



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:52 PM GMT

PDB ID : 1HPL
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

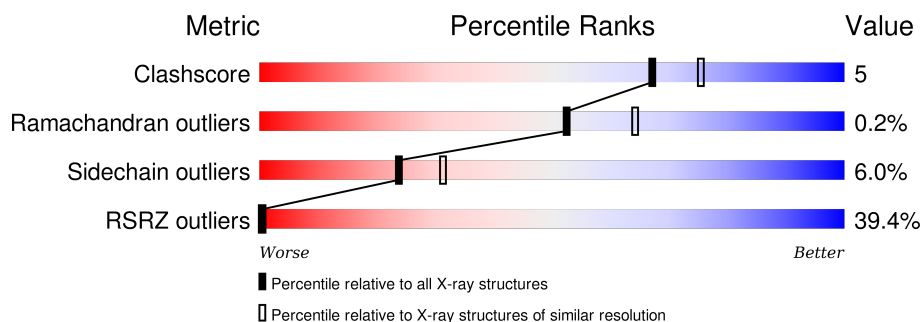
1 Overall quality at a glance

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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>21%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>.</div> </div> </div>
1	B	449	<div> <div>57%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>..</div> </div> </div>

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 (three-letter code: CA) (formula: Ca).

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

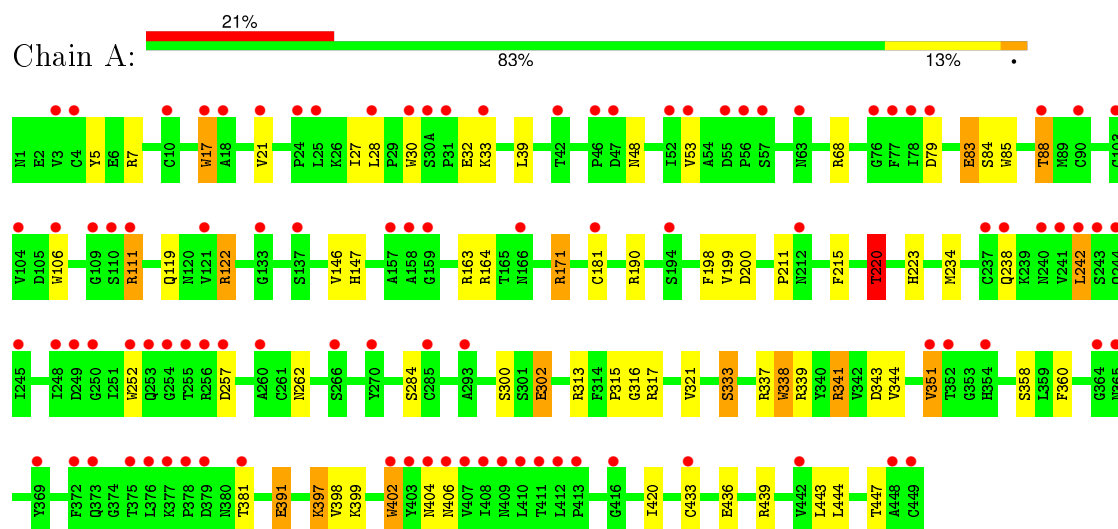
- Molecule 3 is water.

