



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:34 PM UTC

PDB ID : 6WYB / pdb_00006wyb
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 : 4-5-2 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

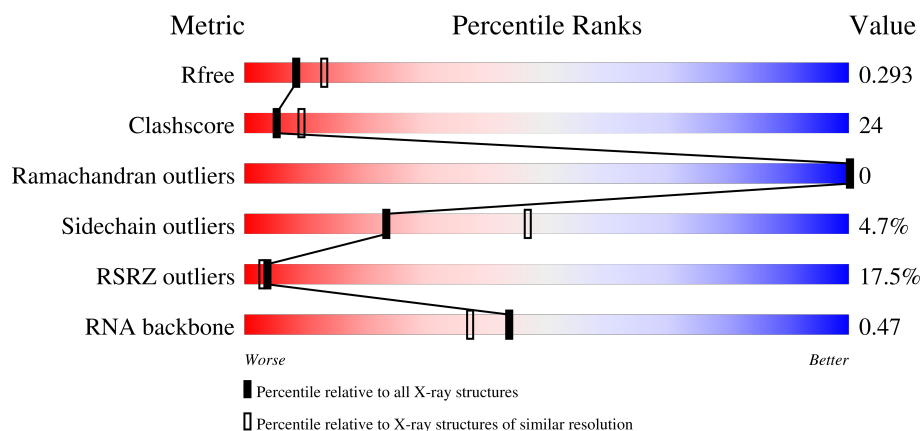
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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	774	
2	B	16	
3	C	13	

2 Entry composition

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
1	A	739	Total	C	N	O	S	0	2	0
			5870	3787	987	1080	16			

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

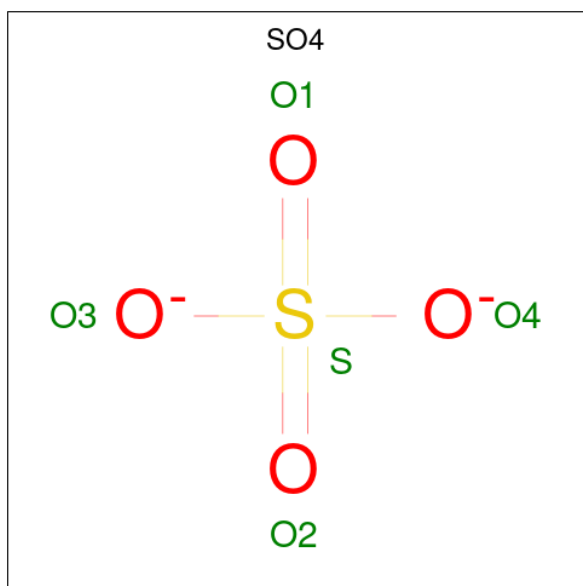
- Molecule 2 is a RNA chain called RNA strand.

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

- Molecule 3 is a DNA chain called DNA strand.

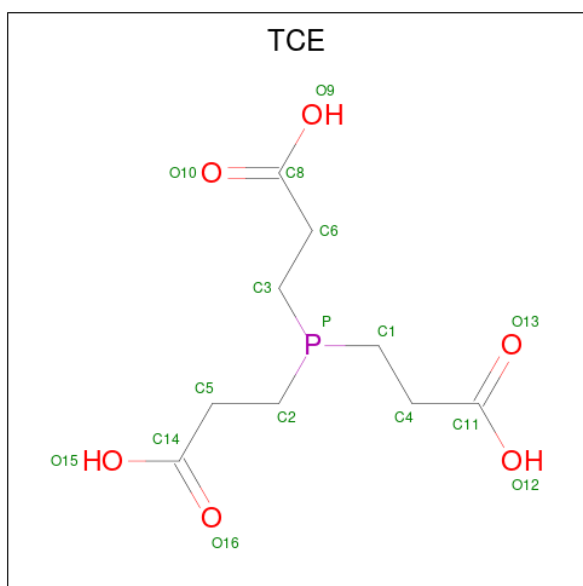
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			243	117	42	73	11			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



