



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:40 AM UTC

PDB ID : 1HPL / pdb_00001hpl
Title : HORSE PANCREATIC LIPASE. THE CRYSTAL STRUCTURE AT 2.3
ANGSTROMS RESOLUTION
Authors : Bourne, Y.; Cambillau, C.
Deposited on : 1993-01-27
Resolution : 2.30 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
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

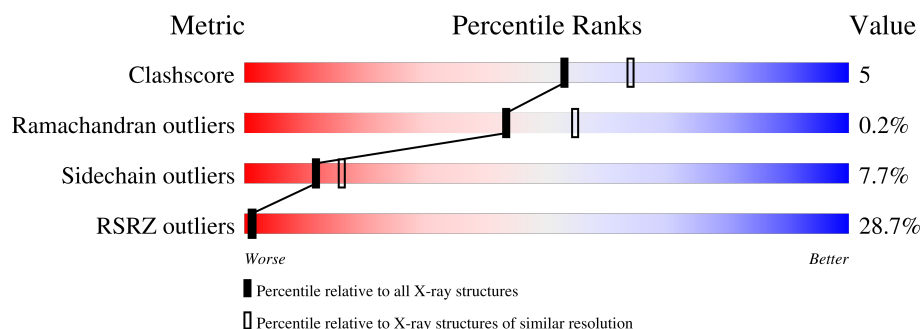
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	449	16% 76% 18% 5%
1	B	449	42% 71% 22% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7709 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 LIPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3501	2205	601	676	19			
1	B	449	Total	C	N	O	S	0	0	0
			3501	2205	601	676	19			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

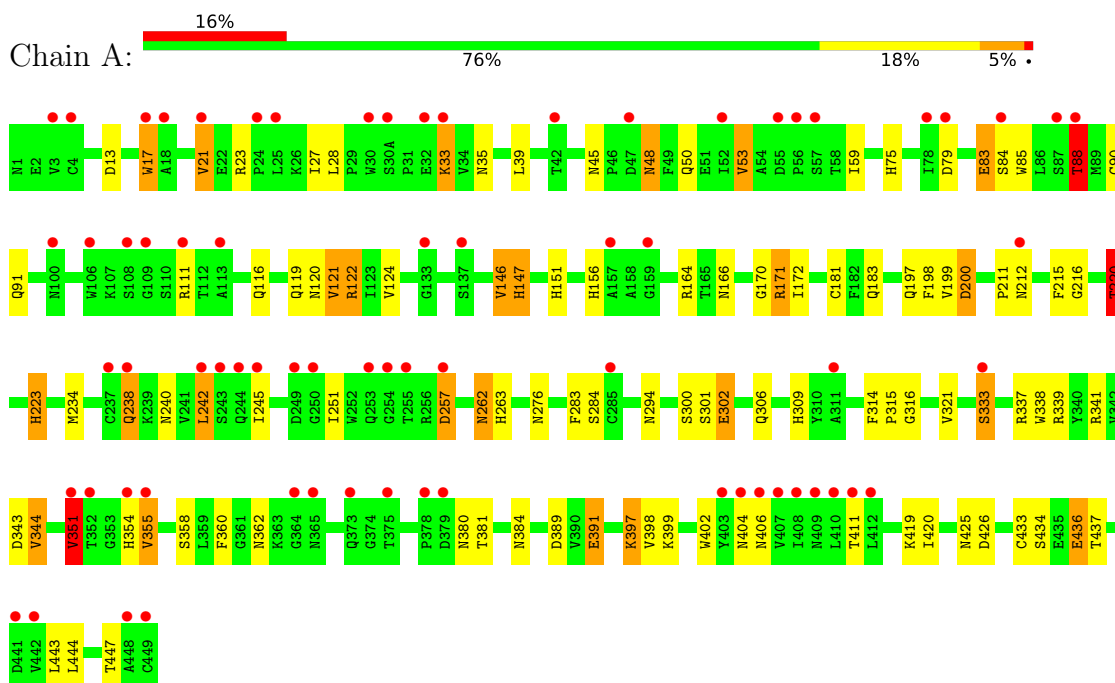
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	397	Total	O	0	0
			397	397		
3	B	308	Total	O	0	0
			308	308		

