



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:45 AM UTC

PDB ID : 4NPA / pdb_00004npa
Title : Scrystal structure of protein with unknown function from Vibrio cholerae at P22121 spacegroup
Authors : Boyko, K.M.; Gorbacheva, M.A.; Rakitina, T.V.; Korgenevsky, D.A.; Dorovatsky, P.V.; Lipkin, A.V.; Minor, W.; Shumilin, I.A.; Popov, V.O.
Deposited on : 2013-11-21
Resolution : 2.10 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
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

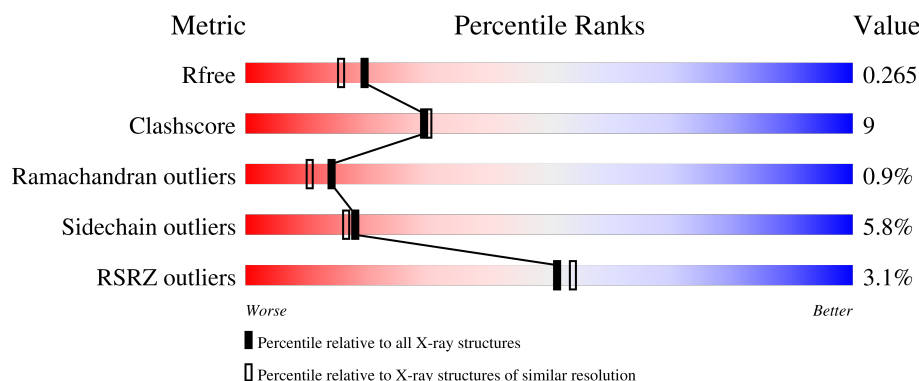
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	456	0% 69% 20% 8%
1	B	456	2% 68% 20% 8%
1	C	456	3% 67% 21% 8%
1	D	456	5% 66% 21% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12881 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3173	2017	557	578	21			
1	B	420	Total	C	N	O	S	0	1	0
			3175	2013	556	585	21			
1	C	418	Total	C	N	O	S	0	1	0
			3164	2011	553	579	21			
1	D	413	Total	C	N	O	S	0	2	0
			3041	1923	537	562	19			

There are 20 discrepancies between the modelled and reference sequences:

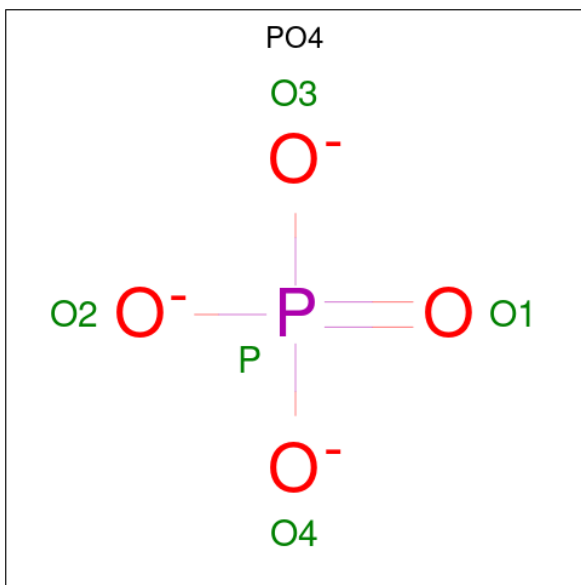
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	expression tag	UNP Q9KTK3
A	5	SER	-	expression tag	UNP Q9KTK3
A	6	LEU	-	expression tag	UNP Q9KTK3
A	458	GLU	-	expression tag	UNP Q9KTK3
A	459	GLY	-	expression tag	UNP Q9KTK3
B	4	MET	-	expression tag	UNP Q9KTK3
B	5	SER	-	expression tag	UNP Q9KTK3
B	6	LEU	-	expression tag	UNP Q9KTK3
B	458	GLU	-	expression tag	UNP Q9KTK3
B	459	GLY	-	expression tag	UNP Q9KTK3
C	4	MET	-	expression tag	UNP Q9KTK3
C	5	SER	-	expression tag	UNP Q9KTK3
C	6	LEU	-	expression tag	UNP Q9KTK3
C	458	GLU	-	expression tag	UNP Q9KTK3
C	459	GLY	-	expression tag	UNP Q9KTK3
D	4	MET	-	expression tag	UNP Q9KTK3
D	5	SER	-	expression tag	UNP Q9KTK3
D	6	LEU	-	expression tag	UNP Q9KTK3
D	458	GLU	-	expression tag	UNP Q9KTK3
D	459	GLY	-	expression tag	UNP Q9KTK3

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			7	4	3		

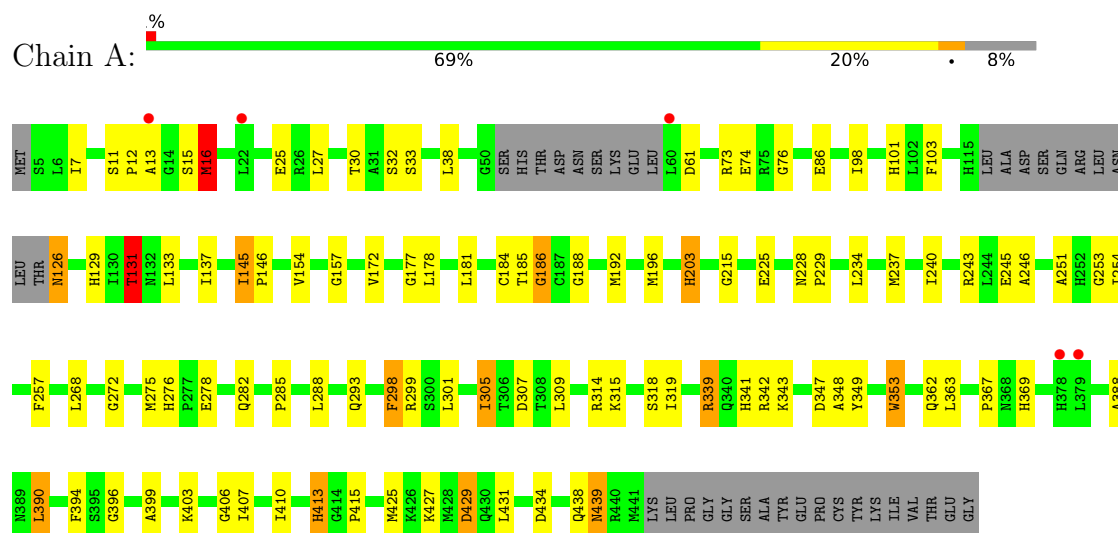
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	93	Total	O	0	0
			93	93		
5	B	91	Total	O	0	0
			91	91		
5	C	78	Total	O	0	0
			78	78		
5	D	39	Total	O	0	0
			39	39		

