



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:23 PM UTC

PDB ID : 1NI4 / pdb_00001ni4
Title : HUMAN PYRUVATE DEHYDROGENASE
Authors : Ciszak, E.; Korotchkina, L.G.; Dominiak, P.M.; Sidhu, S.; Patel, M.S.
Deposited on : 2002-12-20
Resolution : 1.95 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

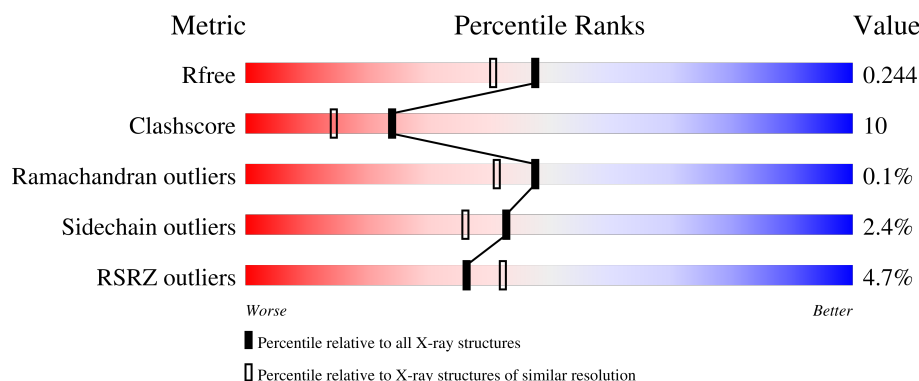
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	365	
1	C	365	
2	B	341	
2	D	341	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11496 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 Pyruvate dehydrogenase E1 component: Alpha subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	Se	0	0	0
			2824	1772	496	532	12	12			
1	C	362	Total	C	N	O	S	Se	0	0	0
			2824	1772	496	532	12	12			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	cloning artifact	UNP P08559
A	-2	ARG	-	cloning artifact	UNP P08559
A	-1	GLY	-	cloning artifact	UNP P08559
A	0	SER	-	cloning artifact	UNP P08559
A	38	MSE	MET	modified residue	UNP P08559
A	39	MSE	MET	modified residue	UNP P08559
A	45	MSE	MET	modified residue	UNP P08559
A	124	MSE	MET	modified residue	UNP P08559
A	126	MSE	MET	modified residue	UNP P08559
A	181	MSE	MET	modified residue	UNP P08559
A	200	MSE	MET	modified residue	UNP P08559
A	228	MSE	MET	modified residue	UNP P08559
A	253	MSE	MET	modified residue	UNP P08559
A	265	MSE	MET	modified residue	UNP P08559
A	289	MSE	MET	modified residue	UNP P08559
A	295	MSE	MET	modified residue	UNP P08559
C	-3	MET	-	cloning artifact	UNP P08559
C	-2	ARG	-	cloning artifact	UNP P08559
C	-1	GLY	-	cloning artifact	UNP P08559
C	0	SER	-	cloning artifact	UNP P08559
C	38	MSE	MET	modified residue	UNP P08559
C	39	MSE	MET	modified residue	UNP P08559
C	45	MSE	MET	modified residue	UNP P08559
C	124	MSE	MET	modified residue	UNP P08559
C	126	MSE	MET	modified residue	UNP P08559

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	181	MSE	MET	modified residue	UNP P08559
C	200	MSE	MET	modified residue	UNP P08559
C	228	MSE	MET	modified residue	UNP P08559
C	253	MSE	MET	modified residue	UNP P08559
C	265	MSE	MET	modified residue	UNP P08559
C	289	MSE	MET	modified residue	UNP P08559
C	295	MSE	MET	modified residue	UNP P08559

- Molecule 2 is a protein called Pyruvate dehydrogenase E1 component: Beta subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	330	Total	C	N	O	S	Se	0	0	0
			2525	1607	428	471	6	13			
2	D	330	Total	C	N	O	S	Se	0	0	0
			2525	1607	428	471	6	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	cloning artifact	UNP P11177
B	-10	ARG	-	cloning artifact	UNP P11177
B	-9	GLY	-	cloning artifact	UNP P11177
B	-8	SER	-	cloning artifact	UNP P11177
B	-7	HIS	-	expression tag	UNP P11177
B	-6	HIS	-	expression tag	UNP P11177
B	-5	HIS	-	expression tag	UNP P11177
B	-4	HIS	-	expression tag	UNP P11177
B	-3	HIS	-	expression tag	UNP P11177
B	-2	HIS	-	expression tag	UNP P11177
B	-1	GLY	-	cloning artifact	UNP P11177
B	0	SER	-	cloning artifact	UNP P11177
B	1	LEU	-	SEE REMARK 999	UNP P11177
B	13	MSE	MET	modified residue	UNP P11177
B	60	MSE	MET	modified residue	UNP P11177
B	71	MSE	MET	modified residue	UNP P11177
B	81	MSE	MET	modified residue	UNP P11177
B	87	MSE	MET	modified residue	UNP P11177
B	103	MSE	MET	modified residue	UNP P11177
B	175	MSE	MET	modified residue	UNP P11177
B	238	MSE	MET	modified residue	UNP P11177
B	244	MSE	MET	modified residue	UNP P11177
B	246	MSE	MET	modified residue	UNP P11177

Continued on next page...

