



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:05 PM GMT

PDB ID : 5BZX
Title : Crystal structure of human phosphatase PTEN treated with a bisperoxovanadium complex
Authors : Lee, C.-U.; Bier, D.; Hennig, S.; Grossmann, T.N.
Deposited on : 2015-06-11
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

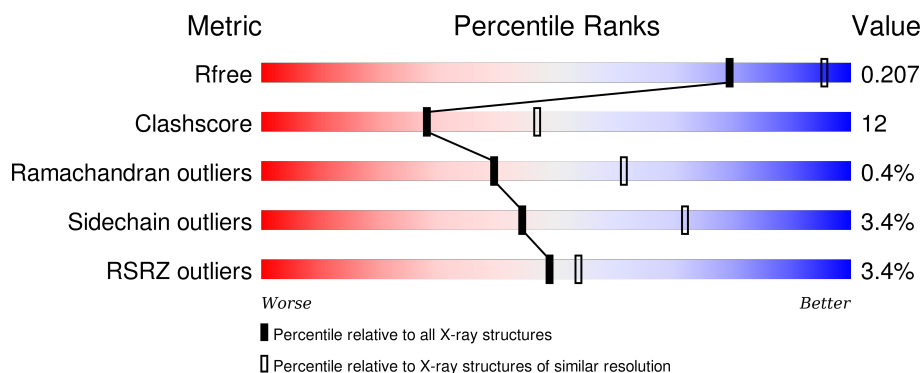
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	314	<div> <div>3%</div> <div>78%</div> <div>19%</div> <div>••</div> </div>
1	B	314	<div> <div>4%</div> <div>81%</div> <div>16%</div> <div>•</div> </div>
1	C	314	<div> <div>3%</div> <div>78%</div> <div>17%</div> <div>•</div> </div>
1	D	314	<div> <div>3%</div> <div>79%</div> <div>19%</div> <div>•</div> </div>

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	VO4	A	401	-	-	X	-
2	VO4	C	402	-	-	-	X
3	TLA	B	401	-	-	X	-
3	TLA	C	401	-	-	-	X
3	TLA	D	401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11230 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 Phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2578	1670	434	458	16			
1	B	314	Total	C	N	O	S	0	0	0
			2580	1672	437	455	16			
1	C	314	Total	C	N	O	S	0	0	0
			2580	1671	436	458	15			
1	D	314	Total	C	N	O	S	0	0	0
			2572	1665	439	453	15			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P60484
A	?	-	SER	deletion	UNP P60484
A	?	-	GLU	deletion	UNP P60484
A	?	-	LYS	deletion	UNP P60484
A	?	-	VAL	deletion	UNP P60484
A	?	-	GLU	deletion	UNP P60484
A	?	-	ASN	deletion	UNP P60484
A	?	-	GLY	deletion	UNP P60484
A	?	-	SER	deletion	UNP P60484
A	?	-	LEU	deletion	UNP P60484
A	?	-	CYS	deletion	UNP P60484
A	?	-	ASP	deletion	UNP P60484
A	?	-	GLN	deletion	UNP P60484
A	?	-	GLU	deletion	UNP P60484
A	?	-	ILE	deletion	UNP P60484
A	?	-	ASP	deletion	UNP P60484
A	?	-	SER	deletion	UNP P60484
A	?	-	ILE	deletion	UNP P60484
A	?	-	CYS	deletion	UNP P60484
A	?	-	SER	deletion	UNP P60484

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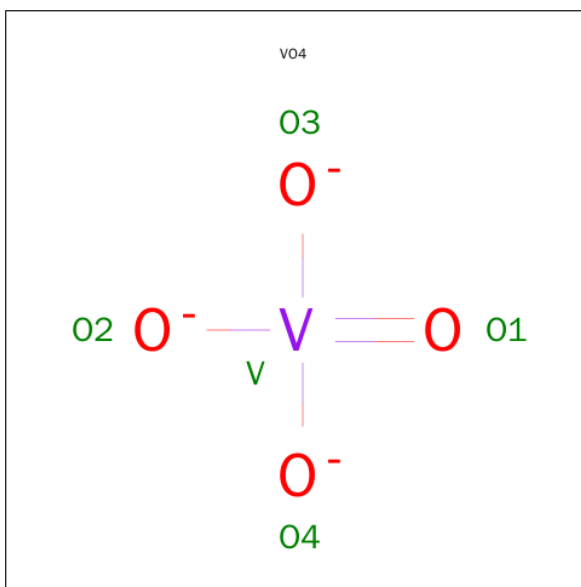
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP P60484
A	?	-	GLU	deletion	UNP P60484
A	?	-	ARG	deletion	UNP P60484
A	?	-	ALA	deletion	UNP P60484
B	?	-	THR	deletion	UNP P60484
B	?	-	SER	deletion	UNP P60484
B	?	-	GLU	deletion	UNP P60484
B	?	-	LYS	deletion	UNP P60484
B	?	-	VAL	deletion	UNP P60484
B	?	-	GLU	deletion	UNP P60484
B	?	-	ASN	deletion	UNP P60484
B	?	-	GLY	deletion	UNP P60484
B	?	-	SER	deletion	UNP P60484
B	?	-	LEU	deletion	UNP P60484
B	?	-	CYS	deletion	UNP P60484
B	?	-	ASP	deletion	UNP P60484
B	?	-	GLN	deletion	UNP P60484
B	?	-	GLU	deletion	UNP P60484
B	?	-	ILE	deletion	UNP P60484
B	?	-	ASP	deletion	UNP P60484
B	?	-	SER	deletion	UNP P60484
B	?	-	ILE	deletion	UNP P60484
B	?	-	CYS	deletion	UNP P60484
B	?	-	SER	deletion	UNP P60484
B	?	-	ILE	deletion	UNP P60484
B	?	-	GLU	deletion	UNP P60484
B	?	-	ARG	deletion	UNP P60484
B	?	-	ALA	deletion	UNP P60484
C	?	-	THR	deletion	UNP P60484
C	?	-	SER	deletion	UNP P60484
C	?	-	GLU	deletion	UNP P60484
C	?	-	LYS	deletion	UNP P60484
C	?	-	VAL	deletion	UNP P60484
C	?	-	GLU	deletion	UNP P60484
C	?	-	ASN	deletion	UNP P60484
C	?	-	GLY	deletion	UNP P60484
C	?	-	SER	deletion	UNP P60484
C	?	-	LEU	deletion	UNP P60484
C	?	-	CYS	deletion	UNP P60484
C	?	-	ASP	deletion	UNP P60484
C	?	-	GLN	deletion	UNP P60484
C	?	-	GLU	deletion	UNP P60484

