



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:27 PM UTC

PDB ID : 4ADD / pdb_00004add
Title : Structural and functional study of succinyl-ornithine transaminase from E. coli
Authors : Newman, J.; Peat, T.S.
Deposited on : 2011-12-23
Resolution : 2.45 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

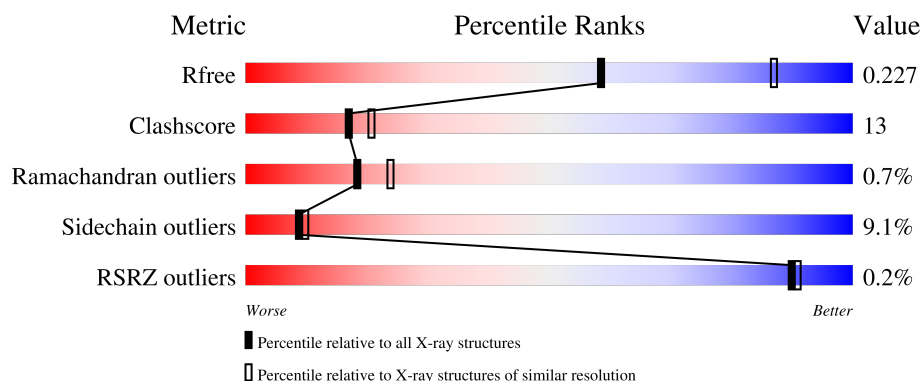
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	406	 67% 27% 5% 1% 2%
1	B	406	 72% 21% 5% 2% 2%
1	C	406	 70% 23% 3% 1% 2%
1	D	406	 69% 24% 5% 2% 2%

2 Entry composition [i](#)

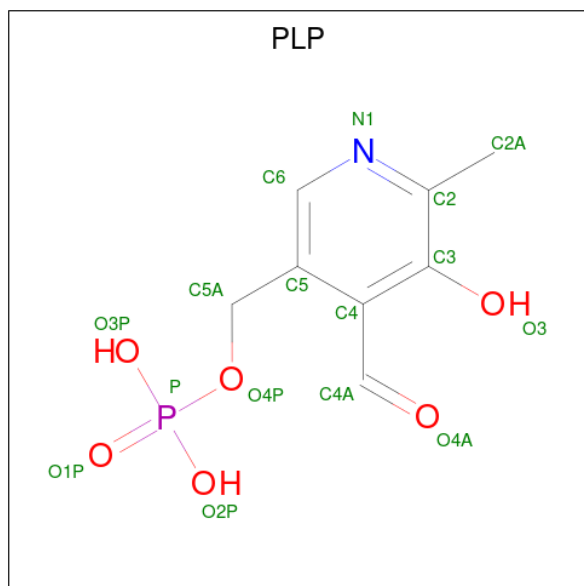
There are 4 unique types of molecules in this entry. The entry contains 12731 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SUCCINYLORNITHINE TRANSAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	5	0
			3074	1945	547	571	11			
1	B	400	Total	C	N	O	S	0	5	0
			3076	1947	546	572	11			
1	C	400	Total	C	N	O	S	0	4	0
			3064	1940	540	573	11			
1	D	400	Total	C	N	O	S	0	6	0
			3073	1947	544	571	11			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



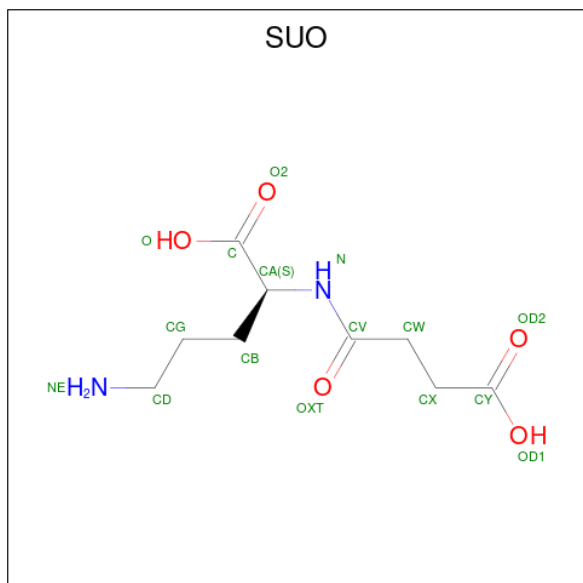
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is N 2 -(3-CARBOXYPROPANOYL)-L-ORNITHINE (CCD ID: SUO) (formula: $C_9H_{16}N_2O_5$).



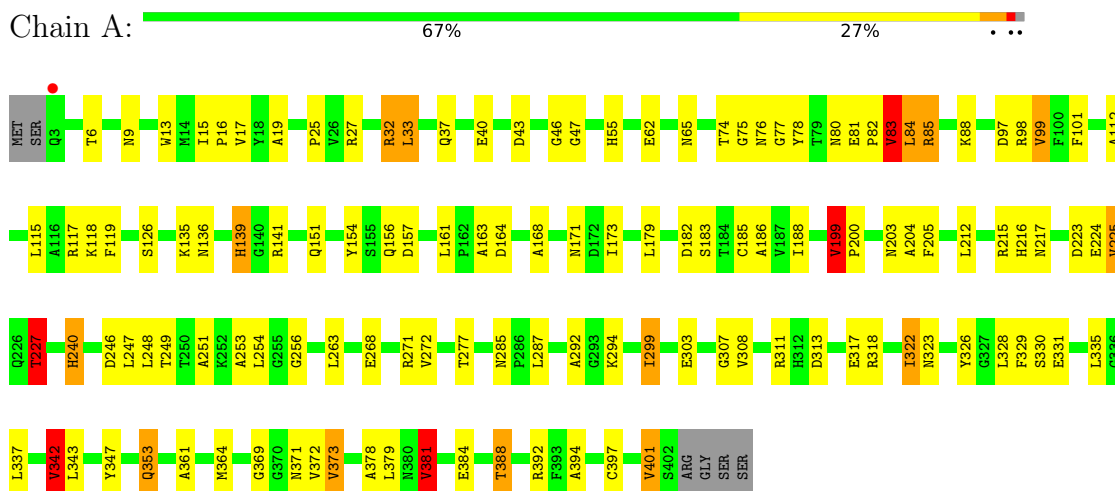
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	50	Total	O	0	0
			50	50		

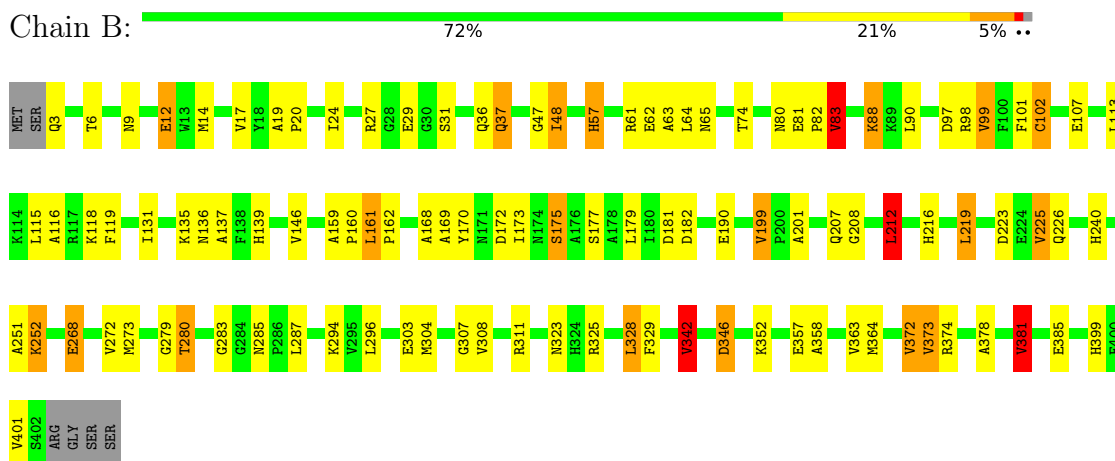
3 Residue-property plots

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: SUCCINYLORNITHINE TRANSAMINASE