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

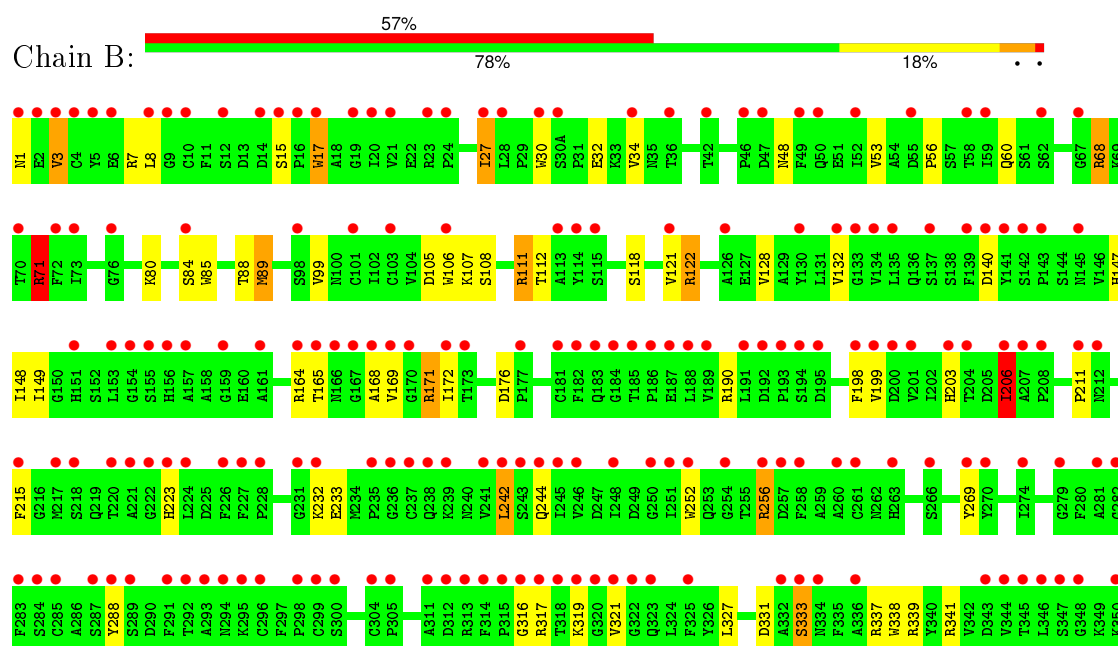
3 Residue-property plots

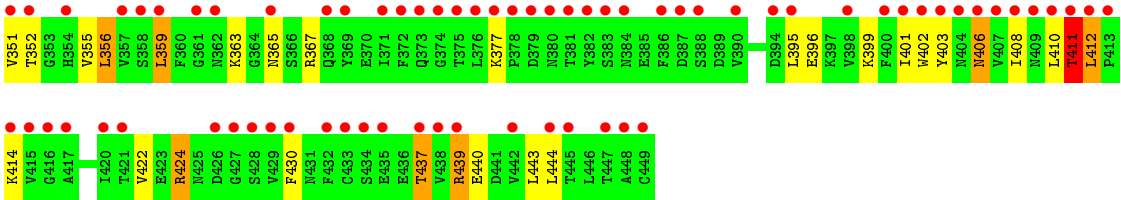
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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 6.05 – 2.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.30) 86.6 (6.05-2.31)	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) (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 99.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ¹	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 40987 reflections (0.005%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.83	1/3587 (0.0%)	1.60	52/4867 (1.1%)
1	B	0.83	0/3587	1.71	67/4867 (1.4%)
All	All	0.83	1/7174 (0.0%)	1.65	119/9734 (1.2%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	VAL	CA-CB	5.60	1.66	1.54

