



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:26 AM UTC

PDB ID : 4QEB / pdb_00004qeb
Title : Dcps in complex with covalent inhibitor targeting Tyrosine
Authors : Liu, S.
Deposited on : 2014-05-15
Resolution : 3.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

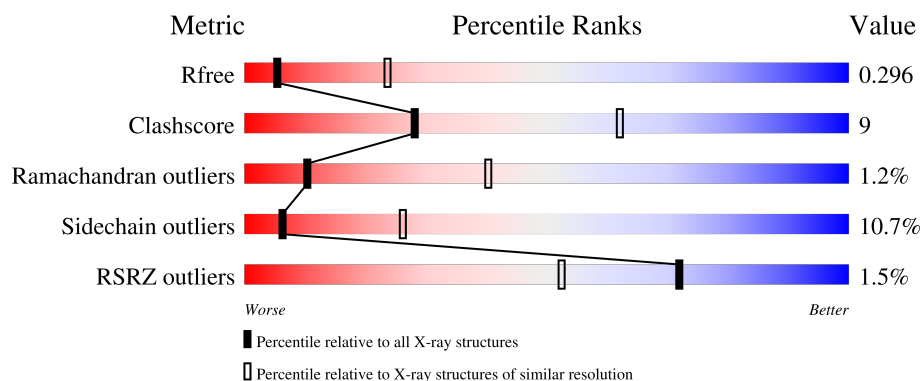
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	337	3% 55% 27% • 15%
1	B	337	53% 29% • 15%
1	C	337	53% 29% • 14%
1	D	337	3% 56% 27% • 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	401	-	X	-	-
2	PO4	B	402	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9617 atoms, of which 13 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 m7GpppX diphosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2377	1523	425	426	3			
1	B	288	Total	C	N	O	S	0	0	0
			2384	1526	427	428	3			
1	C	289	Total	C	N	O	S	0	0	0
			2389	1529	427	430	3			
1	D	292	Total	C	N	O	S	0	0	0
			2411	1542	430	436	3			

There are 4 discrepancies between the modelled and reference sequences:

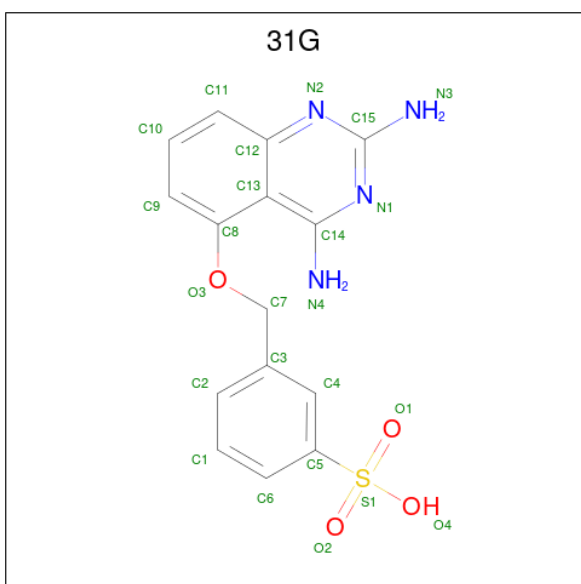
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q96C86
B	1	GLY	-	expression tag	UNP Q96C86
C	1	GLY	-	expression tag	UNP Q96C86
D	1	GLY	-	expression tag	UNP Q96C86

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 3-[[[(2,4-diaminoquinazolin-5-yl)oxy]methyl]benzenesulfonic acid (CCD ID: 31G) (formula: C₁₅H₁₄N₄O₄S).