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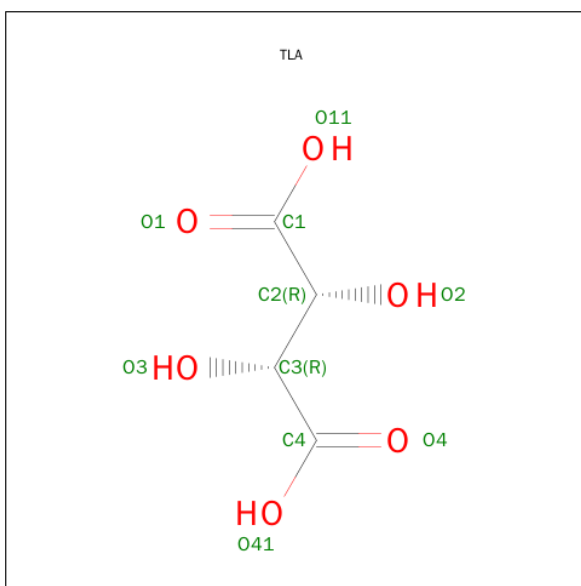
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ILE	deletion	UNP P60484
C	?	-	ASP	deletion	UNP P60484
C	?	-	SER	deletion	UNP P60484
C	?	-	ILE	deletion	UNP P60484
C	?	-	CYS	deletion	UNP P60484
C	?	-	SER	deletion	UNP P60484
C	?	-	ILE	deletion	UNP P60484
C	?	-	GLU	deletion	UNP P60484
C	?	-	ARG	deletion	UNP P60484
C	?	-	ALA	deletion	UNP P60484
D	?	-	THR	deletion	UNP P60484
D	?	-	SER	deletion	UNP P60484
D	?	-	GLU	deletion	UNP P60484
D	?	-	LYS	deletion	UNP P60484
D	?	-	VAL	deletion	UNP P60484
D	?	-	GLU	deletion	UNP P60484
D	?	-	ASN	deletion	UNP P60484
D	?	-	GLY	deletion	UNP P60484
D	?	-	SER	deletion	UNP P60484
D	?	-	LEU	deletion	UNP P60484
D	?	-	CYS	deletion	UNP P60484
D	?	-	ASP	deletion	UNP P60484
D	?	-	GLN	deletion	UNP P60484
D	?	-	GLU	deletion	UNP P60484
D	?	-	ILE	deletion	UNP P60484
D	?	-	ASP	deletion	UNP P60484
D	?	-	SER	deletion	UNP P60484
D	?	-	ILE	deletion	UNP P60484
D	?	-	CYS	deletion	UNP P60484
D	?	-	SER	deletion	UNP P60484
D	?	-	ILE	deletion	UNP P60484
D	?	-	GLU	deletion	UNP P60484
D	?	-	ARG	deletion	UNP P60484
D	?	-	ALA	deletion	UNP P60484

- Molecule 2 is VANADATE ION (three-letter code: VO4) (formula: O₄V).



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

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			10	4	6		

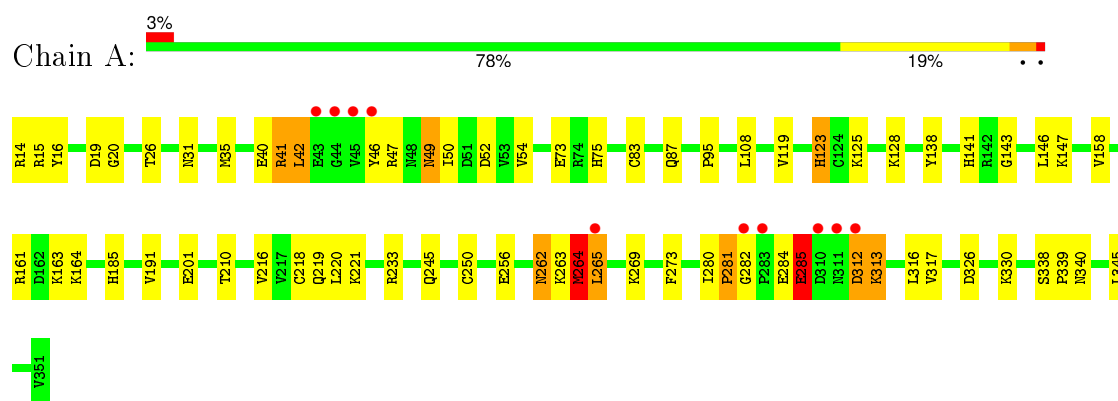
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	203	Total	O	0	0
			203	203		
4	B	224	Total	O	0	0
			224	224		
4	C	209	Total	O	0	0
			209	209		
4	D	244	Total	O	0	0
			244	244		