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	SER	O-C-N	-21.47	88.34	122.70
1	A	333	SER	O-C-N	-19.70	91.19	122.70
1	B	122	ARG	NE-CZ-NH1	19.23	129.91	120.30
1	A	339	ARG	NE-CZ-NH2	-17.82	111.39	120.30
1	B	171	ARG	NE-CZ-NH1	17.45	129.03	120.30
1	B	164	ARG	NE-CZ-NH2	-16.29	112.16	120.30
1	B	122	ARG	NE-CZ-NH2	-15.84	112.38	120.30
1	B	7	ARG	NE-CZ-NH2	-14.68	112.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	ARG	NE-CZ-NH2	-14.28	113.16	120.30
1	B	7	ARG	NE-CZ-NH1	12.68	126.64	120.30
1	A	339	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	B	71	ARG	NE-CZ-NH2	-11.72	114.44	120.30
1	A	164	ARG	NE-CZ-NH1	11.68	126.14	120.30
1	A	122	ARG	NE-CZ-NH1	11.17	125.88	120.30
1	B	171	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	B	339	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	B	317	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	A	171	ARG	NE-CZ-NH2	-10.37	115.11	120.30
1	B	337	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	B	68	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	A	171	ARG	NE-CZ-NH1	9.63	125.11	120.30
1	B	30	TRP	CD1-CG-CD2	9.54	113.93	106.30
1	B	71	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	B	317	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	B	333	SER	CA-C-N	9.28	137.62	117.20
1	B	339	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	A	333	SER	CA-C-N	9.17	137.38	117.20
1	B	68	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	A	122	ARG	NE-CZ-NH2	-8.99	115.81	120.30
1	B	17	TRP	CD1-CG-CD2	8.78	113.32	106.30
1	A	439	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	B	164	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	A	313	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	A	5	TYR	CB-CG-CD1	-8.16	116.10	121.00
1	B	439	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	A	252	TRP	CD1-CG-CD2	8.12	112.80	106.30
1	B	17	TRP	CE2-CD2-CG	-8.02	100.88	107.30
1	A	17	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	B	85	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	B	111	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	337	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	A	402	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	A	30	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	A	17	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	A	341	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	A	85	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	B	402	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	A	17	TRP	CG-CD2-CE3	7.57	140.71	133.90
1	B	30	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	B	85	TRP	CE2-CD2-CG	-7.47	101.32	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	B	424	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	A	338	TRP	CD1-CG-CD2	7.36	112.18	106.30
1	A	163	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	A	85	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	A	30	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	B	256	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	B	338	TRP	CD1-CG-CD2	7.00	111.90	106.30
1	A	7	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	B	402	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	B	3	VAL	CB-CA-C	-6.93	98.23	111.40
1	A	252	TRP	CE2-CD2-CG	-6.92	101.76	107.30
1	A	317	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	B	106	TRP	CE2-CD2-CG	-6.77	101.88	107.30
1	B	424	ARG	CB-CG-CD	-6.72	94.14	111.60
1	B	111	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	B	206	ILE	CA-CB-CG1	-6.64	98.38	111.00
1	B	288	TYR	CB-CG-CD1	-6.62	117.03	121.00
1	A	17	TRP	CB-CG-CD1	-6.62	118.39	127.00
1	B	252	TRP	CD1-CG-CD2	6.52	111.52	106.30
1	B	269	TYR	CB-CG-CD2	-6.45	117.13	121.00
1	B	30	TRP	CG-CD1-NE1	-6.42	103.67	110.10
1	B	411	THR	CA-C-N	-6.40	103.12	117.20
1	B	256	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	300	SER	N-CA-CB	-6.29	101.06	110.50
1	A	338	TRP	CE2-CD2-CG	-6.28	102.28	107.30
1	B	338	TRP	CE2-CD2-CG	-6.27	102.28	107.30
1	A	337	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	190	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	B	17	TRP	CB-CG-CD1	-6.25	118.88	127.00
1	B	8	LEU	CA-C-N	6.23	128.66	116.20
1	B	252	TRP	CE2-CD2-CG	-6.21	102.33	107.30
1	B	367	ARG	CA-CB-CG	6.19	127.02	113.40
1	A	106	TRP	CE2-CD2-CG	-6.17	102.36	107.30
1	B	17	TRP	CG-CD2-CE3	6.14	139.43	133.90
1	A	315	PRO	CA-C-N	6.11	128.42	116.20
1	B	8	LEU	O-C-N	-6.10	112.84	123.20
1	A	337	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	402	TRP	CE2-CD2-CG	-6.07	102.45	107.30
1	B	356	LEU	CA-CB-CG	6.05	129.23	115.30
1	A	402	TRP	CG-CD1-NE1	-5.97	104.13	110.10
1	B	106	TRP	CD1-CG-CD2	5.85	110.98	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	190	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	176	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	397	LYS	CA-CB-CG	5.72	125.99	113.40
1	B	171	ARG	CB-CG-CD	5.67	126.34	111.60
1	A	106	TRP	CD1-CG-CD2	5.66	110.83	106.30
1	B	17	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	B	333	SER	CA-C-O	5.63	131.92	120.10
1	B	341	ARG	CG-CD-NE	-5.57	100.11	111.80
1	A	68	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	30	TRP	CG-CD1-NE1	-5.40	104.70	110.10
1	A	85	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	B	331	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	111	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	B	27	ILE	CA-CB-CG1	-5.34	100.86	111.00
1	A	252	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	B	85	TRP	CB-CG-CD1	-5.29	120.12	127.00
1	B	27	ILE	CA-CB-CG2	5.28	121.46	110.90
1	B	206	ILE	N-CA-CB	-5.27	98.68	110.80
1	A	21	VAL	CA-CB-CG2	-5.23	103.06	110.90
1	B	89	MET	CG-SD-CE	-5.15	91.96	100.20
1	B	363	LYS	CB-CG-CD	-5.15	98.22	111.60
1	A	220	THR	N-CA-CB	-5.14	100.54	110.30
1	A	17	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	A	85	TRP	CA-CB-CG	5.08	123.35	113.70
1	A	300	SER	CA-CB-OG	5.04	124.80	111.20
1	A	338	TRP	CG-CD1-NE1	-5.00	105.10	110.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3501	0	3334	32	2
1	B	3501	0	3334	39	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	66	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 (66) 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
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:H	1:A:242:LEU:HD22	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:412:LEU:HD12	1:B:439:ARG:HD2	1.89	0.55
1:B:171:ARG:HD3	1:B:198:PHE:CD2	2.42	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:B:89:MET:HE3	1:B:149:ILE:HD13	1.93	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:TRP:CZ3	1:A:122:ARG:HD3	2.49	0.48
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:B:223:HIS:HA	1:B:321:VAL:HA	1.96	0.47
1:A:341:ARG:HH11	1:A:341:ARG:HG3	1.80	0.47
1:B:359:LEU:HG	1:B:395:LEU:HD21	1.96	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: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:443:LEU:H	1:B:48:ASN:ND2	2.08	0.44
1:A:33:LYS:HE3	3:A:1032:HOH:O	2.17	0.44
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:B:171:ARG:HA	1:B:198:PHE:O	2.19	0.41
1:A:398:VAL:HG11	1:A:420:ILE:HG21	2.02	0.41
1:A:351:VAL:HG11	1:A:402:TRP:CZ3	2.55	0.41
1:A:171:ARG:HD3	1:A:198:PHE:CD2	2.55	0.41
1:A:83:GLU:CD	1:A:83:GLU:H	2.23	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:238:GLN:H	1:A:238:GLN:CD	2.24	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 sym-