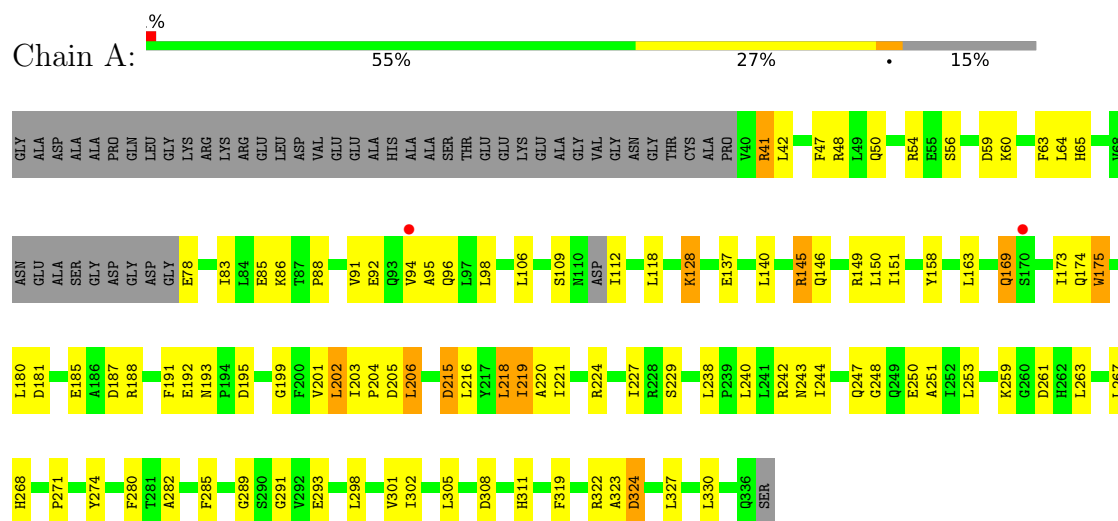


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	S	13	0
			36	15	13	4	3	1		

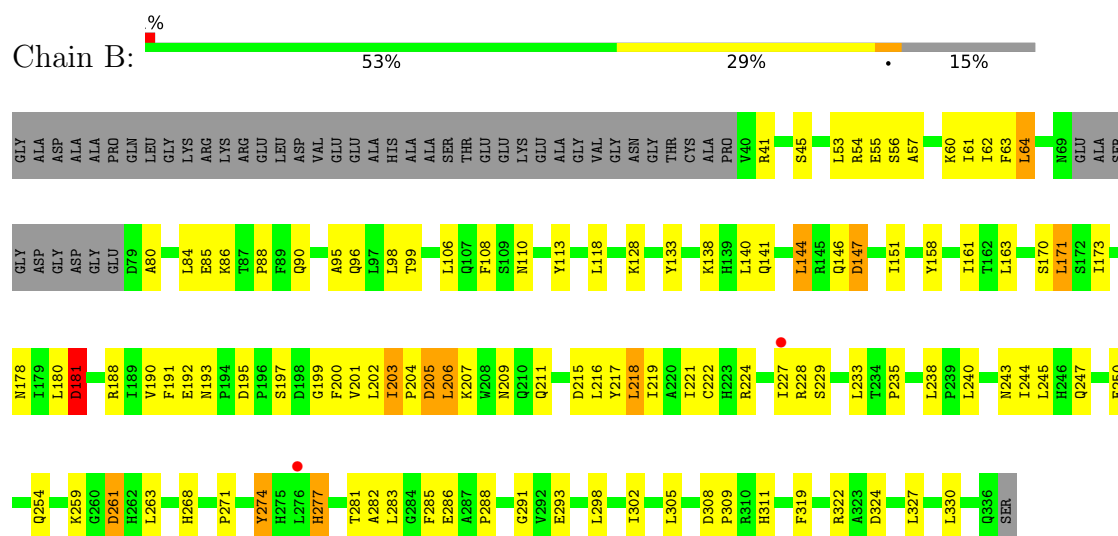
3 Residue-property plots [i](#)

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: m7GpppX diphosphatase

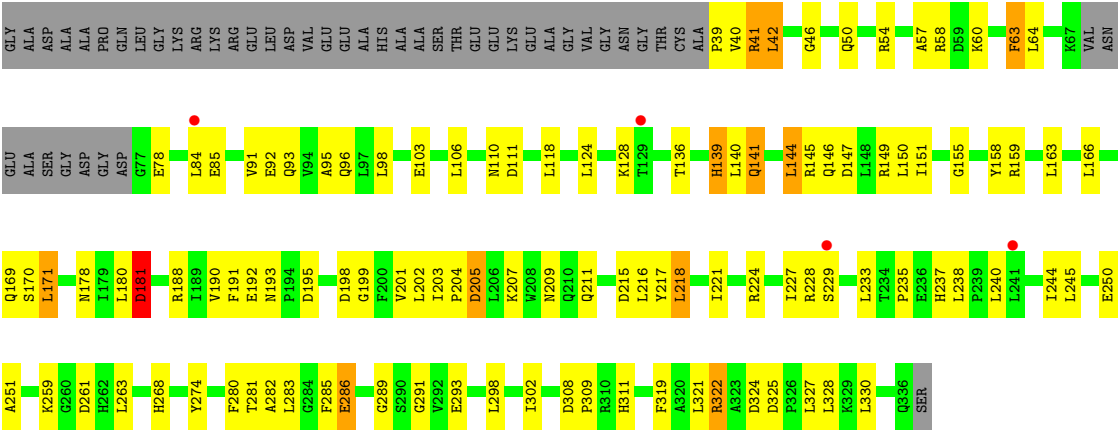


• Molecule 1: m7GpppX diphosphatase

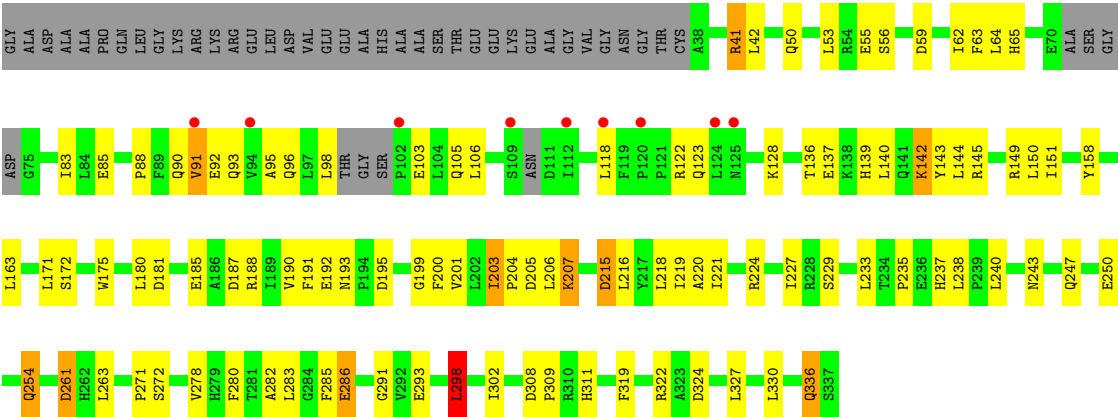


• Molecule 1: m7GpppX diphosphatase





● Molecule 1: m7GpppX diphosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.25Å 105.23Å 139.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.89 – 3.21 33.89 – 3.21	Depositor EDS
% Data completeness (in resolution range)	83.2 (33.89-3.21) 83.4 (33.89-3.21)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.211 , 0.276 0.263 , 0.296	Depositor DCC
R_{free} test set	1069 reflections (4.27%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.752	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 108.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9617	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1064e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PO4, 31G

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	0.95	0/2432	1.45	33/3298 (1.0%)
1	B	0.92	0/2440	1.40	20/3311 (0.6%)
1	C	0.90	0/2446	1.43	19/3318 (0.6%)
1	D	0.93	0/2466	1.45	36/3342 (1.1%)
All	All	0.93	0/9784	1.43	108/13269 (0.8%)

There are no bond length outliers.