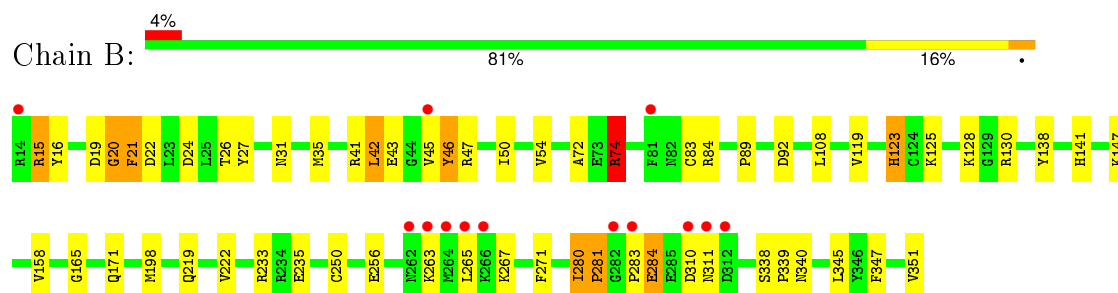
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

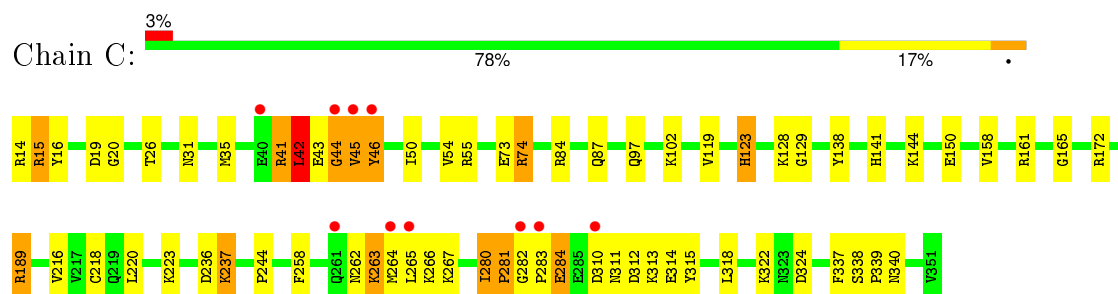
- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN



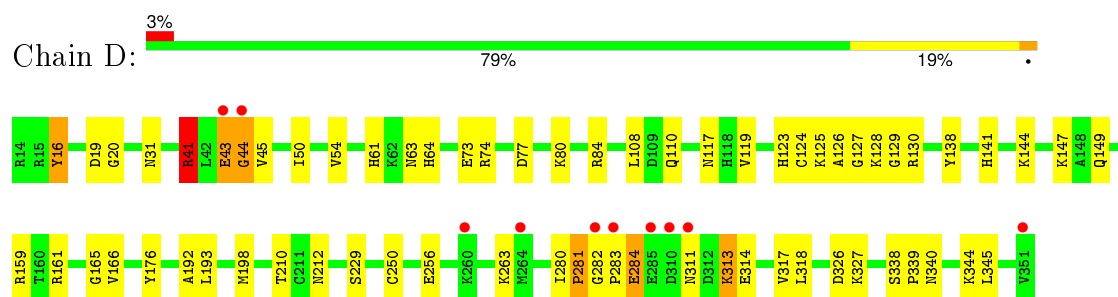
- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN



- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN



- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	207.06 Å 206.90 Å 87.67 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.29 – 2.50 46.29 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.29-2.50) 99.7 (46.29-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.51 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.175 , 0.204 0.178 , 0.207	Depositor DCC
R_{free} test set	3270 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.9	EDS
Estimated twinning fraction	0.501 for H, K, L 0.499 for K, H, -L 0.487 for -k,-h,-l	Xtriage
Reported twinning fraction	0.501 for H, K, L 0.499 for K, H, -L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 65393 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11230	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.73% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: VO4, TLA

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	0.49	0/2652	0.79	0/3585
1	B	0.50	0/2656	0.79	2/3593 (0.1%)
1	C	0.51	0/2656	0.80	2/3594 (0.1%)
1	D	0.50	0/2647	0.76	2/3581 (0.1%)
All	All	0.50	0/10611	0.79	6/14353 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	13
1	B	0	7
1	C	0	11
1	D	0	4
All	All	0	35

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	74	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	D	41	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	74	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	84	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	41	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	D	44	GLY	N-CA-C	-5.05	100.47	113.10