metry 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%)	39	48
All	All	894/898 (100%)	861 (96%)	31 (4%)	2 (0%)	52	64

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%)	364 (94%)	21 (6%)	27	36
1	B	385/385 (100%)	360 (94%)	25 (6%)	21	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	770/770 (100%)	724 (94%)	46 (6%)	24	31

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	32	GLU
1	A	39	LEU
1	A	53	VAL
1	A	83	GLU
1	A	88	THR
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	351	VAL
1	A	391	GLU
1	A	397	LYS
1	A	404	ASN
1	A	406	ASN
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	68	ARG
1	B	80	LYS
1	B	111	ARG
1	B	112	THR
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	327	LEU

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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	406	ASN
1	B	411	THR
1	B	412	LEU
1	B	437	THR
1	B	444	LEU

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

Mol	Chain	Res	Type
1	A	48	ASN
1	A	223	HIS
1	A	262	ASN
1	A	328	ASN
1	A	404	ASN
1	B	48	ASN
1	B	223	HIS
1	B	328	ASN

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 carbohydrates 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	1.39	96 (21%) ⓘ ⓘ	3, 16, 38, 49	0
1	B	449/449 (100%)	2.38	258 (57%) ⓘ ⓘ	3, 16, 38, 57	0
All	All	898/898 (100%)	1.88	354 (39%) ⓘ ⓘ	3, 16, 38, 57	0