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	187	ASP	CA-CB-CG	8.68	121.28	112.60
1	A	187	ASP	CA-CB-CG	8.63	121.23	112.60
1	D	286	GLU	CA-C-N	7.86	132.07	120.83
1	D	286	GLU	C-N-CA	7.86	132.07	120.83
1	A	205	ASP	CA-C-N	7.12	130.13	120.38
1	A	205	ASP	C-N-CA	7.12	130.13	120.38
1	B	286	GLU	CB-CG-CD	6.94	124.39	112.60
1	A	261	ASP	CA-CB-CG	6.69	119.29	112.60
1	C	285	PHE	CA-CB-CG	6.69	120.49	113.80
1	A	285	PHE	CA-CB-CG	6.63	120.43	113.80
1	C	205	ASP	CA-C-N	6.38	129.12	120.38
1	C	205	ASP	C-N-CA	6.38	129.12	120.38
1	B	285	PHE	CA-CB-CG	6.33	120.12	113.80
1	D	285	PHE	CA-CB-CG	6.32	120.12	113.80
1	A	175	TRP	CA-C-N	6.23	128.49	120.70
1	A	175	TRP	C-N-CA	6.23	128.49	120.70
1	D	171	LEU	CA-C-N	6.18	133.35	121.54
1	D	171	LEU	C-N-CA	6.18	133.35	121.54
1	C	63	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	173	ILE	CA-C-N	6.06	133.12	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ILE	C-N-CA	6.06	133.12	121.54
1	D	261	ASP	CA-CB-CG	6.01	118.61	112.60
1	D	271	PRO	CA-C-N	6.00	128.56	120.65
1	D	271	PRO	C-N-CA	6.00	128.56	120.65
1	C	110	ASN	CA-CB-CG	5.92	118.52	112.60
1	A	229	SER	CA-C-N	5.78	128.82	120.38
1	A	229	SER	C-N-CA	5.78	128.82	120.38
1	B	215	ASP	CA-CB-CG	5.76	118.36	112.60
1	B	274	TYR	CA-C-N	5.74	129.37	121.33
1	B	274	TYR	C-N-CA	5.74	129.37	121.33
1	D	175	TRP	CA-C-N	5.70	127.74	120.56
1	D	175	TRP	C-N-CA	5.70	127.74	120.56
1	D	286	GLU	CB-CG-CD	5.69	122.27	112.60
1	A	88	PRO	CA-C-N	5.68	129.17	120.82
1	A	88	PRO	C-N-CA	5.68	129.17	120.82
1	A	248	GLY	CA-C-N	5.66	128.43	120.28
1	A	248	GLY	C-N-CA	5.66	128.43	120.28
1	D	193	ASN	N-CA-C	-5.65	97.32	109.01
1	D	207	LYS	CA-C-N	5.63	129.10	121.05
1	D	207	LYS	C-N-CA	5.63	129.10	121.05
1	B	95	ALA	CA-C-N	5.63	127.82	120.28
1	B	95	ALA	C-N-CA	5.63	127.82	120.28
1	B	193	ASN	N-CA-C	-5.60	97.42	109.01
1	C	215	ASP	CA-CB-CG	5.59	118.19	112.60
1	D	263	LEU	N-CA-C	5.56	118.15	108.76
1	B	181	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	215	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	263	LEU	N-CA-C	5.54	118.12	108.76
1	B	261	ASP	CA-CB-CG	5.53	118.13	112.60
1	C	181	ASP	CA-CB-CG	5.53	118.13	112.60
1	D	122	ARG	CA-C-N	5.53	128.45	120.38
1	D	122	ARG	C-N-CA	5.53	128.45	120.38
1	D	215	ASP	CA-CB-CG	5.52	118.12	112.60
1	C	95	ALA	CA-C-N	5.49	127.63	120.28
1	C	95	ALA	C-N-CA	5.49	127.63	120.28
1	A	305	LEU	CA-C-N	5.47	128.06	120.29
1	A	305	LEU	C-N-CA	5.47	128.06	120.29
1	A	206	LEU	N-CA-CB	-5.45	101.89	110.06
1	D	95	ALA	CA-C-N	5.45	127.52	120.44
1	D	95	ALA	C-N-CA	5.45	127.52	120.44
1	C	263	LEU	N-CA-C	5.44	117.96	108.76
1	C	193	ASN	N-CA-C	-5.43	97.77	109.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	GLY	CA-C-N	5.42	129.50	120.62
1	A	291	GLY	C-N-CA	5.42	129.50	120.62
1	A	158	TYR	CA-C-N	5.41	127.85	120.54
1	A	158	TYR	C-N-CA	5.41	127.85	120.54
1	A	193	ASN	N-CA-C	-5.39	97.85	109.01
1	A	169	GLN	CA-C-N	5.37	131.80	121.54
1	A	169	GLN	C-N-CA	5.37	131.80	121.54
1	C	229	SER	CA-C-N	5.36	128.20	120.38
1	C	229	SER	C-N-CA	5.36	128.20	120.38
1	D	336	GLN	CA-C-N	5.34	131.31	121.70
1	D	336	GLN	C-N-CA	5.34	131.31	121.70
1	B	88	PRO	CA-C-N	5.33	128.66	120.82
1	B	88	PRO	C-N-CA	5.33	128.66	120.82
1	D	291	GLY	CA-C-N	5.32	129.34	120.62
1	D	291	GLY	C-N-CA	5.32	129.34	120.62
1	B	147	ASP	CA-CB-CG	5.29	117.89	112.60
1	D	158	TYR	CA-C-N	5.29	127.68	120.54
1	D	158	TYR	C-N-CA	5.29	127.68	120.54
1	D	298	LEU	CA-C-N	5.28	127.61	120.38
1	D	298	LEU	C-N-CA	5.28	127.61	120.38
1	A	206	LEU	CA-C-N	5.27	131.60	121.54
1	A	206	LEU	C-N-CA	5.27	131.60	121.54
1	D	88	PRO	CA-C-N	5.24	128.52	120.82
1	D	88	PRO	C-N-CA	5.24	128.52	120.82
1	C	286	GLU	CA-C-N	5.23	128.30	120.83
1	C	286	GLU	C-N-CA	5.23	128.30	120.83
1	B	229	SER	CA-C-N	5.22	128.00	120.38
1	B	229	SER	C-N-CA	5.22	128.00	120.38
1	B	158	TYR	CA-C-N	5.20	127.56	120.54
1	B	158	TYR	C-N-CA	5.20	127.56	120.54
1	C	158	TYR	CA-C-N	5.20	127.56	120.54
1	C	158	TYR	C-N-CA	5.20	127.56	120.54
1	A	95	ALA	CA-C-N	5.19	127.23	120.28
1	A	95	ALA	C-N-CA	5.19	127.23	120.28
1	D	91	VAL	CA-C-N	5.19	127.18	120.44
1	D	91	VAL	C-N-CA	5.19	127.18	120.44
1	C	291	GLY	CA-C-N	5.16	129.08	120.62
1	C	291	GLY	C-N-CA	5.16	129.08	120.62
1	B	291	GLY	CA-C-N	5.16	129.08	120.62
1	B	291	GLY	C-N-CA	5.16	129.08	120.62
1	B	263	LEU	N-CA-C	5.13	117.44	108.76
1	D	233	LEU	N-CA-C	5.06	117.02	109.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	229	SER	CA-C-N	5.04	128.74	120.63
1	D	229	SER	C-N-CA	5.04	128.74	120.63
1	A	242	ARG	CA-C-N	5.01	127.41	120.29
1	A	242	ARG	C-N-CA	5.01	127.41	120.29