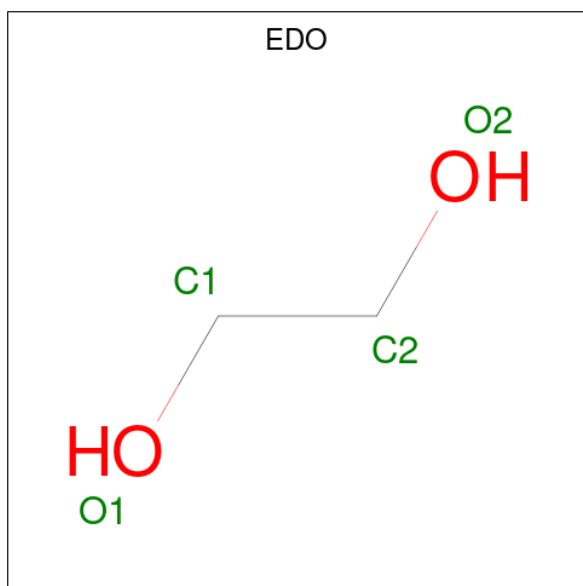
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 3,3',3''-phosphanetriyltripropanoic acid (CCD ID: TCE) (formula: C₉H₁₅O₆P).



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 (CCD ID: 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		

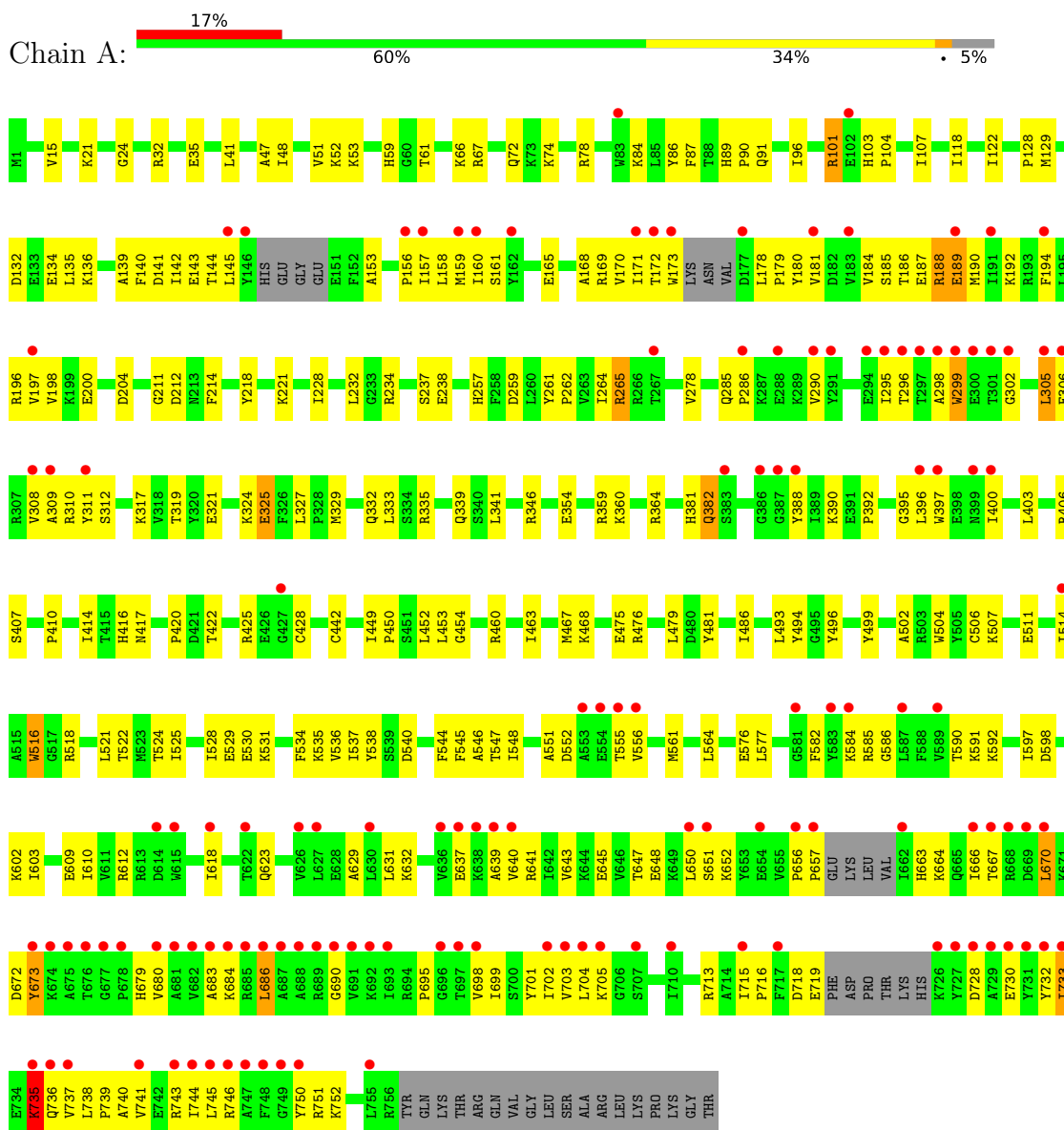
- Molecule 7 is water.