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V365	T250	K128	MET
L366	A251	A137	SER
V371	K252	F138	Q3
V372	A253	H139	P4
V373	L254	G140	T5
R374	L263	R141	T6
A378	L264	P152	N9
V381	A265	A153	V13
L390	T266	V154	M14
E398	E267	S155	V17
H399	A270	Q156	Y18
F400	R271	A159	A19
V401	V272	P160	P20
S402	T280	L161	R27
ARG	L287	D164	R32
GLY	A292	A169	L33
SER	G293	Y170	Y41
SER	L296	N171	G47
	I299	D172	I48
	E303	S183	L53
	G307	P191	R61
	R311	I192	L64
	R318	E195	N65
	L319	V199	Y78
	N320	P200	E81
	L321	A201	P82
	L322	G208	V83
	N323	L212	L84
	Y326	L216	R85
	G327	H216	L86
	L328	L220	A87
	F329	D223	K88
	S330	E224	K89
	E331	V225	L90
	L335	T227	I91
	V342	G230	D97
	A348	E234	R98
	K352	D246	V99
	Q353	L248	S104
	Q356	T249	E107
	E357		K118
	M364		D122

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.94Å 118.26Å 109.24Å 90.00° 96.82° 90.00°	Depositor
Resolution (Å)	108.46 – 2.45 108.46 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (108.46-2.45) 99.8 (108.46-2.45)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.44Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.170 , 0.225 0.172 , 0.227	Depositor DCC
R_{free} test set	4254 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.8	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	0.95	EDS
Total number of atoms	12731	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: PLP, SUO

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	1.35	6/3153 (0.2%)	1.42	32/4282 (0.7%)
1	B	1.34	8/3158 (0.3%)	1.40	20/4288 (0.5%)
1	C	1.23	7/3145 (0.2%)	1.29	30/4271 (0.7%)
1	D	1.17	2/3162 (0.1%)	1.25	11/4295 (0.3%)
All	All	1.28	23/12618 (0.2%)	1.34	93/17136 (0.5%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	137	ALA	C-O	7.47	1.32	1.23
1	A	381	VAL	C-O	6.84	1.30	1.24
1	A	139	HIS	ND1-CE1	6.54	1.39	1.32
1	B	37	GLN	CA-C	-6.37	1.44	1.52
1	A	240	HIS	CG-CD2	5.97	1.42	1.35
1	C	223	ASP	CA-C	5.88	1.60	1.52
1	B	240	HIS	CG-CD2	5.80	1.42	1.35
1	B	219	LEU	C-O	5.65	1.30	1.24
1	A	292	ALA	CA-C	-5.58	1.45	1.52
1	A	55	HIS	CG-CD2	5.55	1.42	1.35
1	B	57	HIS	ND1-CE1	5.50	1.38	1.32
1	C	240	HIS	CG-CD2	5.50	1.41	1.35
1	C	139	HIS	CG-CD2	5.43	1.41	1.35
1	C	399	HIS	CG-CD2	5.43	1.41	1.35
1	C	386	VAL	C-O	5.33	1.30	1.24
1	B	399	HIS	CG-CD2	5.18	1.41	1.35
1	C	221	ILE	CA-C	5.15	1.59	1.52
1	D	20	PRO	CA-C	-5.08	1.46	1.52
1	D	199	VAL	CA-CB	5.07	1.59	1.53
1	B	190	GLU	C-O	-5.06	1.17	1.24
1	B	102	CYS	C-O	-5.05	1.17	1.24
1	A	84	LEU	CA-C	5.03	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	34	TRP	NE1-CE2	-5.03	1.31	1.37