There are no chirality outliers.

There are no planarity outliers.

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	2377	0	2384	45	0
1	B	2384	0	2388	56	0
1	C	2389	0	2391	48	0
1	D	2411	0	2406	41	0
2	A	10	0	0	0	0
2	B	5	0	0	4	0
2	C	5	0	0	1	0
3	B	23	13	13	2	0
All	All	9604	13	9582	171	0

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 9.

All (171) 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:146:GLN:HG3	1:A:324:ASP:HB3	1.63	0.80
1:A:243:ASN:O	1:A:247:GLN:HB2	1.85	0.74
1:C:57:ALA:HB1	1:D:215:ASP:HB3	1.68	0.74
1:B:277:HIS:HE1	2:B:402:PO4:O4	1.70	0.73
1:B:62:ILE:HD12	1:B:64:LEU:HD11	1.75	0.69
1:B:243:ASN:O	1:B:247:GLN:HB2	1.93	0.67
1:B:205:ASP:OD2	1:B:207:LYS:HG2	1.95	0.67
1:A:94:VAL:HG11	1:B:62:ILE:HD11	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:GLN:HA	1:C:144:LEU:HB2	1.77	0.65
1:A:41:ARG:HG3	1:A:42:LEU:N	2.10	0.64
1:A:224:ARG:HD3	1:A:227:ILE:HD11	1.78	0.64
1:C:224:ARG:HD3	1:C:227:ILE:HD11	1.80	0.62
1:C:244:ILE:O	1:C:280:PHE:HZ	1.81	0.62
1:D:41:ARG:HD2	1:D:42:LEU:H	1.65	0.61
1:A:203:ILE:HG13	1:A:204:PRO:HD2	1.82	0.61
1:D:224:ARG:HD3	1:D:227:ILE:HD11	1.80	0.61
1:B:191:PHE:CZ	1:D:254:GLN:HB2	2.36	0.61
1:B:56:SER:HB3	1:B:61:ILE:HG22	1.82	0.60
1:B:217:TYR:CD1	1:B:281:THR:HG22	2.36	0.60
1:A:244:ILE:O	1:A:280:PHE:HZ	1.85	0.60
1:B:180:LEU:HD21	1:B:221:ILE:HG22	1.84	0.59
1:B:224:ARG:HD3	1:B:227:ILE:HD11	1.83	0.59
1:C:198:ASP:HA	1:C:240:LEU:HB2	1.85	0.58
1:A:60:LYS:HG2	1:B:86:LYS:O	2.04	0.58
1:B:113:TYR:HE1	3:B:401:31G:O2	1.85	0.58
1:C:147:ASP:HB3	1:C:149:ARG:HH12	1.68	0.58
1:C:41:ARG:HH12	1:C:42:LEU:HD22	1.68	0.57
1:B:113:TYR:CE1	3:B:401:31G:O2	2.57	0.57
1:B:85:GLU:HB3	1:B:128:LYS:HB3	1.87	0.57
1:D:327:LEU:HA	1:D:330:LEU:HD12	1.86	0.56
1:A:150:LEU:HD13	1:B:283:LEU:HD11	1.87	0.56
1:B:191:PHE:CE2	1:D:254:GLN:HB2	2.40	0.56
1:B:327:LEU:HA	1:B:330:LEU:HD12	1.87	0.56
1:B:209:ASN:HD22	1:B:211:GLN:HE21	1.53	0.56
1:D:85:GLU:HB3	1:D:128:LYS:HB3	1.87	0.56
1:A:240:LEU:O	1:A:244:ILE:HD12	2.06	0.56
1:A:271:PRO:HD2	1:A:274:TYR:HE1	1.70	0.56
1:A:85:GLU:HB3	1:A:128:LYS:HB3	1.87	0.55
1:A:215:ASP:HB3	1:B:57:ALA:HB1	1.88	0.55
1:C:180:LEU:HD21	1:C:221:ILE:HG22	1.88	0.55
1:C:85:GLU:HB3	1:C:128:LYS:HB3	1.88	0.55
1:D:137:GLU:HA	1:D:140:LEU:HD12	1.88	0.55
1:C:327:LEU:HA	1:C:330:LEU:HD12	1.88	0.55
1:C:191:PHE:CD2	1:C:251:ALA:HB2	2.42	0.55
1:C:209:ASN:HD22	1:C:211:GLN:HE21	1.55	0.55
1:A:202:LEU:HA	1:A:219:ILE:O	2.07	0.54
1:A:220:ALA:HB2	1:A:280:PHE:HE1	1.73	0.54
1:B:222:CYS:HB2	1:B:240:LEU:HD11	1.90	0.54
1:B:277:HIS:CE1	2:B:402:PO4:O4	2.55	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:GLN:HE21	1:D:65:HIS:HE1	1.56	0.54
1:A:271:PRO:HD2	1:A:274:TYR:CE1	2.42	0.54
1:C:178:ASN:HA	1:C:181:ASP:OD1	2.08	0.54