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		

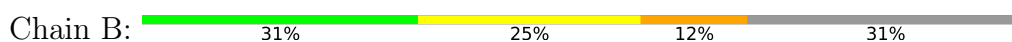
3 Residue-property plots

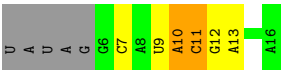
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 2: RNA strand





● Molecule 3: DNA strand



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	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 29.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.97-2.50) 88.6 (29.97-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.267 , 0.283 (Not available) , 0.293	Depositor DCC
R_{free} test set	989 reflections (2.42%)	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)	0.30 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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.*

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: EDO, SO4, TCE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	1/5995 (0.0%)	0.77	3/8118 (0.0%)
2	B	0.25	0/261	0.48	0/404
3	C	0.27	0/271	0.46	0/417
All	All	0.52	1/6527 (0.0%)	0.75	3/8939 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	LEU	C-N	5.77	1.41	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	735	LYS	N-CA-C	7.50	120.92	111.24
1	A	327	LEU	CA-C-N	-5.19	113.19	118.85
1	A	327	LEU	C-N-CA	-5.19	113.19	118.85

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

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	38	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:157:ILE:O	1:A:190:MET:HE1	1.49	1.12
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:159:MET:HE3	1:A:308:VAL:HG12	1.42	1.00
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:159:MET:CE	1:A:308:VAL:HG12	2.16	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:C	1:A:305:LEU:HD23	2.15	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
1:A:89:HIS:ND1	1:A:90:PRO:HD2	2.07	0.70
1:A:157:ILE:O	1:A:190:MET:CE	2.36	0.69
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:159:MET:HE3	1:A:308:VAL:CG1	2.19	0.68
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: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: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
1:A:156:PRO:HB2	1:A:187:GLU:CD	2.22	0.64
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: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:392:PRO:HG3	1:A:590:THR:C	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:156:PRO:CB	1:A:187:GLU:CD	2.75	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
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: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: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: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:145:LEU:HD12	1:A:145:LEU:C	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:128:PRO:HG2	1:A:339:GLN:C	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:157:ILE:C	1:A:190:MET:HE1	2.33	0.50
1:A:159:MET:CE	1:A:308:VAL:CG1	2.84	0.50
1:A:305:LEU:C	1:A:305:LEU:CD2	2.85	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: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: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: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:172:THR:HG1	1:A:299:TRP:HZ2	1.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:663:HIS:HA	1:A:699:ILE:O	2.16	0.46
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:143:GLU:CD	1:A:312:SER:HB2	2.42	0.45
1:A:295:ILE:CB	1:A:308:VAL:HG11	2.47	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:259:ASP:CG	7:A:908:HOH:O	2.60	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: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:211:GLY:C	7:A:908:HOH:O	2.52	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:129:MET:HE2	1:A:341:LEU:HD12	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	576/774 (74%)	563 (98%)	13 (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%)	569 (95%)	29 (5%)	23	46