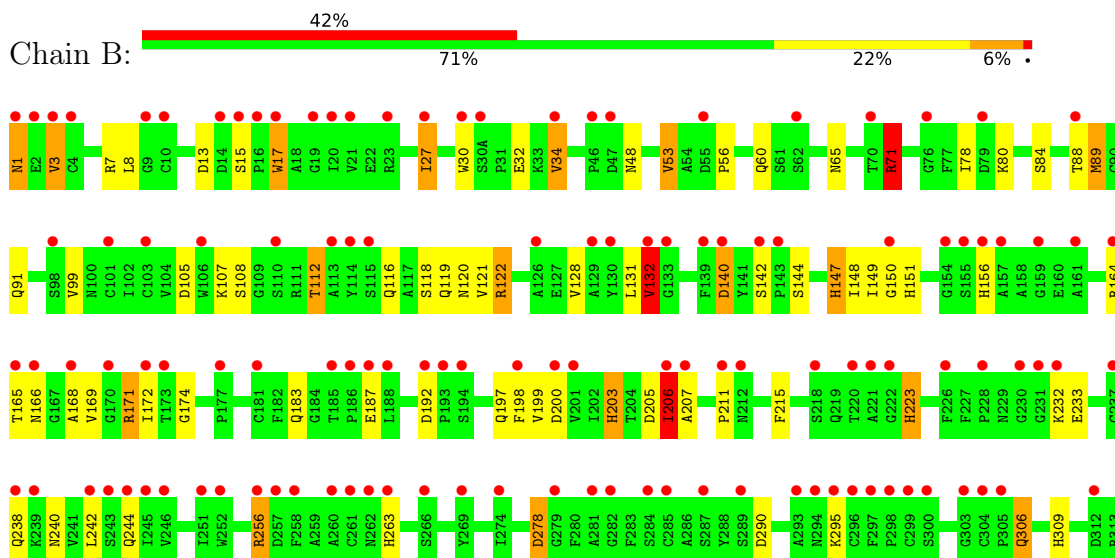
3 Residue-property plots

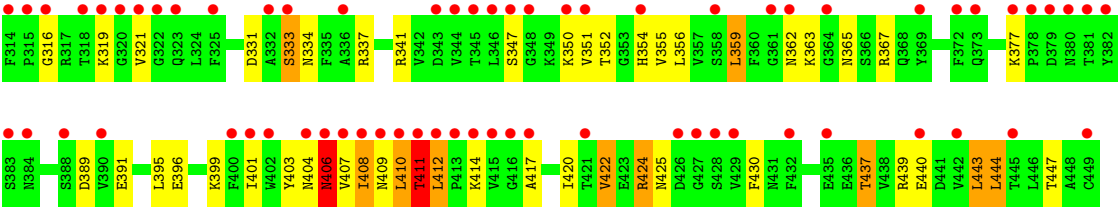
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: LIPASE



• Molecule 1: LIPASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.80Å 97.20Å 145.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30 6.00 – 2.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.30) 81.3 (6.00-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.159 , (Not available) 0.331 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 102.7	EDS
L-test for twinning ¹	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	7709	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2770e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.02	12/3587 (0.3%)	1.79	76/4867 (1.6%)
1	B	1.04	10/3587 (0.3%)	1.85	87/4867 (1.8%)
All	All	1.03	22/7174 (0.3%)	1.82	163/9734 (1.7%)

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
1	B	0	3
All	All	0	5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	VAL	CA-CB	8.40	1.66	1.54
1	B	147	HIS	CD2-NE2	-8.14	1.28	1.37
1	B	223	HIS	CD2-NE2	-7.29	1.29	1.37
1	A	88	THR	CA-CB	7.04	1.65	1.53
1	A	75	HIS	CD2-NE2	-6.88	1.30	1.37
1	A	147	HIS	CD2-NE2	-6.83	1.30	1.37
1	B	263	HIS	CD2-NE2	-6.69	1.30	1.37
1	B	132	VAL	CA-CB	6.49	1.63	1.54
1	B	151	HIS	CD2-NE2	-6.41	1.30	1.37
1	B	354	HIS	CD2-NE2	-6.28	1.30	1.37
1	B	203	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	223	HIS	CD2-NE2	-6.13	1.31	1.37
1	A	354	HIS	CD2-NE2	-5.80	1.31	1.37
1	A	151	HIS	CD2-NE2	-5.70	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	HIS	CG-ND1	-5.63	1.32	1.38
1	B	309	HIS	CD2-NE2	-5.61	1.31	1.37
1	B	156	HIS	CD2-NE2	-5.57	1.31	1.37
1	A	309	HIS	CD2-NE2	-5.54	1.31	1.37
1	A	344	VAL	CA-CB	5.24	1.60	1.54
1	A	351	VAL	CA-CB	5.24	1.61	1.54
1	A	251	ILE	CA-CB	5.17	1.60	1.54
1	A	172	ILE	CA-CB	5.08	1.61	1.54

