



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:18 PM EDT

PDB ID : 4HDS / pdb_00004hds
Title : Crystal Structure of ArsAB in Complex with Phenol.
Authors : Newmister, S.A.; Chan, C.H.; Escalante-Semerena, J.C.; Rayment, I.
Deposited on : 2012-10-02
Resolution : 2.40 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

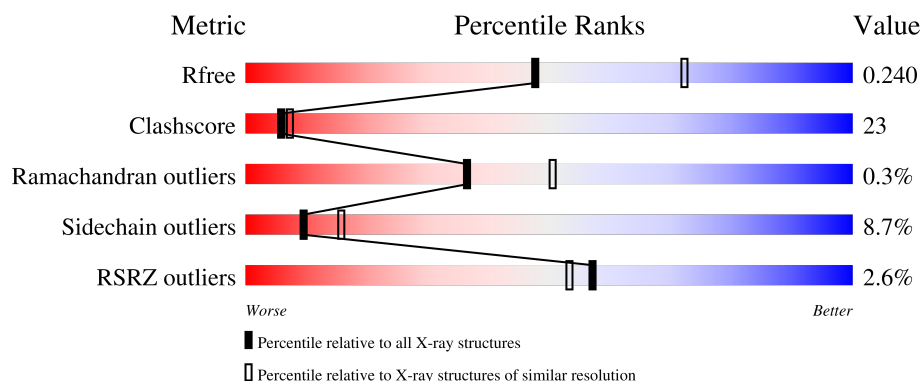
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	348	
2	B	350	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5024 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 ArsA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	4	1	0
			2445	1537	429	461	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP F6MZ55
A	0	GLY	-	expression tag	UNP F6MZ55

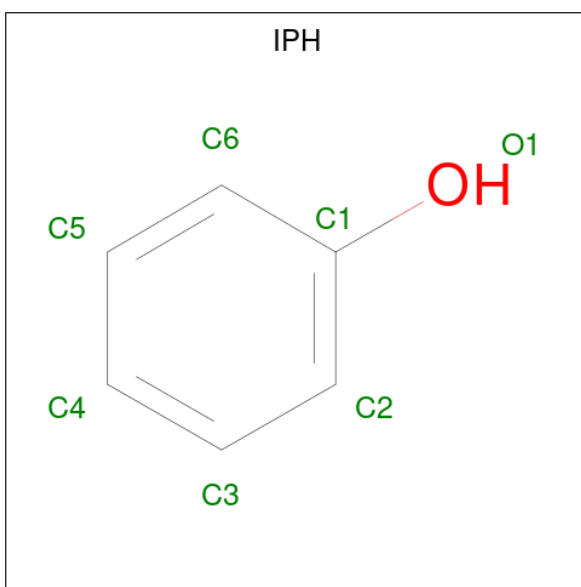
- Molecule 2 is a protein called ArsB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	326	Total	C	N	O	S	0	3	0
			2360	1483	423	434	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP F6MZ56

- Molecule 3 is PHENOL (CCD ID: IPH) (formula: C₆H₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	6	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

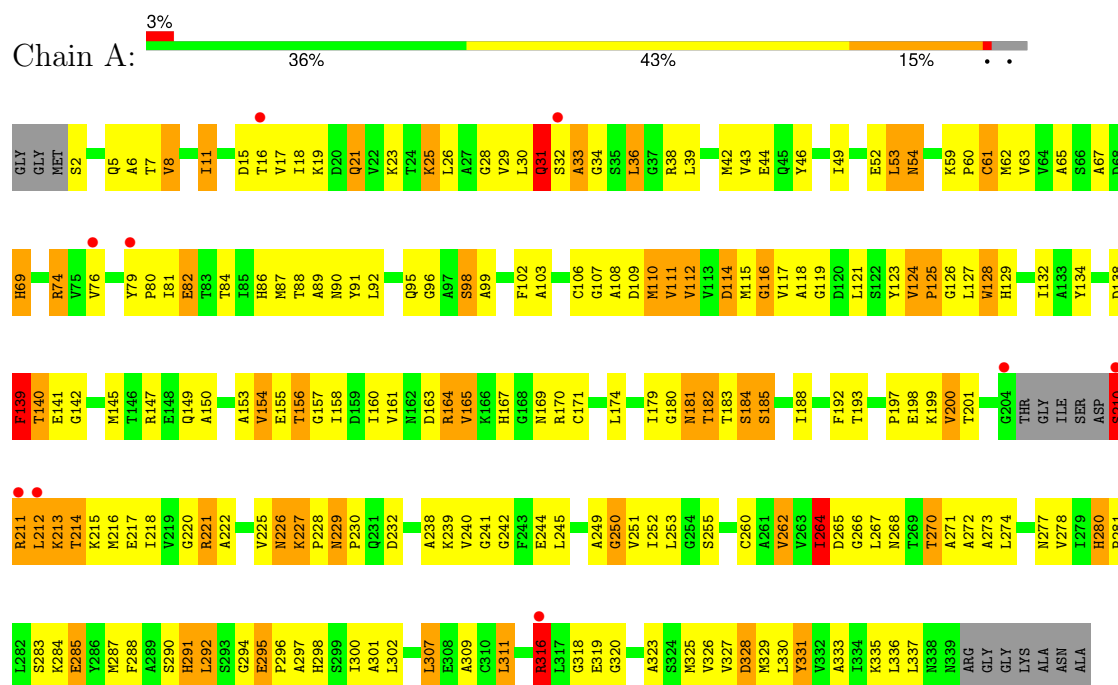
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	66	Total 66	O 66	0	0
5	B	138	Total 138	O 138	0	0

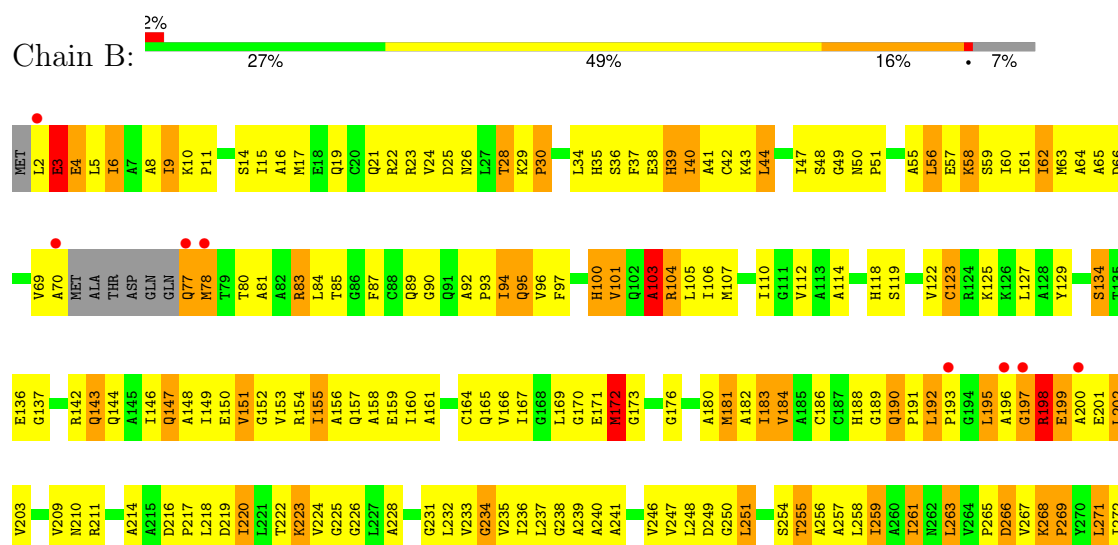
3 Residue-property plots [i](#)