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	HIS	Peptide
1	A	19	ASP	Peptide
1	A	264	MET	Peptide
1	A	265	LEU	Peptide
1	A	280	ILE	Mainchain,Peptide
1	A	282	GLY	Peptide
1	A	285	GLU	Peptide
1	A	312	ASP	Peptide
1	A	313	LYS	Peptide
1	A	40	GLU	Peptide
1	A	41	ARG	Peptide
1	A	42	LEU	Peptide
1	B	123	HIS	Peptide
1	B	19	ASP	Peptide
1	B	20	GLY	Peptide
1	B	21	PHE	Peptide
1	B	280	ILE	Peptide
1	B	284	GLU	Peptide
1	B	311	ASN	Peptide
1	C	123	HIS	Peptide
1	C	19	ASP	Peptide
1	C	280	ILE	Peptide
1	C	282	GLY	Peptide
1	C	283	PRO	Peptide
1	C	310	ASP	Peptide
1	C	312	ASP	Peptide
1	C	41	ARG	Peptide
1	C	42	LEU	Peptide
1	C	44	GLY	Peptide
1	C	46	TYR	Peptide
1	D	123	HIS	Peptide
1	D	19	ASP	Peptide
1	D	263	LYS	Peptide
1	D	281	PRO	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	2578	0	2483	57	0
1	B	2580	0	2476	49	0
1	C	2580	0	2473	68	1
1	D	2572	0	2471	66	1
2	A	5	0	0	2	0
2	C	5	0	0	1	0
3	B	10	0	4	6	0
3	C	10	0	2	2	0
3	D	10	0	4	5	0
4	A	203	0	0	24	0
4	B	224	0	0	17	1
4	C	209	0	0	26	0
4	D	244	0	0	32	1
All	All	11230	0	9913	237	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (237) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:CYS:SG	4:A:599:HOH:O	1.99	1.17
3:C:401:TLA:O1	2:C:402:VO4:O2	1.57	1.17
1:A:312:ASP:O	1:C:265:LEU:CB	2.01	1.08
1:A:250:CYS:SG	4:A:519:HOH:O	2.13	1.06
1:A:42:LEU:HB2	1:A:46:TYR:CB	1.86	1.04
1:B:250:CYS:SG	4:B:526:HOH:O	2.16	1.04
1:D:126:ALA:HB3	4:D:510:HOH:O	1.55	1.03
1:D:283:PRO:HD2	1:D:311:ASN:HA	1.36	1.02
1:A:312:ASP:O	1:C:266:LYS:N	1.97	0.96
1:A:49:ASN:HD21	1:A:52:ASP:CG	1.70	0.95
1:B:15:ARG:NH2	1:B:27:TYR:O	1.99	0.94
1:C:263:LYS:HD2	4:C:535:HOH:O	1.68	0.94
1:C:218:CYS:SG	4:C:531:HOH:O	2.29	0.89
1:C:281:PRO:HG3	1:C:318:LEU:HD13	1.53	0.88
1:B:24:ASP:OD1	4:B:501:HOH:O	1.94	0.86
1:D:127:GLY:O	1:D:159:ARG:NH1	2.08	0.85
1:B:92:ASP:OD1	4:B:502:HOH:O	1.94	0.84
1:A:147:LYS:HG3	4:A:553:HOH:O	1.77	0.84
1:D:283:PRO:HD2	1:D:311:ASN:CA	2.08	0.84
1:A:49:ASN:ND2	1:A:52:ASP:OD2	2.13	0.81
3:B:401:TLA:O41	4:B:503:HOH:O	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:CYS:CB	4:C:531:HOH:O	2.27	0.81
1:C:220:LEU:O	4:C:501:HOH:O	2.00	0.80
1:B:15:ARG:HB2	1:B:158:VAL:O	1.82	0.79
1:A:87:GLN:NE2	4:A:503:HOH:O	2.16	0.78
1:B:281:PRO:HB2	1:B:283:PRO:HD3	1.66	0.77
1:D:84:ARG:NH2	4:D:503:HOH:O	2.16	0.77
1:C:218:CYS:HB3	4:C:531:HOH:O	1.84	0.77
1:A:15:ARG:HB2	1:A:158:VAL:O	1.85	0.77
1:D:283:PRO:CD	1:D:311:ASN:HA	2.13	0.76
1:B:83:CYS:HB3	4:B:633:HOH:O	1.86	0.74
1:A:312:ASP:H	1:C:266:LYS:CB	1.99	0.74
1:C:281:PRO:HG3	1:C:318:LEU:CD1	2.19	0.72
1:A:164:LYS:HE2	4:A:630:HOH:O	1.89	0.71
1:A:49:ASN:ND2	1:A:52:ASP:CG	2.42	0.71
1:C:280:ILE:HG23	1:C:281:PRO:HD3	1.71	0.71
1:C:97:GLN:NE2	4:C:508:HOH:O	2.23	0.70
3:D:401:TLA:O4	4:D:502:HOH:O	2.10	0.69
1:B:280:ILE:HD13	1:B:347:PHE:CE1	2.26	0.69
1:C:55:ARG:NH2	4:C:502:HOH:O	2.09	0.69
1:D:45:VAL:HB	1:D:125:LYS:HB3	1.74	0.69
1:B:351:VAL:HB	4:B:638:HOH:O	1.94	0.67
1:D:327:LYS:HB2	4:D:582:HOH:O	1.95	0.67
1:C:280:ILE:CG2	1:C:281:PRO:HD3	2.25	0.67
1:C:129:GLY:HA3	4:C:542:HOH:O	1.94	0.67
1:D:149:GLN:HG3	4:D:603:HOH:O	1.94	0.66
1:D:327:LYS:N	4:D:501:HOH:O	2.01	0.66
1:D:63:ASN:N	4:D:507:HOH:O	2.22	0.66
1:C:46:TYR:CE2	4:C:504:HOH:O	2.49	0.66
1:C:236:ASP:HB3	1:C:237:LYS:HE2	1.78	0.66
1:D:256:GLU:HG3	4:D:556:HOH:O	1.95	0.65
1:C:46:TYR:CB	4:C:644:HOH:O	2.44	0.65
1:A:20:GLY:HA3	4:A:576:HOH:O	1.96	0.65
1:A:262:ASN:OD1	1:A:264:MET:HB2	1.96	0.65
1:C:237:LYS:NZ	4:C:503:HOH:O	2.13	0.64
1:C:20:GLY:HA3	4:C:560:HOH:O	1.96	0.64
1:A:250:CYS:O	4:A:501:HOH:O	2.14	0.64
1:B:130:ARG:HE	3:B:401:TLA:H2	1.64	0.63
1:B:45:VAL:HG11	1:B:125:LYS:HE3	1.80	0.63
1:B:20:GLY:HA3	4:B:601:HOH:O	1.99	0.62
1:B:147:LYS:HE2	4:B:587:HOH:O	2.00	0.62
1:A:163:LYS:NZ	4:A:510:HOH:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:PRO:HB3	1:D:282:GLY:O	2.00	0.62
