



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2026 – 06:13 PM JST

PDB ID : 9XB8 / pdb_00009xb8
Title : ATP-dependent diazotase Mco01_40450
Authors : Ning, J.; Kawai, S.; Ohnishi, Y.; Katsuyama, Y.
Deposited on : 2025-10-23
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

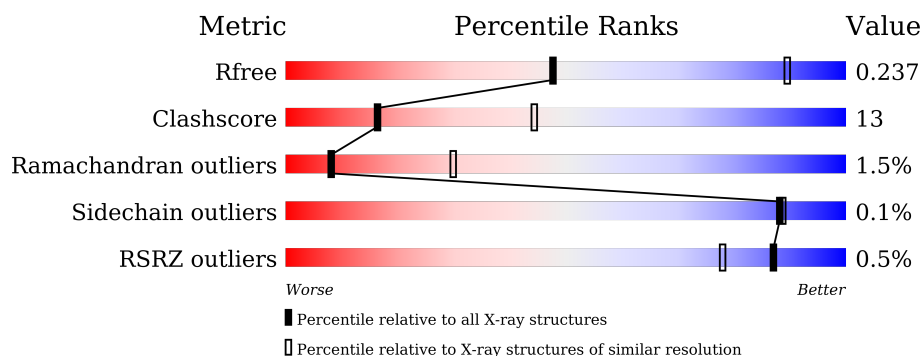
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	577	55% 19% • 25%
1	B	577	53% 21% 25%
1	C	577	% 51% 24% • 25%
1	D	577	% 52% 23% 25%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13384 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 Fatty-acid-CoA ligase FadD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3346	2122	590	624	10			
1	B	433	Total	C	N	O	S	0	0	0
			3346	2122	590	624	10			
1	C	433	Total	C	N	O	S	0	0	0
			3346	2122	590	624	10			
1	D	433	Total	C	N	O	S	0	0	0
			3346	2122	590	624	10			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP A0ABQ4G1Y4
A	-14	ASN	-	expression tag	UNP A0ABQ4G1Y4
A	-13	HIS	-	expression tag	UNP A0ABQ4G1Y4
A	-12	LYS	-	expression tag	UNP A0ABQ4G1Y4
A	-11	VAL	-	expression tag	UNP A0ABQ4G1Y4
A	-10	HIS	-	expression tag	UNP A0ABQ4G1Y4
A	-9	HIS	-	expression tag	UNP A0ABQ4G1Y4
A	-8	HIS	-	expression tag	UNP A0ABQ4G1Y4
A	-7	HIS	-	expression tag	UNP A0ABQ4G1Y4
A	-6	HIS	-	expression tag	UNP A0ABQ4G1Y4
A	-5	HIS	-	expression tag	UNP A0ABQ4G1Y4
A	-4	ILE	-	expression tag	UNP A0ABQ4G1Y4
A	-3	GLU	-	expression tag	UNP A0ABQ4G1Y4
A	-2	GLY	-	expression tag	UNP A0ABQ4G1Y4
A	-1	ARG	-	expression tag	UNP A0ABQ4G1Y4
A	0	HIS	-	expression tag	UNP A0ABQ4G1Y4
B	-15	MET	-	initiating methionine	UNP A0ABQ4G1Y4
B	-14	ASN	-	expression tag	UNP A0ABQ4G1Y4
B	-13	HIS	-	expression tag	UNP A0ABQ4G1Y4
B	-12	LYS	-	expression tag	UNP A0ABQ4G1Y4
B	-11	VAL	-	expression tag	UNP A0ABQ4G1Y4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP A0ABQ4G1Y4
B	-9	HIS	-	expression tag	UNP A0ABQ4G1Y4
B	-8	HIS	-	expression tag	UNP A0ABQ4G1Y4
B	-7	HIS	-	expression tag	UNP A0ABQ4G1Y4
B	-6	HIS	-	expression tag	UNP A0ABQ4G1Y4
B	-5	HIS	-	expression tag	UNP A0ABQ4G1Y4
B	-4	ILE	-	expression tag	UNP A0ABQ4G1Y4
B	-3	GLU	-	expression tag	UNP A0ABQ4G1Y4
B	-2	GLY	-	expression tag	UNP A0ABQ4G1Y4
B	-1	ARG	-	expression tag	UNP A0ABQ4G1Y4
B	0	HIS	-	expression tag	UNP A0ABQ4G1Y4
C	-15	MET	-	initiating methionine	UNP A0ABQ4G1Y4
C	-14	ASN	-	expression tag	UNP A0ABQ4G1Y4
C	-13	HIS	-	expression tag	UNP A0ABQ4G1Y4
C	-12	LYS	-	expression tag	UNP A0ABQ4G1Y4
C	-11	VAL	-	expression tag	UNP A0ABQ4G1Y4
C	-10	HIS	-	expression tag	UNP A0ABQ4G1Y4
C	-9	HIS	-	expression tag	UNP A0ABQ4G1Y4
C	-8	HIS	-	expression tag	UNP A0ABQ4G1Y4
C	-7	HIS	-	expression tag	UNP A0ABQ4G1Y4
C	-6	HIS	-	expression tag	UNP A0ABQ4G1Y4
C	-5	HIS	-	expression tag	UNP A0ABQ4G1Y4
C	-4	ILE	-	expression tag	UNP A0ABQ4G1Y4
C	-3	GLU	-	expression tag	UNP A0ABQ4G1Y4
C	-2	GLY	-	expression tag	UNP A0ABQ4G1Y4
C	-1	ARG	-	expression tag	UNP A0ABQ4G1Y4
C	0	HIS	-	expression tag	UNP A0ABQ4G1Y4
D	-15	MET	-	initiating methionine	UNP A0ABQ4G1Y4
D	-14	ASN	-	expression tag	UNP A0ABQ4G1Y4
D	-13	HIS	-	expression tag	UNP A0ABQ4G1Y4
D	-12	LYS	-	expression tag	UNP A0ABQ4G1Y4
D	-11	VAL	-	expression tag	UNP A0ABQ4G1Y4
D	-10	HIS	-	expression tag	UNP A0ABQ4G1Y4
D	-9	HIS	-	expression tag	UNP A0ABQ4G1Y4
D	-8	HIS	-	expression tag	UNP A0ABQ4G1Y4
D	-7	HIS	-	expression tag	UNP A0ABQ4G1Y4
D	-6	HIS	-	expression tag	UNP A0ABQ4G1Y4
D	-5	HIS	-	expression tag	UNP A0ABQ4G1Y4
D	-4	ILE	-	expression tag	UNP A0ABQ4G1Y4
D	-3	GLU	-	expression tag	UNP A0ABQ4G1Y4
D	-2	GLY	-	expression tag	UNP A0ABQ4G1Y4
D	-1	ARG	-	expression tag	UNP A0ABQ4G1Y4