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: ArsaA



• Molecule 2: ArsB



GLN	H275	V291	VAL
ASP	H276	P292	ALA
GLY	F276	A293	GLY
PRO	A277	Y294	PRO
GLY	A278	L295	GLY
ALA	E279	Q296	ALA
LEU	P280	L297	LEU
ARG	A281	V298	ARG
GLN	H282	H299	GLN
SER	E283	N300	SER
LYS	T284	L301	LYS
ASP	A285	G302	ASP
VAL	L286	E303	VAL
ARG	A287	G304	ARG
ASP		T305	ASP
		G306	
		A307	
		A308	
		L309	
		G310	
		H311	
		S312	
		V313	
		L314	
		N315	
		A316	
		T317	
		L318	
		H319	
		N320	
		L321	
		N322	
		H323	
		K324	
		K325	
		T326	
		F327	
		G328	
		E329	
		A330	
		E331	
		V332	
		A333	
		VAL	
		ALA	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.55Å 77.21Å 151.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.76 – 2.40 75.76 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (75.76-2.40) 99.3 (75.76-2.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.205 , 0.241 0.208 , 0.240	Depositor DCC
R_{free} test set	1260 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.974	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5024	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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: IPH, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.41	109/2481 (4.4%)	1.61	36/3362 (1.1%)
2	B	2.69	197/2399 (8.2%)	1.75	54/3256 (1.7%)
All	All	2.55	306/4880 (6.3%)	1.68	90/6618 (1.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	5
All	All	0	7