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	ALA	CA-C-N	-12.33	104.43	119.84
1	B	19	ALA	C-N-CA	-12.33	104.43	119.84
1	B	83	VAL	CB-CA-C	-9.59	99.61	111.88
1	B	381	VAL	CB-CA-C	-8.72	96.98	111.29
1	A	83	VAL	CB-CA-C	-8.70	100.40	112.14
1	C	81	GLU	CA-C-N	-8.35	109.40	119.84
1	C	81	GLU	C-N-CA	-8.35	109.40	119.84
1	B	161	LEU	CA-C-N	-7.87	111.87	119.90
1	B	161	LEU	C-N-CA	-7.87	111.87	119.90
1	D	381	VAL	CB-CA-C	-7.80	98.61	111.32
1	C	5	ILE	N-CA-C	7.79	119.70	108.48
1	A	369	GLY	N-CA-C	-7.63	101.52	112.81
1	C	381	VAL	CB-CA-C	-7.59	98.84	111.29
1	C	74	THR	N-CA-C	-7.59	105.97	114.62
1	A	75	GLY	N-CA-C	-7.56	103.18	112.33
1	C	15	ILE	CA-C-N	7.56	129.29	119.84
1	C	15	ILE	C-N-CA	7.56	129.29	119.84
1	C	83	VAL	CB-CA-C	-7.50	100.54	112.16
1	A	372	VAL	CA-C-N	-7.48	113.51	122.93
1	A	372	VAL	C-N-CA	-7.48	113.51	122.93
1	A	373	VAL	N-CA-CB	7.47	119.95	110.99
1	B	83	VAL	N-CA-CB	7.44	118.77	110.51
1	B	357	GLU	N-CA-C	-7.29	103.05	112.23
1	A	19	ALA	CA-C-N	-7.27	113.19	120.31
1	A	19	ALA	C-N-CA	-7.27	113.19	120.31
1	A	161	LEU	CA-C-N	-7.21	112.33	119.76
1	A	161	LEU	C-N-CA	-7.21	112.33	119.76
1	A	227	THR	N-CA-CB	-7.10	99.58	110.44
1	C	122	ASP	N-CA-C	7.06	119.06	111.36
1	D	122	ASP	N-CA-C	7.06	118.76	111.14
1	A	156	GLN	N-CA-C	7.03	119.83	111.33
1	A	76	ASN	N-CA-C	7.02	121.69	113.20
1	C	373	VAL	N-CA-CB	6.76	118.09	110.72
1	A	62	GLU	N-CA-C	-6.74	103.40	111.69
1	A	285	ASN	CA-C-N	-6.72	112.78	119.56
1	A	285	ASN	C-N-CA	-6.72	112.78	119.56
1	A	215	ARG	N-CA-C	-6.63	104.13	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	76	ASN	N-CA-C	6.62	121.21	113.20
1	B	199	VAL	CB-CA-C	6.55	118.72	111.18
1	C	221	ILE	N-CA-C	6.53	117.53	107.99
1	B	24	ILE	N-CA-C	6.51	114.57	107.60
1	D	371	ASN	N-CA-C	6.50	121.21	113.28
1	B	373	VAL	N-CA-CB	6.49	117.79	110.72
1	D	83	VAL	CB-CA-C	-6.47	102.14	112.16
1	A	15	ILE	CA-C-N	6.40	127.84	119.84
1	A	15	ILE	C-N-CA	6.40	127.84	119.84
1	C	127	HIS	N-CA-C	-6.33	105.39	113.23
1	C	199	VAL	N-CA-C	6.28	113.27	107.56
1	C	205	PHE	N-CA-C	-6.26	103.77	111.40
1	B	212	LEU	CA-CB-CG	6.25	138.19	116.30
1	C	240	HIS	N-CA-C	-6.23	104.41	111.14
1	B	342	VAL	CB-CA-C	6.20	118.59	110.91
1	C	369	GLY	N-CA-C	-6.14	104.94	112.68
1	A	381	VAL	CB-CA-C	-6.13	102.02	111.71
1	C	362	GLY	CA-C-N	-6.01	114.64	122.99
1	C	362	GLY	C-N-CA	-6.01	114.64	122.99
1	D	14	MET	CG-SD-CE	-5.98	87.74	100.90
1	B	36	GLN	CA-C-N	-5.90	113.28	122.67
1	B	36	GLN	C-N-CA	-5.90	113.28	122.67
1	A	83	VAL	N-CA-CB	5.90	118.56	110.54
1	C	390	LEU	N-CA-C	5.78	118.53	111.82
1	C	83	VAL	N-CA-CB	5.74	120.46	110.65
1	A	186	ALA	N-CA-C	5.71	118.77	109.06
1	C	373	VAL	CB-CA-C	5.65	117.92	110.91
1	A	326	TYR	N-CA-C	5.63	120.30	113.38
1	A	299	ILE	CG1-CB-CG2	-5.59	93.92	110.70
1	A	199	VAL	CA-C-N	5.58	126.01	119.99
1	A	199	VAL	C-N-CA	5.58	126.01	119.99
1	A	82	PRO	CA-C-N	-5.52	112.90	120.46
1	A	82	PRO	C-N-CA	-5.52	112.90	120.46
1	A	246	ASP	N-CA-C	-5.48	104.83	112.45
1	D	357	GLU	N-CA-C	-5.47	104.84	112.45
1	B	372	VAL	CA-C-N	-5.43	115.36	122.37
1	B	372	VAL	C-N-CA	-5.43	115.36	122.37
1	A	342	VAL	CB-CA-C	5.33	118.07	111.15
1	C	272	VAL	CB-CA-C	-5.32	103.91	112.16
1	D	322	ILE	N-CA-C	5.28	116.01	110.62
1	B	285	ASN	CA-C-N	-5.28	114.31	119.64
1	B	285	ASN	C-N-CA	-5.28	114.31	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	291	VAL	N-CA-C	5.28	115.38	110.42
1	A	204	ALA	N-CA-C	-5.22	106.42	112.89
1	C	24	ILE	CA-C-N	-5.21	114.41	119.78
1	C	24	ILE	C-N-CA	-5.21	114.41	119.78
1	A	163	ALA	N-CA-C	5.16	117.19	110.53
1	D	199	VAL	CA-C-N	5.16	124.92	119.76
1	D	199	VAL	C-N-CA	5.16	124.92	119.76
1	D	272	VAL	N-CA-C	5.13	117.51	111.09
1	C	386	VAL	N-CA-C	5.12	115.34	110.42
1	C	21	ALA	CA-C-N	5.12	124.73	119.56
1	C	21	ALA	C-N-CA	5.12	124.73	119.56
1	C	74	THR	CB-CA-C	-5.04	102.58	109.28
1	B	373	VAL	CB-CA-C	5.03	117.15	110.91
1	D	83	VAL	N-CA-CB	5.00	119.20	110.65

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3074	0	3002	97	0
1	B	3076	0	3009	73	0
1	C	3064	0	2996	81	0
1	D	3073	0	3004	87	0
2	A	15	0	7	0	0
2	B	15	0	6	0	0
2	C	15	0	6	2	0
2	D	15	0	7	0	0
3	A	16	0	13	1	0
3	B	16	0	12	3	0
3	C	16	0	12	1	0
3	D	16	0	12	3	0
4	A	118	0	0	5	0
4	B	79	0	0	3	0
4	C	73	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	50	0	0	5	0
All	All	12731	0	12086	312	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 13.