1:C:268:HIS:HB2	2:C:401:PO4:O2	2.08	0.53
1:C:163:LEU:HD11	1:C:228:ARG:NH1	2.24	0.53
1:B:178:ASN:HA	1:B:181:ASP:OD1	2.09	0.53
1:A:149:ARG:HH21	1:B:259:LYS:NZ	2.07	0.53
1:A:327:LEU:HA	1:A:330:LEU:HD12	1.89	0.53
1:B:268:HIS:HB2	2:B:402:PO4:O2	2.08	0.53
1:A:191:PHE:HB3	1:A:202:LEU:HB3	1.90	0.53
1:B:56:SER:HB3	1:B:61:ILE:CG2	2.39	0.53
1:B:188:ARG:NH1	1:B:206:LEU:HG	2.23	0.53
1:A:192:GLU:HG3	1:A:201:VAL:HG22	1.91	0.52
1:C:58:ARG:HD3	1:D:286:GLU:O	2.10	0.52
1:A:94:VAL:HG11	1:B:62:ILE:CD1	2.39	0.52
1:D:180:LEU:HD21	1:D:221:ILE:HG22	1.91	0.52
1:D:56:SER:HB3	1:D:59:ASP:HB2	1.91	0.52
1:C:192:GLU:HG3	1:C:201:VAL:HG22	1.92	0.51
1:D:192:GLU:HG3	1:D:201:VAL:HG22	1.92	0.51
1:A:50:GLN:HE21	1:A:65:HIS:CE1	2.28	0.51
1:C:54:ARG:HG2	1:C:145:ARG:HB2	1.92	0.51
1:C:150:LEU:HD13	1:D:283:LEU:HD11	1.93	0.51
1:A:86:LYS:HD2	1:B:86:LYS:HD2	1.92	0.51
1:B:293:GLU:O	1:B:319:PHE:HA	2.11	0.51
1:A:180:LEU:HD21	1:A:221:ILE:HG22	1.91	0.51
1:B:190:VAL:HG23	1:B:204:PRO:HD3	1.92	0.51
1:B:238:LEU:HD22	1:B:302:ILE:HG23	1.92	0.51
1:C:233:LEU:HA	1:C:237:HIS:ND1	2.26	0.50
1:A:145:ARG:HG2	1:A:145:ARG:HH11	1.76	0.50
1:D:185:GLU:HG2	1:D:188:ARG:HD3	1.93	0.50
1:C:39:PRO:HA	1:D:105:GLN:HG2	1.93	0.50
1:C:283:LEU:HD11	1:D:150:LEU:HD13	1.94	0.50
1:B:233:LEU:HB3	1:B:305:LEU:HD11	1.94	0.49
1:A:191:PHE:HB2	1:A:251:ALA:HB1	1.95	0.49
1:A:195:ASP:O	1:A:199:GLY:HA3	2.13	0.49
1:B:192:GLU:HG3	1:B:201:VAL:HG22	1.94	0.49
1:A:293:GLU:O	1:A:319:PHE:HA	2.11	0.49
1:B:138:LYS:NZ	1:B:141:GLN:HE22	2.11	0.49
1:C:238:LEU:HD22	1:C:302:ILE:HG23	1.93	0.49
1:A:267:LEU:HD12	1:A:301:VAL:HG21	1.95	0.49
1:D:142:LYS:HD2	1:D:322:ARG:HH21	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:GLU:O	1:C:319:PHE:HA	2.13	0.49
1:C:147:ASP:HB3	1:C:149:ARG:NH1	2.27	0.48
1:D:55:GLU:HG3	1:D:62:ILE:HD12	1.94	0.48
1:C:268:HIS:HE2	1:C:289:GLY:CA	2.26	0.48
1:A:268:HIS:HE2	1:A:289:GLY:CA	2.25	0.48
1:B:163:LEU:HD11	1:B:228:ARG:NH1	2.29	0.48
1:D:50:GLN:HE21	1:D:65:HIS:CE1	2.31	0.48
1:D:63:PHE:CD2	1:D:83:ILE:HD12	2.49	0.48
1:D:203:ILE:N	1:D:203:ILE:HD13	2.29	0.48
1:A:63:PHE:CD2	1:A:83:ILE:HD12	2.50	0.47
1:B:235:PRO:HG2	1:B:309:PRO:HB3	1.97	0.47
1:C:204:PRO:HA	1:C:218:LEU:HA	1.97	0.46
1:A:238:LEU:HD22	1:A:302:ILE:HG23	1.96	0.46
1:B:53:LEU:HD23	1:B:144:LEU:HB2	1.96	0.46
1:C:235:PRO:HG2	1:C:309:PRO:HB3	1.97	0.46
1:D:238:LEU:HD22	1:D:302:ILE:HG23	1.97	0.46
1:A:216:LEU:HB3	1:A:282:ALA:HB2	1.97	0.46
1:D:293:GLU:O	1:D:319:PHE:HA	2.14	0.46
1:A:137:GLU:HA	1:A:140:LEU:HD12	1.97	0.46
1:C:141:GLN:HE21	1:C:144:LEU:HD13	1.81	0.46
1:D:41:ARG:HD2	1:D:42:LEU:HG	1.98	0.46
1:C:190:VAL:HG23	1:C:204:PRO:HD3	1.98	0.46
1:C:169:GLN:O	1:C:171:LEU:HD22	2.15	0.46
1:C:155:GLY:O	1:C:159:ARG:HG3	2.16	0.46
1:D:195:ASP:O	1:D:199:GLY:HA3	2.16	0.46