All (306) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200[A]	VAL	N-CA	-21.62	1.20	1.46
1	A	200[B]	VAL	N-CA	-21.62	1.20	1.46
2	B	123[A]	CYS	N-CA	-17.30	1.24	1.46
2	B	123[B]	CYS	N-CA	-17.30	1.24	1.46
2	B	186[A]	CYS	N-CA	-12.72	1.31	1.46
2	B	186[B]	CYS	N-CA	-12.72	1.31	1.46
2	B	246	VAL	C-O	-10.78	1.12	1.24
2	B	104[A]	ARG	N-CA	-10.08	1.33	1.46
2	B	104[B]	ARG	N-CA	-10.08	1.33	1.46
2	B	211	ARG	C-O	-9.63	1.19	1.23
1	A	63	VAL	C-O	-8.90	1.14	1.24
2	B	247	VAL	C-O	-8.89	1.14	1.24
2	B	95	GLN	C-O	-8.85	1.13	1.24
2	B	308	ALA	C-O	-8.75	1.13	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	21	GLN	C-O	-8.68	1.14	1.24
2	B	147	GLN	C-O	-8.60	1.14	1.24
2	B	275	HIS	CD2-NE2	-8.56	1.28	1.37
2	B	39	HIS	CD2-NE2	-8.54	1.28	1.37
2	B	256	ALA	C-O	-8.49	1.14	1.24
2	B	282	HIS	CD2-NE2	-8.46	1.28	1.37
2	B	258	LEU	C-O	-8.44	1.14	1.24
1	A	38	ARG	C-O	-8.43	1.13	1.24
2	B	166	VAL	C-O	-8.31	1.15	1.24
1	A	114	ASP	C-O	-8.27	1.13	1.24
2	B	319	HIS	CD2-NE2	-8.24	1.28	1.37
2	B	36	SER	C-O	-8.20	1.14	1.24
2	B	48	SER	C-O	-8.18	1.14	1.24
2	B	319	HIS	CG-ND1	-8.06	1.29	1.38
2	B	100	HIS	CD2-NE2	-8.02	1.29	1.37
1	A	86	HIS	CG-ND1	-8.00	1.29	1.38
2	B	39	HIS	CG-ND1	-7.99	1.29	1.38
2	B	282	HIS	CG-ND1	-7.92	1.29	1.38
1	A	227	LYS	C-O	-7.88	1.20	1.23
2	B	183	ILE	C-O	-7.87	1.15	1.24
2	B	87	PHE	C-O	-7.84	1.15	1.24
2	B	268	LYS	C-O	-7.75	1.17	1.24
2	B	279	GLU	CA-C	-7.65	1.44	1.52
2	B	143	GLN	C-O	-7.64	1.15	1.24
2	B	250	GLY	C-O	-7.64	1.16	1.23
2	B	35	HIS	CG-ND1	-7.60	1.29	1.38
1	A	156	THR	C-O	-7.59	1.15	1.24
1	A	241	GLY	C-O	-7.53	1.16	1.23
1	A	251	VAL	C-O	-7.50	1.15	1.24
2	B	232	LEU	C-O	-7.49	1.15	1.24
2	B	254	SER	C-O	-7.46	1.15	1.24
1	A	291	HIS	CD2-NE2	-7.45	1.29	1.37
2	B	304	GLY	C-O	-7.43	1.13	1.23
1	A	167	HIS	CG-ND1	-7.42	1.30	1.38
1	A	46	TYR	C-O	-7.40	1.15	1.24
2	B	41	ALA	C-O	-7.36	1.15	1.24
2	B	188	HIS	CG-ND1	-7.32	1.30	1.38
2	B	35	HIS	CD2-NE2	-7.30	1.29	1.37
1	A	86	HIS	CD2-NE2	-7.25	1.29	1.37
2	B	275	HIS	CG-ND1	-7.22	1.30	1.38
2	B	62	ILE	C-O	-7.15	1.16	1.24
2	B	238	GLY	C-O	-7.13	1.15	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	257	ALA	C-O	-7.13	1.15	1.24
2	B	40	ILE	C-O	-7.12	1.15	1.24
2	B	312	SER	C-O	-7.11	1.15	1.24
2	B	306	GLY	C-O	-7.09	1.15	1.23
2	B	97	PHE	C-O	-7.05	1.15	1.24
2	B	61	ILE	C-O	-7.03	1.16	1.24
2	B	218	LEU	C-O	-7.01	1.15	1.24
2	B	154	ARG	C-O	-6.98	1.16	1.24
2	B	322	ASN	C-O	-6.97	1.15	1.24
2	B	317	THR	C-O	-6.97	1.16	1.24
2	B	84	LEU	C-O	-6.95	1.16	1.24
1	A	325	MET	C-O	-6.93	1.16	1.24
1	A	167	HIS	CD2-NE2	-6.92	1.30	1.37
2	B	295	LEU	C-O	-6.91	1.15	1.24
2	B	63	MET	C-O	-6.88	1.15	1.24
2	B	100	HIS	CG-ND1	-6.85	1.30	1.38
2	B	110	ILE	C-O	-6.83	1.17	1.24
1	A	273	ALA	C-O	-6.82	1.16	1.24
1	A	318	GLY	C-O	-6.79	1.14	1.23
2	B	44	LEU	C-O	-6.79	1.16	1.24
2	B	324	MET	C-O	-6.79	1.15	1.23
1	A	89	ALA	C-O	-6.75	1.16	1.24
2	B	60	ILE	C-O	-6.72	1.16	1.24
2	B	292	PRO	C-O	-6.68	1.16	1.23
2	B	188	HIS	CD2-NE2	-6.67	1.30	1.37
2	B	285	ALA	C-O	-6.67	1.16	1.24
1	A	298	HIS	CD2-NE2	-6.66	1.30	1.37
2	B	240	ALA	C-O	-6.65	1.16	1.24
1	A	39	LEU	C-O	-6.61	1.16	1.24
2	B	23	ARG	C-O	-6.60	1.16	1.24
1	A	287	MET	C-O	-6.59	1.15	1.23
1	A	171	CYS	C-O	-6.58	1.16	1.24
1	A	67	ALA	C-O	-6.58	1.15	1.23
2	B	57	GLU	C-O	-6.56	1.16	1.24
1	A	149	GLN	C-O	-6.51	1.16	1.24
2	B	129	TYR	C-O	-6.50	1.16	1.23
2	B	265	PRO	C-O	-6.49	1.16	1.24
1	A	311	LEU	C-O	-6.48	1.16	1.24
1	A	262	VAL	C-O	-6.47	1.17	1.24
1	A	69	HIS	CD2-NE2	-6.45	1.30	1.37
2	B	119	SER	C-O	-6.44	1.17	1.24
2	B	118	HIS	CG-ND1	-6.43	1.31	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	157	GLN	C-O	-6.43	1.16	1.24
1	A	157	GLY	C-O	-6.39	1.16	1.23
2	B	35	HIS	C-O	-6.38	1.16	1.24
1	A	102	PHE	C-O	-6.38	1.16	1.24
2	B	184	VAL	C-O	-6.36	1.16	1.24
1	A	116	GLY	C-O	-6.36	1.15	1.23
1	A	291	HIS	CG-ND1	-6.35	1.31	1.38
2	B	237	LEU	C-O	-6.35	1.16	1.24
2	B	101	VAL	C-O	-6.34	1.17	1.24
1	A	139	PHE	C-O	-6.34	1.15	1.24
2	B	305	THR	C-O	-6.33	1.16	1.24
2	B	153	VAL	C-O	-6.31	1.17	1.24
1	A	128	TRP	NE1-CE2	-6.30	1.30	1.37
2	B	112	VAL	C-O	-6.28	1.17	1.24
2	B	313	VAL	C-O	-6.28	1.16	1.24
1	A	300	ILE	C-O	-6.25	1.17	1.24
1	A	42	MET	C-O	-6.25	1.17	1.24
1	A	245	LEU	C-O	-6.23	1.17	1.24
2	B	291	VAL	C-O	-6.21	1.17	1.24
2	B	114	ALA	C-O	-6.19	1.16	1.23
2	B	318	LEU	C-O	-6.19	1.16	1.24
2	B	125	LYS	C-O	-6.16	1.15	1.23
2	B	164	CYS	C-O	-6.16	1.16	1.23
2	B	331	GLU	C-O	-6.16	1.16	1.24
2	B	251	LEU	C-O	-6.15	1.17	1.24
2	B	272	ILE	C-O	-6.14	1.17	1.24
1	A	267	LEU	C-O	-6.14	1.17	1.24
1	A	82	GLU	C-O	-6.13	1.16	1.24
2	B	269	PRO	C-O	-6.13	1.16	1.24
1	A	129	HIS	CG-ND1	-6.13	1.31	1.38
1	A	11	ILE	C-O	-6.12	1.17	1.24
1	A	98	SER	C-O	-6.09	1.16	1.24
2	B	55	ALA	C-O	-6.09	1.16	1.23
2	B	266	ASP	C-O	-6.08	1.16	1.24
1	A	84	THR	C-O	-6.08	1.17	1.24
1	A	250	GLY	C-O	-6.07	1.16	1.23
2	B	10	LYS	C-O	-6.07	1.16	1.24
1	A	320	GLY	C-O	-6.06	1.16	1.24
1	A	331	TYR	C-O	-6.05	1.17	1.24
2	B	255	THR	C-O	-6.05	1.17	1.24
2	B	225	GLY	C-O	-6.05	1.17	1.23
2	B	302	GLY	C-O	-6.04	1.15	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	22	ARG	C-O	-6.03	1.17	1.24
2	B	287	ALA	C-O	-6.02	1.17	1.24
1	A	153	ALA	C-O	-6.02	1.17	1.24
2	B	105	LEU	C-O	-5.99	1.17	1.24
2	B	159	GLU	C-O	-5.99	1.17	1.24
2	B	226	GLY	C-O	-5.99	1.17	1.23
2	B	30	PRO	C-O	-5.98	1.17	1.23
1	A	298	HIS	CG-ND1	-5.96	1.31	1.38
1	A	249	ALA	C-O	-5.96	1.17	1.24
1	A	242	GLY	C-O	-5.95	1.15	1.23