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	SER	O-C-N	-28.12	88.34	122.65
1	A	333	SER	O-C-N	-27.72	91.19	122.79
1	B	174	GLY	O-C-N	-10.46	116.76	123.35
1	A	45	ASN	CA-CB-CG	8.75	121.35	112.60
1	B	333	SER	CA-C-O	8.71	131.92	121.99
1	A	339	ARG	NE-CZ-NH2	-8.68	111.39	119.20
1	B	406	ASN	CA-CB-CG	-8.63	103.97	112.60
1	B	122	ARG	NE-CZ-NH1	8.41	129.91	121.50
1	B	3	VAL	CB-CA-C	-8.18	98.23	110.82
1	B	8	LEU	N-CA-C	-8.10	100.08	110.53
1	A	301	SER	N-CA-C	8.05	120.97	111.71
1	B	8	LEU	O-C-N	-7.98	112.84	122.65
1	B	164	ARG	NE-CZ-NH2	-7.83	112.16	119.20
1	A	355	VAL	N-CA-CB	-7.80	101.50	111.64
1	A	35	ASN	OD1-CG-ND2	-7.79	114.81	122.60
1	A	404	ASN	OD1-CG-ND2	-7.79	114.81	122.60
1	A	380	ASN	N-CA-C	7.61	120.13	110.24
1	B	122	ARG	NE-CZ-NH2	-7.58	112.38	119.20
1	B	306	GLN	OE1-CD-NE2	-7.58	115.03	122.60
1	B	171	ARG	NE-CZ-NH1	7.53	129.03	121.50
1	B	424	ARG	CB-CG-CD	-7.46	94.14	111.30
1	B	223	HIS	N-CA-C	-7.43	103.27	111.36
1	B	206	ILE	CA-CB-CG1	-7.07	98.38	110.40
1	A	354	HIS	CA-CB-CG	7.00	120.80	113.80
1	A	425	ASN	CA-CB-CG	6.99	119.58	112.60
1	B	389	ASP	CA-CB-CG	6.97	119.57	112.60
1	B	7	ARG	NE-CZ-NH2	-6.93	112.96	119.20
1	A	223	HIS	N-CA-C	-6.90	103.20	111.69
1	A	300	SER	CA-CB-OG	6.85	124.80	111.10
1	A	17	TRP	CG-CD2-CE3	6.81	140.71	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	GLN	OE1-CD-NE2	-6.80	115.80	122.60
1	B	411	THR	CA-C-O	6.79	130.22	120.51
1	B	425	ASN	CA-CB-CG	6.74	119.34	112.60
1	B	404	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	A	164	ARG	NE-CZ-NH2	-6.71	113.16	119.20
1	B	197	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	A	257	ASP	CA-CB-CG	6.55	119.15	112.60
1	B	171	ARG	CB-CG-CD	6.54	126.34	111.30
1	A	314	PHE	CA-C-N	6.53	126.03	119.24
1	A	314	PHE	C-N-CA	6.53	126.03	119.24
1	B	367	ARG	CA-CB-CG	6.46	127.02	114.10
1	B	27	ILE	CA-CB-CG2	6.45	121.46	110.50
1	A	220	THR	N-CA-CB	-6.41	100.54	109.97
1	B	443	LEU	CB-CA-C	-6.36	100.72	110.26
1	B	354	HIS	CA-CB-CG	6.29	120.09	113.80
1	A	426	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	21	VAL	N-CA-CB	-6.26	102.65	110.47
1	B	65	ASN	OD1-CG-ND2	-6.25	116.35	122.60
1	A	404	ASN	CB-CG-ND2	6.22	125.74	116.40
1	B	13	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	384	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	B	347	SER	CA-CB-OG	6.12	123.35	111.10
1	A	240	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	A	294	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	A	212	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	A	50	GLN	OE1-CD-NE2	-6.04	116.56	122.60
1	A	315	PRO	O-C-N	-6.00	115.70	122.18
1	A	23	ARG	CA-C-N	5.98	125.37	118.85
1	A	23	ARG	C-N-CA	5.98	125.37	118.85
1	A	362	ASN	CA-CB-CG	5.97	118.57	112.60
1	B	147	HIS	CA-CB-CG	5.95	119.75	113.80
1	A	397	LYS	CA-CB-CG	5.95	125.99	114.10
1	B	420	ILE	N-CA-C	-5.94	99.57	108.12
1	A	389	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	53	VAL	N-CA-CB	-5.91	101.42	112.36
1	B	112	THR	CB-CA-C	-5.90	99.75	111.91
1	A	35	ASN	CB-CG-ND2	5.89	125.24	116.40
1	B	444	LEU	O-C-N	-5.89	116.50	123.22
1	A	13	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	197	GLN	CG-CD-NE2	5.83	125.15	116.40
1	B	1	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	B	200	ASP	CA-CB-CG	5.80	118.40	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	HIS	CB-CG-CD2	-5.80	123.66	131.20
1	B	334	ASN	N-CA-C	5.75	119.15	110.64
1	B	144	SER	CA-CB-OG	-5.75	99.61	111.10
1	A	75	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	A	306	GLN	OE1-CD-NE2	-5.73	116.87	122.60
1	B	363	LYS	CB-CG-CD	-5.69	98.22	111.30
1	A	437	THR	N-CA-C	-5.68	100.43	109.23
1	B	120	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	A	17	TRP	CB-CG-CD1	-5.67	118.39	126.90