1:D:243:ASN:O	1:D:247:GLN:HB2	2.17	0.45
1:D:201:VAL:HG12	1:D:203:ILE:CD1	2.46	0.45
1:C:93:GLN:HB3	1:C:124:LEU:HD21	1.99	0.45
1:C:195:ASP:O	1:C:199:GLY:HA3	2.16	0.45
1:C:308:ASP:HB3	1:C:311:HIS:HB2	1.98	0.45
1:A:47:PHE:O	1:B:99:THR:HG22	2.16	0.45
1:D:191:PHE:CD2	1:D:200:PHE:CZ	3.04	0.45
1:D:220:ALA:HB2	1:D:280:PHE:HE1	1.81	0.45
1:D:216:LEU:HB3	1:D:282:ALA:HB2	1.98	0.45
1:B:277:HIS:HE1	2:B:402:PO4:P	2.39	0.45
1:D:191:PHE:HD2	1:D:200:PHE:CZ	2.35	0.45
1:A:185:GLU:HG2	1:A:188:ARG:HD3	1.97	0.45
1:B:200:PHE:HE2	1:B:202:LEU:HB2	1.82	0.45
1:B:171:LEU:HD21	1:B:173:ILE:HG23	1.98	0.45
1:C:41:ARG:NH1	1:C:42:LEU:HD22	2.30	0.45
1:C:216:LEU:HB3	1:C:282:ALA:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LEU:HA	1:B:144:LEU:HD12	1.98	0.44
1:C:205:ASP:OD2	1:C:207:LYS:HE2	2.16	0.44
1:B:80:ALA:HB2	1:B:133:TYR:HD1	1.83	0.44
1:A:308:ASP:HB3	1:A:311:HIS:HB2	1.98	0.44
1:D:93:GLN:HG2	1:D:123:GLN:CD	2.42	0.44
1:C:322:ARG:HH21	1:C:325:ASP:HA	1.83	0.44
1:B:195:ASP:O	1:B:199:GLY:HA3	2.18	0.44
1:B:308:ASP:HB3	1:B:311:HIS:HB2	1.99	0.44
1:B:216:LEU:HB3	1:B:282:ALA:HB2	2.00	0.44
1:A:146:GLN:HE21	1:A:323:ALA:HB3	1.83	0.44
1:B:201:VAL:HG12	1:B:203:ILE:HG23	1.99	0.43
1:C:166:LEU:HA	1:C:169:GLN:HE21	1.83	0.43
1:C:217:TYR:CD1	1:C:281:THR:HG22	2.54	0.43
1:A:149:ARG:HH21	1:B:259:LYS:HZ3	1.66	0.42
1:B:204:PRO:HA	1:B:218:LEU:HA	2.00	0.42
1:B:54:ARG:H	1:B:63:PHE:HB2	1.84	0.42
1:B:240:LEU:O	1:B:244:ILE:HG13	2.19	0.42
1:D:308:ASP:HB3	1:D:311:HIS:HB2	2.00	0.42
1:A:206:LEU:HA	1:B:108:PHE:HZ	1.84	0.42
1:C:136:THR:HG23	1:C:139:HIS:H	1.84	0.42
1:C:202:LEU:HD11	1:C:218:LEU:HB3	2.01	0.42
1:D:205:ASP:OD1	1:D:207:LYS:HB2	2.20	0.42
1:A:56:SER:HB3	1:A:59:ASP:HB2	2.02	0.42
1:C:54:ARG:H	1:C:63:PHE:HB2	1.85	0.42
1:A:204:PRO:HA	1:A:218:LEU:HA	2.02	0.42
1:A:253:LEU:HD13	1:A:259:LYS:HA	2.02	0.41
1:A:175:TRP:HB2	1:B:110:ASN:ND2	2.35	0.41
1:B:271:PRO:HD2	1:B:274:TYR:HE1	1.85	0.41
1:A:41:ARG:NH2	1:A:42:LEU:HD12	2.35	0.41
1:C:259:LYS:NZ	1:D:149:ARG:HH21	2.18	0.41
1:D:53:LEU:HD13	1:D:143:TYR:HB2	2.01	0.41
1:C:188:ARG:HH22	1:C:205:ASP:C	2.28	0.41
1:D:235:PRO:HG2	1:D:309:PRO:HB3	2.03	0.41
1:B:197:SER:O	1:B:240:LEU:HD13	2.21	0.40
1:D:190:VAL:HG23	1:D:204:PRO:HD3	2.03	0.40
1:D:237:HIS:O	1:D:240:LEU:HB3	2.22	0.40
1:D:278:VAL:HG11	1:D:298:LEU:HD12	2.03	0.40
1:B:110:ASN:O	1:B:113:TYR:HB2	2.20	0.40
1:C:228:ARG:HB3	1:C:274:TYR:HB3	2.04	0.40
1:C:321:LEU:HB2	1:C:328:LEU:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	281/337 (83%)	251 (89%)	27 (10%)	3 (1%)	11	42
1	B	284/337 (84%)	257 (90%)	24 (8%)	3 (1%)	11	42
1	C	285/337 (85%)	260 (91%)	21 (7%)	4 (1%)	9	37
1	D	284/337 (84%)	254 (89%)	26 (9%)	4 (1%)	9	37
All	All	1134/1348 (84%)	1022 (90%)	98 (9%)	14 (1%)	10	40

