



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:07 AM UTC

PDB ID : 1VI1 / pdb_00001vi1
Title : Crystal structure of a fatty acid/phospholipid synthesis protein
Authors : Structural GenomiX
Deposited on : 2003-12-01
Resolution : 2.95 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

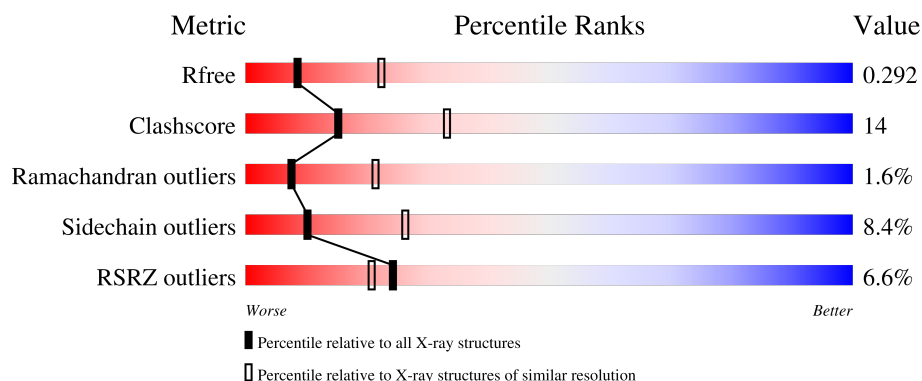
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	345	
1	B	345	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4784 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/phospholipid synthesis protein plsX.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	Se	0	3	0
			2412	1501	419	476	1	15			
1	B	321	Total	C	N	O	S	Se	0	3	0
			2368	1476	410	466	1	15			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	cloning artifact	UNP P71018
A	0	SER	-	cloning artifact	UNP P71018
A	1	LEU	-	cloning artifact	UNP P71018
A	8	MSE	MET	modified residue	UNP P71018
A	80	MSE	MET	modified residue	UNP P71018
A	83	MSE	MET	modified residue	UNP P71018
A	105	MSE	MET	modified residue	UNP P71018
A	157	MSE	MET	modified residue	UNP P71018
A	245	MSE	MET	modified residue	UNP P71018
A	246	MSE	MET	modified residue	UNP P71018
A	250	MSE	MET	modified residue	UNP P71018
A	270	MSE	MET	modified residue	UNP P71018
A	272	MSE	MET	modified residue	UNP P71018
A	274	MSE	MET	modified residue	UNP P71018
A	305	ARG	HIS	modified residue	UNP P71018
A	313	MSE	MET	modified residue	UNP P71018
A	334	GLU	-	cloning artifact	UNP P71018
A	335	GLY	-	cloning artifact	UNP P71018
A	336	GLY	-	cloning artifact	UNP P71018
A	337	SER	-	cloning artifact	UNP P71018
A	338	HIS	-	cloning artifact	UNP P71018
A	339	HIS	-	cloning artifact	UNP P71018
A	340	HIS	-	cloning artifact	UNP P71018
A	341	HIS	-	cloning artifact	UNP P71018
A	342	HIS	-	cloning artifact	UNP P71018

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	343	HIS	-	cloning artifact	UNP P71018
B	-1	MSE	-	cloning artifact	UNP P71018
B	0	SER	-	cloning artifact	UNP P71018
B	1	LEU	-	cloning artifact	UNP P71018
B	8	MSE	MET	modified residue	UNP P71018
B	80	MSE	MET	modified residue	UNP P71018
B	83	MSE	MET	modified residue	UNP P71018
B	105	MSE	MET	modified residue	UNP P71018
B	157	MSE	MET	modified residue	UNP P71018
B	245	MSE	MET	modified residue	UNP P71018
B	246	MSE	MET	modified residue	UNP P71018
B	250	MSE	MET	modified residue	UNP P71018
B	270	MSE	MET	modified residue	UNP P71018
B	272	MSE	MET	modified residue	UNP P71018
B	274	MSE	MET	modified residue	UNP P71018
B	305	ARG	HIS	modified residue	UNP P71018
B	313	MSE	MET	modified residue	UNP P71018
B	334	GLU	-	cloning artifact	UNP P71018
B	335	GLY	-	cloning artifact	UNP P71018
B	336	GLY	-	cloning artifact	UNP P71018
B	337	SER	-	cloning artifact	UNP P71018
B	338	HIS	-	cloning artifact	UNP P71018
B	339	HIS	-	cloning artifact	UNP P71018
B	340	HIS	-	cloning artifact	UNP P71018
B	341	HIS	-	cloning artifact	UNP P71018
B	342	HIS	-	cloning artifact	UNP P71018
B	343	HIS	-	cloning artifact	UNP P71018