1:D:193:LEU:CD1	1:D:280:ILE:HG13	2.30	0.62
1:C:46:TYR:HB2	4:C:644:HOH:O	1.99	0.62
1:A:326:ASP:O	4:A:502:HOH:O	2.16	0.62
3:B:401:TLA:C4	4:B:502:HOH:O	2.47	0.61
1:C:220:LEU:N	4:C:511:HOH:O	2.32	0.61
1:C:43:GLU:OE2	4:C:504:HOH:O	2.16	0.61
1:B:130:ARG:H	3:B:401:TLA:H3	1.65	0.61
1:A:75:HIS:CG	4:A:524:HOH:O	2.54	0.61
1:B:233:ARG:NH1	1:B:235:GLU:OE2	2.34	0.61
1:B:128:LYS:HB3	3:B:401:TLA:O3	2.00	0.61
1:B:83:CYS:CB	4:B:633:HOH:O	2.44	0.61
1:C:44:GLY:C	1:C:46:TYR:H	2.04	0.61
1:B:351:VAL:C	4:B:577:HOH:O	2.40	0.60
1:D:192:ALA:CB	4:D:611:HOH:O	2.47	0.60
1:A:312:ASP:O	1:C:265:LEU:CA	2.49	0.60
1:C:128:LYS:HE3	4:C:641:HOH:O	2.01	0.60
1:B:43:GLU:OE1	1:B:74:ARG:NE	2.35	0.59
1:C:43:GLU:HG2	1:C:44:GLY:H	1.68	0.59
1:A:95:PRO:O	4:A:504:HOH:O	2.16	0.59
1:C:313:LYS:HG2	1:C:315:TYR:HB2	1.84	0.59
1:B:219:GLN:NE2	1:B:250:CYS:O	2.30	0.58
1:D:44:GLY:HA3	1:D:74:ARG:NH1	2.18	0.58
1:A:284:GLU:HG3	1:A:285:GLU:O	2.03	0.58
1:B:45:VAL:CG1	1:B:125:LYS:HE3	2.34	0.57
1:B:84:ARG:NH2	4:B:514:HOH:O	2.37	0.57
1:D:124:CYS:HB3	3:D:401:TLA:O1	2.04	0.57
1:C:172:ARG:NH1	4:C:515:HOH:O	2.37	0.57
1:D:283:PRO:HB3	1:D:317:VAL:HB	1.85	0.57
1:A:312:ASP:O	1:C:265:LEU:C	2.43	0.56
1:B:42:LEU:HB2	1:B:46:TYR:HB2	1.87	0.56
1:B:35:MET:SD	4:B:622:HOH:O	2.58	0.56
1:C:46:TYR:HE2	4:C:504:HOH:O	1.86	0.56
1:A:125:LYS:N	2:A:401:VO4:O1	2.38	0.55
1:D:281:PRO:HB2	1:D:317:VAL:O	2.06	0.55
1:C:15:ARG:HA	4:C:526:HOH:O	2.05	0.55
3:D:401:TLA:C4	4:D:521:HOH:O	2.55	0.55
1:D:117:ASN:O	4:D:504:HOH:O	2.18	0.55
1:D:144:LYS:NZ	4:D:520:HOH:O	2.40	0.54
1:D:149:GLN:HG2	1:D:176:TYR:OH	2.07	0.54
1:D:326:ASP:N	4:D:501:HOH:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:GLU:HG2	1:C:44:GLY:N	2.23	0.54
1:D:283:PRO:HD2	1:D:311:ASN:N	2.23	0.54
1:A:15:ARG:HD2	1:A:26:THR:HG23	1.89	0.54
1:D:20:GLY:HA3	4:D:623:HOH:O	2.07	0.54
1:C:73:GLU:OE1	4:C:505:HOH:O	2.19	0.53
1:B:15:ARG:CB	1:B:158:VAL:O	2.55	0.53
1:D:129:GLY:N	3:D:401:TLA:O3	2.42	0.52
1:C:20:GLY:CA	4:C:560:HOH:O	2.54	0.52
1:B:265:LEU:O	1:B:267:LYS:HG2	2.09	0.52
1:C:313:LYS:HG2	1:C:315:TYR:HD2	1.74	0.52
1:D:339:PRO:O	1:D:340:ASN:HB2	2.10	0.52
1:C:128:LYS:N	3:C:401:TLA:O11	2.41	0.52
1:B:339:PRO:O	1:B:340:ASN:HB2	2.10	0.52
1:A:245:GLN:HG2	4:A:661:HOH:O	2.09	0.51
1:A:312:ASP:C	1:C:265:LEU:CB	2.77	0.51
1:D:128:LYS:CG	4:D:535:HOH:O	2.58	0.51
1:C:339:PRO:O	1:C:340:ASN:CG	2.49	0.51
1:D:344:LYS:NZ	4:D:512:HOH:O	2.30	0.50
1:D:313:LYS:HD2	1:D:314:GLU:H	1.76	0.50
1:D:128:LYS:HG3	4:D:535:HOH:O	2.10	0.50
1:D:16:TYR:CD1	4:D:533:HOH:O	2.54	0.50
1:A:339:PRO:O	1:A:340:ASN:CG	2.50	0.50
1:C:324:ASP:O	4:C:506:HOH:O	2.19	0.50
1:D:281:PRO:HG2	1:D:318:LEU:HA	1.93	0.50
3:B:401:TLA:C4	4:B:503:HOH:O	2.53	0.50
1:D:326:ASP:O	4:D:505:HOH:O	2.19	0.50
1:C:262:ASN:OD1	1:C:264:MET:N	2.45	0.50
1:A:31:ASN:HA	1:A:119:VAL:HG22	1.93	0.49
1:B:222:VAL:HG21	1:C:244:PRO:HG3	1.94	0.49
1:B:108:LEU:HD23	1:B:138:TYR:CG	2.48	0.49
1:A:256:GLU:OE2	1:A:269:LYS:HE3	2.13	0.49
1:B:15:ARG:HG2	1:B:26:THR:HG23	1.95	0.49
1:B:171:GLN:NE2	4:B:503:HOH:O	2.30	0.49
1:C:15:ARG:HB3	1:C:158:VAL:O	2.13	0.49
1:D:198:MET:HG2	1:D:345:LEU:HD22	1.94	0.48
1:D:31:ASN:HA	1:D:119:VAL:HG22	1.95	0.48
1:B:31:ASN:HA	1:B:119:VAL:HG22	1.95	0.48
1:D:41:ARG:HB3	1:D:41:ARG:HH11	1.78	0.48
1:A:108:LEU:HD23	1:A:138:TYR:CG	2.48	0.48
1:C:44:GLY:O	1:C:46:TYR:N	2.30	0.48
1:B:198:MET:HG2	1:B:345:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ARG:HH11	1:C:189:ARG:HG3	1.79	0.47
1:C:102:LYS:NZ	4:C:520:HOH:O	2.45	0.47
1:C:15:ARG:HD2	1:C:26:THR:HG23	1.96	0.47
1:C:338:SER:OG	1:C:339:PRO:O	2.33	0.47
1:C:284:GLU:CB	1:C:311:ASN:OD1	2.63	0.47
1:A:201:GLU:HG2	4:A:518:HOH:O	2.14	0.47
1:D:73:GLU:CD	4:D:525:HOH:O	2.54	0.46
1:A:128:LYS:N	2:A:401:VO4:O2	2.45	0.46
