1	A	736	GLN
1	A	741	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	ASN
1	A	332	GLN

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Mol	Chain	Res	Type
1	A	382	GLN
1	A	439	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	10/16 (62%)	2 (20%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	10	A
2	B	11	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	EDO	A	806	-	3,3,3	0.50	0	2,2,2	0.27	0
6	EDO	A	805	-	3,3,3	0.47	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	TCE	A	802	-	12,15,15	1.85	2 (16%)	12,18,18	2.37	4 (33%)
4	SO4	A	801	-	4,4,4	0.11	0	6,6,6	0.32	0
6	EDO	A	803	-	3,3,3	0.46	0	2,2,2	0.16	0
6	EDO	A	804	-	3,3,3	0.40	0	2,2,2	0.32	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
6	EDO	A	806	-	-	1/1/1/1	-
6	EDO	A	805	-	-	1/1/1/1	-
5	TCE	A	802	-	-	9/15/15/15	-
6	EDO	A	803	-	-	1/1/1/1	-
6	EDO	A	804	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	802	TCE	P-C2	3.97	1.90	1.84
5	A	802	TCE	P-C1	2.30	1.87	1.84

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	802	TCE	C1-P-C2	4.18	114.26	100.95
5	A	802	TCE	C1-P-C3	3.88	113.31	100.95
5	A	802	TCE	C3-P-C2	3.63	112.50	100.95
5	A	802	TCE	O12-C11-C4	2.59	122.36	114.03

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	802	TCE	P-C2-C5-C14
5	A	802	TCE	C6-C3-P-C1
5	A	802	TCE	C4-C1-P-C3
6	A	803	EDO	O1-C1-C2-O2
6	A	804	EDO	O1-C1-C2-O2
6	A	805	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	A	806	EDO	O1-C1-C2-O2
5	A	802	TCE	P-C3-C6-C8
5	A	802	TCE	O12-C11-C4-C1
5	A	802	TCE	C3-C6-C8-O9
5	A	802	TCE	C3-C6-C8-O10
5	A	802	TCE	P-C1-C4-C11
5	A	802	TCE	O13-C11-C4-C1

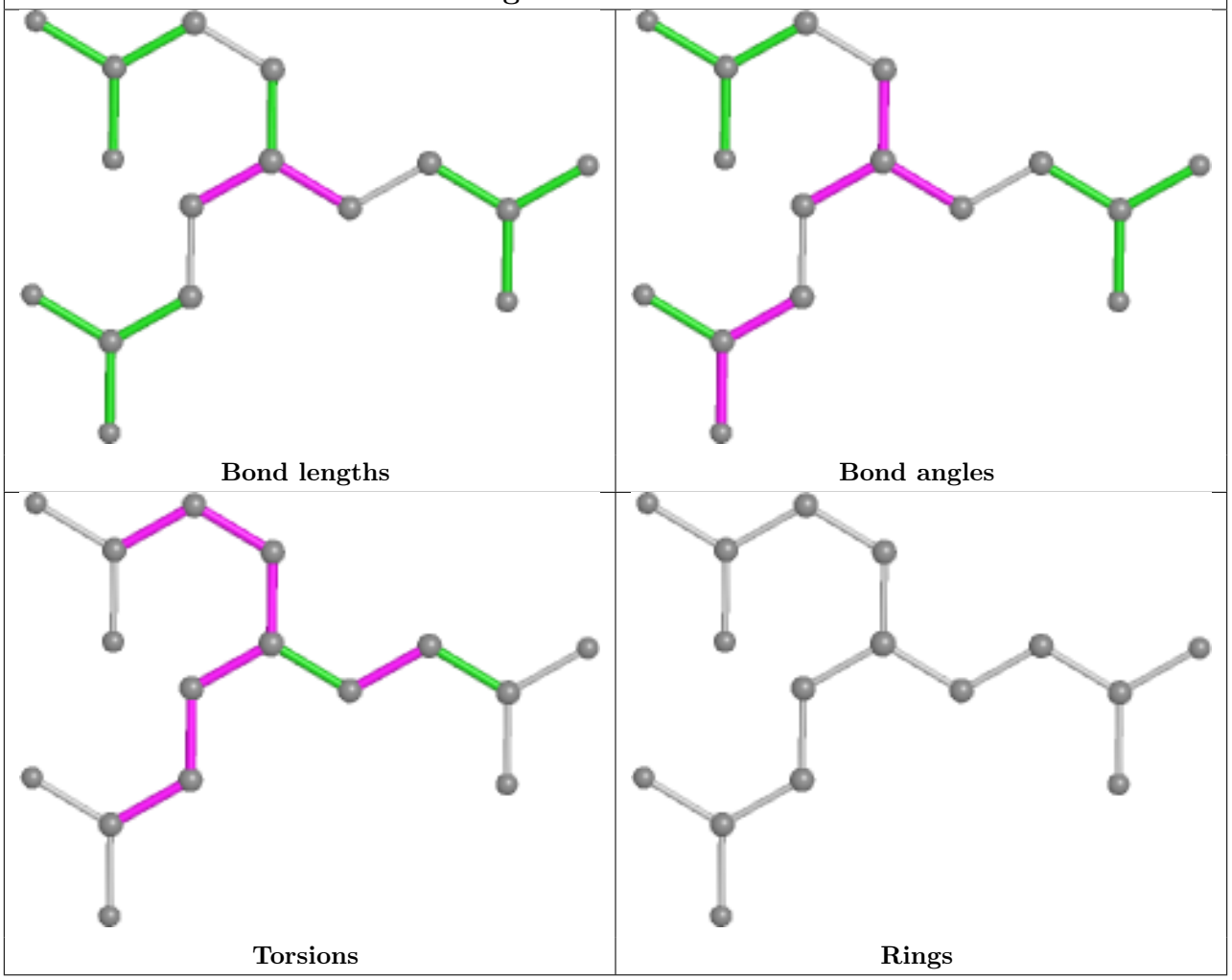
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	806	EDO	1	0
5	A	802	TCE	1	0
6	A	804	EDO	2	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 then 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.