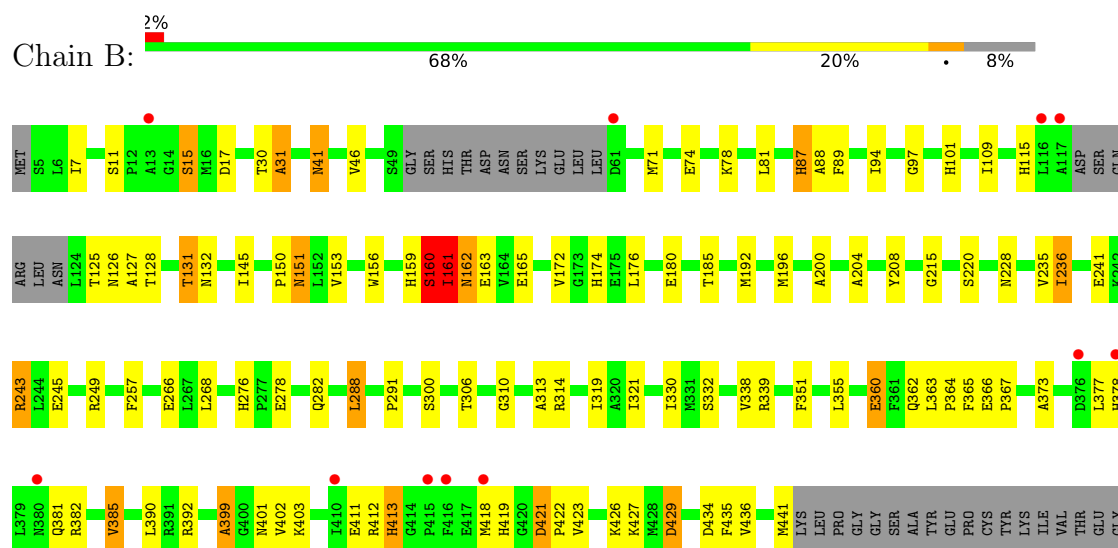
3 Residue-property plots

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: Putative uncharacterized protein

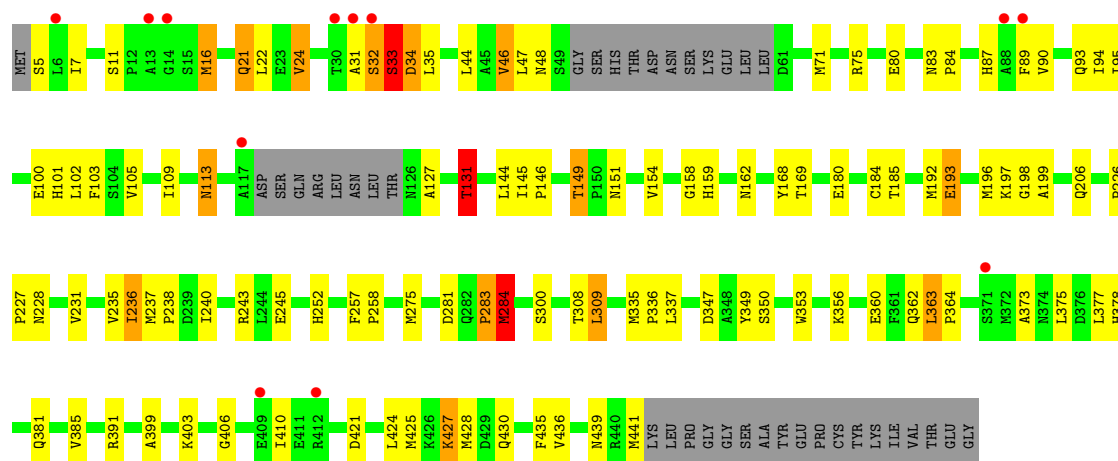


• Molecule 1: Putative uncharacterized protein

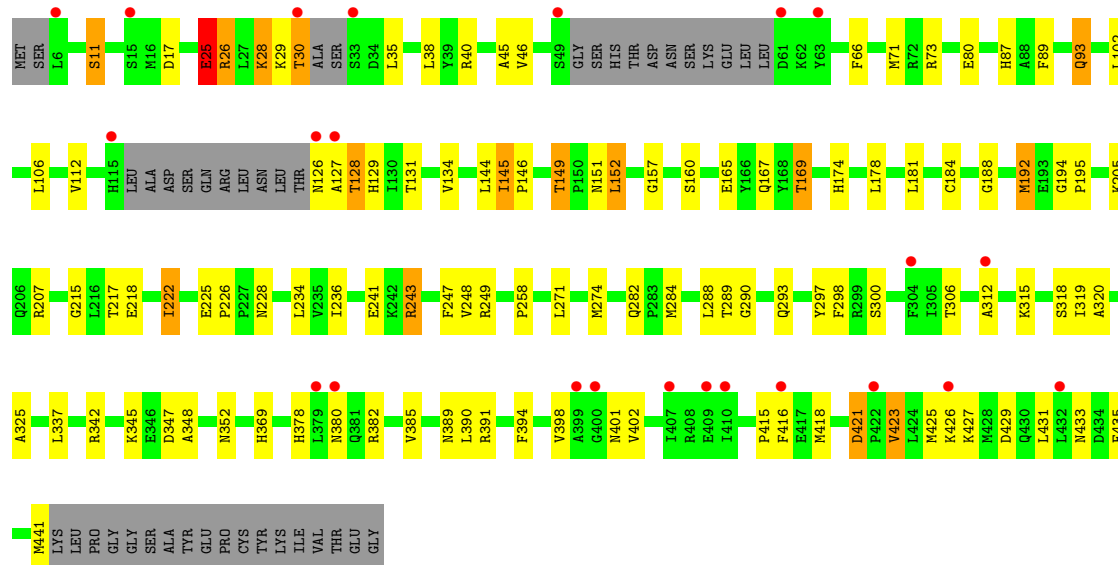


• Molecule 1: Putative uncharacterized protein





• Molecule 1: Putative uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	58.33Å 96.34Å 333.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.74 – 2.10 29.74 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.74-2.10) 99.9 (29.74-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.206 , 0.267 0.206 , 0.265	Depositor DCC
R_{free} test set	5567 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12881	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: PEG, SO4, PO4