1	A	283	PHE	O-C-N	-5.67	116.87	123.27
1	A	48	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	A	121	VAL	N-CA-CB	-5.62	101.72	110.54
1	B	27	ILE	CA-CB-CG1	-5.61	100.86	110.40
1	B	34	VAL	O-C-N	5.57	127.57	121.83
1	A	170	GLY	CA-C-O	-5.56	115.00	121.00
1	A	300	SER	N-CA-CB	-5.54	101.06	109.92
1	B	17	TRP	CG-CD2-CE3	5.53	139.43	133.90
1	B	206	ILE	CA-CB-CG2	5.53	119.89	110.50
1	B	156	HIS	CB-CG-CD2	-5.52	124.02	131.20
1	B	407	VAL	O-C-N	5.51	128.49	122.76
1	B	131	LEU	CA-C-O	-5.48	114.74	120.55
1	A	263	HIS	O-C-N	-5.48	116.31	122.12
1	B	197	GLN	CG-CD-NE2	5.47	124.60	116.40
1	A	183	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	B	410	LEU	N-CA-C	-5.46	99.18	110.80
1	A	263	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	B	223	HIS	CB-CG-ND1	5.43	130.85	122.70
1	B	150	GLY	O-C-N	-5.41	118.61	123.37
1	A	156	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	A	91	GLN	CA-CB-CG	-5.41	103.28	114.10
1	B	341	ARG	CG-CD-NE	-5.40	100.11	112.00
1	A	171	ARG	CB-CG-CD	5.40	123.72	111.30
1	B	140	ASP	CA-CB-CG	-5.40	107.20	112.60
1	A	238	GLN	OE1-CD-NE2	-5.37	117.23	122.60
1	B	417	ALA	N-CA-C	-5.36	99.20	108.69
1	B	17	TRP	CB-CG-CD1	-5.35	118.88	126.90
1	A	200	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	164	ARG	CA-CB-CG	-5.33	103.43	114.10
1	A	434	SER	O-C-N	5.33	129.45	123.27
1	A	436	GLU	N-CA-C	5.32	117.72	110.55
1	B	206	ILE	N-CA-CB	-5.32	98.68	111.23
1	B	263	HIS	CB-CG-CD2	-5.32	124.29	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	B	331	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	71	ARG	NE-CZ-NH2	-5.29	114.44	119.20
1	A	59	ILE	N-CA-C	-5.29	105.34	110.42
1	B	17	TRP	CE2-CD2-CG	-5.26	100.88	107.20
1	A	276	ASN	OD1-CG-ND2	-5.25	117.35	122.60
1	B	91	GLN	N-CA-C	5.25	117.08	111.36
1	B	116	GLN	CG-CD-NE2	5.24	124.26	116.40
1	A	53	VAL	CB-CA-C	5.22	119.12	110.30
1	B	119	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	B	151	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	B	183	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	A	333	SER	CA-C-O	5.20	127.90	121.87
1	A	216	GLY	O-C-N	-5.20	116.98	123.21
1	B	187	GLU	CB-CG-CD	5.18	121.41	112.60
1	A	120	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	B	278	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	411	THR	N-CA-C	-5.15	105.74	111.36
1	A	116	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	A	90	CYS	CB-CA-C	-5.14	102.25	110.79
1	B	7	ARG	NE-CZ-NH1	5.14	126.64	121.50
1	B	142	SER	N-CA-C	5.14	116.16	109.64
1	A	85	TRP	CA-CB-CG	5.13	123.35	113.60
1	B	27	ILE	CB-CG1-CD1	-5.12	103.05	113.80
1	B	238	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	B	362	ASN	CA-CB-CG	5.12	117.72	112.60
1	B	409	ASN	CA-C-N	5.10	131.28	121.54
1	B	409	ASN	C-N-CA	5.10	131.28	121.54
1	B	91	GLN	CA-CB-CG	-5.09	103.91	114.10
1	A	166	ASN	CB-CG-ND2	5.09	124.03	116.40
1	B	206	ILE	CB-CG1-CD1	-5.07	103.15	113.80
1	B	240	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	A	124	VAL	CA-C-N	5.07	125.72	119.99
1	A	124	VAL	C-N-CA	5.07	125.72	119.99
1	B	53	VAL	N-CA-CB	-5.06	103.00	112.36
1	A	309	HIS	CB-CG-CD2	-5.06	124.63	131.20
1	A	245	ILE	N-CA-C	-5.05	100.97	108.45
1	B	205	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	262	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	A	354	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	B	27	ILE	N-CA-CB	-5.04	103.19	111.45
1	B	192	ASP	CA-C-O	-5.03	115.98	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	ASN	CA-C-N	5.03	130.51	121.66
1	B	334	ASN	C-N-CA	5.03	130.51	121.66
1	B	30	TRP	CG-CD1-NE1	-5.02	103.67	110.20
1	B	207	ALA	CA-C-N	5.02	125.30	119.93
1	B	207	ALA	C-N-CA	5.02	125.30	119.93
1	A	17	TRP	CE2-CD2-CG	-5.01	101.19	107.20
1	A	245	ILE	CB-CA-C	5.00	119.37	110.71