Ligand TCE A 802



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	739/774 (95%)	1.20	140 (18%) 1 1	37, 74, 145, 171	0
2	B	11/16 (68%)	0.41	0 100 100	120, 133, 151, 156	0
3	C	12/13 (92%)	0.74	1 (8%) 11 11	116, 131, 137, 138	0
All	All	762/803 (94%)	1.18	141 (18%) 1 1	37, 76, 145, 171	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	690	GLY	15.2
1	A	689	ARG	11.6
1	A	300	GLU	11.4
1	A	707	SER	10.2
1	A	295	ILE	9.4
1	A	301	THR	9.3
1	A	703	VAL	8.8
1	A	708	GLY	8.3
1	A	687	ALA	8.1
1	A	678	PRO	8.0
1	A	668	ARG	6.9
1	A	290	VAL	6.8
1	A	677	GLY	6.7
1	A	296	THR	6.6
1	A	732	TYR	6.4
1	A	666	ILE	5.9
1	A	636	VAL	5.8
1	A	686	LEU	5.6
1	A	702	ILE	5.5
1	A	553	ALA	5.5
1	A	749	GLY	5.5
1	A	299	TRP	5.3
1	A	681	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	615	TRP	5.2
1	A	181	VAL	5.2
1	A	685	ARG	5.2
1	A	696	GLY	5.1
1	A	715	ILE	4.9
1	A	693	ILE	4.8
1	A	630	LEU	4.8
1	A	756	ARG	4.7
1	A	729	ALA	4.6
1	A	699	ILE	4.6
1	A	709	ARG	4.5
1	A	173	TRP	4.4
1	A	388	TYR	4.3
1	A	637	GLU	4.2
1	A	400	ILE	4.1
1	A	688	ALA	4.0
1	A	711	VAL	4.0
1	A	399	ASN	3.9
1	A	387	GLY	3.8
1	A	675	ALA	3.8
1	A	684	LYS	3.8
1	A	589	VAL	3.7
1	A	291	TYR	3.7
1	A	667	THR	3.7
3	C	12	DC	3.6
1	A	194	PHE	3.6
1	A	640	VAL	3.6
1	A	691	VAL	3.6
1	A	738	LEU	3.6
1	A	292	ALA	3.6
1	A	83	TRP	3.6
1	A	745	LEU	3.5
1	A	614	ASP	3.5
1	A	609	GLU	3.5
1	A	389	ILE	3.4
1	A	197	VAL	3.3
1	A	191	ILE	3.3
1	A	57	GLU	3.2
1	A	736	GLN	3.2
1	A	267	THR	3.1
1	A	622	THR	3.1
1	A	397	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	457	LEU	3.0
1	A	694	ARG	3.0
1	A	172	THR	3.0
1	A	453	LEU	3.0
1	A	612	ARG	3.0
1	A	390	LYS	3.0
1	A	157	ILE	2.9
1	A	697	THR	2.9
1	A	302	GLY	2.9
1	A	755	LEU	2.9
1	A	706	GLY	2.9
1	A	305	LEU	2.9
1	A	587	LEU	2.8
1	A	716	PRO	2.8
1	A	650	LEU	2.8
1	A	138	LEU	2.8
1	A	672	ASP	2.8
1	A	579	TYR	2.8
1	A	298	ALA	2.8
1	A	743	ARG	2.8
1	A	683	ALA	2.8
1	A	226	LEU	2.8
1	A	567	ILE	2.7
1	A	747	ALA	2.7
1	A	719	GLU	2.7
1	A	289	LYS	2.7
1	A	306	GLU	2.7
1	A	230	PHE	2.7
1	A	554	GLU	2.6
1	A	674	LYS	2.6
1	A	710	ILE	2.6
1	A	308	VAL	2.6
1	A	219	LEU	2.5
1	A	206	LEU	2.5
1	A	714	ALA	2.5
1	A	525	ILE	2.5
1	A	727	TYR	2.5
1	A	692	LYS	2.4
1	A	162	TYR	2.4
1	A	449	ILE	2.4
1	A	618	ILE	2.4
1	A	717	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	513	VAL	2.4
1	A	695	PRO	2.4
1	A	384	HIS	2.4
1	A	669	ASP	2.3
1	A	730	GLU	2.3
1	A	746	ARG	2.3
1	A	698	VAL	2.3
1	A	740	ALA	2.3
1	A	51	VAL	2.3
1	A	171	ILE	2.3
1	A	297	THR	2.3
1	A	143	GLU	2.2
1	A	327	LEU	2.2
1	A	355	TRP	2.2
1	A	269	ASN	2.2
1	A	728	ASP	2.2
1	A	700	SER	2.2
1	A	159	MET	2.2
1	A	592	LYS	2.2
1	A	627	LEU	2.2
1	A	228	ILE	2.1
1	A	85	LEU	2.1
1	A	341	LEU	2.1
1	A	584	LYS	2.1
1	A	278	VAL	2.1
1	A	412	ILE	2.1
1	A	76	LEU	2.1
1	A	493	LEU	2.1
1	A	608	LEU	2.1
1	A	303	GLU	2.0
1	A	582	PHE	2.0
1	A	626	VAL	2.0
1	A	145	LEU	2.0
1	A	158	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