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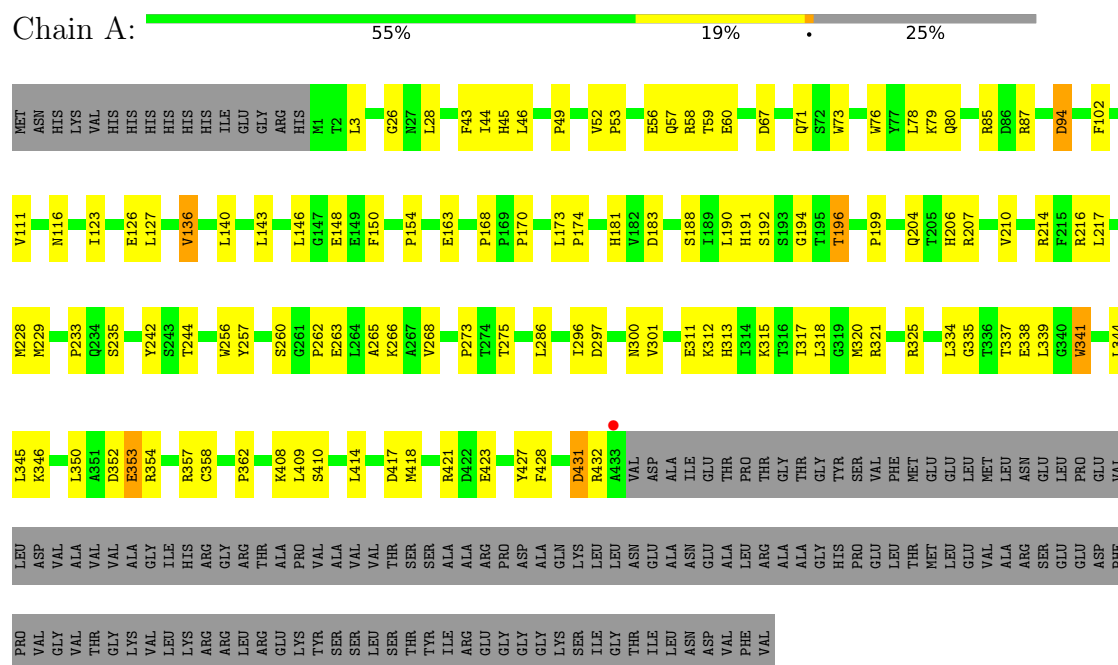
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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP A0ABQ4G1Y4

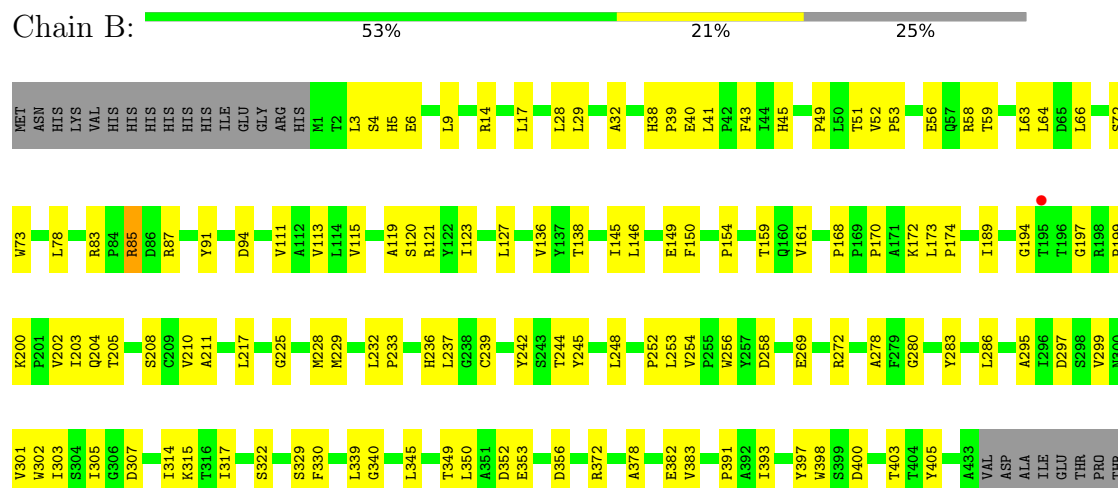
3 Residue-property plots

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: Fatty-acid-CoA ligase FadD



• Molecule 1: Fatty-acid-CoA ligase FadD



ALA	GLY
GLY	THR
GLY	THR
HIS	TYR
PRO	SER
GLU	VAL
LEU	PHE
THR	MET
LEU	GLU
LEU	GLU
VAL	LEU
VAL	MET
ALA	LEU
ARG	ASN
SER	GLU
GLU	LEU
ASP	GLU
PHE	VAL
VAL	LEU
VAL	ASP
GLY	VAL
THR	ALA
GLY	VAL
LYS	GLY
LEU	IIE
LYS	HIS
ARG	ARG
ARG	GLY
LEU	ARG
ARG	THR
GLU	ALA
LYS	PRO
THR	VAL
SER	ALA
SER	VAL
LEU	VAL
LEU	VAL
SER	THR
THR	SER
THR	SER
TYR	ILE
ILE	ALA
ARG	ALA
GLU	ARG
GLY	PRO
GLY	ASP
LYS	ALA
LYS	GLN
SER	LEU
ILE	LEU
GLY	LEU
THR	ASN
ILE	GLU
LEU	ALA
ASN	GLU
ASP	GLU
VAL	ALA
PHE	LEU
VAL	ASP

