



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3QFV / pdb_00003qfv
Title : MRCK beta in complex with TPCA-1
Authors : Heikkila, T.J.; Wheatley, E.; Crichton, D.; Schroder, E.; Boakes, A.; Kaye, S.J.; Mezna, M.; Pang, L.; Rushbrooke, M.; Turnbull, A.; Olson, M.F.
Deposited on : 2011-01-23
Resolution : 2.65 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

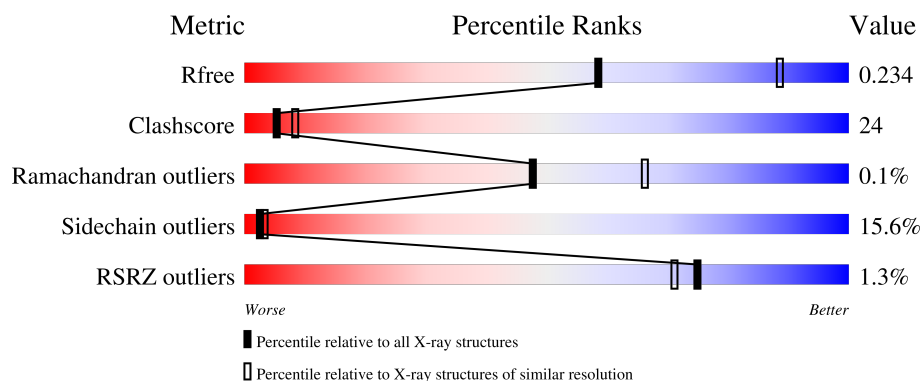
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	415	
1	B	415	

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	NM7	A	416	-	-	X	-

2 Entry composition [i](#)

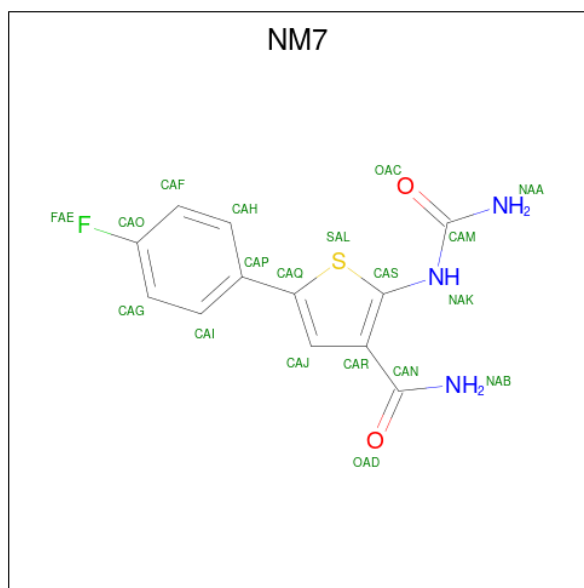
There are 6 unique types of molecules in this entry. The entry contains 6395 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CDC42BPB protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3110	1998	511	581	20			
1	B	396	Total	C	N	O	S	0	0	0
			3116	2006	508	582	20			

- Molecule 2 is 2-(carbamoylamino)-5-(4-fluorophenyl)thiophene-3-carboxamide (CCD ID: NM7) (formula: C₁₂H₁₀FN₃O₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			19	12	1	3	2	1		
2	B	1	Total	C	F	N	O	S	0	0
			19	12	1	3	2	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Cl 2 2	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0

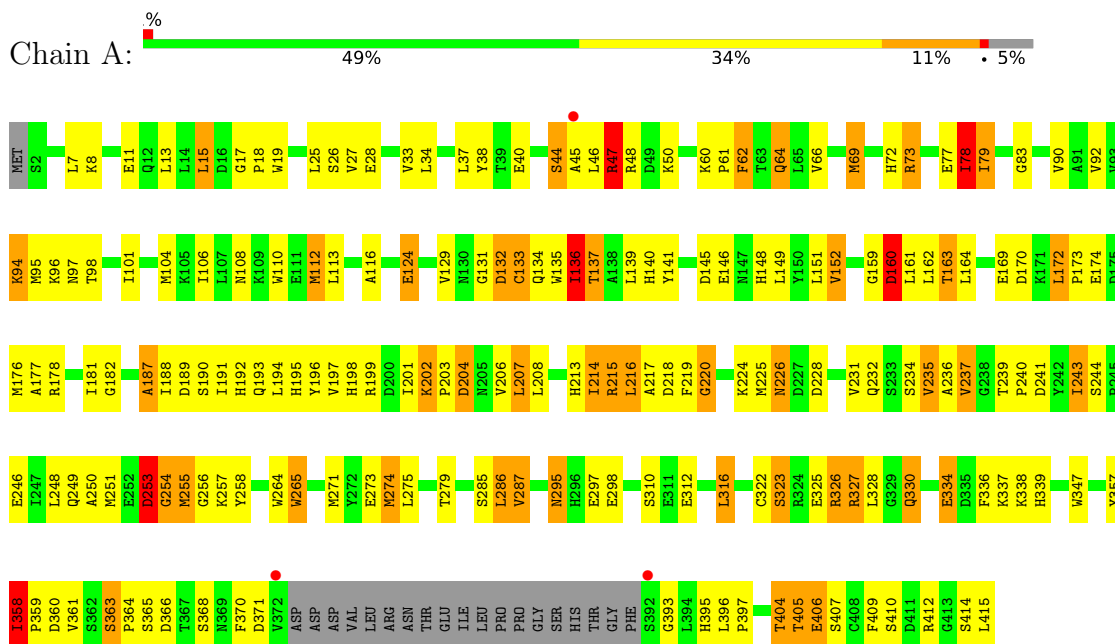
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	53	Total O 53 53	0	0
6	B	63	Total O 63 63	0	0

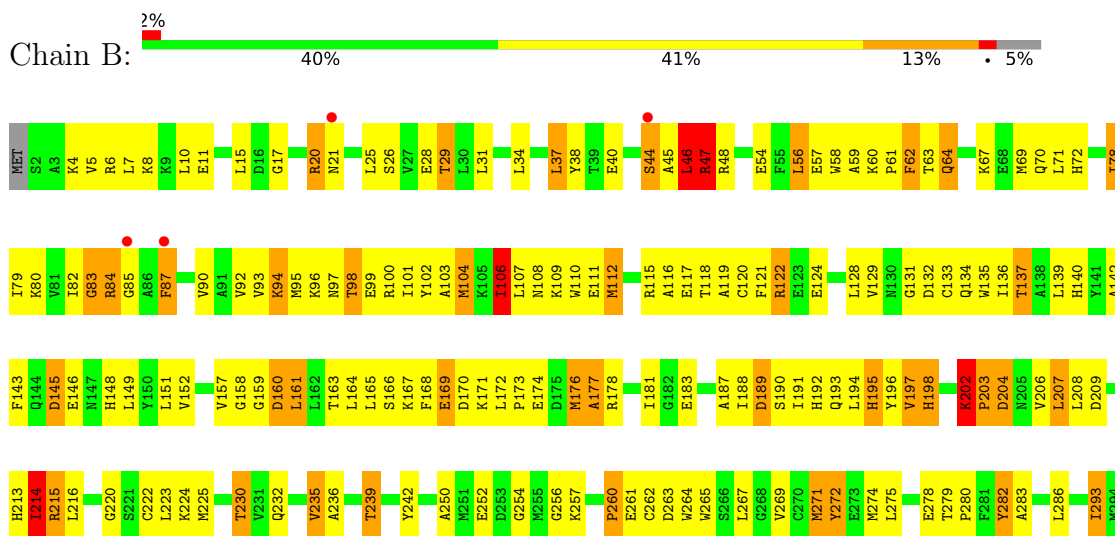
3 Residue-property plots

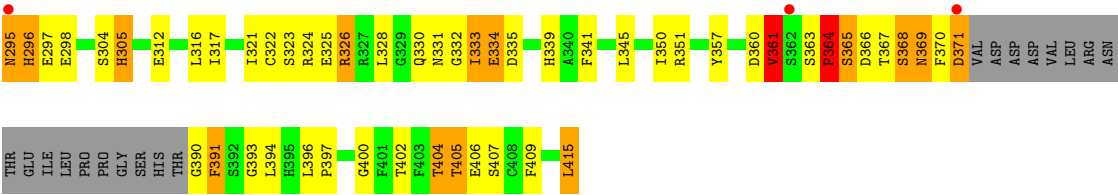
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CDC42BPB protein



• Molecule 1: CDC42BPB protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.81Å 123.36Å 85.49Å 90.00° 100.69° 90.00°	Depositor
Resolution (Å)	39.97 – 2.65 39.97 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.3 (39.97-2.65) 93.9 (39.97-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.192 , 0.268 0.201 , 0.234	Depositor DCC
R_{free} test set	1254 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6395	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CL, NM7, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.08	55/3182 (1.7%)	1.31	39/4315 (0.9%)
1	B	2.12	75/3189 (2.4%)	1.38	46/4323 (1.1%)
All	All	2.10	130/6371 (2.0%)	1.34	85/8638 (1.0%)