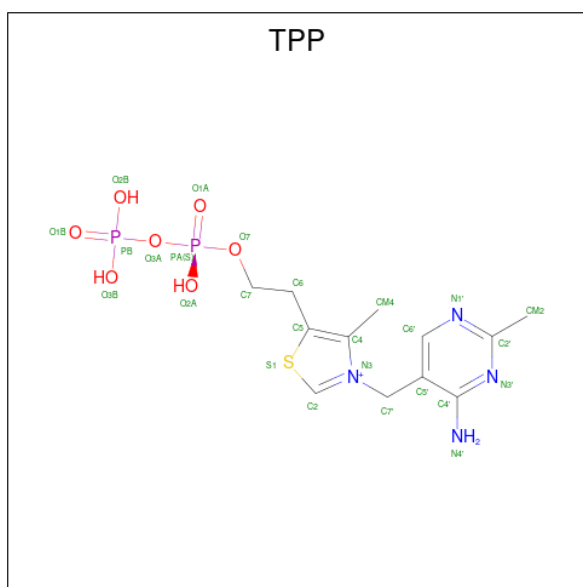
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	254	MSE	MET	modified residue	UNP P11177
B	280	MSE	MET	modified residue	UNP P11177
B	302	MSE	MET	modified residue	UNP P11177
D	-11	MET	-	cloning artifact	UNP P11177
D	-10	ARG	-	cloning artifact	UNP P11177
D	-9	GLY	-	cloning artifact	UNP P11177
D	-8	SER	-	cloning artifact	UNP P11177
D	-7	HIS	-	expression tag	UNP P11177
D	-6	HIS	-	expression tag	UNP P11177
D	-5	HIS	-	expression tag	UNP P11177
D	-4	HIS	-	expression tag	UNP P11177
D	-3	HIS	-	expression tag	UNP P11177
D	-2	HIS	-	expression tag	UNP P11177
D	-1	GLY	-	cloning artifact	UNP P11177
D	0	SER	-	cloning artifact	UNP P11177
D	1	LEU	-	SEE REMARK 999	UNP P11177
D	13	MSE	MET	modified residue	UNP P11177
D	60	MSE	MET	modified residue	UNP P11177
D	71	MSE	MET	modified residue	UNP P11177
D	81	MSE	MET	modified residue	UNP P11177
D	87	MSE	MET	modified residue	UNP P11177
D	103	MSE	MET	modified residue	UNP P11177
D	175	MSE	MET	modified residue	UNP P11177
D	238	MSE	MET	modified residue	UNP P11177
D	244	MSE	MET	modified residue	UNP P11177
D	246	MSE	MET	modified residue	UNP P11177
D	254	MSE	MET	modified residue	UNP P11177
D	280	MSE	MET	modified residue	UNP P11177
D	302	MSE	MET	modified residue	UNP P11177

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

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

- Molecule 4 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
4	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0

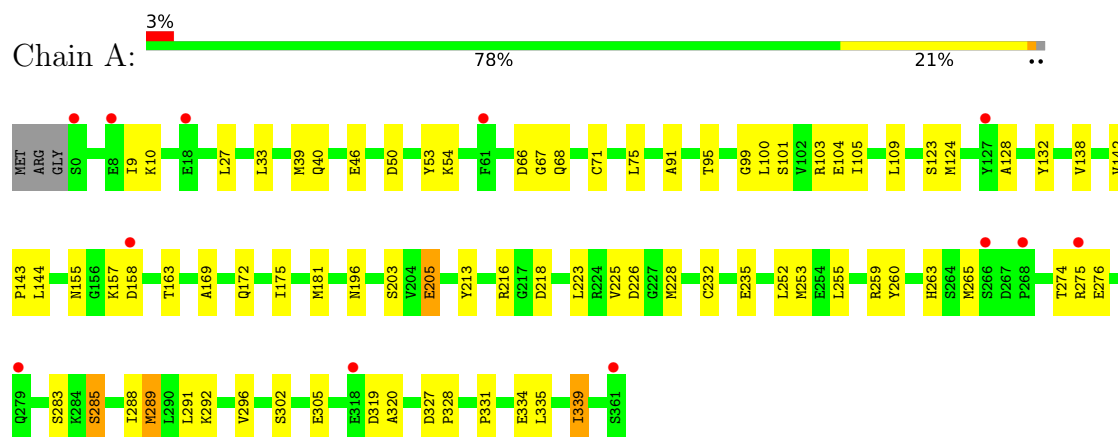
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	203	Total O 203 203	0	0
6	B	179	Total O 179 179	0	0
6	C	177	Total O 177 177	0	0
6	D	183	Total O 183 183	0	0

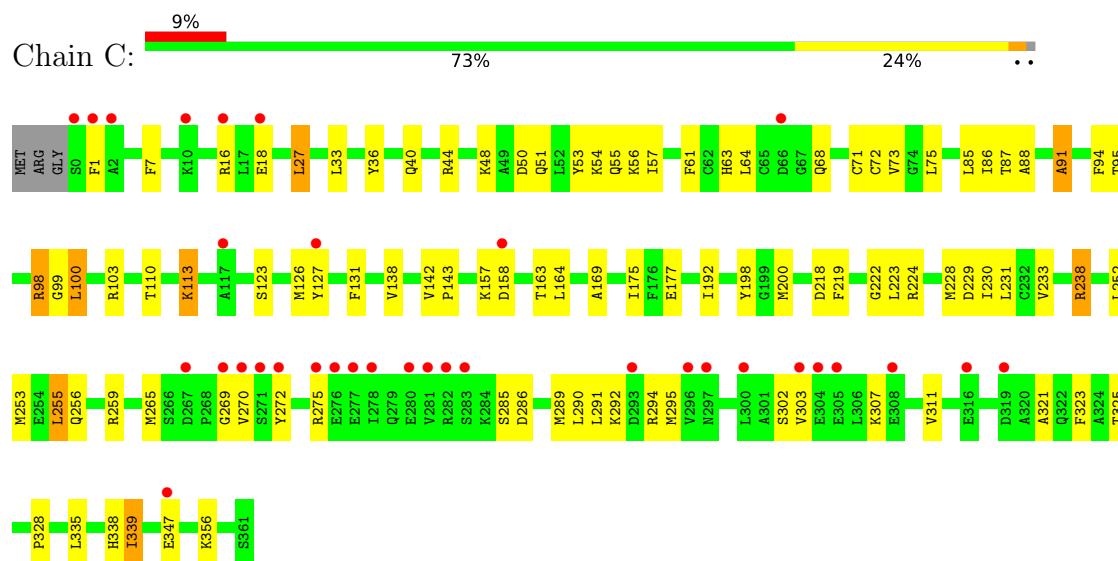
3 Residue-property plots

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.

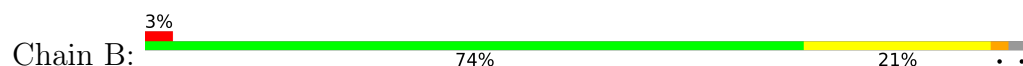
- Molecule 1: Pyruvate dehydrogenase E1 component: Alpha subunit