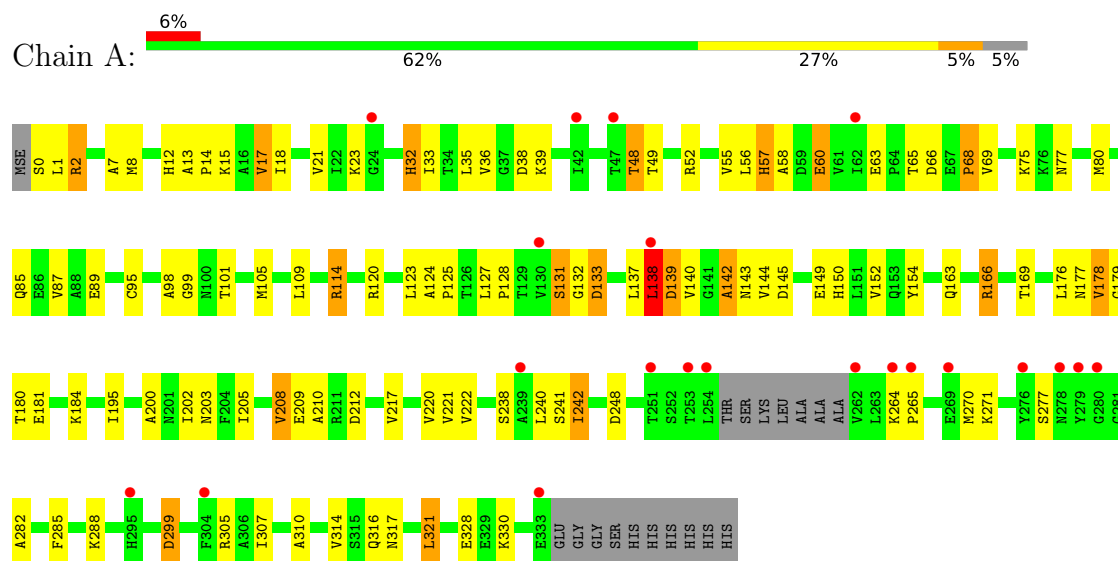
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total O 3 3	0	0
2	B	1	Total O 1 1	0	0

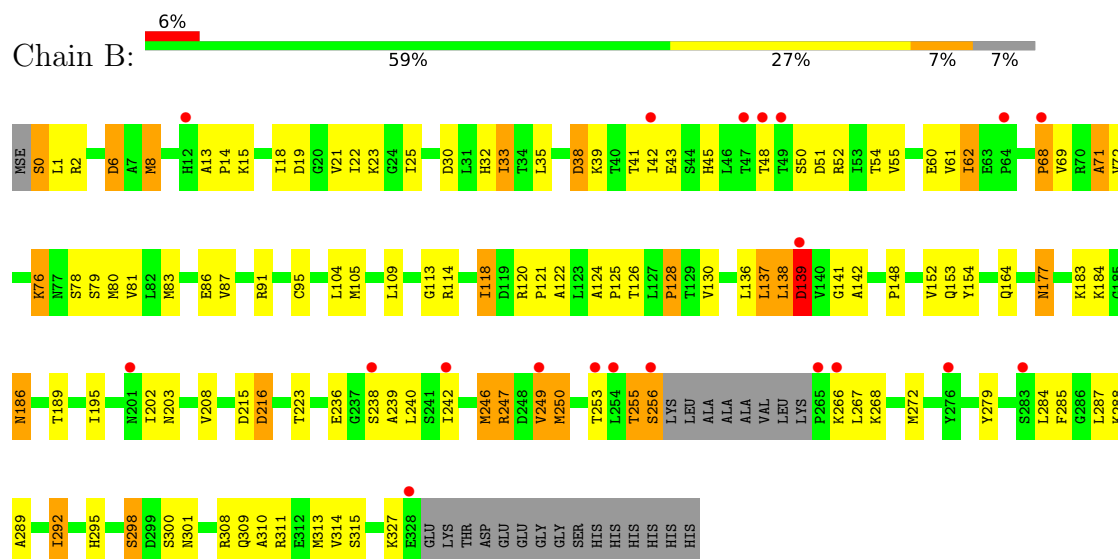
3 Residue-property plots

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/phospholipid synthesis protein plsX