1	A	119	GLY	C-O	-5.94	1.17	1.23
2	B	106	ILE	C-O	-5.94	1.17	1.24
1	A	164	ARG	C-O	-5.93	1.16	1.24
1	A	272	ALA	C-O	-5.92	1.17	1.24
2	B	38	GLU	C-O	-5.92	1.17	1.24
2	B	314	ILE	C-O	-5.90	1.17	1.24
2	B	83	ARG	C-O	-5.89	1.17	1.24
2	B	104[A]	ARG	C-O	-5.89	1.16	1.24
2	B	104[B]	ARG	C-O	-5.89	1.16	1.24
2	B	271	LEU	C-O	-5.88	1.16	1.24
2	B	148	ALA	C-O	-5.87	1.17	1.24
2	B	123[A]	CYS	C-O	-5.86	1.17	1.24
2	B	123[B]	CYS	C-O	-5.86	1.17	1.24
2	B	127	LEU	C-O	-5.82	1.17	1.24
1	A	288	PHE	C-O	-5.82	1.17	1.24
1	A	125	PRO	CA-C	-5.80	1.46	1.52
2	B	172	MET	C-O	-5.80	1.17	1.23
1	A	328	ASP	C-O	-5.79	1.17	1.24
2	B	248	LEU	C-O	-5.79	1.16	1.23
2	B	286	LEU	C-O	-5.79	1.17	1.24
2	B	47	ILE	C-O	-5.79	1.17	1.24
1	A	197	PRO	C-O	-5.79	1.16	1.24
1	A	270	THR	C-O	-5.79	1.17	1.24
2	B	134	SER	C-O	-5.78	1.16	1.24
2	B	17	MET	C-O	-5.77	1.17	1.24
2	B	96	VAL	C-O	-5.76	1.17	1.24
2	B	93	PRO	C-O	-5.76	1.17	1.24
1	A	103	ALA	C-O	-5.75	1.17	1.24
1	A	112	VAL	C-O	-5.75	1.18	1.24
2	B	56	LEU	C-O	-5.75	1.17	1.23
1	A	81	ILE	C-O	-5.74	1.17	1.24
2	B	181	MET	C-O	-5.74	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	94	ILE	C-O	-5.74	1.17	1.24
2	B	42	CYS	C-O	-5.73	1.17	1.24
1	A	184	SER	C-O	-5.73	1.17	1.24
2	B	155	ILE	C-O	-5.73	1.17	1.24
2	B	233	VAL	C-O	-5.72	1.17	1.24
2	B	234	GLY	C-O	-5.72	1.17	1.23
1	A	49	ILE	C-O	-5.71	1.17	1.24
2	B	222	THR	C-O	-5.71	1.17	1.24
2	B	156	ALA	N-CA	-5.70	1.39	1.46
2	B	160	ILE	C-O	-5.70	1.17	1.24
2	B	299	MET	C-O	-5.70	1.17	1.24
2	B	315	ASN	C-O	-5.70	1.17	1.24
1	A	111	VAL	C-O	-5.69	1.18	1.24
1	A	215	LYS	C-O	-5.69	1.17	1.24
1	A	115	MET	C-O	-5.69	1.16	1.24
2	B	321	LEU	C-O	-5.68	1.17	1.24
1	A	59	LYS	C-O	-5.67	1.17	1.24
2	B	59	SER	C-O	-5.65	1.17	1.23
2	B	278	ALA	C-O	-5.64	1.16	1.23
2	B	50	ASN	C-O	-5.63	1.17	1.24
2	B	263	LEU	C-O	-5.62	1.17	1.24
2	B	15	ILE	N-CA	-5.62	1.39	1.46
1	A	110	MET	C-O	-5.60	1.17	1.24
2	B	167	ILE	C-O	-5.60	1.18	1.24
2	B	64	ALA	C-O	-5.59	1.17	1.24
2	B	152	GLY	C-O	-5.59	1.17	1.23
1	A	326	VAL	C-O	-5.56	1.17	1.24
2	B	320	MET	C-O	-5.56	1.17	1.24
1	A	155	GLU	C-O	-5.56	1.17	1.24
2	B	275	HIS	N-CA	-5.55	1.39	1.45
2	B	267	VAL	C-O	-5.54	1.17	1.24
1	A	69	HIS	CG-ND1	-5.53	1.32	1.38
2	B	249	ASP	C-O	-5.53	1.17	1.24
1	A	65	ALA	C-O	-5.53	1.17	1.24
2	B	144	GLN	C-O	-5.53	1.17	1.24
1	A	302	LEU	C-O	-5.50	1.17	1.24
1	A	129	HIS	CD2-NE2	-5.50	1.31	1.37
2	B	29	LYS	C-O	-5.50	1.17	1.24
1	A	6	ALA	N-CA	-5.49	1.39	1.46
2	B	9	ILE	N-CA	-5.49	1.40	1.46
2	B	182	ALA	C-O	-5.48	1.17	1.24
2	B	80	THR	C-O	-5.47	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	SER	C-O	-5.47	1.17	1.24
1	A	106	CYS	C-O	-5.47	1.16	1.24
1	A	297	ALA	C-O	-5.44	1.17	1.24
2	B	43	LYS	C-O	-5.43	1.17	1.24
2	B	211	ARG	CA-C	-5.43	1.50	1.53
2	B	5	LEU	C-O	-5.43	1.17	1.24
2	B	26	ASN	C-O	-5.42	1.16	1.24
1	A	265	ASP	C-O	-5.42	1.17	1.24
2	B	34	LEU	C-O	-5.40	1.16	1.24
1	A	124	VAL	C-O	-5.40	1.17	1.24
2	B	158	ALA	C-O	-5.37	1.17	1.24
1	A	183	THR	C-O	-5.35	1.17	1.24
2	B	169	LEU	C-O	-5.35	1.17	1.23
2	B	276	PHE	C-O	-5.35	1.17	1.23
1	A	327	VAL	C-O	-5.34	1.18	1.24
2	B	161	ALA	C-O	-5.33	1.17	1.24
1	A	319	GLU	C-O	-5.33	1.16	1.24
2	B	300	ASN	C-O	-5.33	1.16	1.24
2	B	332	VAL	C-O	-5.33	1.18	1.24
1	A	99	ALA	C-O	-5.31	1.18	1.24
1	A	222	ALA	C-O	-5.31	1.18	1.24
2	B	220	ILE	C-O	-5.31	1.18	1.24
2	B	316	ALA	C-O	-5.30	1.18	1.24
1	A	331	TYR	CA-C	-5.29	1.46	1.52
1	A	266	GLY	C-O	-5.28	1.17	1.23
1	A	335	LYS	N-CA	-5.28	1.40	1.46
2	B	51	PRO	C-O	-5.28	1.17	1.24
2	B	142	ARG	C-O	-5.28	1.18	1.24
2	B	171	GLU	C-O	-5.28	1.17	1.23
1	A	179	ILE	C-O	-5.26	1.19	1.24
2	B	261	ILE	C-O	-5.25	1.17	1.24
1	A	200[A]	VAL	C-O	-5.24	1.18	1.24
1	A	200[B]	VAL	C-O	-5.24	1.18	1.24
2	B	241	ALA	C-O	-5.24	1.17	1.24
2	B	49	GLY	C-O	-5.23	1.17	1.24
2	B	118	HIS	CD2-NE2	-5.23	1.32	1.37
2	B	319	HIS	C-O	-5.23	1.18	1.24
2	B	325	LYS	C-O	-5.22	1.17	1.23
1	A	182	THR	C-O	-5.21	1.17	1.24
1	A	218	ILE	C-O	-5.21	1.18	1.24
1	A	126	GLY	C-O	-5.21	1.16	1.24
1	A	323	ALA	C-O	-5.21	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	ILE	C-O	-5.20	1.18	1.24
1	A	107	GLY	C-O	-5.20	1.18	1.24
1	A	154	VAL	C-O	-5.20	1.18	1.24
2	B	151	VAL	C-O	-5.20	1.18	1.24
2	B	327	PHE	C-O	-5.19	1.18	1.24
2	B	293	ALA	C-O	-5.18	1.17	1.23
1	A	61	CYS	N-CA	-5.17	1.39	1.46
1	A	180	GLY	C-O	-5.17	1.17	1.24
2	B	19	GLN	C-O	-5.16	1.18	1.24
2	B	16	ALA	C-O	-5.15	1.18	1.24
2	B	14	SER	C-O	-5.15	1.17	1.24
1	A	255	SER	C-O	-5.14	1.18	1.24
2	B	231	GLY	C-O	-5.13	1.17	1.23
2	B	28	THR	C-O	-5.13	1.18	1.23
1	A	283	SER	C-O	-5.13	1.18	1.24
2	B	228	ALA	C-O	-5.12	1.18	1.24
2	B	15	ILE	C-O	-5.11	1.18	1.24
2	B	186[A]	CYS	C-O	-5.10	1.18	1.24
2	B	186[B]	CYS	C-O	-5.10	1.18	1.24
1	A	88	THR	C-O	-5.09	1.18	1.24
2	B	29	LYS	N-CA	-5.09	1.40	1.46
2	B	66	ASP	C-O	-5.09	1.17	1.23
1	A	193	THR	C-O	-5.08	1.17	1.23
1	A	91	TYR	C-O	-5.08	1.17	1.24
2	B	100	HIS	C-O	-5.08	1.18	1.24
2	B	329	GLU	C-O	-5.07	1.18	1.24
2	B	8	ALA	C-O	-5.07	1.17	1.24
2	B	156	ALA	C-O	-5.07	1.18	1.24
1	A	280	HIS	CD2-NE2	-5.06	1.32	1.37
1	A	181	ASN	C-O	-5.06	1.17	1.24
2	B	235	VAL	C-O	-5.05	1.18	1.24
2	B	310	GLY	C-O	-5.04	1.17	1.23
2	B	37	PHE	C-O	-5.04	1.18	1.24
2	B	239	ALA	C-O	-5.04	1.18	1.24
1	A	220	GLY	C-O	-5.02	1.17	1.23
2	B	24	VAL	C-O	-5.02	1.18	1.24
2	B	34	LEU	N-CA	-5.02	1.39	1.46
1	A	271	ALA	C-O	-5.00	1.18	1.24
2	B	25	ASP	C-O	-5.00	1.17	1.24
2	B	176	GLY	C-O	-5.00	1.17	1.23