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	1.41	13/3241 (0.4%)	1.51	35/4397 (0.8%)
1	B	1.47	15/3246 (0.5%)	1.46	35/4404 (0.8%)
1	C	1.38	12/3238 (0.4%)	1.43	28/4398 (0.6%)
1	D	1.26	10/3115 (0.3%)	1.38	29/4241 (0.7%)
All	All	1.38	50/12840 (0.4%)	1.44	127/17440 (0.7%)

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	1
1	B	0	1
1	C	0	1
All	All	0	3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	VAL	C-O	8.78	1.33	1.24
1	C	308	THR	CA-C	-7.98	1.47	1.52
1	D	106	LEU	CA-C	-7.59	1.43	1.52
1	C	284	MET	CA-C	-7.12	1.43	1.52
1	D	226	PRO	CA-C	6.81	1.56	1.52
1	A	253	GLY	C-O	6.26	1.31	1.24
1	D	205	LYS	N-CA	6.24	1.54	1.46
1	C	168	TYR	CA-C	6.22	1.60	1.52
1	B	172	VAL	N-CA	6.14	1.53	1.46
1	D	167	GLN	CA-C	-6.03	1.45	1.52
1	B	145	ILE	CA-C	6.01	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	226	PRO	C-O	-5.97	1.19	1.24
1	C	100	GLU	C-O	-5.93	1.17	1.24
1	D	145	ILE	N-CA	-5.91	1.42	1.46
1	D	243	ARG	CA-CB	-5.79	1.44	1.53
1	D	226	PRO	CA-CB	-5.76	1.49	1.54
1	B	204	ALA	C-O	5.76	1.30	1.24
1	A	157	GLY	N-CA	5.75	1.52	1.45
1	A	178	LEU	N-CA	5.74	1.53	1.46
1	D	165	GLU	CA-C	5.72	1.60	1.52
1	B	288	LEU	C-O	5.64	1.30	1.24
1	A	285	PRO	C-O	5.64	1.30	1.23
1	B	300	SER	CA-C	5.61	1.60	1.52
1	C	144	LEU	C-O	-5.59	1.17	1.24
1	D	248	VAL	CA-CB	5.59	1.61	1.54
1	B	291	PRO	C-O	5.53	1.30	1.23
1	A	390	LEU	CA-C	5.45	1.59	1.52
1	B	332	SER	N-CA	-5.44	1.40	1.46
1	C	238	PRO	C-O	-5.42	1.17	1.24
1	A	396	GLY	N-CA	5.41	1.52	1.45
1	D	290	GLY	N-CA	5.33	1.52	1.44
1	C	84	PRO	CA-C	5.30	1.55	1.52
1	B	235	VAL	C-O	-5.28	1.18	1.24
1	B	15	SER	CA-C	5.26	1.59	1.52
1	A	225	GLU	C-N	5.25	1.39	1.33
1	C	199	ALA	C-O	-5.25	1.17	1.24
1	C	180	GLU	CA-C	-5.25	1.46	1.53
1	A	388	ALA	C-O	5.21	1.30	1.24
1	B	174	HIS	CA-C	5.20	1.59	1.52
1	C	95	ILE	N-CA	-5.17	1.40	1.46
1	A	203	HIS	N-CA	5.13	1.52	1.46
1	B	200	ALA	N-CA	5.13	1.52	1.46
1	B	97	GLY	N-CA	5.09	1.52	1.45
1	A	251	ALA	CA-C	-5.08	1.46	1.52
1	A	298	PHE	N-CA	-5.05	1.40	1.46
1	C	281	ASP	N-CA	5.04	1.52	1.46
1	B	71	MET	C-O	-5.04	1.18	1.24
1	B	236	ILE	C-O	-5.03	1.18	1.24
1	A	203	HIS	C-O	5.02	1.29	1.24
1	A	254	ILE	CA-CB	5.02	1.61	1.54