1:A:185:HIS:CB	1:C:74:ARG:NH2	2.78	0.46
1:A:216:VAL:HG12	4:A:599:HOH:O	2.16	0.46
1:B:50:ILE:O	1:B:54:VAL:HG23	2.16	0.46
1:C:31:ASN:HA	1:C:119:VAL:HG22	1.95	0.46
1:A:191:VAL:C	4:A:519:HOH:O	2.54	0.46
1:A:284:GLU:CG	1:A:285:GLU:O	2.63	0.46
1:C:128:LYS:NZ	1:C:165:GLY:O	2.49	0.46
1:C:50:ILE:O	1:C:54:VAL:HG23	2.16	0.46
1:D:50:ILE:O	1:D:54:VAL:HG23	2.16	0.46
1:A:50:ILE:O	1:A:54:VAL:HG23	2.16	0.46
1:A:15:ARG:NH2	4:A:522:HOH:O	2.48	0.45
1:D:110:GLN:NE2	4:D:517:HOH:O	2.35	0.45
1:D:250:CYS:HB2	4:D:611:HOH:O	2.15	0.45
1:D:61:HIS:HA	4:D:553:HOH:O	2.17	0.45
1:D:192:ALA:HB2	4:D:611:HOH:O	2.14	0.45
1:C:46:TYR:CD2	4:C:504:HOH:O	2.69	0.45
1:D:166:VAL:N	4:D:506:HOH:O	2.22	0.45
1:A:75:HIS:CD2	4:A:524:HOH:O	2.71	0.44
1:C:42:LEU:HG	1:C:42:LEU:O	2.16	0.44
1:D:77:ASP:O	1:D:80:LYS:HB2	2.17	0.44
1:B:281:PRO:CB	1:B:283:PRO:HD3	2.42	0.44
1:C:313:LYS:HG2	1:C:315:TYR:CD2	2.53	0.44
1:B:24:ASP:OD2	1:B:47:ARG:HD3	2.18	0.44
1:A:210:THR:HG21	4:A:611:HOH:O	2.18	0.44
1:C:87:GLN:NE2	4:C:523:HOH:O	2.47	0.43
1:D:210:THR:CB	4:D:531:HOH:O	2.66	0.43
1:B:256:GLU:CG	4:B:530:HOH:O	2.66	0.43
1:D:198:MET:HG2	1:D:345:LEU:CD2	2.49	0.43
1:B:271:PHE:HB2	4:B:504:HOH:O	2.18	0.43
1:C:14:ARG:HA	1:C:161:ARG:HA	2.01	0.43
1:C:46:TYR:HB3	4:C:644:HOH:O	2.16	0.43
1:B:338:SER:OG	1:B:339:PRO:O	2.33	0.43
1:B:198:MET:HG2	1:B:345:LEU:CD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:ASN:OD1	1:D:229:SER:HB3	2.18	0.43
1:D:281:PRO:CB	1:D:282:GLY:O	2.67	0.43
1:D:73:GLU:HG2	1:D:74:ARG:HG3	2.00	0.43
1:D:128:LYS:HG2	4:D:535:HOH:O	2.19	0.43
1:D:193:LEU:HD11	1:D:280:ILE:HG13	1.98	0.43
1:B:35:MET:HG3	1:B:123:HIS:HB3	2.00	0.43
1:D:210:THR:HB	4:D:531:HOH:O	2.18	0.43
1:A:35:MET:HG3	1:A:123:HIS:HB3	2.01	0.43
1:A:281:PRO:CB	4:A:538:HOH:O	2.67	0.43
1:C:144:LYS:HD3	1:C:144:LYS:HA	1.57	0.42
1:B:138:TYR:O	1:B:141:HIS:HB3	2.19	0.42
1:A:143:GLY:HA3	4:A:527:HOH:O	2.19	0.42
1:D:339:PRO:O	1:D:340:ASN:CB	2.67	0.42
1:B:128:LYS:HE2	1:B:165:GLY:O	2.20	0.42
1:D:282:GLY:O	1:D:284:GLU:O	2.37	0.42
1:C:73:GLU:HG2	1:C:74:ARG:HG3	2.00	0.42
1:B:339:PRO:O	1:B:340:ASN:CB	2.67	0.42
1:D:313:LYS:CD	1:D:314:GLU:H	2.32	0.42
1:D:338:SER:OG	1:D:339:PRO:O	2.33	0.42
1:A:73:GLU:OE1	1:A:125:LYS:HE2	2.19	0.42
1:A:281:PRO:HG3	1:A:316:LEU:HD22	2.02	0.42
1:A:312:ASP:N	1:C:266:LYS:CB	2.75	0.42
1:D:256:GLU:CG	4:D:556:HOH:O	2.63	0.42
1:B:74:ARG:HA	1:B:74:ARG:HD2	1.84	0.42
1:A:233:ARG:NH1	4:A:526:HOH:O	2.51	0.42
1:D:64:HIS:CD2	4:D:507:HOH:O	2.73	0.41
1:A:330:LYS:NZ	4:A:514:HOH:O	2.37	0.41
1:C:138:TYR:O	1:C:141:HIS:HB3	2.19	0.41
1:D:138:TYR:O	1:D:141:HIS:HB3	2.19	0.41
1:C:216:VAL:HG13	1:C:223:LYS:HE2	2.02	0.41
1:D:128:LYS:HE2	1:D:165:GLY:O	2.20	0.41
1:C:35:MET:HG3	1:C:123:HIS:HB3	2.03	0.41
1:A:128:LYS:HD3	4:A:572:HOH:O	2.20	0.41
1:D:130:ARG:HB2	3:D:401:TLA:H3	2.01	0.41
1:D:147:LYS:HD2	4:D:603:HOH:O	2.20	0.41
1:B:43:GLU:OE1	1:B:74:ARG:NH2	2.54	0.41
1:D:161:ARG:HD2	4:D:631:HOH:O	2.20	0.41
1:A:219:GLN:HG2	1:A:220:LEU:HD12	2.03	0.41
1:D:280:ILE:HG23	1:D:281:PRO:HD2	2.03	0.41
1:C:322:LYS:HE3	1:C:337:PHE:HB2	2.02	0.41
1:C:258:PHE:HB3	1:C:267:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:HIS:CE1	4:A:524:HOH:O	2.73	0.41
1:B:43:GLU:OE1	1:B:74:ARG:CZ	2.68	0.41
1:A:138:TYR:O	1:A:141:HIS:HB3	2.20	0.41
1:A:285:GLU:HG2	1:A:317:VAL:CG2	2.52	0.40
1:B:46:TYR:CD1	1:B:46:TYR:O	2.75	0.40
1:A:14:ARG:HA	1:A:161:ARG:HA	2.03	0.40
1:A:273:PHE:CE1	1:A:345:LEU:HD21	2.57	0.40
1:C:313:LYS:HG3	1:C:314:GLU:N	2.37	0.40
1:A:338:SER:OG	1:A:339:PRO:O	2.33	0.40
1:D:41:ARG:CB	1:D:41:ARG:HH11	2.33	0.40
1:B:72:ALA:HA	1:B:89:PRO:HB2	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:GLU:CB	4:B:512:HOH:O[1_554]	1.92	0.28
1:C:150:GLU:OE2	1:C:161:ARG:NH1[3_556]	2.15	0.05
4:D:692:HOH:O	4:D:692:HOH:O[4_555]	2.19	0.01