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

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

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	HIS	CG-ND1	-8.20	1.29	1.38
1	B	192	HIS	CG-ND1	-7.83	1.29	1.38
1	A	159	GLY	C-O	-7.76	1.18	1.24
1	A	192	HIS	CG-ND1	-7.66	1.29	1.38
1	B	198	HIS	CG-ND1	-7.63	1.29	1.38
1	B	145	ASP	C-O	-7.41	1.17	1.24
1	A	213	HIS	CG-ND1	-6.76	1.30	1.38
1	A	148	HIS	CD2-NE2	-6.72	1.30	1.37
1	B	72	HIS	CG-ND1	-6.66	1.30	1.38
1	B	339	HIS	CG-ND1	-6.66	1.30	1.38
1	A	339	HIS	CG-ND1	-6.65	1.30	1.38
1	B	140	HIS	CG-ND1	-6.64	1.30	1.38
1	B	148	HIS	CD2-NE2	-6.63	1.30	1.37
1	B	149	LEU	C-O	-6.53	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	HIS	CD2-NE2	-6.39	1.30	1.37
1	B	148	HIS	CG-ND1	-6.37	1.31	1.38
1	B	198	HIS	CD2-NE2	-6.31	1.30	1.37
1	B	159	GLY	C-O	-6.24	1.17	1.24
1	B	191	ILE	C-O	-6.23	1.16	1.24
1	A	140	HIS	CG-ND1	-6.19	1.31	1.38
1	B	213	HIS	CD2-NE2	-6.19	1.31	1.37
1	B	269	VAL	C-O	-6.18	1.16	1.24
1	A	192	HIS	CD2-NE2	-6.16	1.31	1.37
1	B	92	VAL	C-O	-6.15	1.16	1.24
1	B	220	GLY	C-O	-6.12	1.17	1.24
1	B	208	LEU	C-O	-6.11	1.16	1.24
1	A	206	VAL	C-O	-6.11	1.16	1.24
1	B	206	VAL	C-O	-6.05	1.17	1.24
1	B	213	HIS	CG-ND1	-5.96	1.31	1.38
1	A	140	HIS	CD2-NE2	-5.96	1.31	1.37
1	B	216	LEU	C-O	-5.94	1.16	1.23
1	A	148	HIS	CG-ND1	-5.93	1.31	1.38
1	B	215	ARG	C-O	-5.91	1.17	1.24
1	B	151	LEU	C-O	-5.91	1.17	1.24
1	B	104	MET	C-O	-5.90	1.17	1.24
1	B	135	TRP	NE1-CE2	-5.90	1.30	1.37
1	A	145	ASP	C-O	-5.88	1.18	1.24
1	B	197	VAL	C-O	-5.87	1.17	1.24
1	A	316	LEU	C-O	-5.86	1.17	1.24
1	A	110	TRP	NE1-CE2	-5.82	1.31	1.37
1	B	264	TRP	NE1-CE2	-5.77	1.31	1.37
1	A	164	LEU	CA-C	-5.76	1.45	1.52
1	B	223	LEU	C-O	-5.74	1.17	1.23
1	A	347	TRP	NE1-CE2	-5.74	1.31	1.37
1	A	215	ARG	C-O	-5.73	1.17	1.24
1	B	265	TRP	NE1-CE2	-5.73	1.31	1.37
1	A	182	GLY	C-O	-5.70	1.17	1.23
1	A	72	HIS	CG-ND1	-5.70	1.31	1.38
1	A	145	ASP	CA-C	-5.67	1.47	1.53
1	B	260	PRO	C-O	-5.66	1.16	1.24
1	B	208	LEU	CA-C	-5.65	1.45	1.52
1	A	160	ASP	C-O	-5.65	1.17	1.23
1	B	316	LEU	C-O	-5.65	1.17	1.24
1	B	152	VAL	C-O	-5.64	1.18	1.24
1	B	121	PHE	C-O	-5.63	1.17	1.24
1	A	19	TRP	CA-C	-5.63	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	272	TYR	C-O	-5.63	1.17	1.24
1	A	101	ILE	C-O	-5.62	1.18	1.24
1	B	20	ARG	CA-C	-5.59	1.48	1.52
1	A	191	ILE	C-O	-5.59	1.17	1.24
1	A	152	VAL	C-O	-5.58	1.18	1.24
1	A	358	ILE	CA-C	-5.58	1.48	1.53
1	B	262	CYS	C-O	-5.58	1.17	1.24
1	A	264	TRP	NE1-CE2	-5.56	1.31	1.37
1	B	29	THR	C-O	-5.53	1.17	1.24
1	A	187	ALA	C-O	-5.52	1.17	1.24
1	B	188	ILE	C-O	-5.52	1.17	1.24
1	A	201	ILE	C-O	-5.52	1.18	1.24
1	B	34	LEU	C-O	-5.52	1.17	1.24
1	B	72	HIS	CD2-NE2	-5.49	1.31	1.37
1	B	271	MET	C-O	-5.49	1.17	1.24
1	B	72	HIS	CA-C	-5.48	1.45	1.52
1	B	296	HIS	CG-ND1	-5.46	1.32	1.38
1	B	56	LEU	C-O	-5.46	1.17	1.24
1	B	192	HIS	CD2-NE2	-5.44	1.31	1.37
1	B	164	LEU	C-O	-5.44	1.17	1.24
1	A	34	LEU	C-O	-5.44	1.17	1.24
1	A	188	ILE	C-O	-5.43	1.17	1.24
1	A	92	VAL	C-O	-5.42	1.17	1.24
1	B	140	HIS	CD2-NE2	-5.38	1.31	1.37
1	B	190	SER	C-O	-5.37	1.17	1.24
1	B	305	HIS	CG-ND1	-5.37	1.32	1.38
1	B	160	ASP	C-O	-5.34	1.17	1.23
1	B	189	ASP	C-O	-5.34	1.17	1.24
1	B	339	HIS	CA-C	-5.33	1.46	1.52
1	B	339	HIS	CD2-NE2	-5.32	1.31	1.37
1	A	213	HIS	CD2-NE2	-5.32	1.32	1.37
1	B	63	THR	C-O	-5.31	1.17	1.24
1	A	395	HIS	CG-ND1	-5.30	1.32	1.38
1	A	72	HIS	CD2-NE2	-5.25	1.32	1.37
1	B	263	ASP	C-O	-5.24	1.17	1.24
1	A	339	HIS	CD2-NE2	-5.22	1.32	1.37
1	A	196	TYR	C-O	-5.22	1.17	1.23
1	B	143	PHE	C-O	-5.22	1.17	1.23
1	A	226	ASN	CA-C	-5.21	1.46	1.53
1	A	271	MET	C-O	-5.21	1.18	1.24
1	A	273	GLU	C-O	-5.20	1.18	1.24
1	A	135	TRP	NE1-CE2	-5.16	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	122	ARG	C-O	-5.15	1.18	1.24
1	B	142	ALA	C-O	-5.15	1.17	1.24
1	A	151	LEU	C-O	-5.14	1.18	1.24
1	B	62	PHE	C-O	-5.13	1.18	1.24
1	B	134	GLN	C-O	-5.12	1.18	1.24
1	B	267	LEU	C-O	-5.12	1.17	1.24
1	A	197	VAL	C-O	-5.12	1.18	1.24
1	A	124	GLU	C-O	-5.11	1.18	1.24
1	B	37	LEU	C-O	-5.11	1.18	1.24
1	B	110	TRP	NE1-CE2	-5.10	1.31	1.37
1	B	177	ALA	C-O	-5.09	1.17	1.24
1	B	102	TYR	C-O	-5.09	1.17	1.23
1	B	305	HIS	CD2-NE2	-5.09	1.32	1.37
1	A	134	GLN	C-O	-5.09	1.18	1.24
1	B	402	THR	C-O	-5.09	1.17	1.23
1	B	196	TYR	C-O	-5.09	1.17	1.23
1	A	176	MET	C-O	-5.08	1.18	1.24
1	A	258	TYR	C-O	-5.08	1.17	1.23
1	B	106	ILE	C-O	-5.07	1.18	1.24
1	A	149	LEU	C-O	-5.07	1.17	1.24
1	A	357	TYR	CA-C	-5.07	1.46	1.52
1	A	136	ILE	C-O	-5.06	1.18	1.24
1	A	178	ARG	C-O	-5.05	1.18	1.24
1	B	135	TRP	CA-C	-5.04	1.46	1.52
1	A	265	TRP	NE1-CE2	-5.03	1.31	1.37
1	A	106	ILE	C-O	-5.02	1.18	1.24
1	A	220	GLY	C-O	-5.02	1.17	1.23
1	B	116	ALA	C-O	-5.02	1.20	1.24
1	B	103	ALA	C-O	-5.01	1.17	1.24
1	B	203	PRO	C-O	-5.01	1.17	1.24
1	B	174	GLU	C-O	-5.00	1.18	1.24
1	B	400	GLY	C-O	-5.00	1.17	1.24