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	SER	CA-C-N	-12.71	107.12	120.85
1	A	11	SER	C-N-CA	-12.71	107.12	120.85
1	A	257	PHE	CA-C-N	-10.37	109.76	120.03
1	A	257	PHE	C-N-CA	-10.37	109.76	120.03
1	D	225	GLU	CA-C-N	10.18	126.99	119.66
1	D	225	GLU	C-N-CA	10.18	126.99	119.66
1	A	363	LEU	CA-C-N	-9.48	110.27	119.85
1	A	363	LEU	C-N-CA	-9.48	110.27	119.85
1	B	11	SER	CA-C-N	-8.58	111.90	120.31
1	B	11	SER	C-N-CA	-8.58	111.90	120.31
1	A	76	GLY	N-CA-C	-8.43	103.05	111.56
1	D	11	SER	CA-C-N	-8.33	111.58	120.66
1	D	11	SER	C-N-CA	-8.33	111.58	120.66
1	A	237	MET	CA-C-N	-8.31	109.46	119.84
1	A	237	MET	C-N-CA	-8.31	109.46	119.84
1	C	169	THR	N-CA-C	-8.13	102.39	111.82
1	D	241	GLU	N-CA-C	-7.94	102.23	112.23
1	D	145	ILE	N-CA-C	7.87	114.72	107.56
1	A	339	ARG	NE-CZ-NH2	-7.82	112.16	119.20
1	B	385	VAL	CB-CA-C	7.32	121.97	111.65
1	D	401	ASN	N-CA-C	7.23	118.95	111.14
1	C	363	LEU	CA-C-N	-7.22	112.03	119.83
1	C	363	LEU	C-N-CA	-7.22	112.03	119.83
1	C	391	ARG	N-CA-C	-7.17	103.40	111.07
1	A	186	GLY	N-CA-C	-7.11	101.40	112.85
1	C	158	GLY	N-CA-C	7.08	121.27	112.14
1	B	257	PHE	CA-C-N	-7.06	112.50	119.78
1	B	257	PHE	C-N-CA	-7.06	112.50	119.78
1	C	252	HIS	N-CA-C	-6.98	104.64	113.72
1	A	353	TRP	N-CA-C	-6.86	103.86	111.82
1	B	161[A]	ILE	N-CA-C	-6.84	97.84	108.44
1	B	161[B]	ILE	N-CA-C	-6.84	97.84	108.44
1	B	363	LEU	CA-C-N	-6.72	113.04	119.76
1	B	363	LEU	C-N-CA	-6.72	113.04	119.76
1	C	309	LEU	N-CA-C	-6.67	104.08	111.82
1	C	24	VAL	N-CA-C	-6.66	105.63	113.42
1	C	350	SER	N-CA-C	6.62	120.62	112.54
1	B	162	ASN	N-CA-C	-6.60	96.63	110.69
1	B	78	LYS	N-CA-C	-6.50	99.32	109.72
1	B	338	VAL	N-CA-C	-6.49	104.16	110.72
1	B	243	ARG	CB-CG-CD	-6.48	96.39	111.30
1	A	299	ARG	N-CA-C	-6.43	104.19	111.07
1	A	253	GLY	N-CA-C	-6.41	101.36	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	GLY	CA-C-N	6.31	127.73	120.98
1	A	188	GLY	C-N-CA	6.31	127.73	120.98
1	C	283	PRO	N-CA-C	-6.28	100.29	110.40
1	D	127	ALA	N-CA-C	-6.23	103.79	111.33
1	A	305	ILE	CB-CA-C	-6.22	103.87	112.02
1	C	373	ALA	N-CA-C	-6.19	104.43	112.23
1	C	100	GLU	N-CA-C	-6.15	104.58	111.28
1	D	402	VAL	N-CA-C	6.14	119.10	112.96
1	C	235	VAL	N-CA-C	-6.12	99.40	108.45
1	A	16	MET	N-CA-C	6.10	118.62	108.13
1	B	421	ASP	CA-C-N	6.08	125.30	118.97
1	B	421	ASP	C-N-CA	6.08	125.30	118.97
1	A	246	ALA	N-CA-C	-6.04	104.69	111.28
1	D	28	LYS	N-CA-C	-6.03	102.00	110.50
1	B	429	ASP	N-CA-C	6.00	117.82	111.28
1	A	237	MET	N-CA-C	-5.95	103.29	110.13
1	B	426	LYS	N-CA-C	-5.92	104.45	111.03
1	A	145	ILE	N-CA-C	5.87	112.90	107.56
1	D	325	ALA	N-CA-C	5.86	117.67	111.28
1	A	33	SER	N-CA-C	-5.85	100.46	109.76
1	D	144	LEU	CA-C-N	5.84	126.57	122.60
1	D	144	LEU	C-N-CA	5.84	126.57	122.60
1	B	41	ASN	CB-CA-C	-5.83	101.68	110.90
1	C	436	VAL	CB-CA-C	-5.82	104.40	112.02
1	D	25	GLU	N-CA-C	-5.82	105.07	111.82
1	B	160	SER	CB-CA-C	5.81	119.47	111.23
1	D	169	THR	N-CA-C	-5.79	105.05	111.36
1	A	25	GLU	N-CA-C	-5.72	105.13	111.71
1	A	293	GLN	N-CA-C	5.71	119.35	112.38
1	A	86	GLU	N-CA-C	-5.70	106.31	113.72
1	B	115	HIS	N-CA-C	5.70	118.92	107.41
1	D	192	MET	N-CA-C	-5.53	106.54	113.28
1	B	176	LEU	N-CA-C	-5.52	105.34	111.36
1	C	226	PRO	CA-C-N	-5.51	114.25	119.76
1	C	226	PRO	C-N-CA	-5.51	114.25	119.76
1	B	339	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	A	341	HIS	N-CA-C	5.46	117.23	111.28
1	D	228	ASN	CA-C-N	-5.46	114.47	119.82
1	D	228	ASN	C-N-CA	-5.46	114.47	119.82
1	D	382	ARG	CA-C-N	5.43	126.63	119.84
1	D	382	ARG	C-N-CA	5.43	126.63	119.84
1	C	198	GLY	N-CA-C	-5.43	105.92	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ASP	N-CA-C	-5.42	106.74	113.19
1	A	131	THR	N-CA-CB	5.41	118.08	110.12
1	D	290	GLY	CA-C-N	5.39	125.39	120.21
1	D	290	GLY	C-N-CA	5.39	125.39	120.21
1	B	150	PRO	CB-CA-C	-5.39	104.79	111.64
1	B	399	ALA	CA-C-N	5.38	125.95	119.98
1	B	399	ALA	C-N-CA	5.38	125.95	119.98
1	A	309	LEU	N-CA-C	-5.36	106.74	113.28
1	B	215	GLY	N-CA-C	-5.32	100.58	113.18
1	C	240	ILE	N-CA-C	5.30	115.51	110.42
1	A	172	VAL	N-CA-C	-5.30	105.37	110.72
1	D	102	LEU	N-CA-C	-5.29	105.68	111.82
1	C	113	ASN	N-CA-C	5.29	117.13	111.36
1	C	149	THR	CA-C-N	-5.29	114.27	119.93
1	C	149	THR	C-N-CA	-5.29	114.27	119.93
1	C	109	ILE	N-CA-C	-5.29	105.23	110.62
1	C	131	THR	N-CA-CB	5.28	117.97	110.16
1	A	305	ILE	N-CA-C	-5.27	105.58	110.53
1	B	314	ARG	N-CA-C	5.25	117.75	111.71
1	C	127	ALA	CA-C-N	5.22	127.54	120.38
1	C	127	ALA	C-N-CA	5.22	127.54	120.38
1	C	75	ARG	CG-CD-NE	-5.21	100.53	112.00
1	B	161[A]	ILE	CA-C-N	5.21	132.51	122.03
1	B	161[A]	ILE	C-N-CA	5.21	132.51	122.03
1	B	161[B]	ILE	CA-C-N	5.21	132.51	122.03
1	B	161[B]	ILE	C-N-CA	5.21	132.51	122.03
1	B	330	ILE	N-CA-C	-5.20	105.31	110.62
1	B	401	ASN	N-CA-C	5.19	117.02	111.36
1	C	131	THR	CB-CA-C	5.19	119.67	110.85
1	A	318	SER	N-CA-C	5.17	116.52	109.18
1	A	131	THR	CB-CA-C	5.14	119.33	110.79
1	A	282	GLN	CA-C-N	-5.12	114.84	121.04
1	A	282	GLN	C-N-CA	-5.12	114.84	121.04
1	D	271	LEU	N-CA-C	-5.12	105.78	111.36
1	B	313	ALA	N-CA-C	-5.10	105.80	112.23
1	B	288	LEU	N-CA-C	-5.06	101.05	109.46
1	D	318	SER	N-CA-C	5.05	116.35	109.18
1	D	134	VAL	CA-C-N	5.02	127.32	120.54
1	D	134	VAL	C-N-CA	5.02	127.32	120.54
1	D	152	LEU	N-CA-C	5.02	116.91	108.73
1	C	428	MET	N-CA-C	-5.00	105.11	111.11
1	D	149	THR	CB-CA-C	5.00	116.61	109.11