- Molecule 1: Fatty-acid-CoA ligase FadD



SER	VAL	S401	T274	T159	L83	ASN	MET
	VAL	T403		P168	D64	ASN	ASN
THR	THR	R406	M277	P169	D65	HIS	HIS
ILE	ALA	S407	A278	P170	L66	LYS	VAL
ARG	ALA	K408	F779	G280	E68	HIS	HIS
GLU	ARG		G280	P174	L89	HIS	HIS
GLY	GLY	Y420	Y283		V70	HIS	HIS
GLY	ASP				S72	HIS	HIS
LYS	GLN	Q429	A289	R178	W73	HIS	HIS
LYS	ALA	V430	D290	H181	S74	ILE	ILE
SER	LYS	D431	L291	V75		GLU	GLU
GLY	LEU	R432	G294			GLY	GLY
GLY	LEU	A433	G294	L78	L78	ARG	ARG
THR	ASN	VAL	A295	K79	K79		
ILE	ALA	ALA	T296	R85			
LEU	ALA	ILE	D297	P186			
ASN	ASN	ILE		V187			
ASP	GLU	GLU	N300	S188	Y91		
VAL	ALA	ALA					
PHE	LEU	THR	I305	T195	D94		
VAL	LEU	PRO	G306				
	ARG	THR	D307	K200	V100		
	ALA	GLY		P201	H101		
	ALA	THR		V202	F102		
	GLY	GLY	I314	I203			
	HIS	TYR	K315	Q204			
	PRO	SER		T205	I108		
	GLU	VAL	G319	H206	G95		
	GLU	PHE	M320	R207	G28		
	LEU	THR	R321		N116		
	THR	MET	GLU		S117		
	LEU	GLU	E338	R214	L28		
	GLU	LEU	GLU	F215	R121		
	VAL	MET	L344	R216	Y122		
	ALA	LEU	L345		I123		
	ARG	ASN		A226			
	ARG	GLU	R348	L227	E126		
	SER	LEU	T349	M228	L127		
	GLU	LEU	M229	L230	P39		
	GLU	PRO	L350	M230	E40		
	ASP	GLU	T230	L41	L41		
	PHE	VAL	R354	A331	P42		
	PRO	LEU	R355	L232	F43		
	VAL	ASP	D356	T44	P43		
	GLY	VAL	R357		H442		
	VAL	ALA	C358	Y242	L46		
	THR	VAL	V359	S243	G47		
	GLY	VAL	G360	L146	R48		
	LYS	ALA	R361	Y245	P49		
	VAL	GLY	V362	E148			
	LEU	ILE	V363	E149	V52		
	LYS	ARG	G364	F150	P53		
	ARG	ARG	V365	L248	S54		
	ARG	GLY		P255	G55		
	LEU	ARG	N381	V256			
	LEU	THR		Y257			
	ARG	THR		P154			
	GLU	GLU	Y397	D258			
	LYS	PRO	W398	G155			
	VAL	VAL	S260	L156			
	TYR	VAL	S399	R157			
	ALA	ALA	D400	H159			

- Molecule 1: Fatty-acid-CoA ligase FadD



A419	L296	T205	D86	MET
Y420		H206	R87	
R421	V301	V88	A89	HIS
	W302	V210		LYS
N426	I303	A211		VAL
Y427	S304	G212	L92	HIS
F428	I305	P213	H93	HIS
	G306		D94	HIS
A433	D307	L217		HIS
VAL	A308		V111	HIS
ASP	V309	H220	A112	HIS
ALA	H310		V113	ILE
ILE	E311			GLU
THR	A312	Q223	N116	GLY
GLU	H313	P224	S117	ARG
THR	H313	G225		ARG
PRO	A320	A226		HIS
THR	I314			M1
THR		L227	S120	T2
GLY	I317	H228		L3
THR	L318	H229	I123	
GLY	G319	T230		S4
TYR	M320	A231	L127	H5
SER		L232		
VAL	A326	P233	G135	L9
PHE	P327		V136	T10
MET		L237	Y137	
GLU	F330	G238		Q13
GLU		C239	L140	R14
LEU	G335			
MET	T336	S243	L146	L17
LEU	T337	T244		
ASN	E338	Y245	F150	G24
GLU	L339	A246	G25	G25
LEU	G340	V247	W158	G26
PRO		L248		
GLY	V343	G249	E163	L29
VAL				
LEU	R348	P252	P166	H38
ASP	T349		A167	P39
VAL		P255	P168	E40
ALA	D352		P169	L41
VAL		D258	P170	P42
VAL	R357			F43
ALA		E269	H181	I44
GLY	V363			H45
ILE		R272	E184	
HIS	V370	P273		T51
ARG	L371	T274	S188	V52
GLY	R372	T275	I189	P53
ARG		V276	L190	
THR	T376	D277		E56
ALA		A278	G194	
PRO	A392		T195	S62
VAL		Y283	T196	L63
ALA	W398		G197	L64
VAL		L286	R198	D65
VAL	S401		P199	
THR	A289			W73
SER	Y405	D290	V202	
SER		L291	T203	R83
ALA	W418		G204	

ALA	ARG	PRO	PRO	ASP	ALA	GLN	LYS	LEU	LEU	ASN	GLU	ALA	ASN	GLU	ALA	ALA	GLY	HIS	PRO	LEU	LEU	GLU	VAL	ALA	ARG	SER	GLU	GLU	ASP	PHE	PRO	VAL	GLY	LYS	ARG	ARG	LEU	GLU	LYS	TYR	SER	LEU	SER	THR	TYR
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ARG
GLU
GLY
GLY
GLY
LYS
SER
ILE
GLY
THR
ILE
LEU
ASN
ASP
VAL
PHE
VAL

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.19Å 163.99Å 107.69Å 90.00° 99.71° 90.00°	Depositor
Resolution (Å)	49.01 – 3.40 49.01 – 3.40	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.01-3.40) 93.4 (49.01-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.154 , 0.237 0.154 , 0.237	Depositor DCC
R_{free} test set	1856 reflections (6.45%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13384	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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

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	0.42	1/3432 (0.0%)	0.59	0/4684
1	B	0.42	1/3432 (0.0%)	0.61	1/4684 (0.0%)
1	C	0.40	0/3432	0.61	0/4684
1	D	0.41	1/3432 (0.0%)	0.59	0/4684
All	All	0.41	3/13728 (0.0%)	0.60	1/18736 (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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	197	GLY	C-N	7.04	1.48	1.33
1	D	196	THR	CA-C	6.50	1.61	1.52
1	A	196	THR	CA-C	6.08	1.60	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	VAL	N-CA-C	-5.48	108.51	113.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	85	ARG	Sidechain