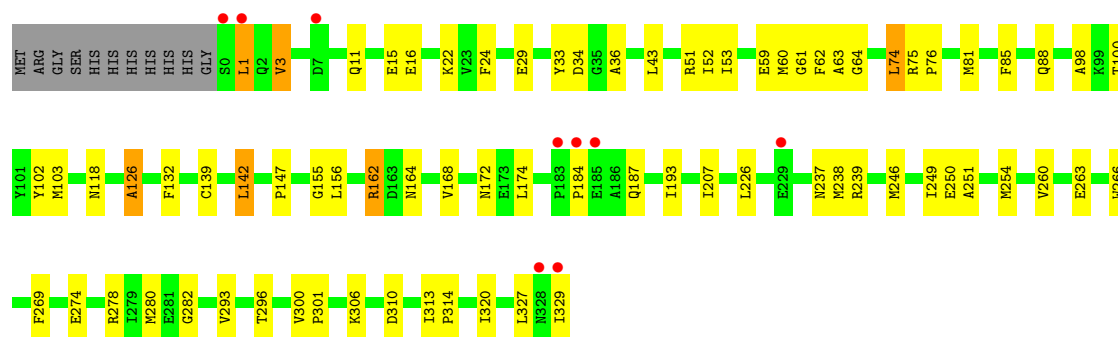


- Molecule 1: Pyruvate dehydrogenase E1 component: Alpha subunit

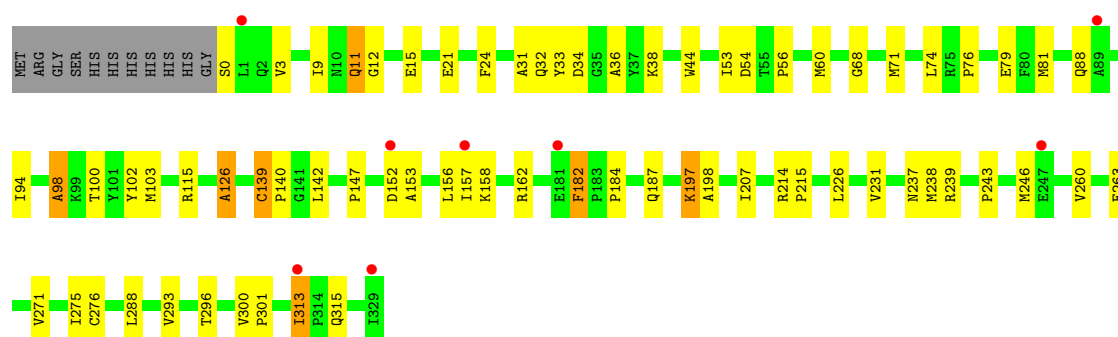
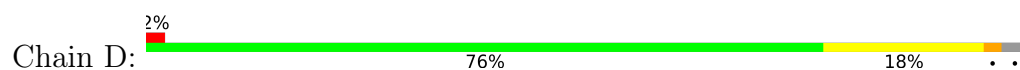


- Molecule 2: Pyruvate dehydrogenase E1 component: Beta subunit





● Molecule 2: Pyruvate dehydrogenase E1 component: Beta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.34Å 126.89Å 190.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.17 – 1.95 45.17 – 1.95	Depositor EDS
% Data completeness (in resolution range)	88.0 (45.17-1.95) 85.2 (45.17-1.95)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.95Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.202 , 0.244 0.208 , 0.244	Depositor DCC
R_{free} test set	17625 reflections (9.34%)	wwPDB-VP
Wilson B-factor (Å ²)	12.6	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11496	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TPP, K

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	0.38	0/2868	0.86	7/3842 (0.2%)
1	C	0.39	0/2868	0.81	7/3842 (0.2%)
2	B	0.41	0/2567	0.95	10/3457 (0.3%)
2	D	0.40	0/2567	0.94	5/3457 (0.1%)
All	All	0.40	0/10870	0.89	29/14598 (0.2%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	98	ALA	N-CA-C	9.21	121.31	111.28
2	D	126	ALA	N-CA-C	9.07	122.31	111.33
2	B	126	ALA	N-CA-C	8.57	121.70	111.33
2	D	53	ILE	N-CA-C	8.13	119.41	107.37
2	B	139	CYS	N-CA-C	7.88	120.19	109.24
1	A	285	SER	N-CA-C	7.70	119.50	110.41
2	B	53	ILE	N-CA-C	7.54	118.73	107.80
1	A	123	SER	N-CA-C	6.75	119.49	111.33
2	D	100	THR	N-CA-C	6.72	118.26	111.07
2	B	266	TRP	CA-C-N	6.69	125.92	118.97
2	B	266	TRP	C-N-CA	6.69	125.92	118.97
1	A	339	ILE	N-CA-C	-6.50	104.69	111.58
2	D	139	CYS	N-CA-C	6.48	118.89	109.04
1	A	91	ALA	N-CA-C	6.15	120.53	111.87
2	B	100	THR	N-CA-C	5.96	117.45	111.07
1	C	339	ILE	N-CA-C	-5.94	105.28	111.58
2	B	98	ALA	N-CA-C	5.68	117.48	111.28
2	B	63	ALA	N-CA-C	-5.59	105.26	111.36
1	A	99	GLY	N-CA-C	5.49	122.26	114.85
1	C	177	GLU	N-CA-C	-5.43	105.44	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	MSE	N-CA-C	5.35	119.86	113.23
1	C	91	ALA	N-CA-C	5.35	118.94	111.56
1	C	99	GLY	N-CA-C	5.28	122.39	114.95
2	B	282	GLY	CA-C-N	5.21	124.82	119.56
2	B	282	GLY	C-N-CA	5.21	124.82	119.56
1	C	123	SER	N-CA-C	5.20	116.95	111.28
1	A	67	GLY	N-CA-C	-5.15	107.88	114.37
1	C	198	TYR	N-CA-C	5.10	117.72	108.69
1	C	338	HIS	N-CA-C	5.01	118.54	111.52

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	2824	0	2780	61	0
1	C	2824	0	2780	67	0
2	B	2525	0	2522	49	0
2	D	2525	0	2522	53	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	26	0	16	1	0
4	C	26	0	16	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	203	0	0	4	0
6	B	179	0	0	5	0
6	C	177	0	0	4	0
6	D	183	0	0	4	0
All	All	11496	0	10636	214	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 10.