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	SER	Peptide
1	B	15	SER	Peptide
1	C	33	SER	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	3173	0	3086	47	0
1	B	3175	0	3057	59	0
1	C	3164	0	3058	58	0
1	D	3041	0	2831	52	0
2	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	D	7	0	10	1	0
5	A	93	0	0	3	0
5	B	91	0	0	2	0
5	C	78	0	0	3	0
5	D	39	0	0	2	0
All	All	12881	0	12042	211	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 (211) 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:30:THR:O	1:B:31:ALA:CB	2.08	0.97
1:B:30:THR:O	1:B:31:ALA:HB2	1.64	0.97
1:C:283:PRO:O	1:C:284:MET:CB	2.11	0.94
1:D:28:LYS:O	1:D:30:THR:HG22	1.70	0.90
1:D:415:PRO:HB3	4:D:502:PEG:H31	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:HIS:CE1	1:B:278:GLU:HG3	2.15	0.82
1:C:283:PRO:O	1:C:284:MET:HB2	1.78	0.82
1:C:33:SER:C	1:C:35:LEU:H	1.90	0.80
1:A:399:ALA:HA	1:A:403:LYS:HD3	1.70	0.74
1:D:425:MET:O	1:D:429:ASP:HB2	1.88	0.74
1:B:161[B]:ILE:HG13	1:B:165:GLU:OE1	1.88	0.73
1:A:185:THR:HG23	1:A:186:GLY:O	1.87	0.72
1:B:192:MET:HA	1:B:192:MET:HE2	1.71	0.72
1:B:436:VAL:HG23	1:B:441:MET:HE3	1.72	0.71
1:A:307:ASP:OD2	1:A:427:LYS:HE2	1.90	0.70
1:A:131:THR:HB	1:A:245:GLU:OE2	1.91	0.70
1:C:131:THR:HB	1:C:245:GLU:OE2	1.91	0.70
1:B:243:ARG:HD3	5:B:621:HOH:O	1.92	0.69
1:B:276:HIS:HE1	1:B:278:GLU:HG3	1.57	0.69
1:C:105:VAL:HA	1:C:236:ILE:HD13	1.73	0.69
1:C:16:MET:HE3	5:C:636:HOH:O	1.92	0.69
1:D:25:GLU:HG2	1:D:26:ARG:N	2.05	0.69
1:C:283:PRO:O	1:C:284:MET:HB3	1.94	0.67
1:A:314:ARG:NH1	1:A:319:ILE:HD12	2.10	0.67
1:C:89:PHE:HA	1:C:93:GLN:O	1.95	0.67
1:A:126:ASN:HA	1:A:129:HIS:HB3	1.76	0.67
1:C:131:THR:HG22	1:C:362:GLN:HE22	1.60	0.66
1:C:71:MET:HE2	1:C:80:GLU:HB2	1.77	0.66
1:B:131:THR:HG22	1:B:362:GLN:NE2	2.10	0.66
1:D:243:ARG:HD3	1:D:247:PHE:CE2	2.31	0.66
1:B:360:GLU:H	1:B:360:GLU:CD	2.04	0.65
1:B:131:THR:HB	1:B:245:GLU:OE2	1.96	0.65
1:C:275:MET:HE1	1:C:309:LEU:HD13	1.79	0.64
1:B:125:THR:O	1:B:127:ALA:N	2.31	0.63
1:D:421:ASP:OD1	1:D:423:VAL:HG23	1.97	0.63
1:B:236:ILE:HD12	1:B:236:ILE:N	2.12	0.63
1:B:192:MET:HE2	1:B:192:MET:CA	2.30	0.62
1:D:217:THR:HG21	1:D:222:ILE:HG13	1.82	0.61
1:C:16:MET:HG3	1:C:103:PHE:HB3	1.82	0.61
1:C:159[B]:HIS:CE1	1:C:192:MET:HG3	2.36	0.60
1:A:438:GLN:O	1:A:439:ASN:HB2	2.01	0.60
1:D:288:LEU:HB3	1:D:298:PHE:CE1	2.36	0.60
1:A:425:MET:O	1:A:429:ASP:HB2	2.00	0.60
1:C:33:SER:C	1:C:35:LEU:N	2.60	0.59
1:A:154:VAL:HA	1:A:184:CYS:O	2.02	0.59
1:C:16:MET:CE	5:C:636:HOH:O	2.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:HIS:CE1	1:A:413:HIS:HB3	2.38	0.58
1:C:275:MET:CE	1:C:309:LEU:HD13	2.33	0.58
1:C:44:LEU:O	1:C:48:ASN:HB2	2.03	0.58
1:A:268:LEU:HD13	1:A:390:LEU:HB3	1.85	0.57
1:B:159:HIS:ND1	3:B:501:PO4:O2	2.26	0.57
1:D:421:ASP:OD1	1:D:421:ASP:C	2.47	0.57
1:B:161[B]:ILE:CG1	1:B:165:GLU:OE1	2.53	0.56
1:C:399:ALA:HA	1:C:403:LYS:HD3	1.88	0.56
1:B:131:THR:HG22	1:B:362:GLN:HE22	1.70	0.56
1:B:88:ALA:O	1:B:94:ILE:HA	2.06	0.56
1:B:185:THR:HG22	1:B:196:MET:HE3	1.87	0.56
1:B:185:THR:CG2	1:B:196:MET:HE3	2.36	0.55
1:B:30:THR:O	1:B:31:ALA:HB3	2.05	0.55
1:D:435:PHE:CB	1:D:441:MET:HE2	2.38	0.54
1:A:131:THR:HG22	1:A:362:GLN:HE22	1.74	0.53
1:D:87:HIS:CD2	1:D:87:HIS:H	2.25	0.53
1:A:98:ILE:HD13	5:A:665:HOH:O	2.09	0.53
1:B:360:GLU:CD	1:B:360:GLU:N	2.66	0.53