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	333	SER	Peptide,Mainchain
1	B	333	SER	Peptide,Mainchain
1	B	71	ARG	Sidechain

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	3501	0	3334	32	2
1	B	3501	0	3334	41	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	397	0	0	7	1
3	B	308	0	0	1	2
All	All	7709	0	6668	68	4

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 5.

All (68) 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:B:165:THR:HG21	1:B:169:VAL:HG23	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:LEU:HD22	1:B:422:VAL:HG11	1.63	0.78
1:A:443:LEU:H	1:B:48:ASN:HD21	1.32	0.77
1:A:111:ARG:HH21	1:B:408:ILE:HG23	1.56	0.70
1:B:399:LYS:HD3	1:B:443:LEU:HD13	1.74	0.68
1:B:84:SER:O	1:B:88:THR:HG23	1.95	0.67
1:B:199:VAL:H	1:B:223:HIS:HD2	1.44	0.64
1:A:84:SER:O	1:A:88:THR:HG23	1.99	0.62
1:A:242:LEU:HD22	1:A:242:LEU:H	1.70	0.56
1:B:232:LYS:HD3	1:B:233:GLU:HG3	1.88	0.56
1:A:147:HIS:CD2	1:A:171:ARG:HG2	2.42	0.55
1:B:171:ARG:HD3	1:B:198:PHE:CD2	2.42	0.55
1:B:412:LEU:HD12	1:B:439:ARG:HD2	1.89	0.55
1:B:147:HIS:CD2	1:B:171:ARG:HG2	2.42	0.55
1:A:360:PHE:CZ	1:A:399:LYS:HE2	2.42	0.54
1:A:199:VAL:H	1:A:223:HIS:HD2	1.57	0.52
1:A:48:ASN:HD21	1:B:443:LEU:H	1.58	0.52
1:A:79:ASP:HA	3:A:1097:HOH:O	2.09	0.52
1:B:71:ARG:HD2	1:B:99:VAL:HG21	1.93	0.51
1:A:223:HIS:HA	1:A:321:VAL:HA	1.93	0.51
1:B:128:VAL:O	1:B:132:VAL:HG13	2.10	0.51
1:B:422:VAL:HG13	1:B:430:PHE:HB2	1.93	0.51
1:A:234:MET:H	1:A:262:ASN:ND2	2.10	0.50
1:A:316:GLY:HA3	3:A:1306:HOH:O	2.12	0.49
1:A:27:ILE:HG13	1:A:119:GLN:HG3	1.95	0.48
1:A:17:TRP:CZ3	1:A:122:ARG:HD3	2.49	0.48
1:B:89:MET:HE3	1:B:149:ILE:HD13	1.96	0.47
1:A:88:THR:HG22	3:A:1038:HOH:O	2.15	0.47
1:B:203:HIS:HB3	1:B:206:ILE:CD1	2.45	0.47
1:A:341:ARG:HH11	1:A:341:ARG:HG3	1.80	0.47
1:B:223:HIS:HA	1:B:321:VAL:HA	1.96	0.47
1:B:359:LEU:HG	1:B:395:LEU:HD21	1.96	0.46
1:A:83:GLU:H	1:A:83:GLU:CD	2.23	0.46
1:B:17:TRP:CZ3	1:B:122:ARG:HD3	2.51	0.46
1:A:220:THR:HG23	3:A:1083:HOH:O	2.17	0.45
1:B:118:SER:O	1:B:121:VAL:HG22	2.16	0.45
1:A:238:GLN:H	1:A:238:GLN:CD	2.24	0.45
1:A:358:SER:OG	1:A:399:LYS:HB2	2.17	0.45
1:B:411:THR:HG22	1:B:412:LEU:HD22	1.99	0.45
1:B:403:TYR:HA	1:B:440:GLU:HG3	1.98	0.44
1:A:33:LYS:HE3	3:A:1032:HOH:O	2.17	0.44
1:A:443:LEU:H	1:B:48:ASN:ND2	2.08	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:LYS:HB3	1:B:437:THR:HB	1.99	0.44
1:B:352:THR:O	1:B:406:ASN:HB2	2.17	0.44
1:A:181:CYS:SG	3:A:968:HOH:O	2.62	0.44
1:A:48:ASN:HD21	1:B:443:LEU:N	2.16	0.44
1:B:165:THR:HG22	1:B:168:ALA:HB3	2.00	0.43
1:B:377:LYS:HD2	3:B:1119:HOH:O	2.17	0.43
1:B:412:LEU:HD12	1:B:439:ARG:CD	2.47	0.43
1:B:316:GLY:HA2	1:B:319:LYS:HG2	2.01	0.42
1:B:34:VAL:O	1:B:108:SER:HB2	2.19	0.42
1:A:171:ARG:HD2	1:A:200:ASP:OD1	2.19	0.42
1:B:105:ASP:OD2	1:B:107:LYS:HE3	2.19	0.42
1:B:401:ILE:HB	1:B:443:LEU:HD23	2.02	0.42
1:A:344:VAL:O	1:A:381:THR:HA	2.20	0.41
1:A:398:VAL:HG11	1:A:420:ILE:HG21	2.02	0.41
1:B:171:ARG:HA	1:B:198:PHE:O	2.19	0.41
1:A:351:VAL:HG11	1:A:402:TRP:CZ3	2.55	0.41
1:B:290:ASP:HA	1:B:295:LYS:HZ2	1.85	0.41
1:A:171:ARG:HD3	1:A:198:PHE:CD2	2.55	0.41
1:B:278:ASP:HA	1:B:306:GLN:CD	2.45	0.41
1:B:351:VAL:HG22	1:B:352:THR:N	2.36	0.41
1:B:424:ARG:HH11	1:B:424:ARG:HD2	1.74	0.41
1:A:338:TRP:CD1	1:A:391:GLU:HG3	2.56	0.40
1:B:148:ILE:O	1:B:172:ILE:HA	2.21	0.40
1:B:56:PRO:O	1:B:60:GLN:HB2	2.21	0.40
1:A:343:ASP:O	1:A:420:ILE:HA	2.22	0.40
1:A:433:CYS:HB3	3:A:1124:HOH:O	2.21	0.40