All (214) 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)
2:B:29:GLU:HG3	1:C:200:MSE:HE2	1.41	1.01
1:C:98:ARG:HG2	1:C:131:PHE:HB2	1.47	0.92
2:D:12:GLY:HA3	2:D:157:ILE:HD11	1.53	0.91
1:C:291:LEU:HG	1:C:295:MSE:HE2	1.51	0.90
2:B:118:ASN:HD21	2:B:132:PHE:H	1.15	0.89
2:B:301:PRO:HG2	2:D:102:TYR:CD2	2.14	0.81
1:A:53:TYR:HB3	1:A:265:MSE:HE2	1.70	0.74
1:C:16:ARG:NH1	1:C:219:PHE:HA	2.02	0.73
1:C:95:THR:HG21	1:C:126:MSE:HE3	1.70	0.73
2:B:88:GLN:HG2	2:D:60:MSE:HE1	1.71	0.73
1:C:286:ASP:HB3	1:C:289:MSE:HG2	1.71	0.72
2:D:147:PRO:HB3	2:D:156:LEU:HD12	1.71	0.71
1:C:95:THR:HG22	1:C:131:PHE:CE2	2.26	0.71
2:B:251:ALA:HA	2:B:254:MSE:HE3	1.71	0.70
2:B:22:LYS:HE3	6:B:1420:HOH:O	1.93	0.69
1:A:339:ILE:HD11	2:D:300:VAL:HG12	1.73	0.68
2:B:300:VAL:HG12	1:C:339:ILE:HD11	1.77	0.66
1:C:71:CYS:O	1:C:75:LEU:HD13	1.96	0.65
2:D:260:VAL:HG22	2:D:293:VAL:HG22	1.78	0.65
2:B:75:ARG:HH22	2:B:164:ASN:ND2	1.94	0.65
2:B:102:TYR:CD2	2:D:301:PRO:HG2	2.32	0.65
2:D:98:ALA:HB2	2:D:142:LEU:HD13	1.79	0.64
2:B:75:ARG:HH22	2:B:164:ASN:HD22	1.45	0.64
2:B:118:ASN:HD21	2:B:132:PHE:N	1.94	0.63
1:A:103:ARG:NH1	1:A:320:ALA:HA	2.14	0.63
1:A:10:LYS:HG2	6:A:2460:HOH:O	1.99	0.62
1:C:50:ASP:OD1	1:C:54:LYS:HE3	2.00	0.62
2:B:22:LYS:HD2	2:B:74:LEU:HD12	1.82	0.61
1:A:103:ARG:HH11	1:A:320:ALA:HA	1.64	0.61
1:A:172:GLN:HB2	1:A:175:ILE:HD13	1.82	0.61
1:A:289:MSE:HE3	6:A:2474:HOH:O	2.00	0.61
1:C:292:LYS:HZ3	1:C:303:VAL:HG23	1.66	0.60
1:A:9:ILE:HB	1:A:232:CYS:SG	2.41	0.60
2:B:327:LEU:O	2:B:329:ILE:HG23	2.02	0.60
2:B:24:PHE:CZ	2:B:76:PRO:HB3	2.36	0.60
1:C:91:ALA:O	1:C:95:THR:HG23	2.02	0.59
1:C:229:ASP:CG	1:C:294:ARG:HH12	2.10	0.59
2:D:79:GLU:CD	2:D:115:ARG:HH12	2.11	0.59
1:A:142:VAL:HG21	1:A:175:ILE:HG13	1.84	0.59
1:A:335:LEU:HD23	1:A:335:LEU:C	2.28	0.59
1:A:283:SER:O	1:A:289:MSE:HE1	2.03	0.58
1:C:57:ILE:HG22	1:C:110:THR:HG22	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:0:SER:HB3	2:D:187:GLN:HE22	1.68	0.58
2:B:142:LEU:HD21	2:B:168:VAL:HG23	1.85	0.58
2:B:155:GLY:HA3	2:B:193:ILE:HG13	1.86	0.58
1:C:238:ARG:HD2	6:C:2477:HOH:O	2.03	0.58
1:A:172:GLN:HE22	2:D:88:GLN:HE22	1.51	0.58
6:B:1450:HOH:O	2:D:243:PRO:HA	2.04	0.58
1:A:50:ASP:OD1	1:A:265:MSE:HE1	2.04	0.57
2:B:260:VAL:HG22	2:B:293:VAL:HG22	1.86	0.57
2:B:313:ILE:HG23	2:B:314:PRO:HD2	1.87	0.57
1:A:253:MSE:HE3	1:A:255:LEU:HD11	1.85	0.57
2:D:33:TYR:O	2:D:34:ASP:HB2	2.05	0.57
1:A:68:GLN:HE21	1:A:259:ARG:HB3	1.68	0.57
1:C:7:PHE:CE2	1:C:294:ARG:HG2	2.40	0.57
1:C:335:LEU:HD23	1:C:335:LEU:O	2.05	0.56
2:D:207:ILE:HD11	2:D:260:VAL:HG23	1.86	0.56
2:D:246:MSE:HE1	2:D:275:ILE:HG23	1.85	0.56
1:A:205:GLU:CD	1:A:205:GLU:H	2.13	0.56
1:A:181:MSE:HE1	2:B:62:PHE:N	2.20	0.56
2:D:139:CYS:HB3	6:D:2510:HOH:O	2.04	0.56
1:A:103:ARG:HG3	6:A:2386:HOH:O	2.05	0.56
1:A:68:GLN:HE22	1:A:196:ASN:HD22	1.53	0.55
1:A:142:VAL:HB	1:A:143:PRO:HD3	1.87	0.55
2:B:60:MSE:HE1	2:D:88:GLN:HG2	1.87	0.55
1:A:144:LEU:HD23	2:B:64:GLY:O	2.07	0.55
1:A:95:THR:CG2	1:A:100:LEU:HD22	2.37	0.55
1:A:142:VAL:HA	1:A:163:THR:HG21	1.87	0.54
1:C:292:LYS:NZ	1:C:303:VAL:HG23	2.22	0.54
2:D:12:GLY:HA3	2:D:157:ILE:CD1	2.34	0.54
1:C:53:TYR:HB3	1:C:265:MSE:HE2	1.90	0.54
1:A:103:ARG:HH11	1:A:103:ARG:HG2	1.73	0.54
1:C:222:GLY:HA2	1:C:252:LEU:O	2.08	0.54
2:B:246:MSE:HE3	2:B:249:ILE:HB	1.90	0.54
1:C:55:GLN:O	1:C:56:LYS:HB2	2.06	0.54
2:B:36:ALA:HB2	2:B:81:MSE:HE2	1.90	0.54
2:B:260:VAL:HG22	2:B:293:VAL:CG2	2.38	0.53
1:C:142:VAL:HA	1:C:163:THR:HG21	1.90	0.53
1:A:327:ASP:OD1	1:A:328:PRO:HD2	2.08	0.53
2:B:207:ILE:HD11	2:B:260:VAL:HG23	1.90	0.53
1:C:95:THR:HG22	1:C:131:PHE:HE2	1.70	0.53
2:B:118:ASN:ND2	2:B:132:PHE:H	1.96	0.52
1:C:103:ARG:HG2	1:C:323:PHE:CD2	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:SER:OG	1:A:305:GLU:HG3	2.09	0.52
1:C:75:LEU:HD11	1:C:255:LEU:HD21	1.91	0.52
2:D:94:ILE:HD12	2:D:139:CYS:SG	2.50	0.52
2:B:11:GLN:O	2:B:15:GLU:HG3	2.10	0.52
1:C:335:LEU:HD23	1:C:335:LEU:C	2.35	0.51
1:C:113:LYS:HB2	1:C:113:LYS:NZ	2.26	0.51
2:D:34:ASP:O	2:D:38:LYS:HA	2.11	0.51
2:D:0:SER:HB3	2:D:187:GLN:NE2	2.26	0.51
2:D:24:PHE:CZ	2:D:76:PRO:HB3	2.45	0.51
2:D:313:ILE:HG23	2:D:315:GLN:HE21	1.76	0.51
1:C:87:THR:HG21	1:C:91:ALA:HB2	1.92	0.50
1:C:113:LYS:HD3	1:C:328:PRO:HG2	1.92	0.50
1:A:213:TYR:HA	1:A:216:ARG:HG2	1.93	0.50
1:C:73:VAL:HG12	1:C:230:ILE:HD11	1.92	0.50
1:A:331:PRO:HG2	1:A:334:GLU:HG3	1.93	0.50
6:B:1456:HOH:O	2:D:60:MSE:HE2	2.12	0.49
2:D:313:ILE:HG23	2:D:315:GLN:NE2	2.27	0.49
1:A:68:GLN:NE2	1:A:259:ARG:HB3	2.26	0.49
1:A:274:THR:OG1	1:A:276:GLU:HG3	2.12	0.49
1:C:228:MSE:HE3	1:C:285:SER:O	2.13	0.49
2:B:250:GLU:O	2:B:254:MSE:HG3	2.12	0.48
2:D:21:GLU:HG2	6:D:2490:HOH:O	2.12	0.48
2:D:31:ALA:HB3	2:D:54:ASP:OD2	2.13	0.48