All (354) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	408	ILE	8.2
1	A	412	LEU	7.8
1	B	411	THR	6.9
1	A	411	THR	6.8
1	B	409	ASN	6.8
1	B	245	ILE	6.6
1	B	410	LEU	6.4
1	B	378	PRO	6.2
1	A	407	VAL	5.9
1	B	351	VAL	5.8
1	B	244	GLN	5.8
1	B	379	ASP	5.8
1	B	372	PHE	5.6
1	A	408	ILE	5.5
1	A	410	LEU	5.3
1	B	402	TRP	5.1
1	B	304	CYS	5.1
1	A	25	LEU	5.1
1	B	416	GLY	4.9
1	A	30	TRP	4.9
1	A	242	LEU	4.9
1	B	333	SER	4.8
1	B	207	ALA	4.8
1	B	373	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	242	LEU	4.7
1	B	332	ALA	4.6
1	B	415	VAL	4.6
1	B	285	CYS	4.5
1	B	299	CYS	4.5
1	B	314	PHE	4.4
1	B	449	CYS	4.4
1	B	381	THR	4.4
1	B	289	SER	4.4
1	B	412	LEU	4.3
1	A	352	THR	4.3
1	B	296	CYS	4.3
1	B	15	SER	4.3
1	B	194	SER	4.3
1	A	3	VAL	4.2
1	A	257	ASP	4.2
1	B	376	LEU	4.2
1	B	407	VAL	4.2
1	B	406	ASN	4.2
1	A	351	VAL	4.1
1	B	261	CYS	4.1
1	A	245	ILE	4.0
1	B	20	ILE	4.0
1	B	246	VAL	4.0
1	B	344	VAL	3.9
1	A	21	VAL	3.9
1	B	400	PHE	3.9
1	B	4	CYS	3.9
1	B	181	CYS	3.9
1	B	14	ASP	3.9
1	B	193	PRO	3.8
1	B	165	THR	3.7
1	B	192	ASP	3.7
1	B	346	LEU	3.7
1	B	445	THR	3.7
1	B	432	PHE	3.6
1	A	241	VAL	3.6
1	B	132	VAL	3.6
1	B	221	ALA	3.6
1	A	254	GLY	3.6
1	B	248	ILE	3.6
1	B	429	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	258	PHE	3.6
1	B	220	THR	3.6
1	B	347	SER	3.6
1	B	448	ALA	3.5
1	B	439	ARG	3.5
1	B	438	VAL	3.5
1	B	404	ASN	3.5
1	B	168	ALA	3.5
1	B	369	TYR	3.5
1	B	126	ALA	3.5
1	B	166	ASN	3.5
1	B	380	ASN	3.5
1	B	421	THR	3.5
1	B	156	HIS	3.5
1	B	21	VAL	3.5
1	B	231	GLY	3.5
1	B	17	TRP	3.5
1	B	142	SER	3.4
1	B	241	VAL	3.4
1	A	255	THR	3.4
1	B	325	PHE	3.4
1	A	373	GLN	3.4
1	A	88	THR	3.4
1	B	1	ASN	3.4
1	B	251	ILE	3.4
1	B	382	TYR	3.4
1	B	442	VAL	3.3
1	B	294	ASN	3.3
1	B	27	ILE	3.3
1	B	218	SER	3.3
1	B	377	LYS	3.3
1	B	143	PRO	3.3
1	B	173	THR	3.3
1	B	185	THR	3.3
1	B	316	GLY	3.3
1	B	177	PRO	3.3
1	B	226	PHE	3.3
1	B	390	VAL	3.3
1	B	322	GLY	3.2
1	A	243	SER	3.2
1	B	298	PRO	3.2
1	B	19	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	269	TYR	3.2
1	A	406	ASN	3.2
1	B	354	HIS	3.2
1	B	186	PRO	3.2
1	B	383	SER	3.2
1	B	345	THR	3.2
1	B	3	VAL	3.2
1	B	101	CYS	3.2
1	A	375	THR	3.2
1	B	187	GLU	3.2
1	B	154	GLY	3.2
1	B	430	PHE	3.1
1	B	134	VAL	3.1
1	B	315	PRO	3.1
1	B	428	SER	3.1
1	A	17	TRP	3.1
1	B	254	GLY	3.1
1	B	437	THR	3.1
1	B	427	GLY	3.1
1	B	295	LYS	3.1