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	312/314 (99%)	289 (93%)	22 (7%)	1 (0%)	46	68
1	B	312/314 (99%)	285 (91%)	26 (8%)	1 (0%)	46	68
1	C	312/314 (99%)	287 (92%)	22 (7%)	3 (1%)	19	34
1	D	312/314 (99%)	286 (92%)	26 (8%)	0	100	100
All	All	1248/1256 (99%)	1147 (92%)	96 (8%)	5 (0%)	39	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	PRO
1	C	45	VAL
1	C	284	GLU
1	B	22	ASP
1	C	281	PRO

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	274/286 (96%)	261 (95%)	13 (5%)	32	56
1	B	273/286 (96%)	263 (96%)	10 (4%)	41	68
1	C	274/286 (96%)	266 (97%)	8 (3%)	50	77
1	D	272/286 (95%)	266 (98%)	6 (2%)	60	84
All	All	1093/1144 (96%)	1056 (97%)	37 (3%)	44	72

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	TYR
1	A	41	ARG
1	A	47	ARG
1	A	49	ASN
1	A	83	CYS
1	A	146	LEU
1	A	221	LYS
1	A	262	ASN
1	A	263	LYS
1	A	264	MET
1	A	265	LEU
1	A	285	GLU
1	A	313	LYS
1	B	15	ARG
1	B	16	TYR
1	B	21	PHE
1	B	42	LEU