1:B:423:VAL:HG12	1:B:427:LYS:HE2	1.91	0.52
1:C:378:HIS:HA	1:C:421:ASP:HB2	1.92	0.52
1:D:347:ASP:OD1	1:D:348:ALA:N	2.43	0.52
1:D:152:LEU:HD11	1:D:184:CYS:HB2	1.91	0.52
1:D:369:HIS:CD2	1:D:416:PHE:HA	2.44	0.51
1:C:47:LEU:HD21	1:C:102:LEU:HD11	1.91	0.51
1:D:157:GLY:O	1:D:192:MET:HE3	2.09	0.51
1:A:12:PRO:HD2	1:A:12:PRO:O	2.10	0.51
1:C:5:SER:HB2	1:C:83:ASN:OD1	2.10	0.51
1:C:378:HIS:H	1:C:381:GLN:HE21	1.57	0.51
1:D:385:VAL:O	1:D:389:ASN:ND2	2.43	0.51
1:B:399:ALA:HA	1:B:403:LYS:HD3	1.92	0.51
1:A:16:MET:HG3	1:A:103:PHE:HB3	1.93	0.51
1:B:74:GLU:HG3	1:C:349:TYR:CZ	2.46	0.51
1:A:192:MET:HE2	1:A:192:MET:HA	1.93	0.50
1:A:399:ALA:O	1:A:406:GLY:HA3	2.12	0.50
1:C:335:MET:N	1:C:336:PRO:CD	2.75	0.50
1:B:365:PHE:CD1	1:B:392:ARG:HD3	2.47	0.50
1:C:237:MET:HG3	1:C:243:ARG:HA	1.94	0.50
1:D:89:PHE:HA	1:D:93:GLN:O	2.12	0.50
1:C:196:MET:HE1	1:C:231:VAL:HG22	1.93	0.50
1:B:249:ARG:HD2	1:B:351:PHE:CZ	2.47	0.50
1:C:46:VAL:HG22	1:C:227:PRO:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:426:LYS:O	1:D:429:ASP:HB3	2.11	0.50
1:D:435:PHE:HB2	1:D:441:MET:HE2	1.93	0.50
1:D:194:GLY:N	1:D:195:PRO:CD	2.74	0.49
1:B:412:ARG:O	1:B:413:HIS:ND1	2.46	0.49
1:B:127:ALA:O	1:B:131:THR:HG23	2.12	0.49
1:A:415:PRO:HB3	5:A:669:HOH:O	2.12	0.49
1:C:231:VAL:O	1:D:207:ARG:NH2	2.46	0.49
1:B:434:ASP:O	1:B:435:PHE:C	2.55	0.48
1:B:282:GLN:HG3	1:B:355:LEU:HD12	1.94	0.48
1:B:288:LEU:O	1:B:319:ILE:HA	2.13	0.48
1:D:274:MET:HE1	1:D:282:GLN:HB2	1.95	0.48
1:D:390:LEU:O	1:D:391:ARG:C	2.56	0.48
1:C:406:GLY:O	1:C:410:ILE:HG12	2.14	0.48
1:A:12:PRO:O	1:A:12:PRO:CD	2.57	0.48
1:B:74:GLU:HB2	1:C:349:TYR:CD1	2.49	0.48
1:B:276:HIS:CE1	1:B:278:GLU:CG	2.92	0.48
1:D:169:THR:HB	1:D:195:PRO:HG3	1.95	0.47
1:D:188:GLY:O	1:D:192:MET:HB2	2.13	0.47
1:A:133:LEU:O	1:A:137:ILE:HG13	2.13	0.47
1:D:345:LYS:CD	1:D:345:LYS:N	2.77	0.47
1:C:32:SER:C	1:C:34:ASP:N	2.71	0.47
1:D:45:ALA:HB3	1:D:222:ILE:HD13	1.96	0.47
1:D:249:ARG:HD3	1:D:352:ASN:O	2.14	0.47
1:A:243:ARG:HB3	5:A:653:HOH:O	2.15	0.47
1:A:301:LEU:O	1:A:305:ILE:HG12	2.15	0.47
1:B:74:GLU:HB2	1:C:349:TYR:CE1	2.50	0.47
1:C:435:PHE:HB2	1:C:441:MET:HE2	1.97	0.47
1:A:185:THR:HG22	1:A:196:MET:HE3	1.97	0.47
1:B:435:PHE:HB2	1:B:441:MET:HE2	1.94	0.47
1:B:192:MET:HE2	1:B:192:MET:N	2.30	0.46
1:C:87:HIS:CD2	5:C:671:HOH:O	2.68	0.46
1:B:180:GLU:HB3	1:B:208:TYR:CD1	2.50	0.46
1:C:185:THR:HG22	1:C:196:MET:HE3	1.96	0.46
1:C:101:HIS:HE1	1:C:228:ASN:O	1.96	0.46
1:D:217:THR:CG2	1:D:236:ILE:HD13	2.46	0.46
1:C:377:LEU:CB	1:C:425:MET:HE1	2.46	0.46
1:B:399:ALA:HA	1:B:403:LYS:CD	2.46	0.46
1:C:105:VAL:HG22	1:C:236:ILE:HD11	1.97	0.46
1:C:427:LYS:HB3	1:C:427:LYS:HE3	1.39	0.46
1:B:412:ARG:O	1:B:413:HIS:CG	2.69	0.46
1:A:215:GLY:O	1:A:234:LEU:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:HIS:HA	1:B:421:ASP:HB2	1.97	0.45
1:D:174:HIS:CE1	1:D:178:LEU:HD11	2.51	0.45
1:B:160:SER:HA	5:B:626:HOH:O	2.16	0.45
1:D:312:ALA:O	1:D:315:LYS:HG2	2.17	0.45
1:A:126:ASN:HD22	1:A:126:ASN:C	2.25	0.45
1:D:215:GLY:O	1:D:234:LEU:HD12	2.16	0.45
1:A:240:ILE:HD13	1:A:240:ILE:HA	1.87	0.45
1:C:192:MET:HA	1:C:192:MET:HE2	1.99	0.45
1:A:177:GLY:HA2	1:A:203:HIS:CD2	2.52	0.44
1:D:194:GLY:N	1:D:195:PRO:HD3	2.31	0.44
1:D:394:PHE:O	1:D:398:VAL:HG23	2.17	0.44
1:C:90:VAL:N	1:C:93:GLN:O	2.41	0.44
1:A:98:ILE:HG13	1:A:229:PRO:HB3	2.00	0.44