All (29) 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	185	SER
1	A	189[A]	GLU
1	A	189[B]	GLU
1	A	265	ARG
1	A	299	TRP
1	A	305	LEU
1	A	310	ARG
1	A	321	GLU
1	A	324	LYS
1	A	325	GLU
1	A	381	HIS
1	A	382	GLN
1	A	390	LYS
1	A	467	MET
1	A	468	LYS
1	A	516	TRP
1	A	667	THR
1	A	670	LEU
1	A	672	ASP
1	A	673	TYR
1	A	686	LEU
1	A	733	ILE
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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	304	ASN
1	A	332	GLN
1	A	382	GLN
1	A	439	HIS
1	A	483	GLN
1	A	736	GLN

5.3.3 RNA [i](#)

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 [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](#)

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	804	-	3,3,3	0.36	0	2,2,2	0.36	0
5	TCE	A	802	-	12,15,15	1.86	2 (16%)	12,18,18	2.38	4 (33%)
6	EDO	A	805	-	3,3,3	0.43	0	2,2,2	0.33	0
6	EDO	A	806	-	3,3,3	0.47	0	2,2,2	0.32	0
6	EDO	A	803	-	3,3,3	0.42	0	2,2,2	0.20	0
4	SO4	A	801	-	4,4,4	0.23	0	6,6,6	0.31	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	804	-	-	1/1/1/1	-
5	TCE	A	802	-	-	9/15/15/15	-
6	EDO	A	805	-	-	1/1/1/1	-
6	EDO	A	806	-	-	1/1/1/1	-
6	EDO	A	803	-	-	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(°)	Ideal(°)
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	2.65	122.36	114.00

There are no chirality outliers.

All (13) torsion outliers are listed below:

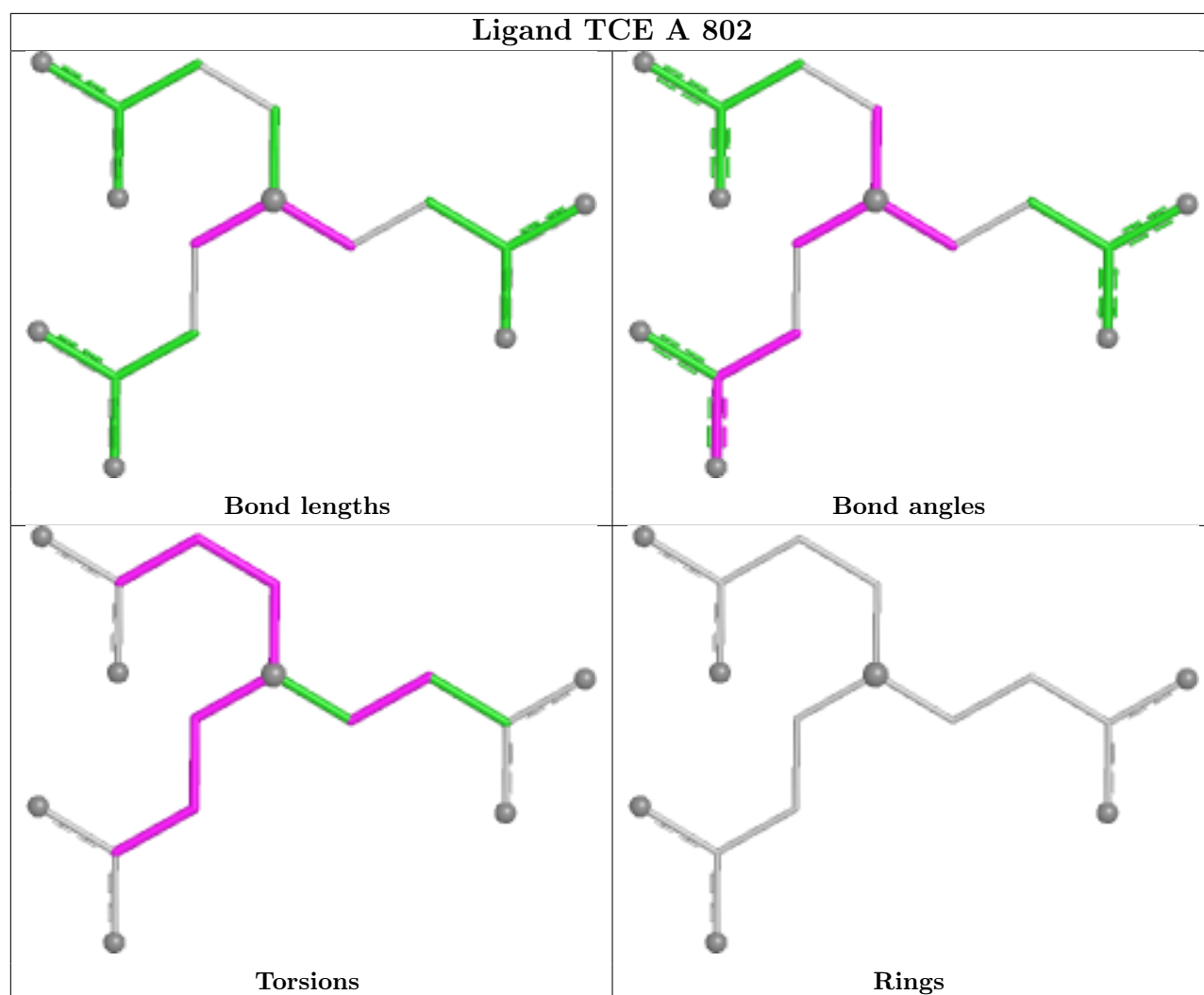
Mol	Chain	Res	Type	Atoms
5	A	802	TCE	P-C2-C5-C14
5	A	802	TCE	C6-C3-P-C1
5	A	802	TCE	C4-C1-P-C3
6	A	804	EDO	O1-C1-C2-O2
6	A	805	EDO	O1-C1-C2-O2
6	A	803	EDO	O1-C1-C2-O2
6	A	806	EDO	O1-C1-C2-O2
5	A	802	TCE	P-C3-C6-C8
5	A	802	TCE	C3-C6-C8-O9
5	A	802	TCE	O12-C11-C4-C1
5	A	802	TCE	C3-C6-C8-O10
5	A	802	TCE	O13-C11-C4-C1
5	A	802	TCE	P-C1-C4-C11

There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

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, 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	739/774 (95%)	1.07	132 (17%) 3 3	37, 74, 145, 171	2 (0%)
2	B	11/16 (68%)	0.91	0 100 100	120, 133, 151, 156	0
3	C	12/13 (92%)	1.09	1 (8%) 17 15	116, 131, 137, 138	0
All	All	762/803 (94%)	1.07	133 (17%) 4 3	37, 76, 145, 171	2 (0%)