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	390	GLY	N-CA-C	-13.78	73.33	113.30
1	A	405	THR	N-CA-C	11.20	123.24	111.14
1	A	78	ILE	CB-CA-C	-10.30	100.11	111.23
1	B	47	ARG	N-CA-C	-10.12	100.03	112.38
1	B	78	ILE	CB-CA-C	-9.88	99.14	111.88
1	A	275	LEU	N-CA-C	9.40	121.61	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	391	PHE	N-CA-C	9.31	123.85	111.28
1	B	405	THR	N-CA-C	9.04	120.82	110.97
1	B	198	HIS	N-CA-C	8.23	120.03	111.14
1	A	218	ASP	N-CA-C	7.75	120.71	111.02
1	B	46	LEU	N-CA-C	-7.62	103.25	112.54
1	B	118	THR	N-CA-C	7.59	119.63	111.36
1	B	83	GLY	N-CA-C	7.42	121.27	110.80
1	A	79	ILE	N-CA-C	7.40	117.49	110.53
1	A	50	LYS	N-CA-C	7.18	118.90	111.14
1	A	47	ARG	N-CA-C	-7.08	103.74	112.38
1	B	214	ILE	N-CA-C	7.05	119.28	109.55
1	B	69	MET	N-CA-C	7.01	119.96	111.82
1	A	198	HIS	N-CA-C	6.93	118.72	111.03
1	B	129	VAL	N-CA-C	6.85	116.97	110.53
1	A	129	VAL	N-CA-C	6.84	116.96	110.53
1	B	202	LYS	N-CA-C	-6.83	102.08	108.22
1	A	412	ARG	N-CA-C	6.80	119.70	111.82
1	A	336	PHE	N-CA-C	6.78	118.75	111.36
1	B	293	ILE	CB-CA-C	-6.75	103.33	111.97
1	B	117	GLU	N-CA-C	6.66	119.37	111.71
1	B	158	GLY	N-CA-C	6.62	121.92	113.24
1	A	62	PHE	N-CA-C	6.54	118.20	111.14
1	A	327	ARG	N-CA-C	6.47	119.86	110.28
1	A	69	MET	N-CA-C	6.43	119.28	111.82
1	A	202	LYS	CA-C-N	6.43	126.35	119.28
1	A	202	LYS	C-N-CA	6.43	126.35	119.28
1	B	161	LEU	N-CA-C	6.36	118.22	111.28
1	B	57	GLU	N-CA-C	-6.31	104.40	111.28
1	B	58	TRP	N-CA-C	6.31	118.23	111.36
1	B	17	GLY	CA-C-N	6.29	125.91	119.56
1	B	17	GLY	C-N-CA	6.29	125.91	119.56
1	A	116	ALA	N-CA-C	6.25	118.10	111.28
1	B	361	VAL	N-CA-C	6.21	116.45	107.88
1	A	214	ILE	N-CA-C	6.16	118.05	109.55
1	B	79	ILE	N-CA-C	6.10	116.27	110.42
1	B	79	ILE	CB-CA-C	-6.07	104.20	111.97
1	B	391	PHE	N-CA-CB	6.06	121.31	111.74
1	A	347	TRP	N-CA-C	6.04	117.95	111.36
1	A	133	CYS	N-CA-C	5.91	117.73	111.28
1	A	363	SER	CA-C-N	5.88	125.75	119.28
1	A	363	SER	C-N-CA	5.88	125.75	119.28
1	A	239	THR	CA-C-N	5.84	125.54	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	THR	C-N-CA	5.84	125.54	119.05
1	B	116	ALA	CB-CA-C	-5.83	109.30	117.23
1	A	45	ALA	N-CA-C	-5.79	106.07	113.02
1	B	78	ILE	N-CA-C	5.70	115.87	107.15
1	A	279	THR	CA-C-N	5.68	125.53	119.28
1	A	279	THR	C-N-CA	5.68	125.53	119.28
1	A	287	VAL	N-CA-C	5.56	116.33	110.72
1	A	256	GLY	N-CA-C	5.54	119.64	112.54
1	B	67	LYS	N-CA-C	5.50	117.36	111.36
1	B	230	THR	N-CA-C	5.43	117.67	109.41
1	B	111	GLU	N-CA-C	-5.42	105.37	111.28
1	B	333	ILE	N-CA-C	-5.39	105.91	112.76
1	B	120	CYS	CA-C-N	5.39	128.04	120.28
1	B	120	CYS	C-N-CA	5.39	128.04	120.28
1	B	85	GLY	N-CA-C	-5.38	100.43	113.18
1	B	239	THR	CA-C-N	5.34	124.98	119.05
1	B	239	THR	C-N-CA	5.34	124.98	119.05
1	A	134	GLN	N-CA-C	5.34	117.10	111.28
1	B	131	GLY	N-CA-C	5.29	119.31	112.54
1	A	172	LEU	CA-C-N	5.23	124.99	119.76
1	A	172	LEU	C-N-CA	5.23	124.99	119.76
1	A	253	ASP	N-CA-C	-5.23	106.95	113.38
1	A	361	VAL	N-CA-C	5.22	115.50	107.77
1	B	364	PRO	N-CA-C	-5.21	107.63	114.03
1	A	17	GLY	CA-C-N	5.18	124.80	119.05
1	A	17	GLY	C-N-CA	5.18	124.80	119.05
1	A	146	GLU	N-CA-C	-5.17	105.54	111.07
1	B	187	ALA	N-CA-C	5.16	116.98	111.36
1	B	275	LEU	N-CA-C	5.16	117.80	111.82
1	B	326	ARG	N-CA-C	5.13	116.96	111.36
1	B	5	VAL	N-CA-C	5.11	115.88	110.72
1	B	298	GLU	N-CA-C	5.07	116.88	111.36
1	B	350	ILE	N-CA-C	5.06	117.38	111.05
1	B	59	ALA	N-CA-C	5.05	119.43	113.16
1	A	131	GLY	N-CA-C	5.05	117.89	112.33
1	B	148	HIS	N-CA-C	5.03	117.31	109.52
1	A	334	GLU	N-CA-C	-5.02	106.42	112.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	253	ASP	Peptide
1	A	254	GLY	Peptide
1	B	115	ARG	Peptide
1	B	254	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3110	0	2950	144	0
1	B	3116	0	2956	160	1
2	A	19	0	10	10	0
2	B	19	0	10	1	0
3	A	4	0	6	1	0
3	B	8	0	12	1	0
4	B	2	0	0	1	0
5	B	1	0	0	0	0
6	A	53	0	0	4	0
6	B	63	0	0	5	0
All	All	6395	0	5944	296	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:MET:O	1:B:98:THR:HB	1.39	1.23
1:A:250:ALA:O	1:A:254:GLY:CA	1.90	1.18
1:A:363:SER:CB	1:A:364:PRO:CD	2.23	1.16
1:B:98:THR:CG2	1:B:100:ARG:H	1.58	1.16
1:A:250:ALA:O	1:A:254:GLY:HA3	1.47	1.15
1:A:363:SER:OG	1:A:364:PRO:HD2	1.47	1.13
1:A:363:SER:CB	1:A:364:PRO:HD3	1.80	1.10
1:B:80:LYS:HD3	1:B:367:THR:HG21	1.24	1.09
1:A:40:GLU:OE2	1:A:393:GLY:HA2	1.53	1.08
1:A:363:SER:HB2	1:A:364:PRO:HD3	1.12	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:GLU:OE2	1:B:169:GLU:HA	1.49	1.07
1:A:78:ILE:HG22	1:A:78:ILE:O	1.55	1.06
1:A:295:ASN:ND2	1:A:298:GLU:CB	2.20	1.05
1:B:98:THR:HG22	1:B:100:ARG:H	1.21	1.04
1:A:163:THR:HG22	1:A:163:THR:O	1.54	1.03
1:A:295:ASN:HD21	1:A:298:GLU:CB	1.72	1.03
1:A:195:HIS:HA	1:A:225:MET:HE3	1.42	1.00
1:A:250:ALA:O	1:A:254:GLY:HA2	1.60	0.99
1:A:370:PHE:CZ	2:A:416:NM7:NAB	2.31	0.98
1:A:195:HIS:O	1:A:225:MET:HG3	1.62	0.98
1:A:363:SER:HB2	1:A:364:PRO:CD	1.88	0.97
1:A:174:GLU:OE2	1:A:310:SER:OG	1.81	0.97
1:B:235:VAL:CG1	1:B:236:ALA:N	2.27	0.96
1:B:177:ALA:O	1:B:181:ILE:HG12	1.69	0.92
1:B:60:LYS:HB3	1:B:61:PRO:HD3	1.50	0.91
1:A:363:SER:OG	1:A:364:PRO:CD	2.19	0.89
1:A:169:GLU:HB2	6:A:456:HOH:O	1.73	0.88
1:A:195:HIS:CA	1:A:225:MET:HE3	2.05	0.87
1:B:282:TYR:C	1:B:282:TYR:CD2	2.51	0.87
1:B:334:GLU:OE2	1:B:334:GLU:HA	1.72	0.87
1:A:161:LEU:HD21	1:A:274:MET:HE2	1.56	0.87
1:A:199:ARG:NH1	1:A:237:VAL:HG21	1.89	0.86
1:B:235:VAL:HG13	1:B:236:ALA:N	1.90	0.86
1:B:215:ARG:NH1	6:B:470:HOH:O	2.09	0.86
1:B:391:PHE:O	1:B:391:PHE:CD1	2.29	0.85
1:B:235:VAL:HG13	1:B:236:ALA:H	1.41	0.85
1:A:28:GLU:OE2	1:A:404:THR:HG23	1.75	0.85
1:A:44:SER:HB3	1:A:46:LEU:HG	1.59	0.84