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	186[A]	CYS	CA-C-O	-17.84	102.27	121.00
2	B	186[B]	CYS	CA-C-O	-17.84	102.27	121.00
1	A	200[A]	VAL	CA-C-O	-16.30	101.56	120.96
1	A	200[B]	VAL	CA-C-O	-16.30	101.56	120.96
2	B	198	ARG	N-CA-C	-12.62	97.52	111.28
2	B	122	VAL	CA-C-N	9.45	136.40	121.66
2	B	122	VAL	C-N-CA	9.45	136.40	121.66
1	A	163	ASP	N-CA-C	9.42	121.31	111.14
2	B	155	ILE	N-CA-C	9.38	119.43	110.42
2	B	223	LYS	N-CA-C	8.94	120.80	111.14
2	B	103	ALA	CA-C-N	8.93	138.60	121.54
2	B	103	ALA	C-N-CA	8.93	138.60	121.54
1	A	201	THR	N-CA-C	8.81	120.97	111.36
2	B	197	GLY	N-CA-C	8.50	122.36	112.50
2	B	322	ASN	N-CA-C	8.01	120.09	111.36
1	A	199	LYS	N-CA-C	7.87	119.86	111.28
1	A	102	PHE	N-CA-C	7.73	119.78	111.36
1	A	239	LYS	N-CA-C	7.53	119.27	111.14
1	A	33	ALA	N-CA-C	7.50	119.53	111.36
1	A	213	LYS	N-CA-C	7.25	120.34	110.55
1	A	15	ASP	CA-C-N	7.13	130.55	120.28
1	A	15	ASP	C-N-CA	7.13	130.55	120.28
1	A	8	VAL	N-CA-C	6.92	117.68	110.62
2	B	228	ALA	N-CA-C	6.88	118.43	111.07
2	B	29	LYS	N-CA-C	-6.87	102.04	108.22
1	A	31	GLN	CB-CA-C	-6.65	107.03	116.34
1	A	311	LEU	N-CA-C	6.63	119.72	108.90
1	A	264	ILE	N-CA-C	6.47	117.11	110.05
2	B	48	SER	N-CA-C	6.47	118.42	111.36
2	B	251	LEU	N-CA-C	6.45	118.31	111.28
2	B	271	LEU	N-CA-C	6.41	119.95	109.76
2	B	122	VAL	N-CA-C	6.39	117.08	107.75
2	B	104[A]	ARG	N-CA-CB	6.31	121.16	110.49
2	B	104[B]	ARG	N-CA-CB	6.31	121.16	110.49
1	A	316	ARG	N-CA-C	6.18	118.09	111.36
2	B	199	GLU	CB-CA-C	-6.15	101.49	110.96
1	A	287	MET	N-CA-C	6.11	119.86	110.20
2	B	123[A]	CYS	CA-C-O	-6.04	113.44	120.62
2	B	123[B]	CYS	CA-C-O	-6.04	113.44	120.62
2	B	199	GLU	N-CA-C	6.02	117.53	110.97
1	A	294	GLY	N-CA-C	-5.96	101.87	111.59
2	B	236	ILE	N-CA-C	5.94	116.12	110.42
1	A	241	GLY	N-CA-C	5.91	121.28	112.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	50	ASN	CA-C-N	5.91	125.78	119.28
2	B	50	ASN	C-N-CA	5.91	125.78	119.28
1	A	226	ASN	CA-C-N	-5.83	116.54	122.83
1	A	226	ASN	C-N-CA	-5.83	116.54	122.83
1	A	210	SER	CA-C-N	5.79	128.59	121.64
1	A	210	SER	C-N-CA	5.79	128.59	121.64
1	A	292	LEU	N-CA-C	5.74	117.61	111.36
2	B	268	LYS	CA-C-N	5.72	125.40	119.56
2	B	268	LYS	C-N-CA	5.72	125.40	119.56
2	B	249	ASP	CA-C-N	5.62	128.73	122.55
2	B	249	ASP	C-N-CA	5.62	128.73	122.55
2	B	192	LEU	CA-C-N	5.61	125.79	119.90
2	B	192	LEU	C-N-CA	5.61	125.79	119.90
1	A	59	LYS	CB-CA-C	5.61	115.49	110.44
1	A	291	HIS	CA-C-N	5.60	128.24	120.29
1	A	291	HIS	C-N-CA	5.60	128.24	120.29
2	B	42	CYS	N-CA-C	5.53	117.31	111.28
2	B	197	GLY	CA-C-N	-5.50	112.91	120.28
2	B	197	GLY	C-N-CA	-5.50	112.91	120.28
2	B	263	LEU	N-CA-C	5.49	117.06	111.14
2	B	246	VAL	N-CA-C	5.44	115.69	107.80
1	A	28	GLY	N-CA-C	5.42	119.71	112.77
2	B	203	VAL	CB-CA-C	-5.42	105.04	111.97
2	B	183	ILE	N-CA-C	5.41	116.14	110.62
1	A	229	ASN	CA-C-N	5.37	125.02	119.05
1	A	229	ASN	C-N-CA	5.37	125.02	119.05
2	B	188	HIS	N-CA-C	5.31	117.15	111.36
2	B	232	LEU	N-CA-C	5.30	117.06	111.28
2	B	190	GLN	CA-C-N	5.29	125.54	119.83
2	B	190	GLN	C-N-CA	5.29	125.54	119.83
1	A	87	MET	N-CA-C	5.28	117.04	111.28
2	B	110	ILE	CB-CA-C	5.25	115.68	111.06
1	A	295	GLU	CA-C-N	5.25	124.87	119.05
1	A	295	GLU	C-N-CA	5.25	124.87	119.05
2	B	64	ALA	N-CA-C	5.22	117.47	109.07
2	B	4	GLU	N-CA-C	5.21	116.77	111.14
1	A	54	ASN	CA-C-N	5.16	125.08	119.76
1	A	54	ASN	C-N-CA	5.16	125.08	119.76
2	B	176	GLY	N-CA-C	5.13	118.89	112.73
2	B	167	ILE	N-CA-C	5.11	115.21	107.80
2	B	169	LEU	CA-C-N	5.10	125.54	121.61
2	B	169	LEU	C-N-CA	5.10	125.54	121.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	ILE	N-CA-C	5.06	115.78	110.62
1	A	74	ARG	CB-CA-C	-5.04	102.91	111.02
2	B	127	LEU	N-CA-C	5.03	116.84	111.36
2	B	155	ILE	CB-CA-C	-5.01	105.55	111.97
2	B	56	LEU	N-CA-C	5.00	117.54	108.69