All (312) 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:C:325:ARG:HH11	1:C:325:ARG:HG3	0.98	1.11
1:D:271[B]:ARG:HH11	1:D:271[B]:ARG:CG	1.65	1.10
1:D:271[B]:ARG:HG2	1:D:271[B]:ARG:NH1	1.65	1.05
1:D:353:GLN:H	1:D:353:GLN:HE21	1.05	1.03
1:D:271[B]:ARG:HH11	1:D:271[B]:ARG:HG2	0.82	0.98
1:C:325:ARG:HG3	1:C:325:ARG:NH1	1.62	0.95
1:C:325:ARG:HH11	1:C:325:ARG:CG	1.79	0.94
1:A:271[A]:ARG:HD2	1:C:271[A]:ARG:HD3	1.48	0.93
1:A:271[A]:ARG:HD2	1:C:271[A]:ARG:CD	2.01	0.91
1:B:182:ASP:OD1	1:B:216:HIS:HD2	1.56	0.88
1:B:323:ASN:ND2	1:B:328:LEU:H	1.72	0.88
1:D:323:ASN:HD21	1:D:329:PHE:H	1.23	0.85
1:B:378:ALA:O	1:B:381:VAL:HG22	1.77	0.84
1:C:304:MET:HE1	1:C:380:ASN:HB3	1.60	0.82
1:A:25:PRO:HB3	1:A:33:LEU:HD11	1.61	0.82
1:D:64:LEU:HD12	1:D:287:LEU:CD2	2.11	0.81
1:D:348:ALA:HB1	1:D:371:ASN:HD21	1.45	0.81
1:D:252:LYS:HZ1	3:D:411:SUA:HD2	1.43	0.80
1:A:323:ASN:HD21	1:A:329:PHE:H	1.31	0.78
1:A:84:LEU:HD23	1:B:14:MET:HE3	1.66	0.78
1:D:353:GLN:HE21	1:D:353:GLN:N	1.82	0.78
3:D:411:SUA:HD1A	4:D:2036:HOH:O	1.84	0.76
1:C:323:ASN:HD21	1:C:329:PHE:H	1.34	0.76
1:D:252:LYS:NZ	3:D:411:SUA:HD2	2.00	0.76
1:B:80:ASN:OD1	1:B:83:VAL:HG22	1.86	0.76
1:A:84:LEU:HD23	1:B:14:MET:CE	2.19	0.73
1:D:3:GLN:N	1:D:4:PRO:HD3	2.04	0.73
1:A:25:PRO:HB3	1:A:33:LEU:CD1	2.19	0.72
1:C:139:HIS:HD2	1:C:223:ASP:OD2	1.73	0.72
1:C:401:VAL:O	1:C:402:SER:OG	2.06	0.72
1:A:343:LEU:O	4:A:2105:HOH:O	2.07	0.71
1:A:157:ASP:HB3	1:B:118:LYS:HG3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:HIS:HD2	1:B:223:ASP:OD2	1.74	0.71
1:B:323:ASN:HD21	1:B:328:LEU:H	1.38	0.70
1:B:64:LEU:HD12	1:B:287:LEU:HD22	1.74	0.69
1:A:318:ARG:O	1:A:322:ILE:HG13	1.93	0.69
1:A:6:THR:H	1:A:9:ASN:HD22	1.41	0.68
1:C:302:PRO:O	1:C:306:ASN:HB2	1.93	0.68
1:A:43:ASP:HA	1:A:364:MET:HE3	1.76	0.68
1:D:191:PRO:HG2	1:D:227:THR:HG21	1.76	0.68
3:A:411:SUA:HD1A	4:A:2087:HOH:O	1.94	0.67
1:C:121:HIS:HE1	1:C:129:SER:OG	1.77	0.67
1:A:139:HIS:HD2	1:A:223:ASP:OD2	1.76	0.67
1:D:271[B]:ARG:CG	1:D:271[B]:ARG:NH1	2.35	0.67
1:C:225:VAL:HB	1:C:251:ALA:HB3	1.78	0.66
1:B:80:ASN:CG	1:B:83:VAL:HG22	2.21	0.66
1:A:271[A]:ARG:CD	1:C:271[A]:ARG:CD	2.73	0.66
1:D:64:LEU:HD12	1:D:287:LEU:HD22	1.78	0.65
1:D:18:TYR:HB2	1:D:20:PRO:HD3	1.80	0.64
1:D:159:ALA:HB1	1:D:160:PRO:HA	1.80	0.64
1:A:322:ILE:HD13	1:A:394:ALA:HB2	1.80	0.64
1:A:388:THR:O	1:A:392:ARG:HG3	1.98	0.64
1:B:116:ALA:HA	1:B:219:LEU:HD12	1.79	0.64
1:A:32:ARG:NH2	1:A:384:GLU:OE1	2.29	0.64
1:A:168:ALA:HB2	1:A:179:LEU:HD12	1.80	0.64
1:C:121:HIS:CE1	1:C:129:SER:OG	2.51	0.64
1:B:29:GLU:HG2	4:B:2004:HOH:O	1.98	0.63
1:B:225:VAL:HG23	1:B:252:LYS:HD2	1.80	0.63
1:D:220:LEU:N	1:D:246:ASP:OD1	2.18	0.63
1:C:115:LEU:C	1:C:115:LEU:HD23	2.25	0.62
1:A:139:HIS:HE1	4:A:2066:HOH:O	1.82	0.61
1:A:384:GLU:OE2	1:A:388:THR:HG21	2.00	0.61
1:B:252:LYS:HZ3	3:B:411:SUA:CD	2.13	0.61
1:D:224:GLU:OE1	1:D:227:THR:HG23	2.00	0.61
1:D:3:GLN:N	1:D:4:PRO:CD	2.64	0.60
1:B:113:LEU:HD22	1:B:131:ILE:HD13	1.83	0.60
1:C:74:THR:O	1:D:47:GLY:HA2	2.02	0.60
1:B:48:ILE:O	1:B:252:LYS:HE3	2.02	0.60
1:A:85:ARG:NH2	1:B:3:GLN:O	2.32	0.59
1:C:157:ASP:HB3	1:D:118:LYS:HG2	1.84	0.59
1:D:366:LEU:HB2	1:D:374:ARG:HB3	1.83	0.59
1:A:271[A]:ARG:HD2	1:C:271[A]:ARG:HD2	1.83	0.59
1:C:177:SER:HA	1:C:212:LEU:HD21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LYS:HZ3	3:B:411:SUA:HD2	1.67	0.59
1:A:47:GLY:HA2	1:B:74:THR:O	2.03	0.59
1:B:223:ASP:OD1	1:B:225:VAL:HG13	2.04	0.58
1:C:18:TYR:C	1:C:20:PRO:HD3	2.28	0.58
1:A:84:LEU:CD2	1:B:14:MET:HE3	2.34	0.58
1:C:378:ALA:O	1:C:381:VAL:HG22	2.03	0.58
1:A:6:THR:H	1:A:9:ASN:ND2	2.00	0.58
1:D:224:GLU:OE1	1:D:227:THR:CG2	2.52	0.58
1:C:133:ALA:O	1:C:167:HIS:HA	2.04	0.57
1:D:323:ASN:HD21	1:D:329:PHE:N	2.00	0.57
1:B:323:ASN:HD21	1:B:328:LEU:N	2.02	0.57
1:C:279:GLY:H	1:D:141:ARG:HG3	1.68	0.57
1:A:97:ASP:C	1:A:98:ARG:HG2	2.29	0.57
1:A:248:LEU:C	1:A:248:LEU:HD23	2.30	0.57
1:D:18:TYR:C	1:D:20:PRO:HD3	2.30	0.57
1:B:280:THR:HG21	1:B:283:GLY:HA3	1.86	0.57
1:C:6:THR:H	1:C:9:ASN:ND2	2.03	0.57
1:B:97:ASP:C	1:B:98:ARG:HG2	2.30	0.56
1:C:90:LEU:HG	1:C:264:LEU:HD11	1.87	0.56
1:D:248:LEU:HD22	1:D:264:LEU:HD22	1.88	0.56
1:A:99:VAL:HG21	1:A:101:PHE:CZ	2.41	0.56
1:D:64:LEU:CD1	1:D:287:LEU:HD22	2.35	0.56
1:A:65[A]:ASN:OD1	1:B:65:ASN:HB2	2.06	0.56
1:D:182:ASP:OD1	1:D:216:HIS:HD2	1.89	0.55
1:B:252:LYS:NZ	3:B:411:SUA:HD2	2.21	0.55
1:C:80:ASN:OD1	1:C:83:VAL:HG22	2.06	0.55
1:C:331:GLU:HG3	4:C:2068:HOH:O	2.06	0.55
1:C:177:SER:HA	1:C:212:LEU:CD2	2.37	0.54
1:D:6:THR:H	1:D:9:ASN:ND2	2.05	0.54
1:D:247:LEU:HD22	1:D:263:LEU:HD11	1.89	0.54
1:C:83:VAL:CG1	1:C:284:GLY:HA2	2.37	0.54
1:A:80:ASN:CG	1:A:83:VAL:HG22	2.33	0.54