All (4) 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:B:1:ASN:OD1	3:A:1307:HOH:O[2_565]	1.68	0.52
1:A:302:GLU:OE2	3:B:1043:HOH:O[2_564]	1.97	0.23
1:B:256:ARG:NH2	1:B:396:GLU:OE2[3_655]	2.12	0.08
1:A:302:GLU:CD	3:B:1043:HOH:O[2_564]	2.18	0.02

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	447/449 (100%)	431 (96%)	16 (4%)	0	100	100
1	B	447/449 (100%)	430 (96%)	15 (3%)	2 (0%)	30	38
All	All	894/898 (100%)	861 (96%)	31 (4%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	410	LEU
1	B	411	THR

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	385/385 (100%)	358 (93%)	27 (7%)	14	19
1	B	385/385 (100%)	353 (92%)	32 (8%)	10	14
All	All	770/770 (100%)	711 (92%)	59 (8%)	12	16

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	28	LEU
1	A	33	LYS
1	A	39	LEU

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Mol	Chain	Res	Type
1	A	53	VAL
1	A	83	GLU
1	A	88	THR
1	A	121	VAL
1	A	122	ARG
1	A	146	VAL
1	A	211	PRO
1	A	215	PHE
1	A	220	THR
1	A	242	LEU
1	A	257	ASP
1	A	284	SER
1	A	302	GLU
1	A	337	ARG
1	A	351	VAL
1	A	355	VAL
1	A	391	GLU
1	A	397	LYS
1	A	406	ASN
1	A	419	LYS
1	A	436	GLU
1	A	444	LEU
1	A	447	THR
1	B	3	VAL
1	B	15	SER
1	B	27	ILE
1	B	32	GLU
1	B	53	VAL
1	B	78	ILE
1	B	80	LYS
1	B	89	MET
1	B	112	THR
1	B	132	VAL
1	B	140	ASP
1	B	206	ILE
1	B	211	PRO
1	B	215	PHE
1	B	242	LEU
1	B	244	GLN
1	B	256	ARG
1	B	337	ARG
1	B	350	LYS