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	A	91	VAL
1	A	174	GLN
1	C	46	GLY
1	C	91	VAL
1	C	146	GLN
1	B	41	ARG
1	B	288	PRO
1	D	91	VAL
1	D	206	LEU
1	B	170	SER
1	D	172	SER
1	C	40	VAL
1	D	336	GLN

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	261/294 (89%)	237 (91%)	24 (9%)	8	32
1	B	262/294 (89%)	231 (88%)	31 (12%)	5	22
1	C	262/294 (89%)	231 (88%)	31 (12%)	5	22
1	D	264/294 (90%)	238 (90%)	26 (10%)	7	30
All	All	1049/1176 (89%)	937 (89%)	112 (11%)	6	26

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	48	ARG
1	A	54	ARG
1	A	64	LEU
1	A	78	GLU
1	A	92	GLU
1	A	96	GLN
1	A	98	LEU
1	A	106	LEU
1	A	109	SER
1	A	112	ILE
1	A	118	LEU
1	A	128	LYS
1	A	145	ARG
1	A	151	ILE
1	A	163	LEU
1	A	181	ASP
1	A	202	LEU
1	A	218	LEU
1	A	219	ILE
1	A	250	GLU
1	A	298	LEU
1	A	322	ARG
1	A	324	ASP
1	B	45	SER
1	B	55	GLU
1	B	60	LYS
1	B	64	LEU
1	B	84	LEU
1	B	90	GLN
1	B	96	GLN
1	B	98	LEU
1	B	106	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	118	LEU
1	B	140	LEU
1	B	144	LEU
1	B	146	GLN
1	B	147	ASP
1	B	151	ILE
1	B	161	ILE
1	B	171	LEU
1	B	181	ASP
1	B	203	ILE
1	B	205	ASP
1	B	206	LEU
1	B	218	LEU
1	B	219	ILE
1	B	245	LEU
1	B	250	GLU
1	B	254	GLN
1	B	261	ASP
1	B	277	HIS
1	B	298	LEU
1	B	322	ARG
1	B	324	ASP
1	C	41	ARG
1	C	42	LEU
1	C	50	GLN
1	C	60	LYS
1	C	64	LEU
1	C	78	GLU
1	C	84	LEU
1	C	92	GLU
1	C	96	GLN
1	C	98	LEU
1	C	103	GLU
1	C	106	LEU
1	C	111	ASP
1	C	118	LEU
1	C	139	HIS
1	C	140	LEU
1	C	141	GLN
1	C	144	LEU
1	C	151	ILE
1	C	170	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	171	LEU
1	C	181	ASP
1	C	203	ILE
1	C	218	LEU
1	C	245	LEU
1	C	250	GLU
1	C	261	ASP
1	C	286	GLU
1	C	298	LEU
1	C	322	ARG
1	C	324	ASP
1	D	41	ARG
1	D	64	LEU
1	D	90	GLN
1	D	92	GLU
1	D	96	GLN
1	D	98	LEU
1	D	103	GLU
1	D	106	LEU
1	D	118	LEU
1	D	136	THR
1	D	139	HIS
1	D	142	LYS
1	D	144	LEU
1	D	145	ARG
1	D	151	ILE
1	D	163	LEU
1	D	181	ASP
1	D	203	ILE
1	D	218	LEU
1	D	219	ILE
1	D	250	GLU
1	D	254	GLN
1	D	261	ASP
1	D	272	SER
1	D	298	LEU
1	D	324	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	90	GLN
1	A	107	GLN
1	A	125	ASN
1	A	146	GLN
1	A	174	GLN
1	A	178	ASN
1	A	246	HIS
1	A	275	HIS
1	A	313	GLN
1	B	50	GLN
1	B	90	GLN
1	B	107	GLN
1	B	110	ASN
1	B	125	ASN
1	B	141	GLN
1	B	193	ASN
1	B	211	GLN
1	B	249	GLN
1	B	275	HIS
1	B	277	HIS
1	B	313	GLN
1	C	96	GLN
1	C	110	ASN
1	C	141	GLN
1	C	169	GLN
1	C	211	GLN
1	C	249	GLN
1	C	262	HIS
1	C	275	HIS
1	C	313	GLN
1	D	65	HIS
1	D	69	ASN
1	D	96	GLN
1	D	107	GLN
1	D	123	GLN
1	D	146	GLN
1	D	169	GLN
1	D	174	GLN
1	D	178	ASN
1	D	193	ASN
1	D	247	GLN
1	D	254	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	313	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
2	PO4	A	402	-	4,4,4	2.57	2 (50%)	6,6,6	0.20	0
3	31G	B	401	1	23,25,26	0.63	1 (4%)	33,35,38	1.78	6 (18%)
2	PO4	C	401	-	4,4,4	1.96	2 (50%)	6,6,6	1.14	1 (16%)
2	PO4	B	402	-	4,4,4	2.77	2 (50%)	6,6,6	1.04	0
2	PO4	A	401	-	4,4,4	2.57	3 (75%)	6,6,6	1.37	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	31G	B	401	1	-	2/9/9/11	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	PO4	P-O1	4.41	1.60	1.50
2	A	402	PO4	P-O1	4.29	1.60	1.50
2	A	401	PO4	P-O1	4.17	1.60	1.50
3	B	401	31G	C5-S1	-2.36	1.75	1.80
2	B	402	PO4	P-O3	2.11	1.60	1.54
2	C	401	PO4	P-O3	2.10	1.60	1.54
2	C	401	PO4	P-O2	2.05	1.60	1.54
2	A	402	PO4	P-O3	2.05	1.60	1.54
2	A	401	PO4	P-O3	2.05	1.60	1.54
2	A	401	PO4	P-O4	2.02	1.60	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	31G	C7-O3-C8	5.40	124.86	117.49
3	B	401	31G	O3-C7-C3	4.29	121.75	109.16
3	B	401	31G	C8-C13-C14	3.72	129.10	126.31
3	B	401	31G	O2-S1-C5	3.53	112.50	104.55
3	B	401	31G	C14-C13-C12	-3.20	112.65	114.90
2	A	401	PO4	O4-P-O3	2.79	116.58	107.91
2	C	401	PO4	O3-P-O2	2.49	115.67	107.91
3	B	401	31G	O3-C8-C13	-2.07	110.79	117.70

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	31G	C13-C8-O3-C7
3	B	401	31G	C9-C8-O3-C7

There are no ring outliers.