1:A:118:LYS:HE3	1:A:277:THR:HG21	1.90	0.54
1:C:180:ILE:HD13	1:C:187:VAL:HG21	1.90	0.54
1:B:280:THR:CG2	1:B:283:GLY:HA3	2.38	0.54
1:A:271[A]:ARG:CD	1:C:271[A]:ARG:HD2	2.37	0.54
1:D:155:SER:HB2	1:D:161:LEU:HD11	1.90	0.54
1:A:224:GLU:OE1	1:A:227:THR:CG2	2.57	0.53
1:A:268:GLU:CD	1:A:268:GLU:H	2.16	0.53
1:A:313:ASP:O	1:A:317:GLU:HB2	2.09	0.53
1:A:74:THR:O	1:B:47:GLY:HA2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:O	1:B:162:PRO:C	2.49	0.53
1:D:48:ILE:O	1:D:252:LYS:HD3	2.08	0.53
1:D:307:GLY:O	1:D:311:ARG:HD2	2.08	0.53
1:A:353:GLN:H	1:A:353:GLN:HE21	1.57	0.53
1:D:91:ILE:O	4:D:2020:HOH:O	2.18	0.53
1:C:350:GLN:HE21	1:C:353:GLN:NE2	2.07	0.53
1:C:352:LYS:O	1:C:356:GLN:HG2	2.08	0.53
1:D:18:TYR:CB	1:D:20:PRO:HD3	2.38	0.53
1:C:115:LEU:HD23	1:C:115:LEU:O	2.10	0.52
1:C:252:LYS:HZ3	2:C:410:PLP:C4A	2.23	0.52
1:B:323:ASN:HD21	1:B:329:PHE:H	1.57	0.52
1:A:401:VAL:O	1:A:401:VAL:CG1	2.58	0.52
1:C:323:ASN:ND2	1:C:329:PHE:H	2.03	0.52
1:D:86:LEU:CD2	1:D:292:ALA:HB3	2.40	0.52
1:A:135:LYS:O	1:A:136:ASN:HB2	2.10	0.52
1:D:89:LYS:HE2	1:D:293:GLY:O	2.08	0.52
1:A:307:GLY:O	1:A:311:ARG:HD2	2.10	0.52
1:A:126:SER:HB3	4:A:2064:HOH:O	2.10	0.52
1:C:225:VAL:HG23	1:C:252:LYS:HD2	1.92	0.51
1:A:77:GLY:C	1:B:20:PRO:HB3	2.36	0.51
1:C:41:TYR:CD1	1:C:41:TYR:N	2.78	0.51
1:B:226:GLN:OE1	1:B:374:ARG:NH1	2.43	0.51
1:D:64:LEU:CD1	1:D:287:LEU:CD2	2.83	0.51
1:A:16:PRO:HG2	1:B:273:MET:O	2.11	0.51
1:A:353:GLN:HE21	1:A:353:GLN:N	2.08	0.51
1:C:170:TYR:OH	1:C:201:ALA:HB2	2.10	0.51
1:A:384:GLU:O	1:A:388:THR:HG23	2.11	0.51
1:A:224:GLU:OE1	1:A:227:THR:HG22	2.11	0.51
1:A:97:ASP:O	1:A:98:ARG:HG2	2.11	0.50
4:B:2071:HOH:O	1:C:183:SER:HB3	2.11	0.50
1:B:57:HIS:O	1:B:61:ARG:HG3	2.11	0.50
1:D:64:LEU:HD12	1:D:287:LEU:HD21	1.93	0.50
1:D:90:LEU:HD13	1:D:296:LEU:HD11	1.93	0.50
1:B:168:ALA:HB2	1:B:179:LEU:HD12	1.92	0.50
1:D:173:ILE:HD13	1:D:208:GLY:HA3	1.92	0.50
1:A:46:GLY:HA2	4:A:2018:HOH:O	2.10	0.50
1:C:80:ASN:CG	1:C:83:VAL:HG22	2.36	0.50
1:B:115:LEU:HD23	1:B:115:LEU:O	2.12	0.50
1:A:247:LEU:HD22	1:A:263:LEU:HD11	1.93	0.49
1:B:6:THR:H	1:B:9:ASN:ND2	2.09	0.49
1:B:182:ASP:OD1	1:B:216:HIS:CD2	2.49	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ILE:HD12	1:C:212:LEU:HD22	1.93	0.49
1:C:208:GLY:O	1:C:212:LEU:HD12	2.11	0.49
1:B:346:ASP:OD1	1:B:346:ASP:N	2.42	0.49
1:A:223:ASP:OD1	1:A:225:VAL:HG13	2.12	0.49
1:A:225:VAL:HB	1:A:251:ALA:HB3	1.93	0.49
1:C:112:ALA:HB2	1:C:263:LEU:HD13	1.94	0.49
1:C:248:LEU:HD22	1:C:264:LEU:HD22	1.94	0.49
1:B:169:ALA:H	1:B:175:SER:HB3	1.76	0.49
1:A:384:GLU:OE2	1:A:388:THR:CG2	2.60	0.49
1:B:99:VAL:HG21	1:B:101:PHE:CZ	2.48	0.49
1:C:295:VAL:HG13	1:C:299:ILE:HD12	1.93	0.49
1:A:77:GLY:O	1:B:20:PRO:HB3	2.13	0.49
1:B:6:THR:O	1:B:9:ASN:HB2	2.13	0.49
1:B:358:ALA:HB1	1:B:363:VAL:HG13	1.94	0.49
1:C:18:TYR:O	1:C:20:PRO:HD3	2.12	0.49
1:D:137:ALA:HB1	1:D:139:HIS:CE1	2.48	0.49
1:A:13:TRP:CE2	1:B:88:LYS:HD3	2.48	0.49
1:C:352:LYS:O	1:C:355:SER:HB3	2.14	0.48
1:B:170:TYR:OH	1:B:201:ALA:HB2	2.13	0.48
1:C:27:ARG:O	1:C:33:LEU:HD12	2.13	0.48
1:C:68:ALA:O	1:D:61:ARG:HD2	2.14	0.48
1:D:169:ALA:HB3	1:D:172:ASP:HB3	1.94	0.48
1:D:225:VAL:O	1:D:252:LYS:HB2	2.13	0.48
1:A:78:TYR:CZ	1:B:364:MET:HE3	2.48	0.48
1:A:364:MET:HE3	1:A:364:MET:HB2	1.65	0.48
1:A:80:ASN:OD1	1:A:83:VAL:HG22	2.14	0.47
1:B:268[B]:GLU:CD	1:B:268[B]:GLU:H	2.22	0.47
1:D:170:TYR:OH	1:D:201:ALA:HB2	2.14	0.47
1:B:31:SER:HB2	1:B:385:GLU:CD	2.39	0.47
1:D:32:ARG:HD3	4:D:2007:HOH:O	2.14	0.47
1:A:240:HIS:CD2	1:A:335:LEU:HD21	2.51	0.47
1:D:139:HIS:HD2	1:D:223:ASP:OD2	1.97	0.46
1:C:117:ARG:NH1	4:C:2044:HOH:O	2.34	0.46
1:A:343:LEU:HD23	1:A:343:LEU:HA	1.77	0.46
1:B:63:ALA:HB2	1:B:294:LYS:HG3	1.98	0.46
1:C:384:GLU:OE2	1:C:388:THR:OG1	2.29	0.46
1:A:401:VAL:O	1:A:401:VAL:HG13	2.15	0.46
1:B:102:CYS:HB2	1:B:107:GLU:OE1	2.16	0.46
1:C:83:VAL:HG11	1:C:284:GLY:HA2	1.98	0.46
1:A:119:PHE:HD2	1:A:272:VAL:HG21	1.80	0.46
1:B:223:ASP:OD1	1:B:223:ASP:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:GLU:OE2	3:C:411:SUA:HD1A	2.16	0.46
1:D:352:LYS:O	1:D:356:GLN:HG3	2.16	0.46
1:D:378:ALA:O	1:D:381:VAL:HG22	2.14	0.46
1:A:99:VAL:CG2	1:A:101:PHE:CZ	2.98	0.46
1:B:139:HIS:HE1	4:B:2045:HOH:O	1.98	0.46
1:B:296:LEU:HD23	1:B:296:LEU:HA	1.74	0.46
1:C:223:ASP:OD1	1:C:223:ASP:C	2.59	0.46
1:D:318:ARG:HG2	1:D:318:ARG:HH11	1.80	0.46
1:A:323:ASN:ND2	1:A:329:PHE:H	2.08	0.46
1:A:117:ARG:HG2	1:A:185:CYS:SG	2.55	0.46
1:C:181:ASP:HB2	4:C:2052:HOH:O	2.15	0.46
1:D:89:LYS:HD3	1:D:296:LEU:HD12	1.98	0.45
1:C:76:ASN:O	1:D:20:PRO:HG3	2.17	0.45
1:D:326:TYR:OH	1:D:398:GLU:OE1	2.32	0.45
1:C:223:ASP:OD1	1:C:225:VAL:HG13	2.16	0.45