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	3346	0	3301	81	1
1	B	3346	0	3301	83	1
1	C	3346	0	3301	95	0
1	D	3346	0	3301	97	0
All	All	13384	0	13204	346	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (346) 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:3:LEU:HD11	1:A:45:HIS:HB2	1.52	0.92
1:D:3:LEU:HD11	1:D:45:HIS:HB2	1.52	0.90
1:B:28:LEU:HD11	1:B:244:THR:HG23	1.54	0.89
1:D:309:VAL:HG13	1:D:314:ILE:HD11	1.56	0.87
1:D:232:LEU:HD22	1:D:305:ILE:HD11	1.55	0.86
1:B:3:LEU:HD21	1:B:45:HIS:HB2	1.61	0.81
1:D:232:LEU:HD11	1:D:239:CYS:HB2	1.65	0.78
1:B:136:VAL:HG13	1:B:159:THR:HG23	1.65	0.77
1:A:417:ASP:HA	1:A:432:ARG:HA	1.69	0.75
1:C:3:LEU:HD11	1:C:45:HIS:HB2	1.68	0.75
1:D:9:LEU:HD12	1:D:249:GLY:HA2	1.68	0.74
1:C:354:ARG:NE	1:C:356:ASP:OD2	2.20	0.73
1:D:39:PRO:HB2	1:D:64:LEU:HD13	1.71	0.71
1:B:315:LYS:NZ	1:B:350:LEU:O	2.23	0.71
1:D:14:ARG:NH2	1:D:245:TYR:OH	2.23	0.71
1:C:17:LEU:HD21	1:C:248:LEU:HB3	1.74	0.70
1:B:301:VAL:HG22	1:B:329:SER:HB2	1.74	0.69
1:B:297:ASP:OD2	1:B:322:SER:OG	2.09	0.69
1:B:4:SER:HB3	1:B:6:GLU:HG3	1.75	0.68
1:C:20:ASP:O	1:C:214:ARG:NH2	2.26	0.68
1:B:228:MET:HG2	1:B:242:TYR:CE2	2.29	0.68
1:C:136:VAL:HG13	1:C:159:THR:HG23	1.75	0.68
1:C:26:GLY:HA3	1:C:181:HIS:NE2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:THR:H	1:D:352:ASP:HB2	1.60	0.66
1:C:232:LEU:HD21	1:C:277:MET:HE2	1.76	0.66
1:D:202:VAL:HG21	1:D:337:THR:HG22	1.78	0.66
1:A:216:ARG:HG3	1:A:341:TRP:HZ2	1.60	0.66
1:B:3:LEU:HB3	1:B:43:PHE:HA	1.78	0.65
1:C:406:ARG:NH2	1:D:86:ASP:OD1	2.29	0.65
1:D:87:ARG:HG3	1:D:111:VAL:HG23	1.78	0.65
1:C:3:LEU:HD21	1:C:45:HIS:HB2	1.78	0.64
1:A:49:PRO:HG3	1:A:59:THR:HG22	1.79	0.63
1:D:190:LEU:HB2	1:D:204:GLN:HE22	1.63	0.63
1:B:149:GLU:OE1	1:B:149:GLU:N	2.29	0.63
1:C:314:ILE:HD13	1:C:348:ARG:HD2	1.79	0.63
1:D:204:GLN:OE1	1:D:204:GLN:N	2.31	0.63
1:B:14:ARG:NH2	1:B:245:TYR:OH	2.32	0.63
1:A:148:GLU:HG3	1:B:345:LEU:O	1.98	0.63
1:A:318:LEU:HB2	1:A:350:LEU:HD13	1.82	0.62
1:D:223:GLN:HB2	1:D:226:ALA:HB2	1.80	0.62
1:A:311:GLU:HG2	1:A:354:ARG:HE	1.65	0.62
1:D:232:LEU:CD1	1:D:239:CYS:HB2	2.29	0.62
1:B:205:THR:H	1:B:208:SER:HB3	1.65	0.61
1:C:28:LEU:HD11	1:C:244:THR:HG23	1.82	0.61
1:B:14:ARG:NH1	1:B:217:LEU:O	2.33	0.61
1:B:45:HIS:HB3	1:B:254:VAL:HG22	1.81	0.61
1:D:62:SER:H	1:D:65:ASP:HB2	1.64	0.61
1:D:73:TRP:CE2	1:D:168:PRO:HD3	2.35	0.61
1:C:319:GLY:O	1:C:321:ARG:N	2.35	0.59
1:A:183:ASP:HB3	1:A:207:ARG:HB2	1.85	0.59
1:C:73:TRP:CE2	1:C:168:PRO:HD3	2.37	0.59
1:C:228:MET:HG2	1:C:242:TYR:CE2	2.37	0.59
1:A:28:LEU:HD11	1:A:244:THR:HG23	1.85	0.59
1:A:335:GLY:HA2	1:A:339:LEU:HD12	1.84	0.59
1:D:26:GLY:HA3	1:D:181:HIS:CD2	2.38	0.59
1:D:188:SER:OG	1:D:204:GLN:HB2	2.03	0.58
1:B:172:LYS:NZ	1:B:173:LEU:O	2.35	0.58
1:B:228:MET:HE1	1:B:303:ILE:HD12	1.85	0.58
1:C:152:LEU:HD12	1:C:152:LEU:O	2.04	0.58
1:A:228:MET:HG2	1:A:242:TYR:CE1	2.39	0.58
1:C:233:PRO:HD3	1:C:258:ASP:HB2	1.85	0.57
1:A:52:VAL:HG11	1:A:58:ARG:HD2	1.84	0.57
1:D:310:HIS:HB2	1:D:313:HIS:ND1	2.19	0.57
1:A:146:LEU:HD22	1:A:150:PHE:CE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ARG:HD2	1:D:405:TYR:O	2.05	0.57
1:D:269:GLU:O	1:D:272:ARG:NE	2.27	0.57
1:C:78:LEU:HD21	1:C:108:ILE:HD12	1.86	0.57
1:B:283:TYR:OH	1:B:303:ILE:O	2.16	0.57
1:D:202:VAL:HG11	1:D:338:GLU:HG3	1.86	0.57
1:A:268:VAL:HA	1:A:273:PRO:HD2	1.87	0.56
1:B:14:ARG:HG2	1:B:217:LEU:HD22	1.86	0.56
1:C:280:GLY:N	1:C:307:ASP:OD1	2.38	0.56
1:C:402:ASP:OD2	1:D:87:ARG:NH1	2.33	0.56
1:D:213:PRO:HB3	1:D:245:TYR:HB2	1.87	0.56
1:C:315:LYS:HD3	1:C:350:LEU:HD12	1.88	0.56
1:D:357:ARG:NH1	1:D:357:ARG:HA	2.21	0.56
1:A:312:LYS:HE2	1:A:313:HIS:CE1	2.41	0.56
1:B:269:GLU:HB2	1:B:295:ALA:HB1	1.86	0.56
1:D:318:LEU:HD11	1:D:330:PHE:HB2	1.88	0.56
1:A:3:LEU:HB3	1:A:43:PHE:HA	1.87	0.55
1:D:24:GLY:HA3	1:D:206:HIS:CE1	2.42	0.55