3 monomers are involved in 7 short contacts:

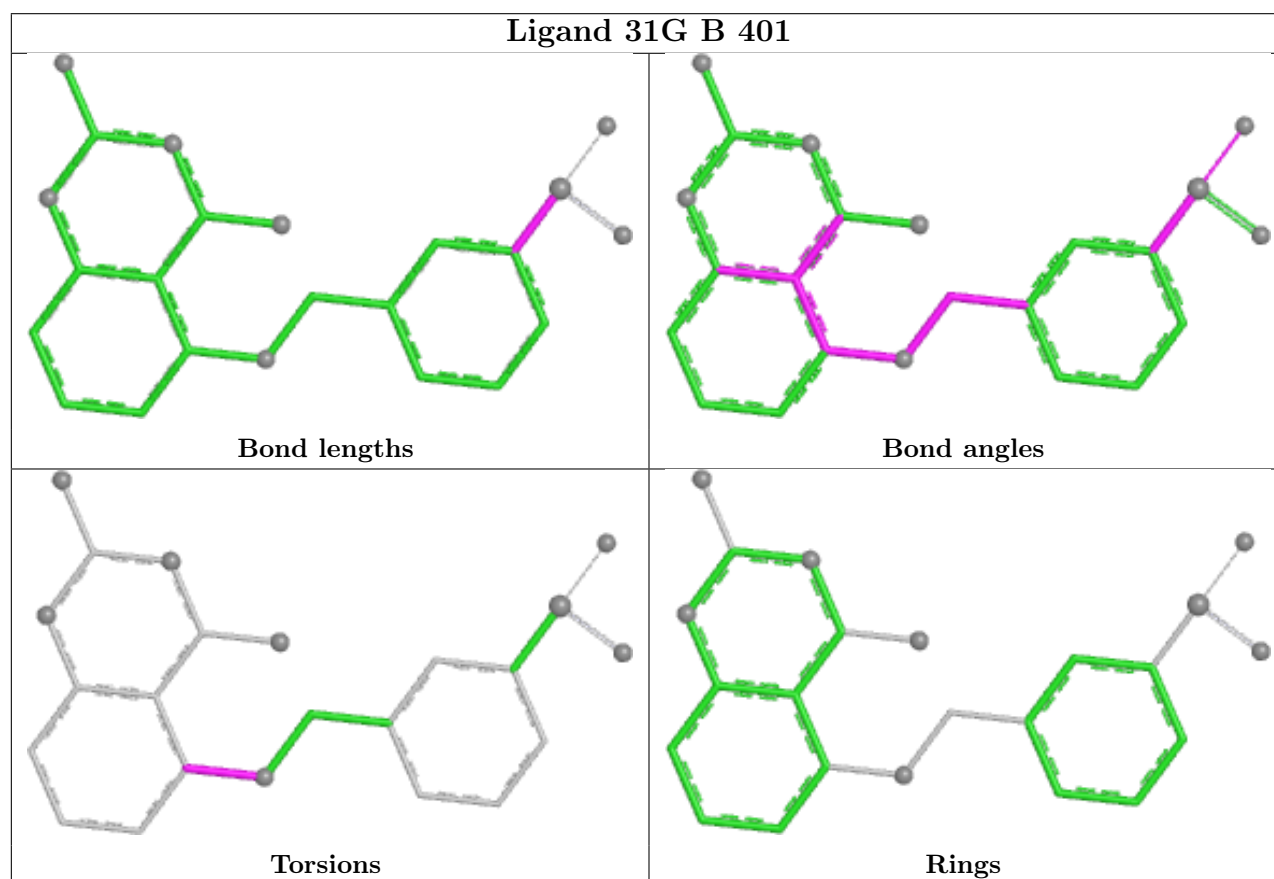
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	31G	2	0
2	C	401	PO4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	PO4	4	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	287/337 (85%)	0.15	2 (0%) 84 70	36, 83, 173, 195	0
1	B	288/337 (85%)	0.10	2 (0%) 84 70	40, 87, 179, 216	0
1	C	289/337 (85%)	0.15	4 (1%) 73 54	59, 96, 186, 198	0
1	D	292/337 (86%)	0.21	9 (3%) 51 33	53, 100, 182, 200	0
All	All	1156/1348 (85%)	0.15	17 (1%) 72 52	36, 93, 183, 216	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	VAL	2.8
1	C	129	THR	2.7
1	D	94	VAL	2.7
1	D	118	LEU	2.5
1	D	91	VAL	2.4
1	D	109	SER	2.4
1	B	227	ILE	2.3
1	C	241	LEU	2.3
1	D	124	LEU	2.3
1	D	102	PRO	2.2
1	A	170	SER	2.2
1	D	125	ASN	2.2
1	D	120	PRO	2.2
1	D	112	ILE	2.1
1	C	229	SER	2.1
1	B	276	LEU	2.0
1	C	84	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

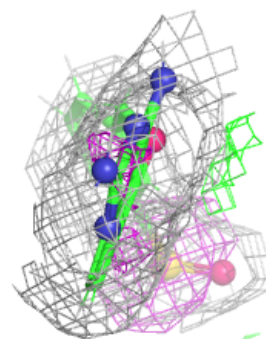
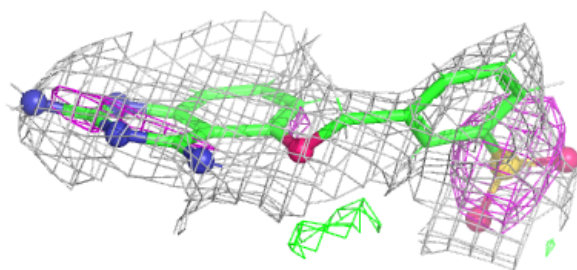
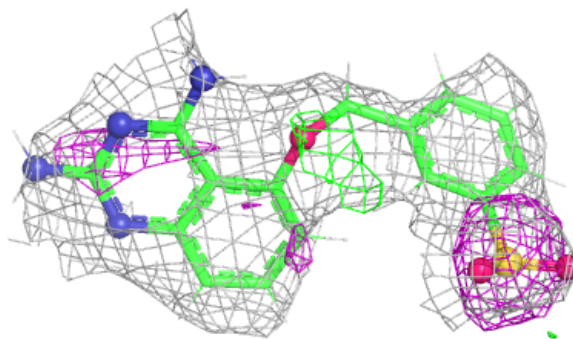
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PO4	C	401	5/5	0.81	0.12	80,84,85,88	0
2	PO4	A	402	5/5	0.83	0.12	106,109,111,111	0
3	31G	B	401	23/24	0.83	0.12	33,45,101,104	13
2	PO4	B	402	5/5	0.90	0.08	51,53,57,59	0
2	PO4	A	401	5/5	0.93	0.09	62,66,67,69	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 31G B 401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.