1:D:86:LEU:HD22	1:D:292:ALA:HB3	1.98	0.45
1:A:199:VAL:HA	1:A:200:PRO:HD3	1.58	0.45
1:C:139:HIS:CD2	1:C:223:ASP:OD2	2.62	0.45
1:D:104:SER:OG	1:D:107:GLU:HG3	2.17	0.45
1:D:128:LYS:HG3	1:D:183:SER:HA	1.98	0.45
1:C:83:VAL:HG13	1:C:289:SER:OG	2.16	0.45
1:C:116:ALA:HA	1:C:219:LEU:HD12	1.98	0.45
1:C:323:ASN:ND2	1:C:328:LEU:H	2.13	0.45
1:D:248:LEU:C	1:D:248:LEU:HD23	2.42	0.45
1:A:188:ILE:O	1:A:188:ILE:HG23	2.17	0.45
1:D:251:ALA:O	1:D:252:LYS:C	2.60	0.45
1:B:304:MET:O	1:B:308:VAL:HG23	2.17	0.44
1:A:80:ASN:ND2	1:A:83:VAL:HG22	2.32	0.44
1:A:331:GLU:HB3	1:A:342:VAL:HG13	1.99	0.44
1:C:325:ARG:NH1	1:C:325:ARG:CG	2.45	0.44
1:A:294:LYS:HB2	1:A:294:LYS:HE2	1.84	0.44
1:B:135:LYS:O	1:B:136:ASN:HB2	2.16	0.44
1:A:81:GLU:HB3	1:A:85:ARG:NH1	2.32	0.44
1:B:208:GLY:O	1:B:212:LEU:HB2	2.18	0.44
1:A:115:LEU:HD23	1:A:115:LEU:C	2.42	0.44
1:C:83:VAL:HG11	1:C:284:GLY:CA	2.48	0.44
1:C:21:ALA:HB1	1:C:23:PHE:CE1	2.52	0.44
1:C:364:MET:HE3	1:D:78:TYR:CZ	2.52	0.44
1:A:253:ALA:O	1:A:254:LEU:C	2.59	0.44
1:C:198:VAL:HG12	1:C:198:VAL:O	2.17	0.43
1:C:329:PHE:CD1	1:C:343:LEU:HD23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:THR:H	1:D:9:ASN:HD22	1.66	0.43
1:C:115:LEU:C	1:C:115:LEU:CD2	2.91	0.43
1:A:216:HIS:O	1:A:217:ASN:HB2	2.17	0.43
1:B:6:THR:H	1:B:9:ASN:HD22	1.64	0.43
1:A:32:ARG:HD3	1:A:40:GLU:CD	2.43	0.43
1:A:43:ASP:CB	1:A:364:MET:CE	2.97	0.43
1:B:323:ASN:HD22	1:B:328:LEU:H	1.60	0.43
1:A:43:ASP:HA	1:A:364:MET:CE	2.45	0.43
1:C:234:GLU:HG3	1:C:240:HIS:HB2	2.00	0.43
1:D:98:ARG:HG3	1:D:270:ALA:CB	2.48	0.43
1:D:230:GLY:HA2	1:D:234:GLU:O	2.19	0.43
1:D:390:LEU:HA	1:D:390:LEU:HD23	1.73	0.43
1:A:308:VAL:HG21	1:A:379:LEU:HD13	2.01	0.43
1:B:169:ALA:HB3	1:B:172:ASP:HB3	2.00	0.43
1:C:225:VAL:HG22	2:C:410:PLP:C2	2.49	0.43
1:D:192:ILE:HG12	1:D:200:PRO:HA	2.00	0.43
1:A:223:ASP:OD1	1:A:223:ASP:C	2.62	0.43
1:D:266:THR:O	1:D:267:GLU:C	2.61	0.43
1:A:328:LEU:HD12	1:A:397:CYS:SG	2.60	0.42
1:B:329:PHE:HA	1:B:342:VAL:O	2.19	0.42
1:A:25:PRO:CB	1:A:33:LEU:HD11	2.42	0.42
1:A:248:LEU:HD23	1:A:249:THR:N	2.34	0.42
1:D:171:ASN:OD1	1:D:201:ALA:HA	2.19	0.42
1:A:32:ARG:HD3	1:A:40:GLU:OE2	2.19	0.42
1:B:80:ASN:ND2	1:B:83:VAL:HG22	2.34	0.42
1:B:81:GLU:N	1:B:82:PRO:CD	2.82	0.42
1:C:128:LYS:HG3	1:C:183:SER:HA	2.02	0.42
1:A:171:ASN:HA	1:A:205:PHE:CG	2.54	0.42
1:A:308:VAL:HG13	1:A:337:LEU:HG	2.01	0.42
1:C:119:PHE:HB2	1:C:272:VAL:HG21	2.01	0.42
1:C:177:SER:CA	1:C:212:LEU:HD21	2.49	0.42
1:D:88:LYS:O	1:D:89:LYS:C	2.63	0.42
1:A:347:TYR:OH	1:A:401:VAL:HG22	2.19	0.42
1:D:199:VAL:HA	1:D:200:PRO:HD3	1.76	0.42
1:A:141:ARG:HG3	1:B:279:GLY:O	2.19	0.42
1:B:177:SER:HA	1:B:212:LEU:HD11	2.01	0.42
1:C:36:GLN:NE2	1:D:81:GLU:OE2	2.51	0.42
1:C:238:TYR:CD1	1:C:238:TYR:C	2.97	0.42
1:A:151:GLN:NE2	1:A:154:TYR:CE2	2.88	0.42
1:C:47:GLY:C	1:C:48:ILE:HG13	2.43	0.42
1:D:41:TYR:CD1	1:D:41:TYR:N	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:LYS:HD2	1:D:272:VAL:HG13	2.01	0.41
1:C:251:ALA:O	1:C:252:LYS:C	2.62	0.41
1:D:53:LEU:HD23	1:D:53:LEU:HA	1.83	0.41
1:D:195:GLU:HG2	4:D:2036:HOH:O	2.19	0.41
1:A:112:ALA:HB2	1:A:263:LEU:HD13	2.01	0.41
1:D:152:PRO:O	1:D:153:ALA:C	2.62	0.41
1:D:320:ASN:O	1:D:321:THR:C	2.63	0.41
1:A:99:VAL:CG2	1:A:101:PHE:CE2	3.04	0.41
1:A:353:GLN:H	1:A:353:GLN:NE2	2.17	0.41
1:A:378:ALA:O	1:A:381:VAL:HG22	2.21	0.41
1:B:159:ALA:HA	1:B:160:PRO:C	2.45	0.41
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.91	0.41
1:D:253:ALA:O	1:D:254:LEU:C	2.64	0.41
1:A:98:ARG:HD3	1:B:12:GLU:O	2.19	0.41
1:C:54:GLY:HA2	4:C:2007:HOH:O	2.19	0.41
1:D:224:GLU:HA	1:D:227:THR:HG22	2.03	0.41
1:D:303[A]:GLU:CD	1:D:303[A]:GLU:H	2.29	0.41
1:B:378:ALA:O	1:B:381:VAL:CG2	2.58	0.41
1:D:155:SER:O	1:D:156:GLN:C	2.63	0.41
1:D:227:THR:HB	4:D:2037:HOH:O	2.20	0.41
1:A:322:ILE:CD1	1:A:394:ALA:HB2	2.51	0.40
1:B:119:PHE:CD1	1:B:119:PHE:C	2.99	0.40
1:B:181:ASP:O	1:B:216:HIS:HB3	2.20	0.40
1:B:342:VAL:HB	1:B:372:VAL:HG22	2.03	0.40
1:D:323:ASN:ND2	1:D:328:LEU:H	2.20	0.40
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.91	0.40
1:A:361:ALA:O	1:A:392:ARG:HB3	2.22	0.40
1:C:225:VAL:O	1:C:252:LYS:HB2	2.22	0.40
1:D:33:LEU:HD12	1:D:364:MET:HE1	2.04	0.40
1:A:32:ARG:HH22	1:A:384:GLU:CD	2.24	0.40
1:B:307:GLY:O	1:B:311:ARG:HD2	2.21	0.40
1:C:3:GLN:O	1:D:85:ARG:NH2	2.55	0.40
1:D:9:ASN:HB3	1:D:13:TRP:CZ3	2.56	0.40
1:D:97:ASP:HB2	1:D:267:GLU:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/406 (99%)	369 (92%)	32 (8%)	2 (0%)	24	32
1	B	403/406 (99%)	380 (94%)	21 (5%)	2 (0%)	24	32
1	C	402/406 (99%)	368 (92%)	30 (8%)	4 (1%)	12	14
1	D	404/406 (100%)	369 (91%)	32 (8%)	3 (1%)	18	24
All	All	1612/1624 (99%)	1486 (92%)	115 (7%)	11 (1%)	18	24