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	690	GLY	7.5
1	A	732	TYR	5.6
1	A	704	LEU	5.5
1	A	295	ILE	5.4
1	A	703	VAL	5.3
1	A	305	LEU	5.0
1	A	689	ARG	5.0
1	A	686	LEU	5.0
1	A	749	GLY	4.9
1	A	729	ALA	4.9
1	A	675	ALA	4.8
1	A	553	ALA	4.7
1	A	300	GLU	4.7
1	A	299	TRP	4.7
1	A	301	THR	4.6
1	A	702	ILE	4.5
1	A	726	LYS	4.4
1	A	687	ALA	4.3
1	A	677	GLY	4.2
1	A	146	TYR	4.2
1	A	173	TRP	4.1
1	A	715	ILE	4.1
1	A	291	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	172	THR	4.0
1	A	298	ALA	3.9
1	A	662	ILE	3.9
1	A	688	ALA	3.8
1	A	181	VAL	3.8
1	A	668	ARG	3.8
1	A	666	ILE	3.8
1	A	705	LYS	3.7
1	A	630	LEU	3.6
1	A	747	ALA	3.6
1	A	197	VAL	3.5
1	A	727	TYR	3.5
1	A	669	ASP	3.5
1	A	290	VAL	3.5
1	A	618	ILE	3.4
1	A	685	ARG	3.4
1	A	296	THR	3.3
1	A	615	TRP	3.3
1	A	667	THR	3.3
1	A	676	THR	3.3
1	A	637	GLU	3.2
1	A	636	VAL	3.2
1	A	744	ILE	3.2
3	C	12	DC	3.2
1	A	741	VAL	3.1
1	A	554	GLU	3.1
1	A	657	PRO	3.0
1	A	302	GLY	3.0
1	A	171	ILE	3.0
1	A	745	LEU	3.0
1	A	400	ILE	3.0
1	A	691	VAL	3.0
1	A	183	VAL	2.9
1	A	191	ILE	2.9
1	A	674	LYS	2.9
1	A	388	TYR	2.9
1	A	737	VAL	2.9
1	A	650	LEU	2.9
1	A	397	TRP	2.9
1	A	614	ASP	2.9
1	A	673	TYR	2.9
1	A	654	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	678	PRO	2.8
1	A	684	LYS	2.8
1	A	162	TYR	2.8
1	A	640	VAL	2.8
1	A	288	GLU	2.8
1	A	194	PHE	2.8
1	A	556	VAL	2.8
1	A	698	VAL	2.8
1	A	102	GLU	2.8
1	A	733	ILE	2.7
1	A	696	GLY	2.7
1	A	693	ILE	2.7
1	A	399	ASN	2.7
1	A	670	LEU	2.7
1	A	267	THR	2.7
1	A	83	TRP	2.7
1	A	622	THR	2.7
1	A	692	LYS	2.6
1	A	748	PHE	2.6
1	A	589	VAL	2.6
1	A	294	GLU	2.6
1	A	189[A]	GLU	2.6
1	A	156	PRO	2.6
1	A	680	VAL	2.6
1	A	587	LEU	2.5
1	A	735	LYS	2.5
1	A	555	THR	2.5
1	A	651	SER	2.5
1	A	746	ARG	2.5
1	A	583	TYR	2.5
1	A	682	VAL	2.5
1	A	743	ARG	2.5
1	A	656	PRO	2.4
1	A	286	PRO	2.4
1	A	728	ASP	2.4
1	A	681	ALA	2.4
1	A	710	ILE	2.4
1	A	731	TYR	2.4
1	A	750	TYR	2.4
1	A	386	GLY	2.4
1	A	177	ASP	2.4
1	A	311	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	717	PHE	2.4
1	A	306	GLU	2.4
1	A	383	SER	2.3
1	A	581	GLY	2.3
1	A	730	GLU	2.3
1	A	396	LEU	2.3
1	A	683	ALA	2.3
1	A	427	GLY	2.2
1	A	145	LEU	2.2
1	A	309	ALA	2.2
1	A	584	LYS	2.2
1	A	159	MET	2.2
1	A	387	GLY	2.2
1	A	639	ALA	2.1
1	A	157	ILE	2.1
1	A	697	THR	2.1
1	A	160	ILE	2.1
1	A	638	LYS	2.1
1	A	308	VAL	2.1
1	A	627	LEU	2.1
1	A	707	SER	2.1
1	A	755	LEU	2.1
1	A	297	THR	2.1
1	A	514	ILE	2.1
1	A	736	GLN	2.0
1	A	626	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