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	200[A]	VAL	Mainchain
1	A	200[B]	VAL	Mainchain
2	B	103	ALA	Peptide
2	B	104[B]	ARG	Mainchain
2	B	123[A]	CYS	Mainchain
2	B	123[B]	CYS	Mainchain

5.2 Too-close contacts [i](#)

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	2445	0	2506	132	0
2	B	2360	0	2456	106	0
3	A	7	0	6	1	0
4	B	8	0	12	1	0
5	A	66	0	0	8	0
5	B	138	0	0	8	0
All	All	5024	0	4980	225	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 23.

All (225) 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:211:ARG:HH11	1:A:211:ARG:CB	1.49	1.23

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:NH1	1:A:211:ARG:HB3	1.60	1.14
1:A:211:ARG:HH11	1:A:211:ARG:HB3	1.02	1.10
2:B:214:ALA:HA	2:B:220:ILE:HD11	1.32	1.09
1:A:221:ARG:HG3	1:A:221:ARG:HH11	1.02	1.08
2:B:196:ALA:O	2:B:199:GLU:HB2	1.53	1.06
1:A:295:GLU:HB2	1:A:296:PRO:HD2	1.31	1.04
2:B:181:MET:CE	2:B:280:PRO:HG2	1.90	1.01
1:A:161:VAL:O	1:A:165:VAL:HG13	1.62	0.99
1:A:33:ALA:HB2	2:B:78:MET:CE	1.94	0.97
1:A:211:ARG:HH11	1:A:211:ARG:CG	1.76	0.97
2:B:181:MET:HE1	2:B:280:PRO:HG2	1.45	0.97
1:A:212:LEU:HD22	1:A:213:LYS:N	1.82	0.94
2:B:197:GLY:O	2:B:201:GLU:HG3	1.68	0.93
1:A:212:LEU:CD2	1:A:213:LYS:N	2.32	0.92
1:A:36:LEU:HD12	2:B:299:MET:HG2	1.52	0.91
1:A:221:ARG:HH11	1:A:221:ARG:CG	1.85	0.90
2:B:181:MET:HE1	2:B:280:PRO:CG	2.02	0.90
1:A:212:LEU:HD23	1:A:213:LYS:H	1.37	0.89
1:A:221:ARG:HG3	1:A:221:ARG:NH1	1.74	0.88
2:B:191:PRO:O	5:B:1038:HOH:O	1.93	0.87
1:A:212:LEU:HD22	1:A:212:LEU:C	2.01	0.85
1:A:295:GLU:HB2	1:A:296:PRO:CD	2.07	0.84
2:B:183:ILE:HG21	2:B:259:ILE:HD11	1.59	0.84
1:A:211:ARG:CB	1:A:211:ARG:NH1	2.30	0.83
1:A:211:ARG:NH1	1:A:212:LEU:N	2.28	0.82
1:A:212:LEU:CD2	1:A:213:LYS:H	1.92	0.81
1:A:21:GLN:NE2	5:A:904:HOH:O	2.12	0.80
2:B:146:ILE:O	2:B:150:GLU:HG3	1.82	0.80
2:B:198:ARG:O	2:B:198:ARG:HD3	1.83	0.78
1:A:212:LEU:CD2	1:A:212:LEU:C	2.57	0.78
2:B:81:ALA:O	2:B:85:THR:HG23	1.82	0.78
2:B:136:GLU:OE2	5:B:1029:HOH:O	2.03	0.77
1:A:150:ALA:O	1:A:154:VAL:HG23	1.86	0.76
1:A:211:ARG:NH1	1:A:211:ARG:CG	2.44	0.73
1:A:69:HIS:HE1	1:A:244:GLU:OE2	1.71	0.73
1:A:33:ALA:HB2	2:B:78:MET:HE3	1.70	0.72
1:A:192:PHE:CE1	1:A:278:VAL:HG21	2.24	0.71
2:B:189:GLY:O	2:B:190:GLN:O	2.09	0.71
1:A:210:SER:OG	1:A:211:ARG:N	2.20	0.70
2:B:196:ALA:O	2:B:200:ALA:N	2.20	0.70
1:A:211:ARG:HH12	1:A:212:LEU:N	1.89	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:THR:HG22	1:A:217:GLU:HB2	1.73	0.68
2:B:181:MET:HE2	2:B:280:PRO:HG2	1.74	0.68
2:B:165:GLN:HG2	5:B:1089:HOH:O	1.93	0.67
2:B:198:ARG:HD3	2:B:198:ARG:C	2.17	0.67
2:B:195:LEU:HD13	2:B:200:ALA:HB2	1.77	0.67
1:A:211:ARG:HH11	1:A:211:ARG:HG2	1.62	0.66
2:B:77:GLN:N	2:B:77:GLN:OE1	2.30	0.65
2:B:181:MET:HE1	2:B:280:PRO:CB	2.26	0.65
2:B:196:ALA:C	2:B:199:GLU:HB2	2.22	0.64
2:B:196:ALA:O	2:B:199:GLU:CB	2.38	0.64
2:B:2:LEU:O	2:B:4:GLU:N	2.30	0.64
1:A:36:LEU:CD1	2:B:299:MET:HG2	2.26	0.64
1:A:198:GLU:OE2	1:A:216:MET:HE1	1.97	0.64
1:A:211:ARG:NH1	1:A:212:LEU:H	1.94	0.64
1:A:182:THR:HA	1:A:268:ASN:HD21	1.64	0.63
1:A:211:ARG:NH1	1:A:211:ARG:HG2	2.13	0.63
1:A:32:SER:CB	2:B:77:GLN:HB3	2.29	0.63
1:A:124:VAL:HG12	1:A:127:LEU:HB2	1.80	0.63
1:A:25:LYS:HD2	1:A:337:LEU:CD1	2.28	0.63
2:B:183:ILE:HG21	2:B:259:ILE:CD1	2.27	0.62
2:B:195:LEU:HD13	2:B:195:LEU:O	1.99	0.62
2:B:251:LEU:O	2:B:255:THR:HG23	1.99	0.62
1:A:138:ASP:OD1	1:A:140:THR:HB	1.99	0.62
1:A:33:ALA:HB2	2:B:78:MET:HE1	1.79	0.62
1:A:36:LEU:HD12	2:B:299:MET:CG	2.28	0.62
1:A:25:LYS:HD2	1:A:337:LEU:HD11	1.81	0.62
1:A:69:HIS:CE1	1:A:181:ASN:HB3	2.35	0.61
2:B:181:MET:HE1	2:B:280:PRO:HB2	1.81	0.61
2:B:184:VAL:HB	2:B:192:LEU:HD11	1.82	0.61
1:A:290:SER:O	1:A:309:ALA:HB1	2.01	0.60
1:A:32:SER:HB3	2:B:77:GLN:HB3	1.84	0.60
1:A:17:VAL:HG13	5:A:904:HOH:O	2.01	0.60
1:A:111:VAL:HG13	1:A:128:TRP:CD1	2.38	0.59
1:A:156:THR:O	1:A:160:ILE:HG13	2.02	0.59
1:A:43:VAL:HB	1:A:333:ALA:HB1	1.85	0.59
1:A:214:THR:CG2	1:A:217:GLU:H	2.16	0.59
1:A:226:ASN:O	1:A:227:LYS:C	2.44	0.59
2:B:217:PRO:HG2	2:B:263:LEU:HD23	1.84	0.58
1:A:214:THR:HG22	1:A:217:GLU:CB	2.33	0.58
2:B:69:VAL:HG12	2:B:70:ALA:N	2.17	0.58
2:B:197:GLY:O	2:B:201:GLU:CG	2.47	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:CYS:HA	1:A:109:ASP:O	2.04	0.58
2:B:58:LYS:NZ	2:B:101:VAL:O	2.37	0.57
1:A:92:LEU:HD11	1:A:112:VAL:HB	1.85	0.57
2:B:39:HIS:HE1	5:B:1084:HOH:O	1.87	0.57
2:B:143:GLN:O	2:B:147:GLN:HG3	2.04	0.57
2:B:210:ASN:HB3	2:B:223:LYS:HD3	1.86	0.56
1:A:21:GLN:HB3	1:A:53:LEU:HD21	1.86	0.56
2:B:134:SER:HA	2:B:137:GLY:O	2.05	0.56
1:A:90:ASN:HA	5:A:945:HOH:O	2.06	0.56
2:B:85:THR:O	2:B:89:GLN:HG3	2.05	0.56
1:A:164:ARG:HB3	1:A:169:ASN:OD1	2.06	0.55
1:A:123:TYR:O	1:A:125:PRO:HD3	2.06	0.55
2:B:251:LEU:HD22	2:B:280:PRO:O	2.07	0.55
1:A:295:GLU:CB	1:A:296:PRO:HD2	2.18	0.55
1:A:170:ARG:HG3	1:A:170:ARG:HH11	1.72	0.54
1:A:211:ARG:HH12	1:A:212:LEU:CA	2.19	0.54
1:A:329:MET:HE2	2:B:297:LEU:HD11	1.88	0.54
2:B:268:LYS:HB3	2:B:269:PRO:HD3	1.89	0.54
1:A:211:ARG:O	1:A:213:LYS:CD	2.56	0.54
1:A:82:GLU:HG3	5:A:944:HOH:O	2.07	0.54
2:B:197:GLY:O	2:B:198:ARG:C	2.42	0.54
2:B:183:ILE:CG2	2:B:259:ILE:HD11	2.33	0.54
2:B:9:ILE:HG22	2:B:266:ASP:HB3	1.90	0.53
2:B:69:VAL:CG1	2:B:70:ALA:N	2.70	0.53
1:A:2:SER:HB3	1:A:5:GLN:HE21	1.74	0.53