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	ALA
1	D	164	ASP
1	D	251	ALA
1	C	251	ALA
1	C	252	LYS
1	A	182	ASP
1	A	256	GLY
1	B	252	LYS
1	C	4	PRO
1	D	401	VAL
1	C	197	GLY

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	311/312 (100%)	282 (91%)	29 (9%)	8	9
1	B	312/312 (100%)	280 (90%)	32 (10%)	7	6
1	C	311/312 (100%)	288 (93%)	23 (7%)	13	16
1	D	312/312 (100%)	279 (89%)	33 (11%)	6	6
All	All	1246/1248 (100%)	1129 (91%)	117 (9%)	9	8

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	27	ARG
1	A	32	ARG
1	A	33	LEU
1	A	37	GLN
1	A	83	VAL
1	A	85	ARG
1	A	88	LYS
1	A	99	VAL
1	A	164	ASP
1	A	173	ILE
1	A	183	SER
1	A	199	VAL
1	A	203	ASN
1	A	212	LEU
1	A	225	VAL
1	A	227	THR
1	A	299	ILE
1	A	303[A]	GLU
1	A	303[B]	GLU
1	A	322	ILE
1	A	330	SER
1	A	342	VAL
1	A	353	GLN
1	A	371	ASN
1	A	373	VAL
1	A	381	VAL
1	A	388	THR
1	A	401	VAL
1	B	12	GLU
1	B	17	VAL
1	B	27[A]	ARG
1	B	27[B]	ARG

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Mol	Chain	Res	Type
1	B	37	GLN
1	B	48	ILE
1	B	62	GLU
1	B	83	VAL
1	B	88	LYS
1	B	90	LEU
1	B	99	VAL
1	B	146	VAL
1	B	173	ILE
1	B	175	SER
1	B	199	VAL
1	B	207	GLN
1	B	212	LEU
1	B	225	VAL
1	B	268[A]	GLU
1	B	268[B]	GLU
1	B	272	VAL
1	B	280	THR
1	B	303[A]	GLU
1	B	303[B]	GLU
1	B	325	ARG
1	B	328	LEU
1	B	342	VAL
1	B	346	ASP
1	B	352	LYS
1	B	373	VAL
1	B	381	VAL
1	B	401	VAL
1	C	14	MET
1	C	17	VAL
1	C	27	ARG
1	C	65	ASN
1	C	83	VAL
1	C	90	LEU
1	C	99	VAL
1	C	175	SER
1	C	207	GLN
1	C	225	VAL
1	C	280	THR
1	C	287	LEU
1	C	297	GLU
1	C	303[A]	GLU