1:D:372:ARG:HD2	1:D:376:THR:OG1	2.07	0.55
1:A:417:ASP:HB3	1:A:432:ARG:HD2	1.89	0.55
1:C:72:SER:HB3	1:C:168:PRO:HG2	1.88	0.55
1:D:286:LEU:HD23	1:D:317:ILE:HD13	1.89	0.55
1:D:146:LEU:HD22	1:D:150:PHE:CD1	2.42	0.55
1:D:210:VAL:C	1:D:213:PRO:HD2	2.32	0.54
1:D:357:ARG:HA	1:D:357:ARG:CZ	2.36	0.54
1:D:229:MET:HE3	1:D:273:PRO:HG3	1.87	0.54
1:B:52:VAL:HG11	1:B:58:ARG:HD2	1.88	0.54
1:D:14:ARG:HD3	1:D:217:LEU:O	2.08	0.54
1:C:44:ILE:HB	1:C:61:LEU:HB2	1.88	0.54
1:B:237:LEU:HD21	1:B:340:GLY:HA2	1.90	0.54
1:A:338:GLU:N	1:A:338:GLU:OE1	2.42	0.53
1:C:408:LYS:HE2	1:D:184:GLU:OE1	2.08	0.53
1:B:229:MET:HA	1:B:254:VAL:O	2.07	0.53
1:C:38:HIS:HB3	1:C:41:LEU:HG	1.91	0.53
1:A:102:PHE:CE1	1:A:188:SER:HB3	2.43	0.53
1:A:357:ARG:HA	1:A:357:ARG:NE	2.23	0.53
1:D:326:ALA:HB1	1:D:327:PRO:HD2	1.90	0.53
1:A:334:LEU:HD22	1:A:344:LEU:HD12	1.91	0.52
1:C:70:VAL:HG22	1:C:100:VAL:HG13	1.90	0.52
1:B:49:PRO:HB3	1:B:59:THR:HG22	1.91	0.52
1:C:123:ILE:O	1:C:127:LEU:HB2	2.08	0.52
1:B:202:VAL:HG12	1:B:204:GLN:NE2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:LEU:HB2	1:B:14:ARG:HG3	1.91	0.52
1:A:53:PRO:HB2	1:A:170:PRO:HG3	1.90	0.52
1:B:146:LEU:HD22	1:B:150:PHE:CE1	2.45	0.52
1:C:357:ARG:HD2	1:C:429:GLN:O	2.10	0.52
1:D:5:HIS:CD2	1:D:225:GLY:HA2	2.44	0.52
1:A:67:ASP:OD1	1:A:71:GLN:HG3	2.09	0.52
1:C:148:GLU:O	1:C:150:PHE:N	2.42	0.52
1:A:87:ARG:HG3	1:A:111:VAL:HB	1.91	0.51
1:B:87:ARG:HG3	1:B:111:VAL:HB	1.92	0.51
1:D:198:ARG:HG3	1:D:199:PRO:HD2	1.91	0.51
1:B:200:LYS:HB3	1:B:397:TYR:CE1	2.46	0.51
1:B:278:ALA:HB3	1:B:283:TYR:CZ	2.45	0.51
1:C:24:GLY:HA3	1:C:206:HIS:CE1	2.46	0.51
1:B:232:LEU:HB2	1:B:233:PRO:HD2	1.92	0.51
1:B:51:THR:HA	1:B:56:GLU:O	2.11	0.51
1:B:280:GLY:HA3	1:B:307:ASP:HB2	1.92	0.51
1:C:3:LEU:HB3	1:C:43:PHE:HA	1.93	0.51
1:D:135:GLY:HA3	1:D:158:TRP:CE2	2.45	0.51
1:A:216:ARG:HG3	1:A:341:TRP:CZ2	2.44	0.50
1:D:296:ILE:HD11	1:D:320:MET:HB2	1.92	0.50
1:B:43:PHE:O	1:B:252:PRO:HA	2.11	0.50
1:B:211:ALA:HB1	1:B:391:PRO:HG2	1.92	0.50
1:A:26:GLY:HA3	1:A:181:HIS:CD2	2.45	0.50
1:A:52:VAL:HB	1:A:53:PRO:HD2	1.92	0.50
1:C:226:ALA:HA	1:C:274:THR:HG21	1.93	0.50
1:D:89:ALA:HA	1:D:113:VAL:HB	1.92	0.50
1:D:94:ASP:OD2	1:D:233:PRO:HA	2.11	0.50
1:D:314:ILE:HD13	1:D:348:ARG:HD2	1.93	0.50
1:D:230:THR:OG1	1:D:255:PRO:HA	2.12	0.50
1:D:87:ARG:HG3	1:D:111:VAL:CG2	2.41	0.49
1:B:38:HIS:HB3	1:B:41:LEU:HG	1.94	0.49
1:B:339:LEU:O	1:B:393:ILE:HD13	2.12	0.49
1:B:353:GLU:H	1:B:353:GLU:CD	2.20	0.49
1:A:192:SER:HB3	1:A:337:THR:OG1	2.12	0.49
1:B:349:THR:H	1:B:352:ASP:CG	2.20	0.49
1:A:146:LEU:HD22	1:A:150:PHE:CD1	2.48	0.49
1:B:115:VAL:HG22	1:B:127:LEU:HD23	1.94	0.49
1:B:17:LEU:HD21	1:B:248:LEU:HD22	1.95	0.49
1:C:116:ASN:OD1	1:C:117:SER:N	2.46	0.49
1:D:204:GLN:HE21	1:D:237:LEU:HD12	1.78	0.49
1:A:418:MET:N	1:A:431:ASP:O	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:PHE:O	1:D:252:PRO:HA	2.13	0.49
1:D:211:ALA:HB3	1:D:392:ALA:HB2	1.95	0.49
1:B:233:PRO:HD3	1:B:258:ASP:HB2	1.95	0.49
1:C:200:LYS:HB3	1:C:397:TYR:CD1	2.48	0.48
1:C:268:VAL:HG11	1:C:296:ILE:HG22	1.93	0.48
1:C:53:PRO:C	1:C:55:GLY:H	2.21	0.48
1:C:344:LEU:HD13	1:C:359:VAL:HG23	1.96	0.48
1:A:421:ARG:HB2	1:A:427:TYR:CE2	2.48	0.48
1:A:94:ASP:OD2	1:A:233:PRO:HA	2.14	0.48
1:C:363:VAL:HG23	1:C:365:VAL:HG12	1.95	0.48
1:C:142:HIS:HA	1:C:145:ILE:HD12	1.95	0.48
1:A:315:LYS:HG3	1:A:354:ARG:HH21	1.78	0.48
1:B:378:ALA:HB1	1:B:382:GLU:HG2	1.95	0.48
1:D:310:HIS:HD2	1:D:313:HIS:HE1	1.62	0.48
1:C:23:LEU:HB3	1:C:214:ARG:NH2	2.29	0.48
1:D:63:LEU:HD23	1:D:63:LEU:HA	1.74	0.48
1:D:232:LEU:HD21	1:D:277:MET:HE3	1.96	0.48
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.67	0.47
1:C:52:VAL:HG11	1:C:58:ARG:HE	1.80	0.47
1:C:94:ASP:OD2	1:C:233:PRO:HA	2.15	0.47
1:C:277:MET:HE3	1:C:305:ILE:HG21	1.97	0.47
1:D:53:PRO:HB2	1:D:170:PRO:HG3	1.97	0.47