2:B:251:LEU:HD13	2:B:282:HIS:HA	1.89	0.53
2:B:2:LEU:HA	2:B:6:ILE:HD12	1.89	0.53
2:B:147:GLN:O	2:B:151:VAL:HG23	2.09	0.53
1:A:139:PHE:HA	1:A:142:GLY:O	2.08	0.53
2:B:151:VAL:O	2:B:155:ILE:HG12	2.09	0.53
1:A:274:LEU:O	1:A:278:VAL:HG23	2.09	0.52
1:A:140:THR:HG22	1:A:141:GLU:HG3	1.91	0.52
2:B:189:GLY:C	2:B:190:GLN:O	2.48	0.52
1:A:147:ARG:NH1	1:A:232:ASP:OD2	2.23	0.52
1:A:74:ARG:O	1:A:212:LEU:HD21	2.09	0.51
1:A:69:HIS:CE1	1:A:181:ASN:CB	2.93	0.51
1:A:62:MET:N	1:A:109:ASP:O	2.35	0.51
1:A:74:ARG:NE	1:A:140:THR:HG21	2.26	0.51
1:A:184:SER:O	1:A:188:ILE:HG13	2.09	0.51
2:B:78:MET:HB3	2:B:83:ARG:HH21	1.74	0.51
2:B:280:PRO:O	2:B:281:ALA:HB3	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ASN:HD21	1:A:284:LYS:NZ	2.08	0.51
1:A:60:PRO:HG2	1:A:108:ALA:HA	1.92	0.50
2:B:198:ARG:HD2	2:B:202:LEU:HD22	1.94	0.50
2:B:181:MET:CE	2:B:280:PRO:CG	2.68	0.49
1:A:2:SER:CB	1:A:5:GLN:HE21	2.25	0.49
2:B:3:GLU:H	2:B:3:GLU:CD	2.20	0.49
1:A:7:THR:HG21	1:A:158:ILE:HG21	1.94	0.49
1:A:291:HIS:HA	1:A:311:LEU:HB2	1.94	0.49
1:A:270:THR:HG22	1:A:301:ALA:HB1	1.94	0.49
1:A:264:ILE:HD11	1:A:307:LEU:HD12	1.95	0.49
1:A:7:THR:HG21	1:A:158:ILE:CG2	2.42	0.48
1:A:69:HIS:HD2	5:A:935:HOH:O	1.96	0.48
1:A:221:ARG:NH1	1:A:225:VAL:HG23	2.27	0.48
1:A:328:ASP:O	1:A:331:TYR:HB2	2.13	0.48
1:A:74:ARG:HE	1:A:140:THR:HG21	1.79	0.47
2:B:83:ARG:HD2	2:B:172:MET:HE3	1.96	0.47
2:B:100:HIS:O	4:B:902:EDO:H22	2.13	0.47
1:A:139:PHE:CD2	1:A:240:VAL:HA	2.49	0.47
1:A:32:SER:HB3	2:B:77:GLN:CB	2.44	0.47
1:A:280:HIS:HA	1:A:281:PRO:HD2	1.67	0.47
2:B:2:LEU:O	2:B:3:GLU:C	2.58	0.47
2:B:2:LEU:HB2	2:B:3:GLU:OE2	2.15	0.47
2:B:90:GLY:HA2	2:B:95:GLN:HE22	1.79	0.47
2:B:149:ILE:O	2:B:234:GLY:HA3	2.15	0.47
2:B:192:LEU:HA	2:B:193:PRO:HD3	1.52	0.47
1:A:30:LEU:O	1:A:31:GLN:HB2	2.14	0.46
2:B:180:ALA:O	2:B:184:VAL:HG23	2.15	0.46
1:A:124:VAL:HA	1:A:125:PRO:HD3	1.76	0.46
1:A:198:GLU:HB2	1:A:216:MET:HE3	1.97	0.46
1:A:19:LYS:HB3	1:A:44:GLU:HG2	1.96	0.46
1:A:214:THR:HG22	1:A:217:GLU:H	1.81	0.46
2:B:333:ALA:HB2	5:B:1011:HOH:O	2.16	0.46
1:A:154:VAL:O	1:A:250:GLY:HA3	2.16	0.46
1:A:214:THR:CG2	1:A:216:MET:HG2	2.46	0.46
2:B:11:PRO:HA	5:B:1066:HOH:O	2.16	0.45
1:A:145:MET:HG2	1:A:238:ALA:HA	1.99	0.45
2:B:216:ASP:HB3	2:B:219:ASP:HB2	1.98	0.45
1:A:252:ILE:HG12	1:A:262:VAL:HG21	1.98	0.45
2:B:62:ILE:HG12	2:B:170:GLY:HA3	1.99	0.45
2:B:332:VAL:O	2:B:332:VAL:HG12	2.16	0.45
2:B:327:PHE:O	2:B:331:GLU:HG3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:O	1:A:213:LYS:HD3	2.17	0.45
1:A:174:LEU:HD11	1:A:252:ILE:HD11	1.99	0.45
2:B:198:ARG:O	2:B:201:GLU:HB2	2.16	0.45
1:A:170:ARG:HA	1:A:260:CYS:SG	2.57	0.45
1:A:31:GLN:HB3	1:A:32:SER:H	1.26	0.45
2:B:78:MET:HB3	2:B:83:ARG:NH2	2.32	0.45
1:A:90:ASN:O	1:A:95:GLN:N	2.44	0.44
1:A:214:THR:HG23	1:A:217:GLU:H	1.81	0.44
1:A:32:SER:CB	2:B:77:GLN:CB	2.93	0.44
3:A:801:IPH:C3	2:B:30:PRO:HG3	2.48	0.44
2:B:83:ARG:CG	2:B:172:MET:HE3	2.47	0.44
1:A:211:ARG:HH12	1:A:212:LEU:HB2	1.82	0.44
1:A:307:LEU:HA	1:A:307:LEU:HD23	1.65	0.44
1:A:18:ILE:HD13	1:A:18:ILE:HA	1.67	0.44
2:B:94:ILE:HG12	2:B:303:GLU:O	2.18	0.43
2:B:77:GLN:N	2:B:77:GLN:CD	2.74	0.43
1:A:114:ASP:OD1	1:A:117:VAL:HG23	2.18	0.43
1:A:232:ASP:OD1	5:A:961:HOH:O	2.21	0.43
1:A:316:ARG:N	5:A:958:HOH:O	2.52	0.43
2:B:28:THR:HG22	2:B:327:PHE:CD1	2.54	0.43
2:B:92:ALA:H	2:B:95:GLN:NE2	2.17	0.43
1:A:277:ASN:HD21	1:A:284:LYS:HZ2	1.67	0.43
2:B:90:GLY:HA2	2:B:95:GLN:NE2	2.34	0.43
1:A:214:THR:HG22	1:A:217:GLU:CG	2.49	0.43
1:A:227:LYS:N	1:A:228:PRO:CD	2.81	0.43
1:A:214:THR:O	1:A:217:GLU:HB2	2.18	0.42
2:B:268:LYS:HA	2:B:271:LEU:HD12	2.01	0.42
1:A:292:LEU:HA	1:A:309:ALA:HB3	2.00	0.42
1:A:212:LEU:HD23	1:A:213:LYS:N	2.05	0.42
2:B:220:ILE:O	2:B:224:VAL:HG22	2.19	0.42
2:B:107:MET:HE1	2:B:172:MET:SD	2.60	0.42
2:B:56:LEU:HD12	2:B:318:LEU:HD11	2.00	0.42
2:B:195:LEU:O	2:B:195:LEU:CD1	2.65	0.42
2:B:44:LEU:HD23	2:B:44:LEU:HA	1.88	0.42
1:A:60:PRO:O	1:A:109:ASP:N	2.45	0.42
2:B:40:ILE:O	2:B:44:LEU:HG	2.20	0.42
2:B:83:ARG:HG2	2:B:172:MET:HE3	2.01	0.42
2:B:195:LEU:HD22	2:B:200:ALA:HA	2.01	0.42
1:A:96:GLY:HA3	2:B:325:LYS:CG	2.50	0.41
1:A:8:VAL:HA	1:A:11:ILE:HD12	2.02	0.41
1:A:79:TYR:HA	1:A:80:PRO:HD2	1.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PRO:O	1:A:230:PRO:HD3	2.20	0.41
2:B:65:ALA:O	2:B:173:GLY:HA3	2.20	0.41
1:A:62:MET:O	1:A:110:MET:HA	2.19	0.41
1:A:328:ASP:HA	1:A:331:TYR:CD2	2.55	0.41
2:B:103:ALA:O	5:B:1018:HOH:O	2.22	0.41
2:B:195:LEU:HD13	2:B:195:LEU:C	2.46	0.41
1:A:34:GLY:HA3	2:B:301:LEU:HA	2.01	0.41
2:B:268:LYS:HD3	2:B:268:LYS:C	2.44	0.41
1:A:69:HIS:CD2	5:A:935:HOH:O	2.73	0.41
1:A:185:SER:OG	1:A:268:ASN:HA	2.21	0.41
1:A:229:ASN:HA	1:A:230:PRO:HD2	1.78	0.41
1:A:214:THR:HG23	1:A:216:MET:HG2	2.03	0.41
2:B:197:GLY:C	2:B:199:GLU:N	2.68	0.41
2:B:197:GLY:O	2:B:201:GLU:CB	2.69	0.40
2:B:327:PHE:HE2	5:B:1010:HOH:O	2.05	0.40
1:A:118:ALA:HA	1:A:134:TYR:CD1	2.57	0.40
1:A:121:LEU:HD22	1:A:124:VAL:HG21	2.03	0.40
1:A:285:GLU:H	1:A:285:GLU:HG2	1.43	0.40
2:B:28:THR:HA	2:B:327:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/348 (95%)	323 (98%)	6 (2%)	1 (0%)	36	50
2	B	325/350 (93%)	314 (97%)	10 (3%)	1 (0%)	36	50
All	All	655/698 (94%)	637 (97%)	16 (2%)	2 (0%)	36	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3	GLU
1	A	116	GLY