1:B:209:ASP:OD2	6:B:470:HOH:O	1.94	0.84
1:A:195:HIS:C	1:A:225:MET:HE3	2.02	0.84
1:A:194:LEU:O	1:A:195:HIS:HB2	1.78	0.83
1:A:325:GLU:H	1:A:325:GLU:CD	1.87	0.83
1:A:28:GLU:OE2	1:A:404:THR:CG2	2.27	0.83
1:B:44:SER:HB2	1:B:391:PHE:H	1.45	0.82
1:A:161:LEU:HD21	1:A:274:MET:CE	2.10	0.81
1:A:235:VAL:HG13	1:A:236:ALA:N	1.94	0.81
2:A:416:NM7:SAL	2:A:416:NM7:OAC	2.36	0.80
1:B:98:THR:HG22	1:B:100:ARG:N	1.94	0.80
1:A:73:ARG:O	1:A:73:ARG:HG2	1.81	0.80
1:B:44:SER:OG	1:B:46:LEU:HD22	1.82	0.80
1:A:69:MET:HE2	1:B:6:ARG:HG2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:GLU:OE1	3:B:421:EDO:H21	1.81	0.80
1:B:334:GLU:OE2	1:B:334:GLU:CA	2.30	0.79
1:A:323:SER:HB3	1:A:325:GLU:OE2	1.82	0.79
1:A:60:LYS:HB3	1:A:61:PRO:HD3	1.64	0.79
1:A:240:PRO:HA	1:A:243:ILE:HG13	1.62	0.79
1:B:96:LYS:O	1:B:97:ASN:HB2	1.83	0.79
1:B:169:GLU:OE2	1:B:169:GLU:CA	2.29	0.79
1:A:370:PHE:HZ	2:A:416:NM7:NAB	1.80	0.77
1:A:226:ASN:HB3	1:A:228:ASP:H	1.48	0.77
1:B:44:SER:O	1:B:45:ALA:HB3	1.83	0.77
1:A:249:GLN:O	1:A:253:ASP:OD1	2.04	0.76
1:A:11:GLU:OE1	1:B:407:SER:HA	1.86	0.76
1:B:98:THR:CG2	1:B:100:ARG:N	2.44	0.76
1:B:178:ARG:NH1	1:B:341:PHE:O	2.19	0.75
1:B:60:LYS:CB	1:B:61:PRO:HD3	2.17	0.75
1:B:371:ASP:CG	1:B:371:ASP:O	2.29	0.75
1:A:160:ASP:OD1	1:A:160:ASP:C	2.30	0.74
1:B:40:GLU:OE2	1:B:393:GLY:HA2	1.87	0.74
1:B:46:LEU:O	1:B:48:ARG:N	2.20	0.74
1:B:46:LEU:C	1:B:48:ARG:H	1.95	0.73
1:B:235:VAL:HG12	1:B:236:ALA:N	2.03	0.73
1:B:367:THR:O	1:B:367:THR:HG22	1.87	0.73
1:A:364:PRO:HD2	1:A:365:SER:H	1.53	0.73
1:A:132:ASP:C	1:A:132:ASP:OD1	2.29	0.72
1:B:157:VAL:O	1:B:369:ASN:ND2	2.22	0.72
1:A:334:GLU:OE2	1:A:337:LYS:HD2	1.89	0.72
1:B:109:LYS:HE3	1:B:145:ASP:O	1.88	0.72
1:A:136:ILE:O	1:A:215:ARG:NH1	2.22	0.72
1:B:391:PHE:O	1:B:391:PHE:HD1	1.71	0.72
1:B:98:THR:HG21	1:B:100:ARG:HB2	1.73	0.71
1:B:46:LEU:C	1:B:48:ARG:N	2.42	0.71
1:A:396:LEU:N	1:A:397:PRO:CD	2.54	0.70
1:B:98:THR:HG23	1:B:100:ARG:HG3	1.74	0.70
4:B:418:CL:CL	6:B:483:HOH:O	2.46	0.70
1:B:70:GLN:OE1	6:B:459:HOH:O	2.09	0.69
1:A:363:SER:CB	1:A:364:PRO:HD2	2.07	0.69
1:A:235:VAL:CG1	1:A:236:ALA:N	2.54	0.69
1:B:90:VAL:HG21	2:B:416:NM7:HAI	1.74	0.69
1:A:415:LEU:O	6:A:447:HOH:O	2.11	0.69
1:B:202:LYS:HE3	1:B:239:THR:OG1	1.93	0.69
1:A:338:LYS:O	1:A:338:LYS:HG2	1.90	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:THR:HG23	1:B:100:ARG:H	1.55	0.68
1:A:90:VAL:HG11	2:A:416:NM7:HAI	1.77	0.67
1:B:98:THR:CG2	1:B:99:GLU:N	2.58	0.67
1:B:168:PHE:O	1:B:169:GLU:HB2	1.95	0.67
1:B:363:SER:O	1:B:366:ASP:HB2	1.94	0.67
1:B:370:PHE:O	1:B:371:ASP:C	2.39	0.66
1:B:325:GLU:CD	1:B:325:GLU:H	2.03	0.66
1:B:332:GLY:C	1:B:334:GLU:H	2.04	0.65
1:A:236:ALA:HB2	1:A:251:MET:SD	2.36	0.65
1:A:95:MET:HB3	1:A:98:THR:OG1	1.97	0.65
1:B:360:ASP:O	1:B:361:VAL:HG12	1.97	0.65
1:A:235:VAL:HG13	1:A:236:ALA:H	1.63	0.64
1:B:282:TYR:C	1:B:282:TYR:HD2	2.03	0.64
1:A:60:LYS:HB3	1:A:61:PRO:CD	2.27	0.64
1:A:163:THR:O	1:A:163:THR:CG2	2.29	0.64
1:B:160:ASP:C	1:B:160:ASP:OD1	2.41	0.64
1:A:312:GLU:N	1:A:312:GLU:OE1	2.30	0.64
1:B:98:THR:CG2	1:B:100:ARG:HG3	2.28	0.64
1:A:322:CYS:SG	1:A:326:ARG:HB2	2.38	0.63
1:B:250:ALA:HA	1:B:256:GLY:HA3	1.80	0.63
1:B:366:ASP:OD1	1:B:368:SER:OG	2.16	0.63
1:A:69:MET:HE2	1:B:6:ARG:CG	2.28	0.63
1:B:60:LYS:HB3	1:B:61:PRO:CD	2.27	0.63
1:B:95:MET:O	1:B:98:THR:CB	2.33	0.63
1:A:90:VAL:HG21	2:A:416:NM7:HAI	1.79	0.62
1:A:18:PRO:HG3	1:A:26:SER:HB3	1.80	0.62
1:B:128:LEU:CD2	1:B:137:THR:HG22	2.29	0.62
1:B:112:MET:HA	1:B:112:MET:HE2	1.81	0.62
1:B:406:GLU:N	1:B:406:GLU:OE1	2.29	0.62
1:A:172:LEU:HD12	1:A:274:MET:HG2	1.81	0.62
1:A:226:ASN:HB3	1:A:228:ASP:N	2.13	0.62
1:B:360:ASP:C	1:B:361:VAL:CG1	2.73	0.61
1:B:137:THR:HG22	1:B:137:THR:O	2.00	0.61
1:A:396:LEU:N	1:A:397:PRO:HD3	2.16	0.61
1:B:80:LYS:CD	1:B:367:THR:HG21	2.15	0.61
1:A:253:ASP:OD1	1:A:253:ASP:N	2.30	0.60
1:A:338:LYS:O	1:A:338:LYS:CG	2.47	0.60
1:B:108:ASN:O	1:B:112:MET:HG2	2.02	0.60
1:B:80:LYS:HD3	1:B:367:THR:CG2	2.16	0.60
1:B:87:PHE:N	1:B:87:PHE:CD2	2.69	0.60
1:B:405:THR:HG23	1:B:406:GLU:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:HD12	1:B:62:PHE:CD2	2.38	0.59
1:B:20:ARG:O	1:B:21:ASN:C	2.40	0.59
1:B:204:ASP:OD1	1:B:204:ASP:N	2.29	0.59
1:B:323:SER:OG	1:B:325:GLU:OE1	2.17	0.59
1:A:96:LYS:O	1:A:97:ASN:HB2	2.03	0.59
1:B:15:LEU:HA	1:B:415:LEU:HD12	1.84	0.59
1:B:94:LYS:HB3	1:B:101:ILE:HD13	1.85	0.59
1:A:364:PRO:CD	1:A:365:SER:H	2.15	0.58
1:B:166:SER:OG	1:B:167:LYS:HG2	2.03	0.58
1:B:98:THR:HG21	1:B:100:ARG:CB	2.33	0.58
1:B:282:TYR:CD2	1:B:283:ALA:N	2.71	0.58
1:A:216:LEU:HD12	1:A:217:ALA:H	1.68	0.58
1:B:10:LEU:HD12	1:B:10:LEU:O	2.03	0.58
1:B:194:LEU:O	1:B:195:HIS:HB2	2.03	0.58
1:B:44:SER:O	1:B:45:ALA:CB	2.51	0.57
1:B:332:GLY:C	1:B:334:GLU:N	2.58	0.57
1:B:295:ASN:CG	1:B:295:ASN:O	2.47	0.57
1:A:255:MET:O	6:A:457:HOH:O	2.17	0.57
1:A:37:LEU:HD13	1:B:37:LEU:HD13	1.86	0.56
1:A:108:ASN:O	1:A:112:MET:HG2	2.04	0.56
1:B:321:ILE:O	1:B:321:ILE:HG22	2.05	0.56
1:B:272:TYR:CD1	1:B:280:PRO:HD3	2.40	0.56
1:A:169:GLU:O	1:A:170:ASP:HB2	2.06	0.56
1:A:83:GLY:HA3	2:A:416:NM7:CAG	2.36	0.56
1:B:173:PRO:HG2	1:B:176:MET:HB2	1.88	0.56
1:A:189:ASP:O	1:A:193:GLN:HG2	2.07	0.55
1:B:45:ALA:C	1:B:47:ARG:H	2.14	0.55
1:A:325:GLU:CD	1:A:325:GLU:N	2.63	0.55
1:A:366:ASP:OD2	1:A:368:SER:OG	2.21	0.54
1:B:214:ILE:O	1:B:351:ARG:NH2	2.39	0.54
1:A:204:ASP:OD1	1:A:204:ASP:N	2.40	0.54
1:A:160:ASP:OD1	1:A:162:LEU:N	2.40	0.54
1:B:312:GLU:OE1	1:B:312:GLU:N	2.30	0.54
1:A:133:CYS:O	1:A:215:ARG:NH1	2.41	0.53
1:B:332:GLY:O	1:B:334:GLU:N	2.41	0.53
1:A:40:GLU:CD	1:A:393:GLY:HA2	2.30	0.53