1:C:253:MSE:HE3	1:C:255:LEU:HD11	1.96	0.48
1:C:270:VAL:HG22	1:C:270:VAL:O	2.13	0.48
1:A:235:GLU:HG2	6:A:2407:HOH:O	2.13	0.48
2:D:11:GLN:O	2:D:15:GLU:HG3	2.12	0.48
1:A:142:VAL:HA	1:A:163:THR:CG2	2.44	0.48
1:A:203:SER:HB2	1:A:205:GLU:OE2	2.13	0.48
1:A:223:LEU:HD23	1:A:252:LEU:O	2.14	0.48
2:B:16:GLU:OE1	2:B:162:ARG:HD2	2.13	0.48
2:B:184:PRO:HA	2:B:187:GLN:NE2	2.29	0.47
2:B:238:MSE:O	2:B:239:ARG:HB2	2.13	0.47
2:D:68:GLY:HA2	2:D:71:MSE:HE2	1.95	0.47
2:D:313:ILE:HD12	6:D:2485:HOH:O	2.13	0.47
2:B:269:PHE:HE1	2:D:271:VAL:HA	1.80	0.47
1:C:289:MSE:HG3	1:C:290:LEU:N	2.28	0.47
2:D:238:MSE:O	2:D:239:ARG:HB2	2.13	0.47
1:C:87:THR:CG2	1:C:91:ALA:HB2	2.45	0.47
1:C:224:ARG:HD2	1:C:256:GLN:NE2	2.30	0.47
1:A:138:VAL:HG13	1:A:169:ALA:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:LEU:HD12	2:B:3:VAL:CG1	2.45	0.46
2:B:147:PRO:HB3	2:B:156:LEU:HD12	1.96	0.46
1:C:68:GLN:HE21	1:C:259:ARG:HB3	1.80	0.46
1:A:100:LEU:HD13	1:A:128:ALA:HB2	1.98	0.46
1:C:356:LYS:N	1:C:356:LYS:HD2	2.31	0.46
1:A:9:ILE:CD1	1:A:235:GLU:HG3	2.46	0.46
1:A:68:GLN:NE2	1:A:196:ASN:HD22	2.13	0.46
2:D:79:GLU:HG3	2:D:115:ARG:NH1	2.31	0.46
1:C:1:PHE:HZ	1:C:302:SER:HB3	1.81	0.46
2:D:152:ASP:OD1	2:D:239:ARG:NE	2.47	0.45
1:A:95:THR:HG22	1:A:100:LEU:HB2	1.98	0.45
2:B:33:TYR:O	2:B:34:ASP:HB2	2.16	0.45
1:A:95:THR:HG23	1:A:100:LEU:HD22	1.99	0.45
2:B:280:MSE:CE	2:D:276:CYS:HB3	2.46	0.45
1:C:142:VAL:HB	1:C:143:PRO:HD3	1.98	0.45
1:C:321:ALA:O	1:C:325:THR:HG23	2.16	0.45
2:D:0:SER:HB2	2:D:184:PRO:HD3	1.99	0.45
2:B:51:ARG:O	2:B:52:ILE:HD13	2.17	0.44
1:C:91:ALA:HA	6:C:2379:HOH:O	2.17	0.44
1:A:39:MSE:CE	1:A:291:LEU:HD22	2.47	0.44
2:B:22:LYS:HG3	6:B:1500:HOH:O	2.16	0.44
2:B:274:GLU:O	2:B:278:ARG:HG2	2.17	0.44
6:B:1439:HOH:O	2:D:88:GLN:HG3	2.17	0.44
1:C:40:GLN:O	1:C:44:ARG:HG2	2.18	0.44
1:A:225:VAL:HG12	1:A:226:ASP:N	2.33	0.44
1:A:132:TYR:N	1:A:132:TYR:CD1	2.86	0.44
2:B:306:LYS:HD3	2:B:310:ASP:OD1	2.18	0.44
1:A:181:MSE:HE1	2:B:61:GLY:C	2.43	0.43
1:C:53:TYR:CG	1:C:265:MSE:HG3	2.52	0.43
2:D:157:ILE:HG13	2:D:158:LYS:N	2.33	0.43
2:B:263:GLU:HG2	2:B:296:THR:HG22	2.00	0.43
1:C:127:TYR:N	1:C:127:TYR:CD1	2.86	0.43
2:D:56:PRO:HA	6:D:2455:HOH:O	2.18	0.43
1:A:39:MSE:HE1	1:A:291:LEU:HD22	2.00	0.43
1:A:105:ILE:O	1:A:109:LEU:HD13	2.18	0.43
2:D:153:ALA:O	2:D:157:ILE:HG23	2.18	0.43
1:A:50:ASP:OD2	1:A:54:LYS:NZ	2.51	0.43
2:B:103:MSE:SE	2:D:126:ALA:HB3	2.68	0.43
2:B:226:LEU:HD21	2:B:320:ILE:HG23	2.00	0.43
2:D:237:ASN:C	2:D:237:ASN:HD22	2.26	0.43
1:C:61:PHE:HB3	1:C:63:HIS:CE1	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:VAL:HG13	1:C:169:ALA:HB2	2.00	0.43
2:B:172:ASN:HD21	2:B:174:LEU:HB2	1.82	0.43
1:C:94:PHE:O	1:C:98:ARG:HB2	2.19	0.43
1:C:100:LEU:HD12	1:C:100:LEU:HA	1.89	0.43
1:C:269:GLY:HA2	1:C:272:TYR:CE1	2.54	0.43
1:C:270:VAL:HG21	1:C:275:ARG:NH1	2.34	0.43
2:D:9:ILE:HA	2:D:157:ILE:HD13	2.00	0.43
2:D:226:LEU:HB3	2:D:231:VAL:HB	2.01	0.43
1:A:71:CYS:SG	1:A:255:LEU:HD23	2.59	0.43
1:C:36:TYR:HB2	1:C:295:MSE:HE1	2.01	0.43
1:C:307:LYS:O	1:C:311:VAL:HG23	2.19	0.42
2:D:139:CYS:HA	2:D:140:PRO:HD3	1.82	0.42
1:A:66:ASP:OD1	1:A:260:TYR:HB2	2.18	0.42
2:D:214:ARG:N	2:D:215:PRO:HD2	2.34	0.42
1:A:275:ARG:HH11	1:A:275:ARG:HG2	1.84	0.42
1:C:85:LEU:HD23	1:C:86:ILE:N	2.35	0.42
1:C:157:LYS:O	1:C:158:ASP:HB2	2.19	0.42
2:D:197:LYS:HD2	2:D:198:ALA:O	2.19	0.42
2:D:197:LYS:HD3	2:D:198:ALA:N	2.35	0.42
1:A:100:LEU:HD13	1:A:128:ALA:CB	2.49	0.42
1:A:101:SER:OG	1:A:104:GLU:HG3	2.19	0.41
1:A:172:GLN:CB	1:A:175:ILE:HD13	2.50	0.41
1:A:263:HIS:CE1	4:A:2330:TPP:S1	3.13	0.41
1:C:103:ARG:NH1	6:C:2506:HOH:O	2.52	0.41
1:C:27:LEU:HG	1:C:231:LEU:HD21	2.02	0.41
1:C:53:TYR:CD2	1:C:265:MSE:HG3	2.55	0.41
2:B:126:ALA:HB3	2:D:103:MSE:SE	2.71	0.41
1:C:48:LYS:NZ	1:C:51:GLN:NE2	2.68	0.41
2:B:59:GLU:HG2	2:B:85:PHE:O	2.21	0.41
1:C:88:ALA:HB3	6:C:2356:HOH:O	2.21	0.41
2:D:36:ALA:HB2	2:D:81:MSE:HE2	2.01	0.41
1:A:157:LYS:O	1:A:158:ASP:HB3	2.20	0.41
1:C:72:CYS:HA	1:C:94:PHE:CE1	2.54	0.41
1:C:223:LEU:N	1:C:223:LEU:HD23	2.35	0.41
1:A:103:ARG:HH12	1:A:319:ASP:C	2.29	0.41
1:A:228:MSE:HE3	1:A:285:SER:O	2.21	0.41
1:A:292:LYS:O	1:A:296:VAL:HG23	2.21	0.41
1:C:64:LEU:HD22	1:C:64:LEU:N	2.36	0.41
1:C:142:VAL:HG21	1:C:175:ILE:HG12	2.02	0.41
2:D:32:GLN:HG2	2:D:44:TRP:CH2	2.56	0.41
1:C:75:LEU:HD12	1:C:233:VAL:CG1	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:VAL:HG21	2:D:182:PHE:CG	2.56	0.40
2:D:263:GLU:HG2	2:D:296:THR:HG22	2.03	0.40
1:C:164:LEU:HG	1:C:192:ILE:HB	2.04	0.40
1:C:259:ARG:HG3	1:C:259:ARG:O	2.21	0.40
1:A:46:GLU:OE1	1:A:46:GLU:HA	2.21	0.40
1:A:155:ASN:OD1	2:B:22:LYS:HE2	2.21	0.40
1:A:40:GLN:HE21	1:A:288:ILE:HD13	1.86	0.40
2:B:237:ASN:HD22	2:B:237:ASN:C	2.29	0.40