- Molecule 1: Fatty acid/phospholipid synthesis protein plsX



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	170.31Å 170.31Å 187.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.94 – 2.95 47.94 – 2.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.94-2.95) 100.0 (47.94-2.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.95 (at 2.96Å)	Xtriage
Refinement program	REFMAC 4.0	Depositor
R, R_{free}	0.285 , 0.334 0.241 , 0.292	Depositor DCC
R_{free} test set	1116 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.2	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	0.91	EDS
Total number of atoms	4784	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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	0.89	2/2439 (0.1%)	1.65	35/3283 (1.1%)
1	B	0.87	0/2395	1.61	24/3223 (0.7%)
All	All	0.88	2/4834 (0.0%)	1.63	59/6506 (0.9%)

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	5
1	B	0	11
All	All	0	16

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	ASP	N-CA	-6.15	1.38	1.46
1	A	221	VAL	N-CA	5.12	1.52	1.46

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	ASP	CA-CB-CG	11.68	124.28	112.60
1	A	52	ARG	CD-NE-CZ	8.81	136.74	124.40
1	A	178	VAL	N-CA-CB	-7.76	101.95	112.28
1	A	12	HIS	N-CA-C	7.76	122.75	113.28
1	B	137	LEU	CA-C-O	7.42	128.26	120.54
1	B	292	ILE	N-CA-C	7.34	118.45	108.17
1	B	139	ASP	CA-CB-CG	-7.30	105.30	112.60
1	A	203	ASN	CA-CB-CG	7.23	119.83	112.60
1	B	301	ASN	CA-CB-CG	-6.85	105.75	112.60
1	B	164	GLN	N-CA-C	6.76	118.73	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ARG	NE-CZ-NH1	-6.68	114.82	121.50
1	A	299	ASP	CA-CB-CG	-6.67	105.93	112.60
1	A	200	ALA	CA-C-N	6.44	130.90	120.60
1	A	200	ALA	C-N-CA	6.44	130.90	120.60
1	B	203	ASN	CA-CB-CG	6.34	118.94	112.60
1	A	144	VAL	N-CA-C	6.32	122.58	113.16
1	A	52	ARG	NE-CZ-NH2	6.24	124.82	119.20
1	A	58	ALA	CA-C-N	6.16	129.15	120.28
1	A	58	ALA	C-N-CA	6.16	129.15	120.28
1	A	114	ARG	NE-CZ-NH2	6.11	124.70	119.20
1	A	138	LEU	O-C-N	6.08	130.13	123.13
1	B	52	ARG	CD-NE-CZ	6.07	132.90	124.40
1	A	32	HIS	CA-CB-CG	6.06	119.86	113.80
1	A	139	ASP	N-CA-CB	6.02	120.67	110.49
1	B	216	ASP	CA-CB-CG	-5.97	106.63	112.60
1	A	220	VAL	CA-C-N	-5.96	115.80	123.19
1	A	220	VAL	C-N-CA	-5.96	115.80	123.19
1	B	289	ALA	O-C-N	-5.91	117.33	121.65
1	A	138	LEU	CA-C-N	5.79	132.59	121.54
1	A	138	LEU	C-N-CA	5.79	132.59	121.54
1	A	98	ALA	N-CA-C	-5.78	104.95	113.61
1	A	208	VAL	CA-CB-CG1	5.72	120.12	110.40
1	A	142	ALA	CA-C-O	-5.69	114.55	120.92
1	B	202	ILE	N-CA-C	5.61	117.20	109.46
1	B	177	ASN	OD1-CG-ND2	5.57	128.17	122.60
1	A	32	HIS	CA-C-O	-5.53	114.64	121.11
1	A	321	LEU	CA-C-O	-5.46	114.77	120.55
1	B	118	ILE	N-CA-C	5.36	116.08	107.73
1	B	186	ASN	N-CA-CB	-5.26	101.60	110.49
1	A	166	ARG	CD-NE-CZ	5.26	131.76	124.40
1	B	51	ASP	N-CA-C	-5.25	106.83	113.18
1	A	87	VAL	CA-C-N	5.24	127.30	120.28
1	A	87	VAL	C-N-CA	5.24	127.30	120.28
1	B	184	LYS	N-CA-C	5.24	117.94	109.40
1	A	248	ASP	N-CA-C	-5.21	105.66	112.23
1	B	52	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	B	287	LEU	O-C-N	-5.17	116.96	122.85
1	A	2	ARG	CD-NE-CZ	5.16	131.62	124.40
1	A	109	LEU	N-CA-C	5.15	116.58	111.07
1	A	57	HIS	N-CA-C	5.15	116.65	108.67
1	B	128	PRO	CB-CA-C	-5.14	104.49	111.12
1	A	145	ASP	CA-CB-CG	5.11	117.71	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	HIS	CA-CB-CG	5.08	118.88	113.80
1	B	38	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	6	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	87	VAL	CA-C-N	5.05	127.31	120.38
1	B	87	VAL	C-N-CA	5.05	127.31	120.38
1	A	209	GLU	CA-C-O	-5.01	116.10	121.56
1	A	208	VAL	N-CA-CB	-5.01	104.58	111.99