1:A:220:GLY:HA3	3:A:417:EDO:H11	1.91	0.53
1:A:44:SER:O	1:A:47:ARG:HG3	2.07	0.53
1:A:199:ARG:HH11	1:A:237:VAL:HG21	1.71	0.53
1:B:98:THR:HG22	1:B:99:GLU:N	2.22	0.53
1:A:195:HIS:C	1:A:225:MET:CE	2.79	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ASN:ND2	1:A:295:ASN:O	2.37	0.53
1:B:104:MET:SD	1:B:106:ILE:HD11	2.49	0.53
1:B:163:THR:O	1:B:167:LYS:HG3	2.09	0.52
1:B:183:GLU:HB3	1:B:214:ILE:HG12	1.91	0.52
1:B:232:GLN:HG3	1:B:257:LYS:HG2	1.92	0.52
1:B:137:THR:O	1:B:137:THR:CG2	2.53	0.52
1:B:293:ILE:O	1:B:296:HIS:HB3	2.10	0.52
1:A:60:LYS:O	1:A:64:GLN:HB2	2.10	0.52
1:A:161:LEU:HD21	1:A:274:MET:HE1	1.91	0.52
1:B:360:ASP:C	1:B:361:VAL:HG13	2.33	0.52
1:A:177:ALA:O	1:A:181:ILE:HG12	2.10	0.51
1:A:327:ARG:HG2	1:A:328:LEU:O	2.11	0.51
1:B:169:GLU:O	1:B:170:ASP:HB2	2.09	0.51
1:B:371:ASP:C	1:B:371:ASP:OD2	2.52	0.51
1:A:194:LEU:O	1:A:195:HIS:CB	2.54	0.51
1:B:60:LYS:CB	1:B:61:PRO:CD	2.86	0.51
1:B:46:LEU:O	1:B:47:ARG:C	2.53	0.51
1:A:316:LEU:HD12	1:A:316:LEU:O	2.10	0.51
1:A:334:GLU:OE2	1:A:337:LYS:CD	2.58	0.50
1:B:370:PHE:O	1:B:371:ASP:O	2.30	0.50
1:B:371:ASP:O	1:B:371:ASP:OD2	2.29	0.50
1:B:145:ASP:O	1:B:146:GLU:C	2.53	0.50
1:B:360:ASP:O	1:B:361:VAL:CG1	2.59	0.50
1:B:25:LEU:HD22	1:B:29:THR:HG21	1.94	0.49
1:B:60:LYS:N	1:B:61:PRO:CD	2.74	0.49
1:B:176:MET:HE2	1:B:357:TYR:HB2	1.95	0.49
1:B:28:GLU:OE1	1:B:404:THR:HG23	2.11	0.49
1:A:232:GLN:HG2	1:A:255:MET:HG3	1.95	0.49
1:B:38:TYR:OH	1:B:60:LYS:HG3	2.12	0.49
1:B:109:LYS:O	1:B:112:MET:HB2	2.12	0.49
1:B:83:GLY:C	1:B:84:ARG:HG2	2.35	0.49
1:B:60:LYS:O	1:B:64:GLN:HB2	2.12	0.48
1:B:78:ILE:HA	1:B:93:VAL:HG12	1.95	0.48
1:A:202:LYS:HE3	1:A:204:ASP:HB2	1.94	0.48
1:A:38:TYR:C	1:A:38:TYR:CD2	2.92	0.48
1:B:198:HIS:HA	1:B:222:CYS:SG	2.54	0.48
1:B:391:PHE:CD1	1:B:391:PHE:C	2.91	0.48
1:B:172:LEU:HD22	1:B:176:MET:SD	2.53	0.48
1:A:161:LEU:CD2	1:A:274:MET:HE2	2.37	0.48
1:A:46:LEU:N	1:A:46:LEU:HD23	2.28	0.48
1:A:83:GLY:HA3	2:A:416:NM7:CAO	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:GLU:H	1:B:406:GLU:CD	2.19	0.47
1:A:207:LEU:H	1:A:207:LEU:HG	1.52	0.47
1:A:195:HIS:HA	1:A:225:MET:CE	2.31	0.47
1:A:187:ALA:O	1:A:190:SER:HB3	2.15	0.47
1:B:45:ALA:C	1:B:47:ARG:N	2.72	0.47
1:B:197:VAL:HG22	1:B:260:PRO:HA	1.97	0.46
1:B:396:LEU:N	1:B:397:PRO:CD	2.78	0.46
1:A:46:LEU:C	1:A:48:ARG:N	2.66	0.46
1:A:405:THR:HG23	1:A:406:GLU:N	2.30	0.46
1:B:46:LEU:HA	1:B:46:LEU:HD12	1.55	0.46
1:A:241:ASP:OD1	1:A:241:ASP:N	2.45	0.46
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.68	0.46
1:A:60:LYS:CB	1:A:61:PRO:CD	2.92	0.46
1:B:202:LYS:HG3	1:B:204:ASP:OD1	2.16	0.46
1:A:246:GLU:HA	6:A:464:HOH:O	2.16	0.46
1:B:304:SER:O	1:B:305:HIS:HB2	2.14	0.46
1:A:104:MET:HE2	1:A:152:VAL:HG22	1.98	0.46
1:B:98:THR:CG2	1:B:100:ARG:CB	2.94	0.46
1:B:100:ARG:HG2	1:B:100:ARG:HH21	1.81	0.46
1:B:272:TYR:CD1	1:B:272:TYR:C	2.94	0.46
1:B:367:THR:O	1:B:367:THR:CG2	2.60	0.45
1:A:124:GLU:HG3	1:A:219:PHE:HB2	1.98	0.45
1:A:202:LYS:HB2	1:A:203:PRO:HD2	1.99	0.45
1:B:165:LEU:HD23	1:B:172:LEU:HG	1.99	0.45
1:A:104:MET:HE2	1:A:152:VAL:CG2	2.47	0.45
1:A:286:LEU:HD12	1:A:286:LEU:HA	1.62	0.45
1:A:27:VAL:HB	1:A:409:PHE:HB3	1.98	0.45
1:A:90:VAL:CG1	2:A:416:NM7:HAI	2.45	0.45
1:B:282:TYR:HD2	1:B:282:TYR:O	2.00	0.45
1:A:44:SER:C	1:A:46:LEU:H	2.24	0.45
1:A:265:TRP:CD1	1:A:265:TRP:C	2.95	0.45
1:A:295:ASN:O	1:A:298:GLU:N	2.49	0.45
1:B:98:THR:HG21	1:B:100:ARG:CG	2.47	0.45
1:B:132:ASP:OD1	1:B:132:ASP:C	2.60	0.44
1:A:15:LEU:CD1	1:B:409:PHE:CZ	3.01	0.44
1:A:69:MET:CE	1:B:6:ARG:CG	2.95	0.44
1:B:165:LEU:O	1:B:170:ASP:N	2.49	0.44
1:B:189:ASP:O	1:B:193:GLN:HG2	2.17	0.44
1:B:98:THR:CG2	1:B:100:ARG:CG	2.95	0.44
1:A:90:VAL:CB	2:A:416:NM7:HAI	2.48	0.44
1:A:251:MET:HB3	1:A:251:MET:HE2	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:PRO:CD	1:A:365:SER:N	2.77	0.43
1:A:234:SER:HB3	1:A:255:MET:SD	2.59	0.43
1:B:328:LEU:CD2	1:B:335:ASP:HB3	2.48	0.43
1:A:407:SER:HA	1:B:11:GLU:OE2	2.19	0.43
1:B:203:PRO:HD3	1:B:242:TYR:CE2	2.52	0.43
1:A:46:LEU:O	1:A:47:ARG:C	2.60	0.43
1:A:137:THR:O	1:A:137:THR:HG22	2.17	0.43
1:B:98:THR:HG23	1:B:99:GLU:N	2.32	0.43
1:B:332:GLY:O	1:B:333:ILE:C	2.60	0.43
1:B:363:SER:C	1:B:365:SER:N	2.76	0.43
1:B:322:CYS:SG	1:B:326:ARG:HB2	2.59	0.42
1:B:71:LEU:HD23	1:B:71:LEU:HA	1.78	0.42
1:B:195:HIS:C	1:B:225:MET:HE3	2.44	0.42
1:B:195:HIS:HA	1:B:225:MET:HE3	2.01	0.42
1:A:405:THR:HG23	1:A:406:GLU:HG3	2.01	0.42
1:B:363:SER:HA	1:B:364:PRO:HD2	1.87	0.42
1:A:172:LEU:HA	1:A:173:PRO:HD3	1.78	0.42
1:B:122:ARG:HB2	6:B:425:HOH:O	2.19	0.42
1:A:60:LYS:N	1:A:61:PRO:HD2	2.35	0.41
1:A:62:PHE:CD2	1:B:25:LEU:HD12	2.55	0.41
1:A:69:MET:CE	1:B:6:ARG:HG3	2.50	0.41
1:A:207:LEU:C	1:A:208:LEU:HD23	2.45	0.41
1:A:231:VAL:O	1:A:257:LYS:HA	2.20	0.41
1:B:394:LEU:HA	1:B:394:LEU:HD23	1.80	0.41
1:A:327:ARG:O	1:A:330:GLN:HG2	2.20	0.41
1:B:194:LEU:HD23	1:B:194:LEU:HA	1.87	0.41
1:B:405:THR:CG2	1:B:406:GLU:N	2.83	0.41
1:A:90:VAL:HG21	2:A:416:NM7:CAI	2.46	0.41
1:A:139:LEU:HD11	1:A:141:TYR:O	2.21	0.41
1:B:112:MET:CE	1:B:119:ALA:HB1	2.50	0.41
1:A:232:GLN:HG2	1:A:255:MET:CG	2.50	0.41
1:B:161:LEU:HD21	1:B:274:MET:HE2	2.03	0.41
1:A:202:LYS:HB2	1:A:203:PRO:CD	2.51	0.41
1:A:79:ILE:HD11	1:A:94:LYS:HB3	2.03	0.40
1:B:165:LEU:CD2	1:B:172:LEU:HG	2.50	0.40
1:A:113:LEU:HA	1:A:113:LEU:HD23	1.87	0.40
1:B:160:ASP:HA	1:B:207:LEU:HA	2.03	0.40
1:A:136:ILE:HG21	1:A:136:ILE:HD13	1.89	0.40
1:A:47:ARG:HG3	1:A:47:ARG:H	1.36	0.40
1:A:358:ILE:HA	1:A:359:PRO:HD2	1.95	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LYS:NZ	1:B:331:ASN:OD1[1_655]	2.11	0.09