There are no symmetry-related clashes.

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	360/365 (99%)	349 (97%)	10 (3%)	1 (0%)	36	28
1	C	360/365 (99%)	349 (97%)	10 (3%)	1 (0%)	36	28
2	B	328/341 (96%)	316 (96%)	12 (4%)	0	100	100
2	D	328/341 (96%)	317 (97%)	11 (3%)	0	100	100
All	All	1376/1412 (98%)	1331 (97%)	43 (3%)	2 (0%)	48	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	218	ASP
1	A	218	ASP

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	295/285 (104%)	290 (98%)	5 (2%)	53	49
1	C	295/285 (104%)	286 (97%)	9 (3%)	35	26
2	B	269/265 (102%)	263 (98%)	6 (2%)	45	40
2	D	269/265 (102%)	262 (97%)	7 (3%)	40	33
All	All	1128/1100 (102%)	1101 (98%)	27 (2%)	43	36

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	33	LEU
1	A	75	LEU
1	A	205	GLU
1	A	289	MSE
2	B	1	LEU
2	B	3	VAL
2	B	43	LEU
2	B	74	LEU
2	B	142	LEU
2	B	162	ARG
1	C	18	GLU
1	C	27	LEU
1	C	33	LEU
1	C	98	ARG
1	C	100	LEU
1	C	113	LYS
1	C	238	ARG
1	C	255	LEU
1	C	347	GLU
2	D	11	GLN
2	D	74	LEU
2	D	162	ARG
2	D	182	PHE
2	D	197	LYS
2	D	288	LEU
2	D	313	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	55	GLN
1	A	68	GLN
1	A	80	ASN
1	A	130	ASN
1	A	174	GLN
1	A	256	GLN
1	A	297	ASN
1	A	353	GLN
2	B	32	GLN
2	B	88	GLN
2	B	118	ASN
2	B	164	ASN
2	B	172	ASN
2	B	187	GLN
2	B	237	ASN
2	B	328	ASN
1	C	3	ASN
1	C	40	GLN
1	C	51	GLN
1	C	55	GLN
1	C	68	GLN
1	C	80	ASN
1	C	125	HIS
1	C	256	GLN
1	C	299	ASN
2	D	88	GLN
2	D	187	GLN
2	D	237	ASN
2	D	286	ASN
2	D	315	GLN
2	D	328	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	TPP	A	2330	3	26,27,27	1.80	5 (19%)	38,40,40	1.40	5 (13%)
4	TPP	C	1330	3	26,27,27	1.92	5 (19%)	38,40,40	1.38	6 (15%)