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	GLU	Mainchain
1	A	17	VAL	Mainchain
1	A	299	ASP	Mainchain
1	A	32	HIS	Mainchain
1	A	95	CYS	Mainchain
1	B	0	SER	Mainchain
1	B	126	THR	Mainchain
1	B	130	VAL	Mainchain
1	B	139	ASP	Mainchain
1	B	183	LYS	Mainchain
1	B	216	ASP	Mainchain
1	B	246[A]	MSE	Mainchain
1	B	246[B]	MSE	Mainchain
1	B	253	THR	Mainchain
1	B	71	ALA	Mainchain
1	B	86	GLU	Mainchain

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	2412	0	2373	58	0
1	B	2368	0	2358	71	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4784	0	4731	129	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 14.

All (129) 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:13:ALA:HB1	1:A:14:PRO:HA	1.33	1.04
1:B:309:GLN:HG2	1:B:313:MSE:HE2	1.46	0.98
1:B:13:ALA:HB1	1:B:14:PRO:HA	1.49	0.95
1:A:138:LEU:HD23	1:A:154:TYR:HB3	1.63	0.80
1:A:1:LEU:HD12	1:A:2:ARG:H	1.45	0.79
1:B:15:LYS:HD2	1:B:45:HIS:HE1	1.48	0.77
1:A:13:ALA:HB1	1:A:14:PRO:CA	2.14	0.75
1:A:264:LYS:N	1:A:265:PRO:HD2	2.03	0.73
1:B:246[A]:MSE:HE3	1:B:250[A]:MSE:HE3	1.73	0.70
1:B:122:ALA:HB1	1:B:138:LEU:HD22	1.74	0.69
1:B:124:ALA:HB2	1:B:138:LEU:CD2	2.24	0.67
1:B:138:LEU:HD13	1:B:154:TYR:HB3	1.76	0.67
1:B:8:MSE:SE	1:B:38:ASP:H	2.29	0.66
1:B:139:ASP:HB3	1:B:223:THR:O	1.96	0.66
1:A:120:ARG:HD3	1:A:150:HIS:CE1	2.32	0.65
1:B:105:MSE:HA	1:B:284:LEU:HD21	1.79	0.64
1:A:177:ASN:OD1	1:A:178:VAL:HG12	1.96	0.63
1:A:176:LEU:HD11	1:A:210:ALA:HB2	1.80	0.63
1:A:138:LEU:HD23	1:A:154:TYR:CB	2.29	0.62
1:B:152:VAL:HG21	1:B:195:ILE:HG21	1.81	0.62
1:A:152:VAL:HG21	1:A:195:ILE:HG21	1.81	0.62
1:A:7:ALA:HA	1:A:17:VAL:HG11	1.81	0.61
1:A:238:SER:O	1:A:242:ILE:HG13	2.00	0.61
1:A:125:PRO:HB3	1:A:282:ALA:HB2	1.84	0.60
1:A:2:ARG:HH21	1:A:2:ARG:HG3	1.66	0.60
1:B:62:ILE:HG12	1:B:71:ALA:HB1	1.83	0.60
1:A:212:ASP:CB	1:A:217:VAL:HG11	2.32	0.60
1:A:270[A]:MSE:HG3	1:A:271:LYS:N	2.18	0.58
1:B:246[A]:MSE:HE3	1:B:250[A]:MSE:CE	2.33	0.58
1:B:128:PRO:HA	1:B:279:TYR:CZ	2.39	0.57
1:B:15:LYS:HD2	1:B:45:HIS:CE1	2.35	0.57
1:A:1:LEU:HD12	1:A:2:ARG:N	2.19	0.56