1:D:73:TRP:CZ2	1:D:168:PRO:HD3	2.50	0.47
1:D:189:ILE:HA	1:D:202:VAL:O	2.14	0.47
1:B:73:TRP:CE2	1:B:168:PRO:HD3	2.50	0.47
1:D:228:MET:HE1	1:D:277:MET:HB2	1.96	0.47
1:A:286:LEU:HD23	1:A:317:ILE:HD13	1.97	0.47
1:B:91:TYR:OH	1:B:119:ALA:O	2.29	0.47
1:B:233:PRO:HG2	1:B:236:HIS:HB2	1.97	0.47
1:B:314:ILE:HG23	1:B:330:PHE:CD2	2.50	0.47
1:B:383:VAL:HG23	1:C:381:ASN:O	2.13	0.47
1:C:48:ARG:NH1	1:C:94:ASP:O	2.48	0.47
1:C:85:ARG:NH2	1:C:185:ASP:OD1	2.47	0.47
1:C:148:GLU:C	1:C:150:PHE:H	2.23	0.47
1:D:3:LEU:CD1	1:D:45:HIS:HB2	2.35	0.47
1:A:73:TRP:CE2	1:A:168:PRO:HD3	2.50	0.47
1:C:121:ARG:NE	1:C:145:ILE:O	2.42	0.47
1:A:188:SER:OG	1:A:204:GLN:HB2	2.15	0.47
1:A:300:ASN:OD1	1:A:321:ARG:NH2	2.45	0.47
1:A:408:LYS:HB3	1:A:408:LYS:HE2	1.64	0.46
1:C:49:PRO:HG3	1:C:59:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ILE:O	1:D:127:LEU:HB2	2.14	0.46
1:C:12:GLU:OE1	1:C:12:GLU:N	2.48	0.46
1:C:126:GLU:O	1:C:130:GLN:HG3	2.16	0.46
1:D:10:THR:HG23	1:D:13:GLN:OE1	2.16	0.46
1:C:294:GLY:HA2	1:C:297:ASP:OD1	2.15	0.46
1:A:297:ASP:HB3	1:A:325:ARG:HD3	1.98	0.46
1:B:28:LEU:HD11	1:B:244:THR:CG2	2.35	0.46
1:B:40:GLU:HA	1:B:64:LEU:HD12	1.98	0.46
1:D:228:MET:HE1	1:D:277:MET:CB	2.46	0.46
1:B:73:TRP:HA	1:B:168:PRO:HG3	1.98	0.46
1:B:83:ARG:HA	1:B:83:ARG:HD3	1.77	0.46
1:B:299:VAL:HG11	1:B:302:TRP:CD2	2.51	0.46
1:A:229:MET:HE3	1:A:273:PRO:HG3	1.97	0.46
1:B:39:PRO:HB2	1:B:64:LEU:HG	1.98	0.46
1:C:202:VAL:HG12	1:C:204:GLN:HE22	1.81	0.46
1:C:29:LEU:HD11	1:C:66:LEU:HG	1.97	0.46
1:C:259:THR:OG1	1:C:260:SER:N	2.49	0.46
1:A:190:LEU:HD23	1:A:235:SER:O	2.16	0.45
1:A:210:VAL:HG23	1:A:214:ARG:NH1	2.31	0.45
1:D:14:ARG:NH1	1:D:220:HIS:O	2.49	0.45
1:D:140:LEU:HD23	1:D:140:LEU:HA	1.66	0.45
1:D:418:MET:HB3	1:D:418:MET:HE2	1.51	0.45
1:A:183:ASP:CG	1:A:207:ARG:HD3	2.41	0.45
1:B:372:ARG:HD3	1:B:382:GLU:OE2	2.16	0.45
1:C:40:GLU:H	1:C:40:GLU:CD	2.25	0.45
1:D:120:SER:OG	1:D:123:ILE:HG12	2.17	0.45
1:D:127:LEU:HD13	1:D:199:PRO:HB2	1.97	0.45
1:B:356:ASP:OD1	1:B:356:ASP:N	2.47	0.45
1:D:38:HIS:HB3	1:D:41:LEU:HG	1.99	0.45
1:A:358:CYS:HB2	1:A:428:PHE:CE2	2.51	0.45
1:B:120:SER:OG	1:B:123:ILE:HG12	2.16	0.45
1:B:85:ARG:HG3	1:B:85:ARG:HH11	1.82	0.45
1:C:319:GLY:C	1:C:321:ARG:H	2.24	0.45
1:D:343:VAL:O	1:D:363:VAL:HG22	2.16	0.45
1:A:262:PRO:O	1:A:265:ALA:HB3	2.17	0.45
1:C:107:GLN:OE1	1:C:178:ARG:NH1	2.44	0.45
1:D:17:LEU:HD21	1:D:248:LEU:HB3	1.99	0.45
1:D:278:ALA:HB3	1:D:283:TYR:CE2	2.52	0.45
1:A:85:ARG:HA	1:A:85:ARG:HD3	1.80	0.44
1:B:202:VAL:HG12	1:B:204:GLN:HE22	1.81	0.44
1:C:156:LEU:HD12	1:C:157:ARG:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:SER:N	1:D:401:SER:OG	2.50	0.44
1:A:116:ASN:HA	1:A:235:SER:OG	2.17	0.44
1:C:200:LYS:HB3	1:C:397:TYR:CE1	2.52	0.44
1:D:233:PRO:HD3	1:D:258:ASP:HB2	1.98	0.44
1:B:173:LEU:HD12	1:B:174:PRO:HD2	1.98	0.44
1:B:286:LEU:HD23	1:B:317:ILE:HG12	1.99	0.44
1:A:143:LEU:HA	1:A:146:LEU:HD12	1.99	0.44
1:A:262:PRO:O	1:A:266:LYS:HG3	2.17	0.44
1:D:335:GLY:HA2	1:D:339:LEU:HD12	1.99	0.44
1:D:420:TYR:CE2	1:D:428:PHE:HB2	2.52	0.44
1:B:113:VAL:HG22	1:B:189:ILE:HB	2.00	0.44
1:C:229:MET:HE2	1:C:256:TRP:CG	2.52	0.44
1:C:350:LEU:HD12	1:C:350:LEU:HA	1.61	0.44
1:D:87:ARG:HD3	1:D:87:ARG:N	2.32	0.44
1:A:296:ILE:HD11	1:A:320:MET:HB3	1.98	0.44
1:D:51:THR:HA	1:D:56:GLU:O	2.18	0.44
1:D:283:TYR:HE1	1:D:302:TRP:CE3	2.36	0.44
1:A:256:TRP:CD1	1:A:257:TYR:H	2.35	0.44
1:B:232:LEU:CD1	1:B:239:CYS:HB2	2.48	0.44
1:C:216:ARG:HD3	1:C:245:TYR:CZ	2.53	0.44
1:D:311:GLU:OE1	1:D:348:ARG:HD3	2.18	0.44
1:B:121:ARG:NE	1:B:145:ILE:O	2.50	0.43
1:D:275:THR:HG23	1:D:301:VAL:O	2.18	0.43
1:A:260:SER:OG	1:A:263:GLU:HG3	2.18	0.43
1:C:64:LEU:HA	1:C:64:LEU:HD23	1.68	0.43
1:B:49:PRO:HB3	1:B:59:THR:CG2	2.47	0.43
1:C:46:LEU:HD21	1:C:61:LEU:HD12	2.01	0.43
1:D:232:LEU:CD2	1:D:305:ILE:HD11	2.39	0.43
1:A:76:TRP:O	1:A:79:LYS:N	2.52	0.43