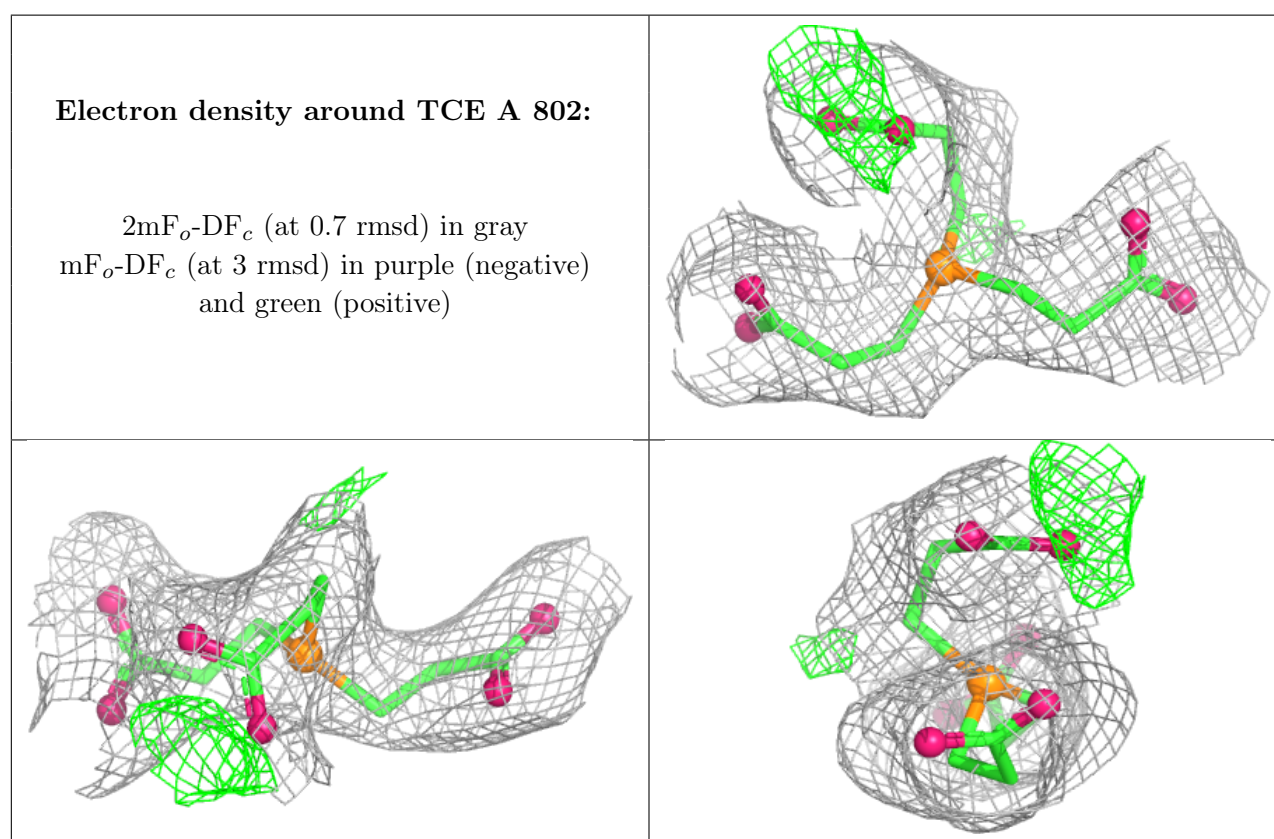
There are no oligosaccharides in this entry.

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
6	EDO	A	806	4/4	0.54	0.16	74,79,79,79	0
6	EDO	A	805	4/4	0.66	0.20	57,76,83,99	0
6	EDO	A	803	4/4	0.71	0.21	53,53,53,59	0
6	EDO	A	804	4/4	0.71	0.21	53,57,57,70	0
5	TCE	A	802	16/16	0.81	0.12	53,53,70,74	0
4	SO4	A	801	5/5	0.92	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.