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
4	TPP	A	2330	3	-	1/17/17/17	0/2/2/2
4	TPP	C	1330	3	-	1/17/17/17	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1330	TPP	PA-O3A	-5.87	1.53	1.59
4	A	2330	TPP	PA-O3A	-5.20	1.53	1.59
4	C	1330	TPP	C4-N3	4.39	1.48	1.39
4	A	2330	TPP	C4-N3	3.91	1.47	1.39
4	C	1330	TPP	C2-N3	2.71	1.38	1.32
4	A	2330	TPP	C2-N3	2.63	1.38	1.32
4	A	2330	TPP	CM4-C4	2.35	1.54	1.49
4	C	1330	TPP	CM4-C4	2.31	1.54	1.49
4	C	1330	TPP	C2-S1	2.14	1.75	1.69
4	A	2330	TPP	C2-S1	2.08	1.75	1.69

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2330	TPP	C4-C5-S1	3.33	115.75	110.56
4	C	1330	TPP	C4-C5-S1	3.15	115.47	110.56
4	A	2330	TPP	C6-C5-S1	-3.13	113.58	120.90
4	A	2330	TPP	C6'-N1'-C2'	3.10	121.16	116.07
4	C	1330	TPP	C6-C5-S1	-3.07	113.72	120.90
4	C	1330	TPP	C6'-N1'-C2'	3.02	121.03	116.07
4	A	2330	TPP	N4'-C4'-N3'	-2.20	114.06	117.03
4	C	1330	TPP	O3B-PB-O3A	2.17	111.90	104.64
4	A	2330	TPP	CM2-C2'-N3'	2.12	120.30	117.13
4	C	1330	TPP	N4'-C4'-N3'	-2.06	114.24	117.03
4	C	1330	TPP	C5'-C4'-N3'	2.01	124.27	121.31

There are no chirality outliers.

All (2) torsion outliers are listed below:

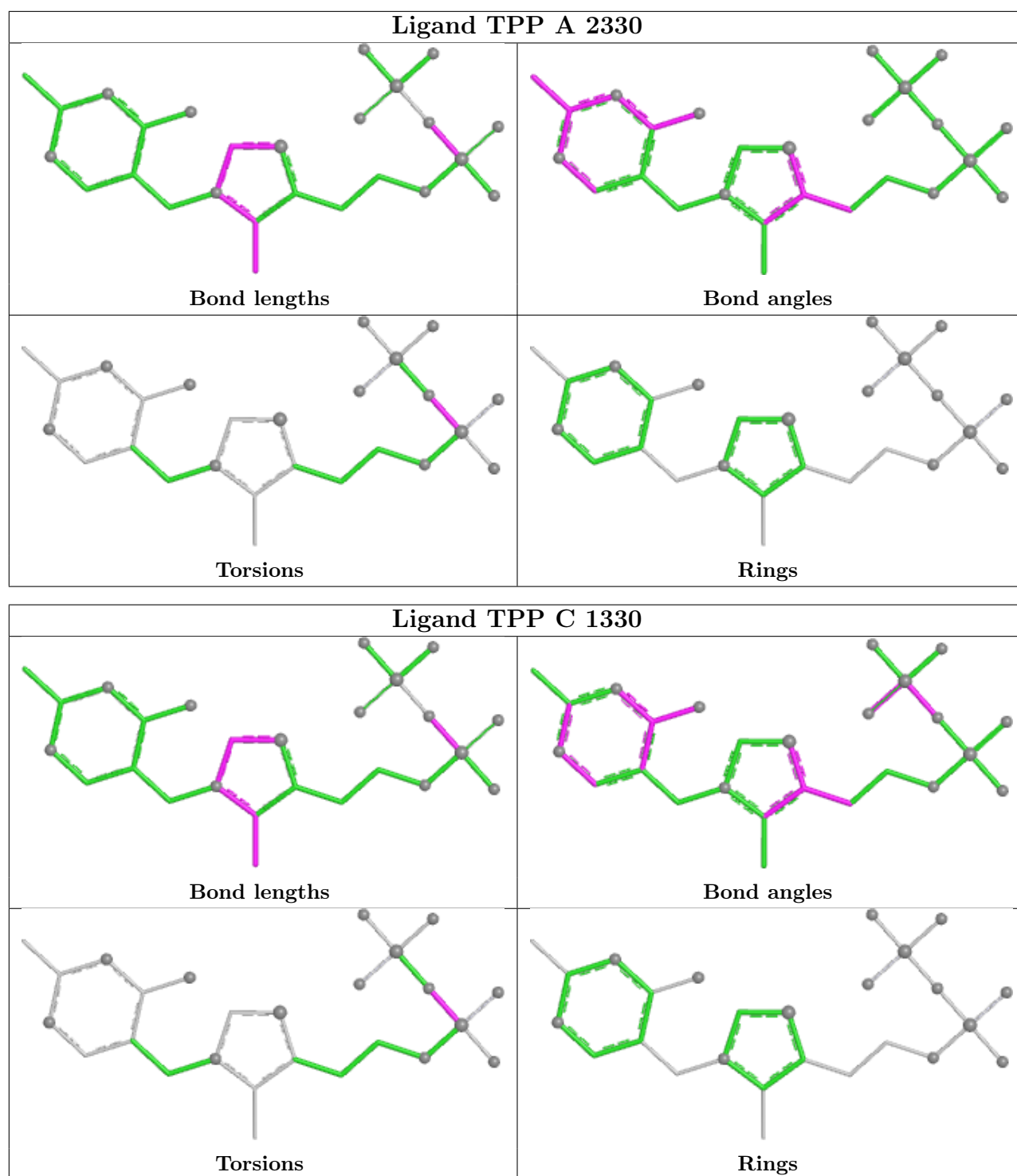
Mol	Chain	Res	Type	Atoms
4	A	2330	TPP	PB-O3A-PA-O7
4	C	1330	TPP	PB-O3A-PA-O7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2330	TPP	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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	350/365 (95%)	0.54	12 (3%) 48 54	5, 17, 30, 42	0
1	C	350/365 (95%)	0.78	34 (9%) 13 15	5, 19, 40, 50	0
2	B	317/341 (92%)	0.37	9 (2%) 55 62	5, 14, 27, 49	0
2	D	317/341 (92%)	0.37	8 (2%) 58 65	5, 14, 27, 37	0
All	All	1334/1412 (94%)	0.52	63 (4%) 36 42	5, 16, 33, 50	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	0	SER	4.3
2	D	329	ILE	4.0
1	C	270	VAL	4.0
1	C	303	VAL	4.0
1	C	278	ILE	3.7
1	C	281	VAL	3.7
2	D	1	LEU	3.6
1	C	276	GLU	3.6
2	D	181	GLU	3.6
2	B	1	LEU	3.2
1	A	279	GLN	3.2
1	C	18	GLU	3.2
1	C	304	GLU	3.2
1	A	18	GLU	3.1
2	B	7	ASP	3.0
2	B	185	GLU	3.0
1	C	0	SER	2.9
2	B	329	ILE	2.9
1	C	280	GLU	2.9
1	C	347	GLU	2.9
1	C	1	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	319	ASP	2.8
1	C	2	ALA	2.7
2	D	152	ASP	2.7
1	C	293	ASP	2.7
1	A	127	TYR	2.6
2	B	184	PRO	2.6
1	A	8	GLU	2.5
1	C	275	ARG	2.5
1	C	300	LEU	2.5
2	D	89	ALA	2.5
2	B	229	GLU	2.5
1	A	361	SER	2.4
1	C	297	ASN	2.4
1	C	10	LYS	2.4
1	C	296	VAL	2.4
2	D	157	ILE	2.4
2	D	247	GLU	2.4
2	B	183	PRO	2.4
1	A	266	SER	2.4
1	A	158	ASP	2.3
1	A	275	ARG	2.3
2	B	328	ASN	2.3
1	C	117	ALA	2.3
2	D	313	ILE	2.3
1	A	61	PHE	2.2
1	A	0	SER	2.2
1	C	16	ARG	2.2
1	C	269	GLY	2.2
1	C	158	ASP	2.2
1	C	271	SER	2.2
1	C	272	TYR	2.2
1	C	305	GLU	2.2
1	C	316	GLU	2.1
1	C	282	ARG	2.1
1	C	308	GLU	2.1
1	A	268	PRO	2.1
1	C	66	ASP	2.1
1	A	318	GLU	2.0
1	C	127	TYR	2.0
1	C	267	ASP	2.0
1	C	277	GLU	2.0
1	C	283	SER	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](#)