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Mol	Chain	Res	Type
1	B	46	TYR
1	B	74	ARG
1	B	263	LYS
1	B	281	PRO
1	B	284	GLU
1	B	310	ASP
1	C	15	ARG
1	C	16	TYR
1	C	41	ARG
1	C	42	LEU
1	C	45	VAL
1	C	189	ARG
1	C	237	LYS
1	C	263	LYS
1	D	16	TYR
1	D	41	ARG
1	D	43	GLU
1	D	108	LEU
1	D	284	GLU
1	D	313	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	D	272	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 carbohydrates 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	VO4	A	401	-	1,4,4	4.29	1 (100%)	0,6,6	0.00	-
3	TLA	B	401	-	3,9,9	0.72	0	6,12,12	0.76	0
3	TLA	C	401	2	3,9,9	0.70	0	6,12,12	1.21	1 (16%)
2	VO4	C	402	3	1,4,4	4.50	1 (100%)	0,6,6	0.00	-
3	TLA	D	401	-	3,9,9	0.48	0	6,12,12	1.36	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VO4	A	401	-	-	0/0/0/0	0/0/0/0
3	TLA	B	401	-	-	0/4/12/12	0/0/0/0
3	TLA	C	401	2	-	0/4/12/12	0/0/0/0
2	VO4	C	402	3	-	0/0/0/0	0/0/0/0
3	TLA	D	401	-	-	0/4/12/12	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	VO4	O1-V	4.29	1.90	1.63
2	C	402	VO4	O1-V	4.50	1.91	1.63

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	TLA	C1-C2-C3	-2.93	107.33	113.35
3	C	401	TLA	C4-C3-C2	2.11	117.68	113.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	VO4	2	0
3	B	401	TLA	6	0
3	C	401	TLA	2	0
2	C	402	VO4	1	0
3	D	401	TLA	5	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

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	314/314 (100%)	0.05	10 (3%) 51 56	38, 57, 108, 135	0
1	B	314/314 (100%)	0.04	13 (4%) 41 46	39, 57, 103, 137	2 (0%)
1	C	314/314 (100%)	0.03	10 (3%) 51 56	38, 55, 105, 133	0
1	D	314/314 (100%)	-0.01	10 (3%) 51 56	36, 56, 105, 144	1 (0%)
All	All	1256/1256 (100%)	0.03	43 (3%) 49 54	36, 56, 106, 144	3 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	44	GLY	10.9
1	B	283	PRO	8.6
1	A	45	VAL	7.9
1	C	265	LEU	7.2
1	B	14	ARG	6.2
1	C	282	GLY	5.7
1	C	264	MET	5.2
1	B	45	VAL	4.7
1	B	282	GLY	4.7
1	D	283	PRO	4.5
1	D	285	GLU	4.5
1	A	44	GLY	4.1
1	B	265	LEU	3.9
1	A	282	GLY	3.9
1	C	283	PRO	3.7
1	C	310	ASP	3.7
1	D	264	MET	3.5
1	A	311	ASN	3.5
1	D	311	ASN	3.4
1	D	351	VAL	3.4
1	A	265	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	310	ASP	3.3
1	B	312	ASP	3.2
1	A	46	TYR	3.2
1	A	312	ASP	3.1
1	B	264	MET	3.1
1	D	43	GLU	3.1
1	B	263	LYS	3.0
1	D	310	ASP	2.9
1	C	40	GLU	2.9
1	D	282	GLY	2.8
1	B	310	ASP	2.7
1	A	283	PRO	2.7
1	C	261	GLN	2.5
1	B	81	PHE	2.5
1	B	311	ASN	2.5
1	C	46	TYR	2.4
1	B	262	ASN	2.3
1	C	45	VAL	2.2
1	D	44	GLY	2.2
1	A	43	GLU	2.2
1	D	260	LYS	2.0
1	B	266	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	VO4	C	402	5/5	0.96	0.27	3.77	65,65,65,68	5
3	TLA	C	401	10/10	0.95	0.23	2.78	56,63,64,69	10
2	VO4	A	401	5/5	0.96	0.14	-0.58	70,77,88,90	5
3	TLA	B	401	10/10	0.95	0.11	-1.40	41,48,56,59	0
3	TLA	D	401	10/10	0.96	0.10	-2.49	37,42,45,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.