1:A:264:LYS:N	1:A:265:PRO:CD	2.67	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:HD11	1:A:285:PHE:CD1	2.40	0.56
1:A:127:LEU:HB3	1:A:128:PRO:HD2	1.88	0.56
1:B:13:ALA:CB	1:B:14:PRO:HA	2.25	0.55
1:A:85:GLN:O	1:A:89:GLU:HG3	2.05	0.55
1:A:317:ASN:O	1:A:321:LEU:HG	2.07	0.55
1:B:118:ILE:HA	1:B:153:GLN:HE22	1.73	0.54
1:B:13:ALA:HB1	1:B:14:PRO:CA	2.32	0.54
1:B:148:PRO:O	1:B:152:VAL:HG23	2.08	0.53
1:B:61:VAL:HG12	1:B:61:VAL:O	2.09	0.53
1:A:14:PRO:HB2	1:A:18:ILE:HD11	1.90	0.53
1:A:212:ASP:HB2	1:A:217:VAL:HG11	1.90	0.53
1:A:179:GLY:HA3	1:A:184:LYS:HG3	1.91	0.53
1:A:181:GLU:H	1:A:181:GLU:CD	2.17	0.53
1:A:212:ASP:HB3	1:A:217:VAL:HG11	1.91	0.53
1:B:125:PRO:HD2	1:B:137:LEU:O	2.08	0.52
1:B:42:ILE:HD11	1:B:55:VAL:HG13	1.90	0.52
1:A:8:MSE:SE	1:A:38:ASP:H	2.42	0.52
1:A:114:ARG:O	1:A:288:LYS:HE3	2.08	0.52
1:B:124:ALA:HB2	1:B:138:LEU:HD21	1.91	0.52
1:B:0:SER:OG	1:B:30:ASP:HB2	2.10	0.52
1:A:152:VAL:HG21	1:A:195:ILE:CG2	2.41	0.51
1:A:131:SER:OG	1:A:132:GLY:N	2.42	0.51
1:B:114:ARG:HH11	1:B:114:ARG:HG3	1.75	0.51
1:B:1:LEU:HD22	1:B:311:ARG:HG3	1.93	0.50
1:B:113:GLY:HA3	1:B:288:LYS:NZ	2.27	0.50
1:B:124:ALA:HB2	1:B:138:LEU:HD23	1.92	0.50
1:B:236:GLU:HG2	1:B:236:GLU:O	2.10	0.50
1:B:1:LEU:CD2	1:B:311:ARG:HG3	2.42	0.50
1:B:310:ALA:O	1:B:314:VAL:HG23	2.12	0.50
1:B:18:ILE:HG12	1:B:35:LEU:HD11	1.93	0.50
1:A:124:ALA:HB2	1:A:138:LEU:CD1	2.42	0.49
1:B:122:ALA:HB1	1:B:138:LEU:CD2	2.41	0.49
1:B:292:ILE:HD11	1:B:313:MSE:CE	2.43	0.49
1:A:105:MSE:SE	1:A:142:ALA:HA	2.62	0.49
1:A:212:ASP:HB3	1:A:217:VAL:CG1	2.42	0.49
1:B:122:ALA:HB2	1:B:154:TYR:CE2	2.48	0.48
1:B:21:VAL:HG13	1:B:33:ILE:HG13	1.95	0.48
1:B:136:LEU:HD21	1:B:285:PHE:CE1	2.49	0.48
1:B:21:VAL:HG11	1:B:33:ILE:HG21	1.96	0.48
1:A:14:PRO:HB2	1:A:18:ILE:CD1	2.43	0.48
1:A:0:SER:OG	1:A:1:LEU:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:MSE:SE	1:B:104:LEU:HD13	2.64	0.48
1:A:33:ILE:HD11	1:A:307:ILE:HD13	1.96	0.48
1:B:238:SER:O	1:B:242:ILE:HG13	2.14	0.48
1:B:138:LEU:HD23	1:B:138:LEU:HA	1.64	0.47
1:B:2:ARG:HD3	1:B:91:ARG:O	2.14	0.47
1:B:295:HIS:O	1:B:298:SER:HB2	2.14	0.47
1:B:109:LEU:HD13	1:B:121:PRO:HG2	1.96	0.47