1:A:344:LEU:HD23	1:A:362:PRO:HA	1.99	0.43
1:D:163:GLU:O	1:D:166:PRO:HD3	2.18	0.43
1:D:291:LEU:HD12	1:D:320:MET:SD	2.59	0.43
1:B:29:LEU:HD21	1:B:66:LEU:HD23	2.00	0.43
1:C:230:THR:OG1	1:C:255:PRO:HA	2.19	0.43
1:A:127:LEU:HD13	1:A:199:PRO:HB2	2.00	0.43
1:B:5:HIS:NE2	1:B:225:GLY:HA2	2.33	0.43
1:B:228:MET:O	1:B:253:LEU:HD12	2.18	0.43
1:B:397:TYR:CE2	1:B:403:THR:HG22	2.54	0.43
1:C:53:PRO:HD2	1:C:68:GLU:OE1	2.19	0.43
1:C:62:SER:H	1:C:65:ASP:HB2	1.84	0.43
1:C:344:LEU:HD23	1:C:362:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:TRP:CZ3	1:A:80:GLN:HG3	2.54	0.43
1:A:126:GLU:HG2	1:A:199:PRO:HD2	2.00	0.43
1:C:91:TYR:CE2	1:C:146:LEU:HD21	2.54	0.43
1:D:40:GLU:HG2	1:D:41:LEU:HD23	2.01	0.43
1:D:116:ASN:OD1	1:D:117:SER:N	2.52	0.43
1:D:340:GLY:HA3	1:D:392:ALA:O	2.18	0.43
1:A:217:LEU:HD23	1:A:217:LEU:HA	1.77	0.42
1:A:423:GLU:N	1:A:423:GLU:OE1	2.50	0.42
1:C:102:PHE:CE1	1:C:188:SER:HB3	2.54	0.42
1:C:117:SER:O	1:C:142:HIS:NE2	2.48	0.42
1:C:278:ALA:HB3	1:C:283:TYR:CE2	2.54	0.42
1:D:29:LEU:HD23	1:D:29:LEU:HA	1.84	0.42
1:D:73:TRP:HA	1:D:168:PRO:HG3	2.01	0.42
1:A:73:TRP:HA	1:A:168:PRO:HG3	2.01	0.42
1:B:78:LEU:HD23	1:B:78:LEU:HA	1.73	0.42
1:C:45:HIS:O	1:C:255:PRO:HD2	2.19	0.42
1:A:275:THR:HG23	1:A:301:VAL:HG13	2.01	0.42
1:C:183:ASP:CG	1:C:207:ARG:HD3	2.44	0.42
1:D:278:ALA:O	1:D:304:SER:HA	2.17	0.42
1:A:46:LEU:HD13	1:A:49:PRO:HA	2.01	0.42
1:A:56:GLU:HG2	1:A:57:GLN:O	2.19	0.42
1:A:136:VAL:HG11	1:A:150:PHE:HE2	1.85	0.42
1:C:294:GLY:HA2	1:C:297:ASP:CG	2.44	0.42
1:A:183:ASP:CB	1:A:207:ARG:HB2	2.49	0.42
1:B:232:LEU:HD22	1:B:305:ILE:HD11	2.01	0.42
1:B:269:GLU:HG2	1:B:272:ARG:HH21	1.84	0.42
1:D:83:ARG:HD2	1:D:83:ARG:HA	1.88	0.42
1:C:2:THR:HB	1:C:3:LEU:H	1.70	0.42
1:C:41:LEU:HA	1:C:42:PRO:HD3	1.83	0.42
1:A:191:HIS:CD2	1:A:191:HIS:N	2.88	0.42
1:B:383:VAL:HG21	1:C:420:TYR:CD1	2.55	0.42
1:D:310:HIS:HB2	1:D:313:HIS:CE1	2.54	0.42
1:A:350:LEU:HD12	1:A:350:LEU:HA	1.73	0.42
1:C:149:GLU:H	1:C:149:GLU:HG3	1.65	0.42
1:A:140:LEU:HG	1:A:163:GLU:HG3	2.01	0.41
1:A:409:LEU:HD12	1:A:410:SER:N	2.34	0.41
1:B:353:GLU:CD	1:B:353:GLU:N	2.78	0.41
1:C:53:PRO:HB2	1:C:170:PRO:HB3	2.00	0.41
1:D:243:SER:O	1:D:247:VAL:HG23	2.19	0.41
1:A:345:LEU:HD12	1:A:346:LYS:N	2.34	0.41
1:D:92:LEU:HD11	1:D:137:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:O	1:A:60:GLU:HA	2.21	0.41
1:A:352:ASP:O	1:A:353:GLU:O	2.38	0.41
1:D:421:ARG:HA	1:D:426:ASN:O	2.21	0.41
1:A:46:LEU:HB2	1:A:59:THR:O	2.21	0.41
1:A:414:LEU:HA	1:A:414:LEU:HD23	1.85	0.41
1:C:274:THR:HB	1:C:300:ASN:ND2	2.35	0.41
1:C:289:ALA:HB3	1:C:291:LEU:HD21	2.03	0.41
1:C:338:GLU:OE1	1:C:338:GLU:N	2.51	0.41
1:A:346:LYS:NZ	1:A:358:CYS:O	2.53	0.41
1:B:63:LEU:HA	1:B:63:LEU:HD23	1.74	0.41
1:C:345:LEU:O	1:C:360:GLY:HA3	2.20	0.41
1:D:226:ALA:O	1:D:252:PRO:HG2	2.20	0.41
1:B:32:ALA:HB2	1:B:248:LEU:HD23	2.02	0.41
1:B:203:ILE:HD11	1:B:398:TRP:HA	2.03	0.41
1:C:307:ASP:OD1	1:C:307:ASP:N	2.54	0.41
1:A:78:LEU:HA	1:A:78:LEU:HD23	1.55	0.41
1:B:72:SER:HB3	1:B:168:PRO:HG2	2.02	0.41
1:B:127:LEU:HD13	1:B:199:PRO:HB2	2.02	0.41
1:B:400:ASP:OD2	1:B:403:THR:HB	2.21	0.41
1:C:85:ARG:HD2	1:D:405:TYR:C	2.46	0.41
1:C:186:PRO:HG3	1:D:405:TYR:CZ	2.55	0.41
1:D:289:ALA:O	1:D:291:LEU:HG	2.20	0.41
1:C:75:VAL:HG12	1:C:79:LYS:HE3	2.03	0.41
1:B:53:PRO:O	1:B:170:PRO:HD3	2.21	0.40
1:A:140:LEU:HD12	1:A:163:GLU:HG3	2.02	0.40
1:A:346:LYS:HE2	1:A:346:LYS:HB3	1.53	0.40
1:B:229:MET:HE2	1:B:256:TRP:HB2	2.02	0.40
1:C:156:LEU:HD12	1:C:157:ARG:N	2.35	0.40
1:C:400:ASP:OD2	1:C:403:THR:HB	2.21	0.40
1:A:173:LEU:HD12	1:A:174:PRO:HD2	2.02	0.40
1:A:260:SER:OG	1:A:262:PRO:HD2	2.21	0.40
1:B:138:THR:O	1:B:161:VAL:HA	2.21	0.40
1:C:31:LYS:HA	1:C:31:LYS:HD3	1.77	0.40
1:C:40:GLU:OE1	1:C:40:GLU:N	2.52	0.40
1:C:203:ILE:HG21	1:C:203:ILE:HD13	1.86	0.40
1:D:370:VAL:HG23	1:D:427:TYR:HE2	1.86	0.40