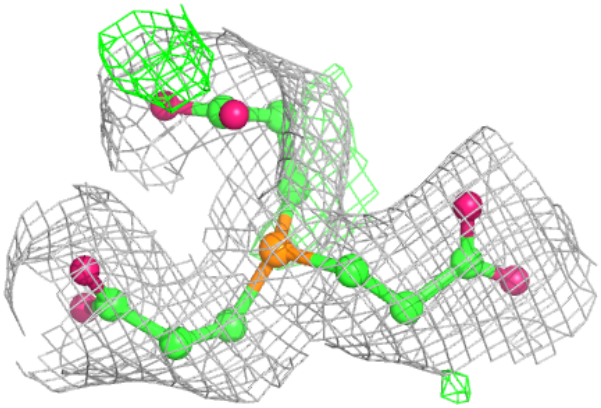
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

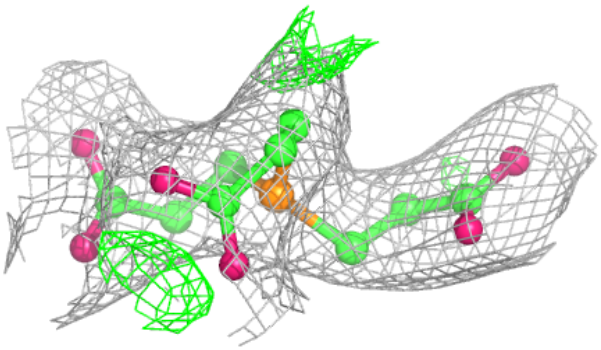
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	A	806	4/4	0.22	0.27	74,79,79,79	0
6	EDO	A	804	4/4	0.67	0.27	53,57,57,70	0
6	EDO	A	805	4/4	0.70	0.18	57,76,83,99	0
6	EDO	A	803	4/4	0.78	0.23	53,53,53,59	0
5	TCE	A	802	16/16	0.84	0.17	53,53,70,74	0
4	SO4	A	801	5/5	0.97	0.12	54,60,66,73	0

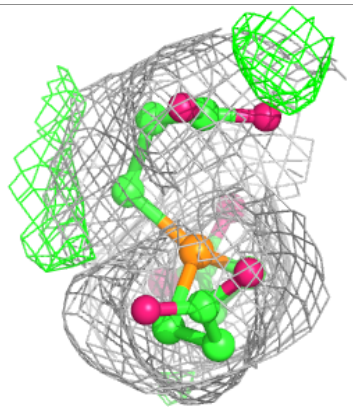
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TCE A 802:

$2mF_o$-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.