1:B:8:MSE:HA	1:B:8:MSE:CE	2.45	0.47
1:B:19:ASP:O	1:B:23:LYS:HG3	2.14	0.47
1:B:255:THR:OG1	1:B:256:SER:N	2.47	0.47
1:B:71:ALA:O	1:B:72:VAL:C	2.58	0.46
1:A:36:VAL:HG13	1:A:56:LEU:HD23	1.96	0.46
1:B:266:LYS:O	1:B:267:LEU:C	2.59	0.45
1:B:78:SER:OG	1:B:81:VAL:HG23	2.15	0.45
1:B:136:LEU:HD21	1:B:285:PHE:CZ	2.52	0.45
1:A:63:GLU:HA	1:A:63:GLU:OE1	2.17	0.45
1:A:139:ASP:OD1	1:A:143:ASN:ND2	2.50	0.45
1:A:139:ASP:OD2	1:A:142:ALA:HB3	2.17	0.45
1:B:76:LYS:HZ1	1:B:76:LYS:HA	1.81	0.45
1:A:2:ARG:HG3	1:A:2:ARG:NH2	2.32	0.45
1:B:113:GLY:HA3	1:B:288:LYS:HZ3	1.82	0.45
1:A:277:SER:O	1:A:305:ARG:NH2	2.45	0.44
1:B:22:ILE:O	1:B:23:LYS:C	2.60	0.44
1:B:39:LYS:O	1:B:43:GLU:HB2	2.17	0.43
1:B:139:ASP:HB2	1:B:154:TYR:CE1	2.53	0.43
1:A:310:ALA:O	1:A:314:VAL:HG23	2.18	0.43
1:B:109:LEU:HD11	1:B:114:ARG:HD3	2.00	0.43
1:B:38:ASP:OD2	1:B:41:THR:OG1	2.29	0.43
1:B:240:LEU:HD23	1:B:240:LEU:HA	1.91	0.43
1:A:23:LYS:HA	1:A:23:LYS:HE2	2.01	0.43
1:A:60:GLU:OE1	1:A:75:LYS:HD3	2.18	0.43
1:B:23:LYS:HE3	1:B:300:SER:HB2	2.01	0.42
1:A:240:LEU:O	1:A:241:SER:C	2.62	0.42
1:A:131:SER:OG	1:A:133:ASP:OD2	2.27	0.42
1:B:83:MSE:HE3	1:B:95:CYS:SG	2.59	0.42
1:A:80:MSE:HE1	1:A:99:GLY:HA3	2.02	0.42
1:A:123:LEU:HD23	1:A:140:VAL:HG23	2.02	0.42
1:B:60:GLU:O	1:B:78:SER:HA	2.19	0.42
1:B:21:VAL:CG1	1:B:33:ILE:HG21	2.50	0.42
1:B:22:ILE:O	1:B:25:ILE:N	2.50	0.41
1:A:63:GLU:HB2	1:A:66:ASP:OD1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ALA:HB2	1:A:138:LEU:HD11	2.01	0.41
1:B:268:LYS:O	1:B:272:MSE:HB2	2.21	0.41
1:B:38:ASP:HB3	1:B:41:THR:HB	2.03	0.41
1:B:239:ALA:O	1:B:240:LEU:C	2.64	0.41
1:A:21:VAL:HG21	1:A:35:LEU:HD21	2.03	0.41
1:A:68:PRO:O	1:A:69:VAL:C	2.62	0.40
1:B:15:LYS:HB2	1:B:45:HIS:CE1	2.56	0.40
1:A:125:PRO:HD2	1:A:137:LEU:O	2.21	0.40
1:A:264:LYS:H	1:A:265:PRO:HD2	1.85	0.40
1:A:180:THR:O	1:A:181:GLU:C	2.65	0.40
1:A:39:LYS:H	1:A:57:HIS:CD2	2.40	0.40
1:B:177:ASN:ND2	1:B:189:THR:CG2	2.85	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	326/345 (94%)	296 (91%)	27 (8%)	3 (1%)	14	34
1	B	320/345 (93%)	284 (89%)	29 (9%)	7 (2%)	5	15
All	All	646/690 (94%)	580 (90%)	56 (9%)	10 (2%)	7	23