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Mol	Chain	Res	Type
1	B	355	VAL
1	B	356	LEU
1	B	359	LEU
1	B	365	ASN
1	B	391	GLU
1	B	406	ASN
1	B	408	ILE
1	B	411	THR
1	B	412	LEU
1	B	422	VAL
1	B	437	THR
1	B	444	LEU
1	B	447	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	48	ASN
1	A	60	GLN
1	A	119	GLN
1	A	223	HIS
1	A	262	ASN
1	A	328	ASN
1	A	404	ASN
1	B	48	ASN
1	B	116	GLN
1	B	197	GLN
1	B	223	HIS
1	B	328	ASN
1	B	380	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	449/449 (100%)	1.21	71 (15%)	5 5	3, 16, 38, 49	0
1	B	449/449 (100%)	1.89	187 (41%)	0 0	3, 16, 38, 57	0
All	All	898/898 (100%)	1.55	258 (28%)	1 1	3, 16, 38, 57	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	378	PRO	5.7
1	B	411	THR	5.3
1	A	412	LEU	5.1
1	B	409	ASN	4.8
1	B	351	VAL	4.8
1	B	416	GLY	4.6
1	B	408	ILE	4.6
1	B	402	TRP	4.6
1	A	411	THR	4.5
1	B	379	ASP	4.5
1	A	30	TRP	4.3
1	A	410	LEU	4.2
1	B	192	ASP	4.1
1	A	257	ASP	4.0
1	B	14	ASP	4.0
1	B	15	SER	4.0
1	B	207	ALA	3.9
1	B	126	ALA	3.8
1	B	143	PRO	3.7
1	A	408	ILE	3.7
1	B	314	PHE	3.7
1	B	415	VAL	3.7
1	B	372	PHE	3.7
1	A	407	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	373	GLN	3.6
1	B	20	ILE	3.5
1	A	365	ASN	3.5
1	B	404	ASN	3.5
1	B	320	GLY	3.5
1	B	220	THR	3.5
1	A	25	LEU	3.4
1	B	142	SER	3.4
1	B	294	ASN	3.4
1	A	3	VAL	3.4
1	B	400	PHE	3.3
1	B	373	GLN	3.3
1	B	154	GLY	3.3
1	B	429	VAL	3.3
1	A	254	GLY	3.2
1	B	427	GLY	3.2
1	B	261	CYS	3.2
1	B	321	VAL	3.2
1	B	369	TYR	3.2
1	B	322	GLY	3.2
1	B	417	ALA	3.2
1	B	410	LEU	3.2
1	B	194	SER	3.1
1	B	187	GLU	3.1
1	B	348	GLY	3.1
1	B	380	ASN	3.1
1	B	245	ILE	3.1
1	B	285	CYS	3.1
1	A	57	SER	3.1
1	B	325	PHE	3.1
1	A	442	VAL	3.1
1	B	345	THR	3.0
1	B	246	VAL	3.0
1	B	347	SER	3.0
1	B	166	ASN	3.0
1	B	242	LEU	3.0
1	B	407	VAL	3.0
1	B	343	ASP	3.0
1	B	350	LYS	3.0
1	A	30(A)	SER	3.0
1	A	364	GLY	3.0
1	B	244	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	245	ILE	2.9
1	B	9	GLY	2.9
1	B	221	ALA	2.9
1	B	3	VAL	2.9
1	A	352	THR	2.9
1	A	137	SER	2.9
1	B	232	LYS	2.9
1	B	449	CYS	2.9
1	B	435	GLU	2.9
1	B	354	HIS	2.9
1	B	113	ALA	2.9
1	B	332	ALA	2.9
1	A	55	ASP	2.9
1	A	333	SER	2.8
1	B	157	ALA	2.8
1	B	344	VAL	2.8
1	B	132	VAL	2.8
1	B	106	TRP	2.8
1	B	252	TRP	2.8
1	B	165	THR	2.8
1	B	243	SER	2.8
1	B	231	GLY	2.8
1	B	46	PRO	2.8
1	B	442	VAL	2.8
1	A	255	THR	2.7
1	B	289	SER	2.7
1	B	299	CYS	2.7
1	B	304	CYS	2.7
1	A	351	VAL	2.7
1	A	42	THR	2.7
1	B	383	SER	2.7
1	B	193	PRO	2.7
1	B	284	SER	2.7
1	B	377	LYS	2.7
1	B	101	CYS	2.7
1	A	403	TYR	2.7
1	B	323	GLN	2.7
1	A	52	ILE	2.7
1	B	133	GLY	2.7
1	B	413	PRO	2.7
1	B	296	CYS	2.7
1	A	17	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	441	ASP	2.6
1	B	1	ASN	2.6
1	B	140	ASP	2.6
1	A	242	LEU	2.6