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	391/415 (94%)	377 (96%)	14 (4%)	0	100	100
1	B	392/415 (94%)	378 (96%)	13 (3%)	1 (0%)	36	52
All	All	783/830 (94%)	755 (96%)	27 (3%)	1 (0%)	48	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	195	HIS

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	321/368 (87%)	276 (86%)	45 (14%)	3	5
1	B	321/368 (87%)	266 (83%)	55 (17%)	2	2
All	All	642/736 (87%)	542 (84%)	100 (16%)	2	3

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	8	LYS
1	A	13	LEU
1	A	15	LEU
1	A	33	VAL
1	A	44	SER
1	A	47	ARG
1	A	64	GLN
1	A	66	VAL
1	A	73	ARG
1	A	77	GLU
1	A	78	ILE
1	A	94	LYS
1	A	112	MET
1	A	132	ASP
1	A	136	ILE
1	A	137	THR
1	A	160	ASP
1	A	163	THR
1	A	204	ASP
1	A	207	LEU
1	A	214	ILE
1	A	216	LEU
1	A	224	LYS
1	A	235	VAL
1	A	237	VAL
1	A	243	ILE
1	A	244	SER
1	A	255	MET
1	A	274	MET
1	A	285	SER
1	A	286	LEU
1	A	287	VAL
1	A	295	ASN
1	A	297	GLU
1	A	323	SER
1	A	326	ARG
1	A	330	GLN
1	A	358	ILE
1	A	360	ASP
1	A	371	ASP
1	A	404	THR
1	A	406	GLU

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Mol	Chain	Res	Type
1	A	410	SER
1	A	414	SER
1	B	4	LYS
1	B	7	LEU
1	B	8	LYS
1	B	26	SER
1	B	31	LEU
1	B	44	SER
1	B	46	LEU
1	B	47	ARG
1	B	54	GLU
1	B	56	LEU
1	B	64	GLN
1	B	82	ILE
1	B	84	ARG
1	B	87	PHE
1	B	94	LYS
1	B	98	THR
1	B	106	ILE
1	B	107	LEU
1	B	112	MET
1	B	133	CYS
1	B	136	ILE
1	B	137	THR
1	B	139	LEU
1	B	169	GLU
1	B	171	LYS
1	B	176	MET
1	B	202	LYS
1	B	204	ASP
1	B	207	LEU
1	B	214	ILE
1	B	224	LYS
1	B	230	THR
1	B	235	VAL
1	B	252	GLU
1	B	261	GLU
1	B	271	MET
1	B	278	GLU
1	B	279	THR
1	B	282	TYR
1	B	286	LEU

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Mol	Chain	Res	Type
1	B	295	ASN
1	B	297	GLU
1	B	317	ILE
1	B	324	ARG
1	B	330	GLN
1	B	334	GLU
1	B	345	LEU
1	B	361	VAL
1	B	364	PRO
1	B	365	SER
1	B	368	SER
1	B	369	ASN
1	B	371	ASP
1	B	404	THR
1	B	415	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	72	HIS
1	A	134	GLN
1	A	193	GLN
1	A	211	ASN
1	A	232	GLN
1	A	249	GLN
1	A	295	ASN
1	B	70	GLN
1	B	148	HIS
1	B	211	ASN
1	B	232	GLN
1	B	369	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NM7	B	416	-	20,20,20	2.74	7 (35%)	27,28,28	2.87	6 (22%)
3	EDO	B	421	-	3,3,3	0.45	0	2,2,2	0.07	0
2	NM7	A	416	-	20,20,20	3.70	8 (40%)	27,28,28	2.74	6 (22%)
3	EDO	B	420	-	3,3,3	0.52	0	2,2,2	0.31	0
3	EDO	A	417	-	3,3,3	0.65	0	2,2,2	0.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NM7	B	416	-	-	0/12/12/12	0/2/2/2
3	EDO	B	421	-	-	1/1/1/1	-
2	NM7	A	416	-	-	0/12/12/12	0/2/2/2
3	EDO	B	420	-	-	1/1/1/1	-
3	EDO	A	417	-	-	0/1/1/1	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	416	NM7	CAR-CAN	-10.08	1.33	1.49
2	B	416	NM7	CAR-CAN	-8.25	1.36	1.49
2	A	416	NM7	CAS-SAL	-7.35	1.64	1.73
2	A	416	NM7	CAP-CAQ	-7.08	1.33	1.47
2	B	416	NM7	CAP-CAQ	-6.09	1.35	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	416	NM7	CAS-NAK	-4.46	1.33	1.38
2	A	416	NM7	CAM-NAK	-4.19	1.34	1.40
2	A	416	NM7	CAJ-CAR	-3.27	1.35	1.42
2	B	416	NM7	CAM-NAK	-3.22	1.35	1.40
2	A	416	NM7	CAR-CAS	-3.11	1.34	1.37
2	B	416	NM7	CAJ-CAR	-3.03	1.35	1.42
2	B	416	NM7	CAS-SAL	2.56	1.76	1.73
2	B	416	NM7	FAE-CAO	2.51	1.42	1.36
2	A	416	NM7	CAQ-SAL	-2.20	1.63	1.73
2	B	416	NM7	CAS-NAK	-2.05	1.36	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	416	NM7	CAR-CAS-SAL	-12.83	107.15	111.64
2	A	416	NM7	CAR-CAS-SAL	-10.87	107.83	111.64
2	A	416	NM7	CAS-NAK-CAM	-4.53	116.98	124.29
2	A	416	NM7	CAJ-CAR-CAS	3.83	115.03	111.67
2	B	416	NM7	CAJ-CAR-CAS	3.74	114.95	111.67
2	A	416	NM7	CAQ-SAL-CAS	3.70	95.27	90.92
2	A	416	NM7	CAR-CAS-NAK	3.35	129.44	125.01
2	B	416	NM7	CAP-CAQ-SAL	2.22	126.69	121.02
2	B	416	NM7	SAL-CAS-NAK	2.19	125.63	122.95
2	A	416	NM7	CAG-CAO-CAF	-2.11	120.03	122.80
2	B	416	NM7	CAQ-SAL-CAS	2.08	93.37	90.92
2	B	416	NM7	CAG-CAO-CAF	-2.07	120.09	122.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	420	EDO	O1-C1-C2-O2
3	B	421	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 13 short contacts:

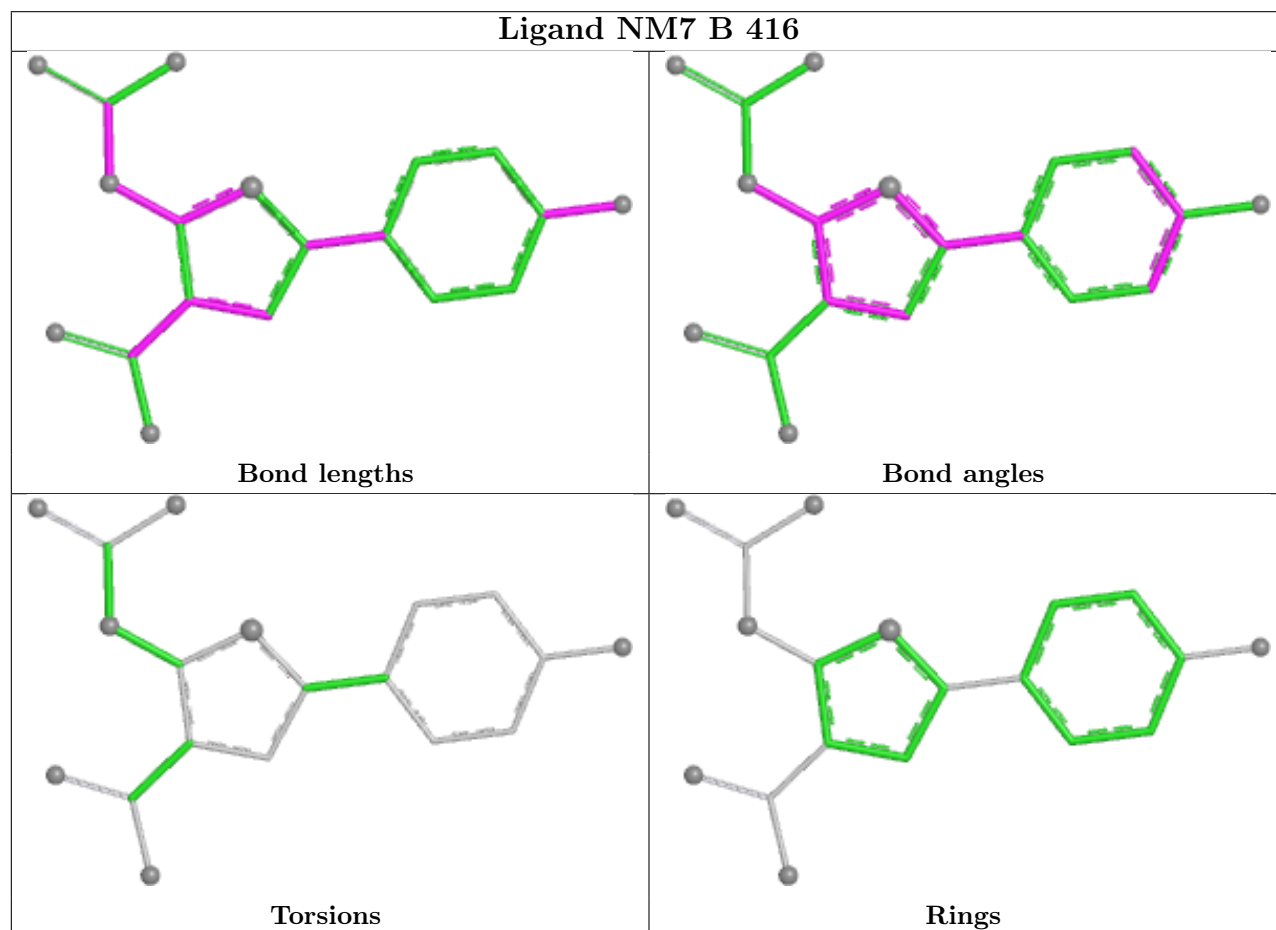
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	416	NM7	1	0
3	B	421	EDO	1	0
2	A	416	NM7	10	0

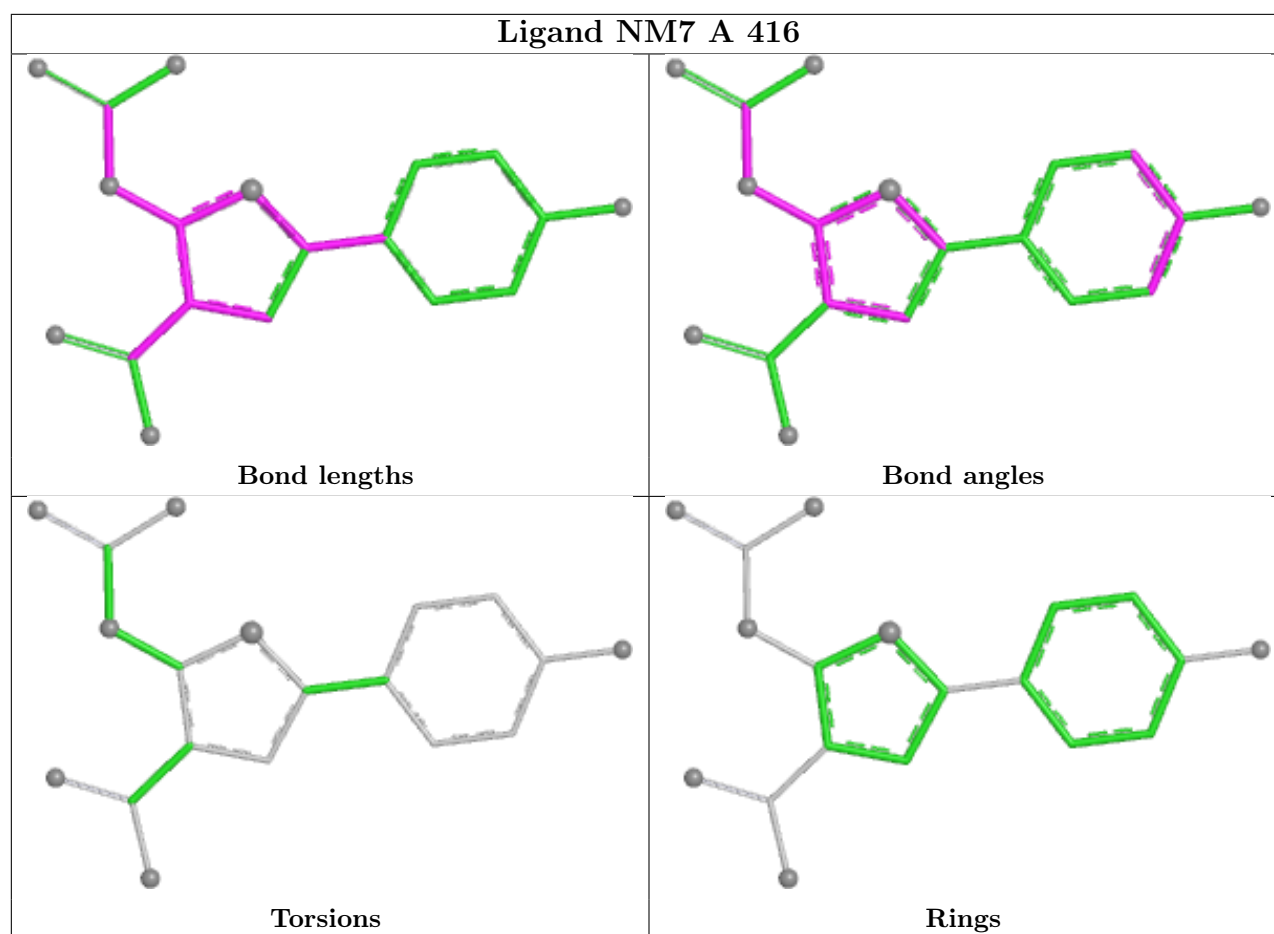
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	417	EDO	1	0