1:A:276:HIS:ND1	1:A:278:GLU:HB2	2.32	0.44
1:C:131:THR:HG22	1:C:362:GLN:NE2	2.32	0.44
1:A:131:THR:HG22	1:A:362:GLN:NE2	2.33	0.44
1:C:162:ASN:C	1:C:162:ASN:OD1	2.60	0.43
1:B:399:ALA:CB	1:B:403:LYS:HD3	2.47	0.43
1:A:101:HIS:HE1	1:A:228:ASN:O	2.00	0.43
1:A:145:ILE:O	1:A:146:PRO:C	2.60	0.43
1:A:288:LEU:HB3	1:A:298:PHE:CE1	2.54	0.43
1:B:87:HIS:CD2	1:B:87:HIS:H	2.33	0.43
1:D:40:ARG:NH1	1:D:66:PHE:O	2.49	0.43
1:D:421:ASP:OD1	1:D:423:VAL:CG2	2.65	0.43
1:C:7:ILE:HG23	1:C:80:GLU:HG2	2.00	0.43
1:C:257:PHE:HB3	1:C:258:PRO:CD	2.49	0.43
1:B:101:HIS:HE1	1:B:228:ASN:O	2.02	0.43
1:B:185:THR:HG22	1:B:196:MET:CE	2.48	0.43
1:C:35:LEU:HD12	1:C:35:LEU:HA	1.73	0.43
1:C:154:VAL:HA	1:C:184:CYS:O	2.18	0.43
1:D:390:LEU:HD23	1:D:390:LEU:HA	1.82	0.43
1:B:306:THR:O	1:B:310:GLY:HA2	2.19	0.43
1:D:145:ILE:HA	1:D:146:PRO:HD3	1.86	0.43
1:D:284:MET:HE3	5:D:610:HOH:O	2.18	0.43
1:A:272:GLY:HA2	1:A:275:MET:HE2	2.00	0.42
1:C:360:GLU:OE1	1:C:360:GLU:HA	2.18	0.42
1:A:342:ARG:HD2	1:A:348:ALA:O	2.19	0.42
1:B:377:LEU:HD23	1:B:377:LEU:HA	1.85	0.42
1:B:128:THR:O	1:B:132:ASN:ND2	2.52	0.42
1:B:421:ASP:HA	1:B:422:PRO:HD3	1.77	0.42
1:D:128:THR:HG22	1:D:129:HIS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:ASP:OD1	1:C:353:TRP:HB2	2.19	0.42
1:C:185:THR:CG2	1:C:196:MET:HE3	2.50	0.42
1:C:375:LEU:HD23	1:C:375:LEU:HA	1.86	0.42
1:C:363:LEU:O	1:C:364:PRO:C	2.60	0.42
1:B:366:GLU:HA	1:B:367:PRO:HD2	1.91	0.42
1:B:7:ILE:HA	1:B:81:LEU:O	2.19	0.42
1:D:195:PRO:HD2	5:D:615:HOH:O	2.19	0.42
1:D:274:MET:HE1	1:D:282:GLN:CB	2.50	0.42
1:A:73:ARG:HA	1:A:73:ARG:HD3	1.86	0.41
1:A:343:LYS:HD3	1:A:349:TYR:OH	2.20	0.41
1:C:145:ILE:O	1:C:146:PRO:C	2.63	0.41
1:C:193:GLU:HG3	1:C:197:LYS:HE3	2.02	0.41
1:D:35:LEU:HD12	1:D:35:LEU:HA	1.73	0.41
1:A:347:ASP:OD1	1:A:353:TRP:HB2	2.20	0.41
1:B:87:HIS:C	1:B:89:PHE:H	2.28	0.41
1:D:151:ASN:HB2	1:D:181:LEU:HD23	2.02	0.41
1:D:258:PRO:HA	1:D:297:TYR:CE2	2.55	0.41
1:B:381:GLN:O	1:B:382:ARG:C	2.61	0.41
1:A:268:LEU:CD1	1:A:394:PHE:HE2	2.33	0.41
1:A:268:LEU:CD1	1:A:394:PHE:CE2	3.04	0.41
1:A:407:ILE:O	1:A:410:ILE:N	2.54	0.41
1:C:21:GLN:O	1:C:22:LEU:C	2.63	0.41
1:D:71:MET:HE2	1:D:80:GLU:HB2	2.02	0.41
1:B:268:LEU:HD13	1:B:390:LEU:HB3	2.03	0.41
1:D:429:ASP:O	1:D:433:ASN:CG	2.64	0.41
1:C:377:LEU:HB3	1:C:424:LEU:HD23	2.03	0.41
1:B:373:ALA:O	1:B:419:HIS:CE1	2.74	0.41
1:C:356:LYS:HA	1:C:356:LYS:HD2	1.93	0.41
1:D:289:THR:HA	1:D:320:ALA:O	2.20	0.41
1:A:410:ILE:HD12	1:A:415:PRO:HA	2.02	0.41
1:D:342:ARG:HD2	1:D:348:ALA:O	2.21	0.41
1:D:378:HIS:C	1:D:380:ASN:N	2.77	0.41
1:D:73:ARG:HD3	1:D:73:ARG:HA	1.83	0.40
1:A:367:PRO:HG2	1:A:399:ALA:CB	2.51	0.40
1:C:71:MET:CE	1:C:80:GLU:HB2	2.49	0.40
1:A:74:GLU:HA	1:D:347:ASP:O	2.21	0.40
1:A:399:ALA:O	1:A:403:LYS:HB2	2.21	0.40
1:B:180:GLU:HB3	1:B:208:TYR:CE1	2.56	0.40
1:A:431:LEU:O	1:A:434:ASP:HB2	2.22	0.40
1:B:156:TRP:CE3	1:B:266:GLU:HB3	2.56	0.40
1:A:181:LEU:HA	1:A:181:LEU:HD23	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:GLU:CD	1:B:364:PRO:HA	2.46	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	412/456 (90%)	397 (96%)	13 (3%)	2 (0%)	24	22
1	B	415/456 (91%)	387 (93%)	22 (5%)	6 (1%)	9	5
1	C	413/456 (91%)	384 (93%)	24 (6%)	5 (1%)	10	7
1	D	407/456 (89%)	376 (92%)	29 (7%)	2 (0%)	24	22
All	All	1647/1824 (90%)	1544 (94%)	88 (5%)	15 (1%)	14	10