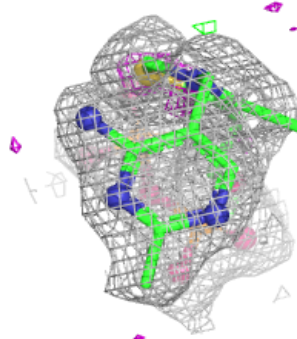
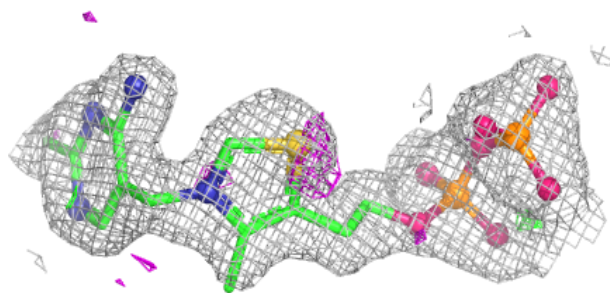
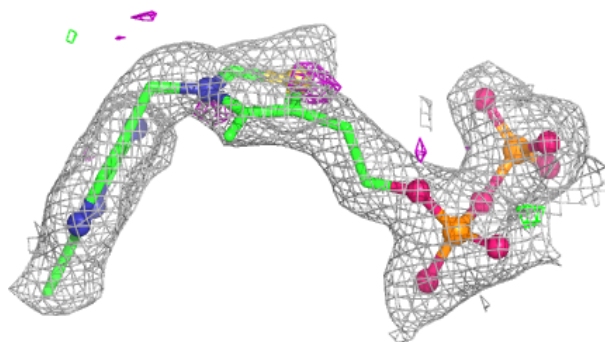
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	MG	A	1331	1/1	0.94	0.06	5,5,5,5	0
3	MG	C	2331	1/1	0.96	0.11	5,5,5,5	0
4	TPP	C	1330	26/26	0.96	0.09	8,19,25,27	0
4	TPP	A	2330	26/26	0.97	0.08	6,16,22,24	0
5	K	B	1332	1/1	0.98	0.02	12,12,12,12	0
5	K	D	2332	1/1	0.98	0.04	12,12,12,12	0

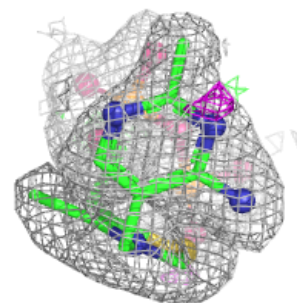
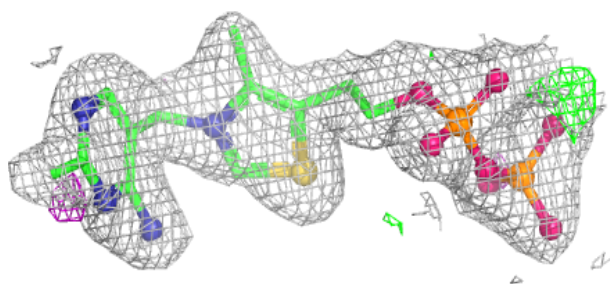
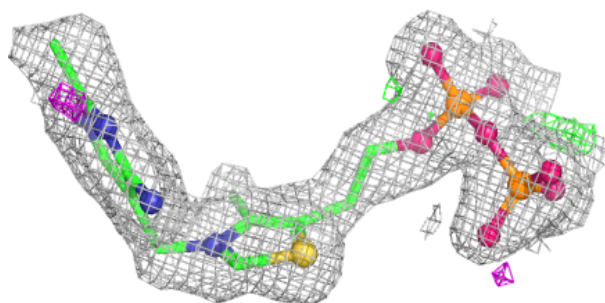
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP C 1330:

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

**Electron density around TPP A 2330:**

$2mF_o-DF_c$ (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.