All (1) 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:A:85:ARG:NH1	1:B:405:TYR:O[1_655]	2.16	0.04

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	431/577 (75%)	394 (91%)	28 (6%)	9 (2%)	5	24
1	B	431/577 (75%)	395 (92%)	33 (8%)	3 (1%)	18	47
1	C	431/577 (75%)	400 (93%)	23 (5%)	8 (2%)	6	26
1	D	431/577 (75%)	393 (91%)	33 (8%)	5 (1%)	10	35
All	All	1724/2308 (75%)	1582 (92%)	117 (7%)	25 (2%)	8	30

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	353	GLU
1	A	431	ASP
1	C	154	PRO
1	C	320	MET
1	A	206	HIS
1	C	248	LEU
1	D	194	GLY
1	D	195	THR
1	A	94	ASP
1	A	123	ILE
1	A	194	GLY
1	A	196	THR
1	A	341	TRP
1	B	94	ASP
1	B	154	PRO
1	C	149	GLU
1	C	174	PRO

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Mol	Chain	Res	Type
1	C	431	ASP
1	C	2	THR
1	D	196	THR
1	D	307	ASP
1	D	398	TRP
1	C	54	SER
1	B	194	GLY
1	A	154	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	352/471 (75%)	351 (100%)	1 (0%)	86	84
1	B	352/471 (75%)	352 (100%)	0	100	100
1	C	352/471 (75%)	351 (100%)	1 (0%)	86	84
1	D	352/471 (75%)	352 (100%)	0	100	100
All	All	1408/1884 (75%)	1406 (100%)	2 (0%)	88	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	VAL
1	C	195	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	381	ASN
1	B	80	GLN
1	B	107	GLN
1	B	130	GLN
1	B	142	HIS

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Mol	Chain	Res	Type
1	D	36	ASN
1	D	310	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	433/577 (75%)	-0.44	1 (0%) 91 87	16, 36, 81, 99	0
1	B	433/577 (75%)	-0.52	1 (0%) 91 87	17, 35, 66, 98	0
1	C	433/577 (75%)	-0.46	3 (0%) 84 73	15, 36, 71, 110	0
1	D	433/577 (75%)	-0.36	4 (0%) 81 68	18, 38, 86, 121	0
All	All	1732/2308 (75%)	-0.44	9 (0%) 87 78	15, 36, 78, 121	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	196	THR	3.8
1	D	195	THR	3.5
1	D	2	THR	3.4
1	C	176	GLU	3.2
1	C	4	SER	2.6
1	D	1	MET	2.4
1	B	195	THR	2.4
1	A	433	ALA	2.1
1	C	2	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.