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	126	ASN
1	B	162	ASN
1	B	411	GLU
1	C	31	ALA
1	C	34	ASP
1	C	284	MET
1	B	31	ALA
1	B	413	HIS
1	C	32	SER
1	D	26	ARG
1	D	29	LYS
1	A	13	ALA
1	B	151	ASN
1	C	151	ASN

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Mol	Chain	Res	Type
1	A	32	SER

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	322/385 (84%)	310 (96%)	12 (4%)	30	33
1	B	322/385 (84%)	304 (94%)	18 (6%)	19	18
1	C	322/385 (84%)	303 (94%)	19 (6%)	18	16
1	D	291/385 (76%)	266 (91%)	25 (9%)	10	7
All	All	1257/1540 (82%)	1183 (94%)	74 (6%)	18	16

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	16	MET
1	A	27	LEU
1	A	30	THR
1	A	38	LEU
1	A	126	ASN
1	A	131	THR
1	A	315	LYS
1	A	339	ARG
1	A	413	HIS
1	A	429	ASP
1	A	439	ASN
1	B	17	ASP
1	B	41	ASN
1	B	46	VAL
1	B	87	HIS
1	B	109	ILE
1	B	131	THR
1	B	151	ASN
1	B	160	SER

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Mol	Chain	Res	Type
1	B	161[A]	ILE
1	B	161[B]	ILE
1	B	163	GLU
1	B	220	SER
1	B	321	ILE
1	B	360	GLU
1	B	385	VAL
1	B	402	VAL
1	B	418	MET
1	B	429	ASP
1	C	11	SER
1	C	16	MET
1	C	21	GLN
1	C	24	VAL
1	C	33	SER
1	C	46	VAL
1	C	94	ILE
1	C	113	ASN
1	C	131	THR
1	C	149	THR
1	C	193	GLU
1	C	206	GLN
1	C	236	ILE
1	C	300	SER
1	C	337	LEU
1	C	385	VAL
1	C	427	LYS
1	C	430	GLN
1	C	439	ASN
1	D	11	SER
1	D	17	ASP
1	D	25	GLU
1	D	30	THR
1	D	38	LEU
1	D	46	VAL
1	D	93	GLN
1	D	112	VAL
1	D	126	ASN
1	D	128	THR
1	D	131	THR
1	D	149	THR
1	D	160	SER

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Mol	Chain	Res	Type
1	D	218	GLU
1	D	222	ILE
1	D	293	GLN
1	D	300	SER
1	D	306	THR
1	D	319	ILE
1	D	337	LEU
1	D	418	MET
1	D	421	ASP
1	D	423	VAL
1	D	427	LYS
1	D	431	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	93	GLN
1	A	101	HIS
1	A	126	ASN
1	A	140	ASN
1	A	167	GLN
1	A	316	HIS
1	A	333	ASN
1	A	362	GLN
1	B	41	ASN
1	B	87	HIS
1	B	115	HIS
1	B	151	ASN
1	B	333	ASN
1	B	362	GLN
1	B	419	HIS
1	C	101	HIS
1	C	140	ASN
1	C	333	ASN
1	C	362	GLN
1	C	381	GLN
1	C	389	ASN
1	D	101	HIS
1	D	126	ASN
1	D	293	GLN
1	D	316	HIS

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 ⓘ

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	SO4	A	501	-	4,4,4	0.57	0	6,6,6	0.60	0
3	PO4	B	501	-	4,4,4	1.21	0	6,6,6	0.94	0
3	PO4	C	501	-	4,4,4	1.08	0	6,6,6	1.40	1 (16%)
4	PEG	D	502	-	6,6,6	0.57	0	5,5,5	0.58	0
3	PO4	D	501	-	4,4,4	0.47	0	6,6,6	1.54	2 (33%)

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	PEG	D	502	-	-	3/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	PO4	O3-P-O2	2.99	117.22	107.91
3	D	501	PO4	O2-P-O1	2.64	120.28	110.95
3	D	501	PO4	O3-P-O1	-2.08	103.60	110.95

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	502	PEG	O2-C3-C4-O4
4	D	502	PEG	O1-C1-C2-O2
4	D	502	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	PO4	1	0
4	D	502	PEG	1	0

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	418/456 (91%)	-0.19	5 (1%) 76 78	15, 30, 56, 81	0
1	B	420/456 (92%)	-0.16	11 (2%) 57 60	12, 29, 67, 93	1 (0%)
1	C	418/456 (91%)	-0.07	12 (2%) 53 56	18, 33, 62, 87	1 (0%)
1	D	413/456 (90%)	0.33	23 (5%) 30 32	20, 39, 72, 94	2 (0%)
All	All	1669/1824 (91%)	-0.02	51 (3%) 51 54	12, 33, 67, 94	4 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	416	PHE	6.6
1	D	410	ILE	4.3
1	B	117	ALA	4.2
1	B	116	LEU	3.9
1	C	31	ALA	3.9
1	A	60	LEU	3.9
1	A	378	HIS	3.5
1	D	407	ILE	3.5
1	B	13	ALA	3.3
1	D	61	ASP	3.3
1	D	6	LEU	3.1
1	B	61	ASP	3.0
1	D	127	ALA	3.0
1	D	33	SER	2.9
1	D	380	ASN	2.9
1	C	32	SER	2.8
1	B	376	ASP	2.7
1	C	14	GLY	2.7
1	A	13	ALA	2.6
1	C	412	ARG	2.5
1	B	415	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	380	ASN	2.5
1	C	88	ALA	2.5
1	A	22	LEU	2.5
1	C	409	GLU	2.4
1	C	13	ALA	2.4
1	D	422	PRO	2.4
1	D	304	PHE	2.4
1	D	432	LEU	2.3
1	D	115	HIS	2.3
1	D	409	GLU	2.3
1	D	63	TYR	2.3
1	B	416	PHE	2.3
1	C	117	ALA	2.3
1	D	379	LEU	2.2
1	B	378	HIS	2.2
1	C	89	PHE	2.2
1	A	379	LEU	2.2
1	C	6	LEU	2.2
1	D	312	ALA	2.2
1	C	371	SER	2.2
1	B	418	MET	2.2
1	D	30	THR	2.2
1	D	399	ALA	2.1
1	D	15	SER	2.1
1	D	49	SER	2.1
1	D	126	ASN	2.1
1	B	410	ILE	2.1
1	D	426	LYS	2.0
1	C	30	THR	2.0
1	D	400	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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
4	PEG	D	502	7/7	0.63	0.18	58,65,73,76	0
2	SO4	A	501	5/5	0.94	0.12	31,37,39,44	0
3	PO4	D	501	5/5	0.95	0.08	33,36,46,46	0
3	PO4	C	501	5/5	0.97	0.11	32,35,38,42	0
3	PO4	B	501	5/5	0.98	0.10	32,32,35,38	0

6.5 Other polymers

There are no such residues in this entry.