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	257/264 (97%)	229 (89%)	28 (11%)	6	9
2	B	240/256 (94%)	225 (94%)	15 (6%)	16	29
All	All	497/520 (96%)	454 (91%)	43 (9%)	9	16

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	21	GLN
1	A	23	LYS
1	A	25	LYS
1	A	26	LEU
1	A	29	VAL
1	A	31	GLN
1	A	36	LEU
1	A	52	GLU
1	A	53	LEU
1	A	54	ASN
1	A	76	VAL
1	A	98	SER
1	A	139	PHE
1	A	140	THR
1	A	165	VAL
1	A	210	SER
1	A	211	ARG
1	A	212	LEU
1	A	214	THR
1	A	221	ARG
1	A	253	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	264	ILE
1	A	285	GLU
1	A	307	LEU
1	A	316	ARG
1	A	330	LEU
1	A	336	LEU
2	B	3	GLU
2	B	58	LYS
2	B	77	GLN
2	B	78	MET
2	B	172	MET
2	B	195	LEU
2	B	198	ARG
2	B	202	LEU
2	B	209	VAL
2	B	259	ILE
2	B	261	ILE
2	B	275	HIS
2	B	284	THR
2	B	303	GLU
2	B	312	SER

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

Mol	Chain	Res	Type
1	A	5	GLN
1	A	31	GLN
1	A	69	HIS
1	A	129	HIS
1	A	268	ASN
1	A	277	ASN
1	A	306	GLN
2	B	19	GLN
2	B	39	HIS
2	B	91	GLN
2	B	95	GLN
2	B	188	HIS
2	B	190	GLN

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 ⓘ

3 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	IPH	A	801	-	7,7,7	0.46	0	8,8,8	0.39	0
4	EDO	B	902	-	3,3,3	0.54	0	2,2,2	0.35	0
4	EDO	B	901	-	3,3,3	0.48	0	2,2,2	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IPH	A	801	-	-	-	0/1/1/1
4	EDO	B	902	-	-	1/1/1/1	-
4	EDO	B	901	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	902	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	IPH	1	0
4	B	902	EDO	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	333/348 (95%)	0.21	9 (2%) 56 52	10, 22, 45, 84	1 (0%)
2	B	326/350 (93%)	0.04	8 (2%) 58 54	4, 14, 43, 77	3 (0%)
All	All	659/698 (94%)	0.13	17 (2%) 57 53	4, 19, 45, 84	4 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	GLY	5.7
2	B	70	ALA	3.7
2	B	196	ALA	3.6
2	B	197	GLY	3.2
2	B	2	LEU	3.1
1	A	32	SER	3.0
2	B	77	GLN	2.5
2	B	78	MET	2.4
2	B	193	PRO	2.4
1	A	212	LEU	2.4
1	A	76	VAL	2.4
1	A	16	THR	2.3
1	A	210	SER	2.3
1	A	79	TYR	2.3
1	A	211	ARG	2.2
2	B	200	ALA	2.1
1	A	316	ARG	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](#)

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
4	EDO	B	901	4/4	0.77	0.16	40,42,49,54	0
3	IPH	A	801	7/7	0.88	0.12	12,15,17,19	0
4	EDO	B	902	4/4	0.89	0.09	14,15,15,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.