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 [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	395/415 (95%)	-0.08	3 (0%) 82 79	17, 41, 67, 80	0
1	B	396/415 (95%)	-0.04	7 (1%) 67 63	16, 43, 71, 94	0
All	All	791/830 (95%)	-0.06	10 (1%) 75 71	16, 42, 70, 94	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	ALA	3.6
1	B	85	GLY	3.4
1	B	362	SER	3.3
1	B	295	ASN	2.7
1	A	372	VAL	2.6
1	B	371	ASP	2.3
1	B	87	PHE	2.3
1	B	21	ASN	2.1
1	A	392	SER	2.1
1	B	44	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](#)

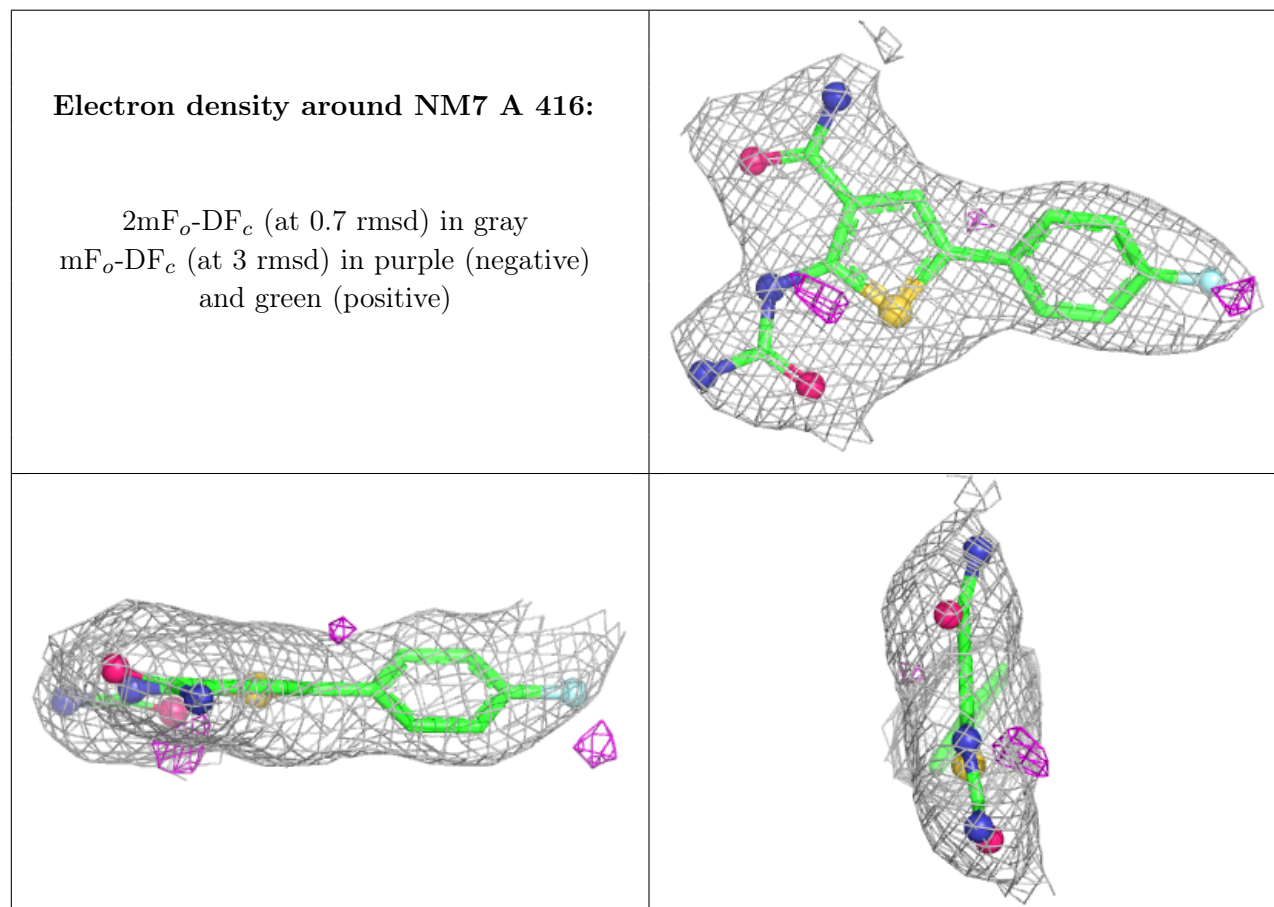
There are no oligosaccharides in this entry.

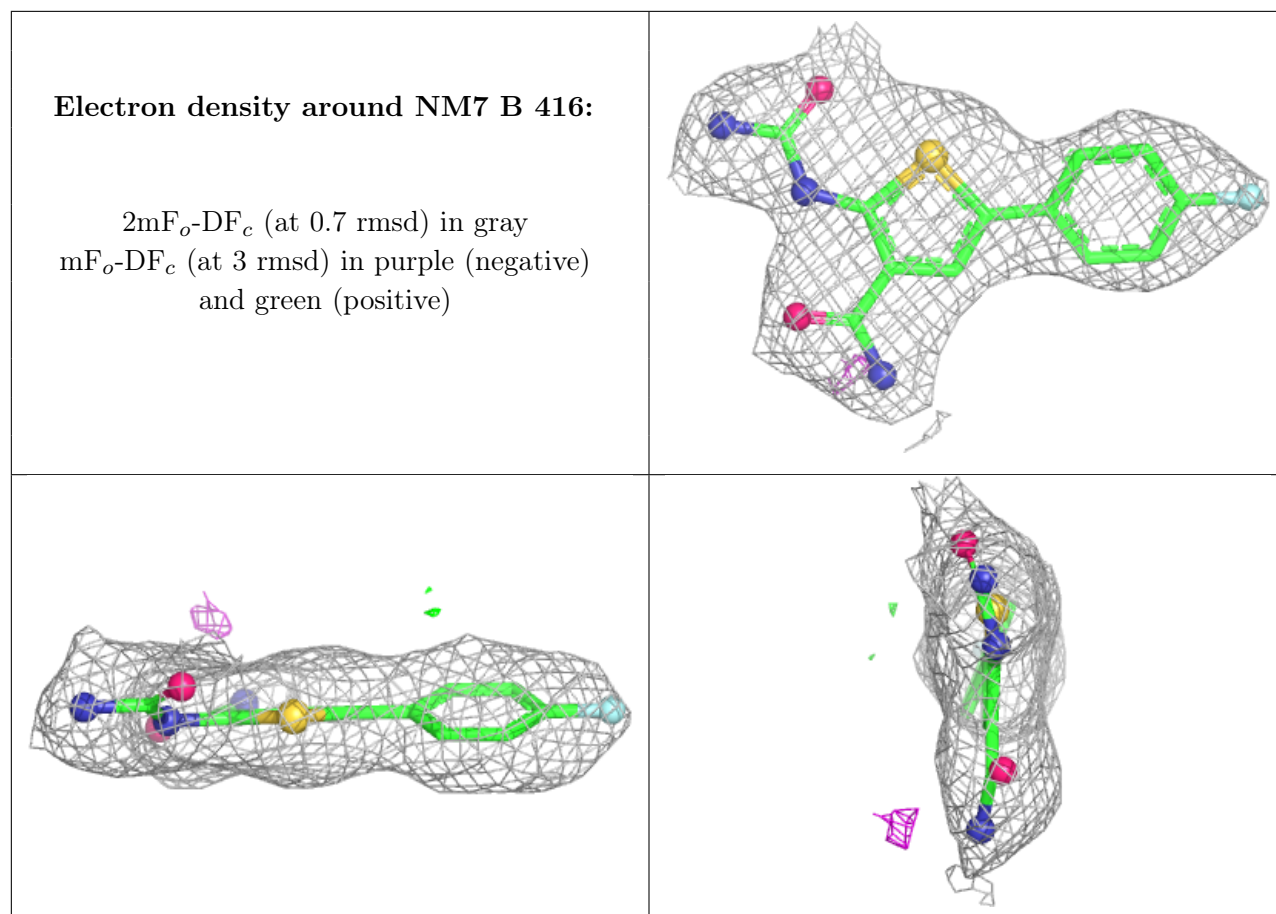
6.4 Ligands ⓘ

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(Å ²)	Q<0.9
3	EDO	B	420	4/4	0.64	0.18	69,71,71,71	0
3	EDO	A	417	4/4	0.79	0.16	42,46,50,51	0
2	NM7	A	416	19/19	0.93	0.09	27,41,45,45	0
2	NM7	B	416	19/19	0.94	0.08	22,34,47,50	0
4	CL	B	417	1/1	0.94	0.14	56,56,56,56	0
4	CL	B	418	1/1	0.94	0.15	57,57,57,57	0
5	MG	B	419	1/1	0.95	0.12	26,26,26,26	0
3	EDO	B	421	4/4	0.96	0.08	33,33,34,38	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.