1	B	293	ALA	2.6
1	B	432	PHE	2.6
1	A	111	ARG	2.6
1	B	164	ARG	2.6
1	A	109	GLY	2.6
1	B	421	THR	2.6
1	B	333	SER	2.6
1	A	244	GLN	2.6
1	A	249	ASP	2.6
1	B	185	THR	2.6
1	B	201	VAL	2.6
1	B	282	GLY	2.6
1	B	316	GLY	2.6
1	B	115	SER	2.6
1	B	300	SER	2.6
1	A	379	ASP	2.6
1	B	21	VAL	2.6
1	B	130	TYR	2.6
1	B	206	ILE	2.6
1	A	448	ALA	2.5
1	B	16	PRO	2.5
1	B	76	GLY	2.5
1	B	88	THR	2.5
1	B	173	THR	2.5
1	B	222	GLY	2.5
1	B	230	GLY	2.5
1	B	381	THR	2.5
1	B	358	SER	2.5
1	B	414	LYS	2.5
1	B	27	ILE	2.5
1	B	168	ALA	2.5
1	A	250	GLY	2.5
1	B	279	GLY	2.5
1	A	88	THR	2.5
1	B	226	PHE	2.5
1	A	409	ASN	2.5
1	A	159	GLY	2.5
1	B	303	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	258	PHE	2.5
1	B	428	SER	2.5
1	B	156	HIS	2.5
1	B	177	PRO	2.5
1	B	390	VAL	2.4
1	A	113	ALA	2.4
1	B	161	ALA	2.4
1	A	375	THR	2.4
1	B	70	THR	2.4
1	B	318	THR	2.4
1	B	181	CYS	2.4
1	B	269	TYR	2.4
1	B	262	ASN	2.4
1	B	445	THR	2.4
1	B	30(A)	SER	2.4
1	B	10	CYS	2.4
1	B	17	TRP	2.4
1	B	159	GLY	2.4
1	B	198	PHE	2.4
1	A	212	ASN	2.3
1	B	312	ASP	2.3
1	B	382	TYR	2.3
1	B	62	SER	2.3
1	B	110	SER	2.3
1	A	237	CYS	2.3
1	A	106	TRP	2.3
1	B	239	LYS	2.3
1	A	133	GLY	2.3
1	B	266	SER	2.3
1	A	354	HIS	2.3
1	A	285	CYS	2.3
1	B	4	CYS	2.3
1	B	346	LEU	2.3
1	B	212	ASN	2.3
1	B	412	LEU	2.3
1	B	237	CYS	2.3
1	B	362	ASN	2.3
1	B	298	PRO	2.3
1	B	315	PRO	2.3
1	A	84	SER	2.3
1	A	243	SER	2.3
1	A	79	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	404	ASN	2.2
1	A	406	ASN	2.2
1	A	449	CYS	2.2
1	B	406	ASN	2.2
1	B	170	GLY	2.2
1	B	361	GLY	2.2
1	B	129	ALA	2.2
1	B	155	SER	2.2
1	B	257	ASP	2.2
1	A	56	PRO	2.2
1	A	32	GLU	2.2
1	A	157	ALA	2.2
1	B	172	ILE	2.2
1	A	21	VAL	2.2
1	B	139	PHE	2.2
1	A	47	ASP	2.2
1	B	79	ASP	2.2
1	B	364	GLY	2.2
1	B	251	ILE	2.2
1	B	200	ASP	2.2
1	B	228	PRO	2.2
1	B	388	SER	2.2
1	B	274	ILE	2.1
1	A	24	PRO	2.1
1	B	2	GLU	2.1
1	A	4	CYS	2.1
1	A	87	SER	2.1
1	B	260	ALA	2.1
1	B	287	SER	2.1
1	B	336	ALA	2.1
1	B	23	ARG	2.1
1	B	114	TYR	2.1
1	B	188	LEU	2.1
1	B	295	LYS	2.1
1	A	378	PRO	2.1
1	B	186	PRO	2.1
1	B	211	PRO	2.1
1	B	103	CYS	2.1
1	A	311	ALA	2.1
1	B	19	GLY	2.1
1	A	18	ALA	2.1
1	B	319	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	100	ASN	2.1
1	A	253	GLN	2.1
1	B	384	ASN	2.1
1	B	401	ILE	2.1
1	B	305	PRO	2.1
1	B	150	GLY	2.1
1	B	297	PHE	2.1
1	A	108	SER	2.0
1	B	238	GLN	2.0
1	A	78	ILE	2.0
1	A	355	VAL	2.0
1	B	34	VAL	2.0
1	B	30	TRP	2.0
1	B	98	SER	2.0
1	B	218	SER	2.0
1	B	440	GLU	2.0
1	B	281	ALA	2.0
1	A	238	GLN	2.0
1	B	263	HIS	2.0
1	B	47	ASP	2.0
1	B	55	ASP	2.0
1	B	426	ASP	2.0
1	B	256	ARG	2.0
1	A	33	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
2	CA	B	970	1/1	0.66	0.12	21,21,21,21	0
2	CA	A	960	1/1	0.67	0.08	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.