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Mol	Chain	Res	Type
1	C	303[B]	GLU
1	C	325	ARG
1	C	331	GLU
1	C	335	LEU
1	C	342	VAL
1	C	352	LYS
1	C	356	GLN
1	C	373	VAL
1	C	381	VAL
1	D	14	MET
1	D	17	VAL
1	D	20	PRO
1	D	27	ARG
1	D	32	ARG
1	D	33	LEU
1	D	61	ARG
1	D	65	ASN
1	D	83	VAL
1	D	85	ARG
1	D	90	LEU
1	D	99	VAL
1	D	156	GLN
1	D	173	ILE
1	D	199	VAL
1	D	212	LEU
1	D	225	VAL
1	D	227	THR
1	D	246	ASP
1	D	250	THR
1	D	263	LEU
1	D	272	VAL
1	D	280	THR
1	D	287	LEU
1	D	299	ILE
1	D	331	GLU
1	D	335	LEU
1	D	342	VAL
1	D	352	LYS
1	D	353	GLN
1	D	371	ASN
1	D	373	VAL
1	D	381	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	103	ASN
1	A	121	HIS
1	A	139	HIS
1	A	203	ASN
1	A	300	ASN
1	A	323	ASN
1	A	353	GLN
1	A	371	ASN
1	B	9	ASN
1	B	57	HIS
1	B	139	HIS
1	B	151	GLN
1	B	214	ASN
1	B	216	HIS
1	B	310	GLN
1	B	323	ASN
1	B	399	HIS
1	C	3	GLN
1	C	9	ASN
1	C	51	ASN
1	C	103	ASN
1	C	121	HIS
1	C	139	HIS
1	C	151	GLN
1	C	214	ASN
1	C	216	HIS
1	C	323	ASN
1	C	353	GLN
1	C	371	ASN
1	D	9	ASN
1	D	37	GLN
1	D	51	ASN
1	D	65	ASN
1	D	139	HIS
1	D	156	GLN
1	D	216	HIS
1	D	312	HIS
1	D	323	ASN
1	D	353	GLN
1	D	371	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	$\# Z > 2$
3	SUO	C	411	2	15,15,15	0.93	0	18,18,18	1.35	1 (5%)
3	SUO	B	411	2	15,15,15	1.42	3 (20%)	18,18,18	1.71	6 (33%)
3	SUO	D	411	2	15,15,15	1.16	0	18,18,18	1.43	2 (11%)
2	PLP	A	410	3	15,15,16	2.56	5 (33%)	21,22,23	1.49	3 (14%)
2	PLP	C	410	3	15,15,16	3.10	4 (26%)	21,22,23	1.64	4 (19%)
3	SUO	A	411	2	15,15,15	0.96	0	18,18,18	2.27	7 (38%)
2	PLP	B	410	3	15,15,16	2.82	3 (20%)	21,22,23	1.66	5 (23%)
2	PLP	D	410	3	15,15,16	2.56	5 (33%)	21,22,23	1.48	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SUO	C	411	2	-	2/17/17/17	-
3	SUO	B	411	2	-	1/17/17/17	-
3	SUO	D	411	2	-	4/17/17/17	-
2	PLP	A	410	3	-	1/6/6/8	0/1/1/1
2	PLP	C	410	3	-	0/6/6/8	0/1/1/1
3	SUO	A	411	2	-	1/17/17/17	-
2	PLP	B	410	3	-	2/6/6/8	0/1/1/1
2	PLP	D	410	3	-	3/6/6/8	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	410	PLP	C3-C2	8.18	1.49	1.41
2	B	410	PLP	C5-C4	7.28	1.48	1.40
2	C	410	PLP	C5-C4	6.93	1.48	1.40
2	D	410	PLP	C3-C2	6.83	1.48	1.41
2	A	410	PLP	C3-C2	6.55	1.47	1.41
2	B	410	PLP	C3-C2	6.08	1.47	1.41
2	A	410	PLP	C5-C4	4.63	1.45	1.40
2	B	410	PLP	C3-C4	4.59	1.48	1.40
2	D	410	PLP	C5-C4	4.37	1.45	1.40
2	A	410	PLP	C3-C4	4.34	1.48	1.40
2	C	410	PLP	C3-C4	4.12	1.48	1.40
2	D	410	PLP	C4A-C4	-3.41	1.44	1.51
2	D	410	PLP	C3-C4	3.26	1.46	1.40
2	A	410	PLP	C4A-C4	-2.51	1.46	1.51
3	B	411	SUO	O2-C	2.40	1.29	1.22
2	A	410	PLP	P-O3P	-2.29	1.46	1.54
2	D	410	PLP	C2A-C2	-2.22	1.46	1.50
2	C	410	PLP	C4A-C4	-2.22	1.47	1.51
3	B	411	SUO	CW-CV	2.21	1.55	1.51
3	B	411	SUO	OXT-CV	2.15	1.27	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	410	PLP	O2P-P-O4P	-4.55	94.82	106.67
2	C	410	PLP	O2P-P-O4P	-4.47	95.02	106.67
3	A	411	SUO	C-CA-N	4.28	120.49	110.57
3	A	411	SUO	CB-CA-N	-4.18	102.64	110.91
2	A	410	PLP	C6-N1-C2	3.49	125.53	119.20
3	B	411	SUO	C-CA-N	3.31	118.25	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	411	SUO	O-C-CA	3.18	124.27	113.51
3	A	411	SUO	O-C-O2	-3.16	116.92	124.08
3	D	411	SUO	CA-N-CV	3.12	129.51	121.68
3	D	411	SUO	CX-CW-CV	3.11	119.07	112.67
3	C	411	SUO	CB-CA-N	-3.09	104.79	110.91
3	B	411	SUO	CB-CA-N	-3.09	104.79	110.91
2	C	410	PLP	O2P-P-O1P	2.92	122.22	110.83
2	B	410	PLP	C6-N1-C2	2.91	124.47	119.20
2	D	410	PLP	C4A-C4-C5	-2.85	118.00	120.94
2	A	410	PLP	C3-C2-N1	-2.73	117.52	120.96
3	A	411	SUO	CX-CW-CV	-2.72	107.06	112.67
3	A	411	SUO	CB-CG-CD	-2.72	102.57	112.62
2	D	410	PLP	C6-N1-C2	2.68	124.05	119.20
3	B	411	SUO	O-C-O2	-2.55	118.29	124.08
2	C	410	PLP	O3P-P-O2P	2.54	117.32	107.80
2	B	410	PLP	C2A-C2-C3	2.43	123.64	120.80
3	B	411	SUO	CG-CD-NE	-2.40	96.08	112.60
3	A	411	SUO	OD2-CY-CX	-2.38	115.54	123.09
2	A	410	PLP	O3-C3-C2	2.37	122.50	117.58
2	B	410	PLP	O2P-P-O1P	2.28	119.73	110.83
2	D	410	PLP	C4-C3-C2	-2.16	116.66	119.89
3	B	411	SUO	CW-CX-CY	2.11	119.26	113.67
2	B	410	PLP	O3P-P-O2P	2.10	115.67	107.80
3	B	411	SUO	OD1-CY-CX	2.09	120.59	114.00
2	C	410	PLP	C3-C4-C5	-2.06	116.12	118.59

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	410	PLP	C5A-O4P-P-O1P
2	D	410	PLP	C5A-O4P-P-O2P
2	A	410	PLP	C5A-O4P-P-O1P
2	B	410	PLP	C5A-O4P-P-O1P
3	D	411	SUO	CV-CW-CX-CY
3	B	411	SUO	C-CA-CB-CG
3	C	411	SUO	NE-CD-CG-CB
3	D	411	SUO	NE-CD-CG-CB
3	A	411	SUO	NE-CD-CG-CB
2	B	410	PLP	C5A-O4P-P-O2P
2	D	410	PLP	C5A-O4P-P-O3P
3	D	411	SUO	CW-CX-CY-OD2

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Mol	Chain	Res	Type	Atoms
3	D	411	SUO	CW-CX-CY-OD1
3	C	411	SUO	CW-CX-CY-OD2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	411	SUO	1	0
3	B	411	SUO	3	0
3	D	411	SUO	3	0
2	C	410	PLP	2	0
3	A	411	SUO	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	400/406 (98%)	-0.80	1 (0%) 90 91	9, 22, 36, 77	20 (5%)
1	B	400/406 (98%)	-0.81	0 100 100	9, 21, 37, 55	22 (5%)
1	C	400/406 (98%)	-0.66	1 (0%) 90 91	16, 27, 46, 76	23 (5%)
1	D	400/406 (98%)	-0.48	2 (0%) 87 88	16, 32, 54, 76	25 (6%)
All	All	1600/1624 (98%)	-0.69	4 (0%) 90 91	9, 26, 46, 77	90 (5%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	GLN	11.0
1	C	3	GLN	6.9
1	A	3	GLN	2.9
1	D	399[A]	HIS	2.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SUO	D	411	16/16	0.91	0.09	26,46,53,56	0
3	SUO	B	411	16/16	0.92	0.09	22,33,39,41	0
3	SUO	C	411	16/16	0.93	0.08	33,50,54,60	0
3	SUO	A	411	16/16	0.93	0.07	25,32,41,45	0
2	PLP	D	410	15/16	0.98	0.05	15,17,21,23	0
2	PLP	C	410	15/16	0.99	0.04	20,25,27,28	0
2	PLP	A	410	15/16	0.99	0.04	15,17,18,21	0
2	PLP	B	410	15/16	0.99	0.03	11,12,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.