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	327	LYS
1	B	139	ASP
1	B	141	GLY
1	B	142	ALA
1	B	186	ASN
1	A	169	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	48	THR
1	B	68	PRO
1	B	62	ILE
1	A	68	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	252/270 (93%)	231 (92%)	21 (8%)	10	27
1	B	252/270 (93%)	230 (91%)	22 (9%)	9	25
All	All	504/540 (93%)	461 (92%)	43 (8%)	10	25

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

Mol	Chain	Res	Type
1	A	15	LYS
1	A	48	THR
1	A	49	THR
1	A	55	VAL
1	A	60	GLU
1	A	65	THR
1	A	77	ASN
1	A	101	THR
1	A	131	SER
1	A	133	ASP
1	A	138	LEU
1	A	163	GLN
1	A	166	ARG
1	A	202	ILE
1	A	205	ILE
1	A	208	VAL
1	A	222	VAL
1	A	242	ILE
1	A	316	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	328	GLU
1	A	330	LYS
1	B	6	ASP
1	B	8	MSE
1	B	33	ILE
1	B	48	THR
1	B	50	SER
1	B	54	THR
1	B	68	PRO
1	B	69	VAL
1	B	76	LYS
1	B	79	SER
1	B	120	ARG
1	B	138	LEU
1	B	208	VAL
1	B	247	ARG
1	B	249	VAL
1	B	250[A]	MSE
1	B	250[B]	MSE
1	B	255	THR
1	B	256	SER
1	B	298	SER
1	B	308	ARG
1	B	315	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	32	HIS
1	A	57	HIS
1	A	85	GLN
1	A	201	ASN
1	A	295	HIS
1	A	323	GLN
1	B	32	HIS
1	B	45	HIS
1	B	194	GLN
1	B	278	ASN
1	B	316	GLN
1	B	317	ASN
1	B	323	GLN

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	315/345 (91%)	0.49	21 (6%) 24 20	30, 64, 86, 93	0
1	B	309/345 (89%)	0.62	20 (6%) 25 21	35, 66, 86, 93	0
All	All	624/690 (90%)	0.55	41 (6%) 24 21	30, 65, 86, 93	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	LEU	5.0
1	A	265	PRO	4.2
1	B	276	TYR	3.9
1	A	280	GLY	3.6
1	A	253	THR	3.6
1	A	276	TYR	3.5
1	B	253	THR	3.5
1	B	139	ASP	3.4
1	B	12	HIS	3.4
1	B	266	LYS	3.3
1	B	254	LEU	3.2
1	A	279	TYR	3.2
1	B	328	GLU	3.2
1	B	242	ILE	2.8
1	B	68	PRO	2.7
1	B	201	ASN	2.7
1	B	42	ILE	2.6
1	A	239	ALA	2.6
1	A	304	PHE	2.6
1	B	64	PRO	2.5
1	B	256	SER	2.4
1	A	333	GLU	2.4
1	A	62	ILE	2.4
1	A	47	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	49	THR	2.3
1	A	24	GLY	2.3
1	B	283	SER	2.3
1	A	278	ASN	2.3
1	A	130	VAL	2.3
1	B	47	THR	2.3
1	A	262	VAL	2.3
1	B	249	VAL	2.3
1	B	265	PRO	2.3
1	A	295	HIS	2.2
1	A	42	ILE	2.2
1	A	138	LEU	2.2
1	A	269	GLU	2.2
1	B	238	SER	2.2
1	A	264	LYS	2.1
1	A	251	THR	2.1
1	B	48	THR	2.1

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.