1	B	447	THR	3.1
1	B	139	PHE	3.1
1	A	409	ASN	3.1
1	B	10	CYS	3.1
1	B	257	ASP	3.1
1	B	76	GLY	3.0
1	B	350	LYS	3.0
1	B	211	PRO	3.0
1	A	78	ILE	3.0
1	B	252	TRP	3.0
1	B	103	CYS	3.0
1	B	172	ILE	3.0
1	B	106	TRP	3.0
1	A	55	ASP	3.0
1	A	260	ALA	3.0
1	B	318	THR	3.0
1	B	164	ARG	3.0
1	B	130	TYR	3.0
1	B	155	SER	3.0
1	B	222	GLY	3.0
1	A	212	ASN	2.9
1	A	449	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	343	ASP	2.9
1	A	364	GLY	2.9
1	B	16	PRO	2.9
1	A	244	GLN	2.9
1	B	348	GLY	2.9
1	B	232	LYS	2.9
1	B	113	ALA	2.9
1	B	417	ALA	2.9
1	A	57	SER	2.9
1	B	198	PHE	2.9
1	A	111	ARG	2.9
1	A	53	VAL	2.9
1	A	106	TRP	2.9
1	A	109	GLY	2.9
1	A	237	CYS	2.9
1	B	5	TYR	2.8
1	B	274	ILE	2.8
1	A	376	LEU	2.8
1	B	243	SER	2.8
1	B	414	LYS	2.8
1	B	320	GLY	2.8
1	A	378	PRO	2.8
1	B	413	PRO	2.8
1	B	201	VAL	2.8
1	B	321	VAL	2.8
1	B	67	GLY	2.8
1	B	352	THR	2.8
1	A	137	SER	2.7
1	B	206	ILE	2.7
1	A	249	ASP	2.7
1	A	433	CYS	2.7
1	B	287	SER	2.7
1	B	375	THR	2.7
1	B	9	GLY	2.7
1	B	239	LYS	2.7
1	A	293	ALA	2.7
1	B	312	ASP	2.7
1	B	36	THR	2.7
1	B	266	SER	2.7
1	B	170	GLY	2.7
1	B	270	TYR	2.7
1	A	377	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	167	GLY	2.7
1	A	238	GLN	2.7
1	A	256	ARG	2.7
1	B	115	SER	2.7
1	A	24	PRO	2.7
1	B	398	VAL	2.7
1	B	228	PRO	2.6
1	B	371	ILE	2.6
1	B	200	ASP	2.6
1	A	181	CYS	2.6
1	B	300	SER	2.6
1	A	354	HIS	2.6
1	B	362	ASN	2.6
1	A	402	TRP	2.6
1	B	317	ARG	2.6
1	A	56	PRO	2.6
1	B	223	HIS	2.6
1	A	442	VAL	2.6
1	B	212	ASN	2.6
1	A	33	LYS	2.6
1	B	34	VAL	2.6
1	A	52	ILE	2.6
1	B	358	SER	2.5
1	B	403	TYR	2.5
1	B	157	ALA	2.5
1	B	435	GLU	2.5
1	B	401	ILE	2.5
1	B	420	ILE	2.5
1	B	23	ARG	2.5
1	B	263	HIS	2.5
1	B	70	THR	2.5
1	B	195	ASP	2.5
1	B	359	LEU	2.5
1	B	323	GLN	2.5
1	B	46	PRO	2.5
1	A	18	ALA	2.5
1	A	133	GLY	2.5
1	B	55	ASP	2.5
1	B	374	GLY	2.5
1	A	365	ASN	2.5
1	B	140	ASP	2.5
1	B	256	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	30(A)	SER	2.4
1	B	334	ASN	2.4
1	B	188	LEU	2.4
1	B	183	GLN	2.4
1	A	76	GLY	2.4
1	A	404	ASN	2.4
1	B	281	ALA	2.4
1	B	305	PRO	2.4
1	B	49	PHE	2.4
1	B	313	ARG	2.4
1	B	224	LEU	2.4
1	B	433	CYS	2.4
1	B	426	ASP	2.4
1	B	141	TYR	2.4
1	A	166	ASN	2.4
1	A	4	CYS	2.4
1	B	151	HIS	2.4
1	B	159	GLY	2.4
1	B	384	ASN	2.4
1	A	30(A)	SER	2.4
1	B	284	SER	2.4
1	A	381	THR	2.4
1	B	24	PRO	2.4
1	B	2	GLU	2.3
1	B	292	THR	2.3
1	B	30	TRP	2.3
1	A	10	CYS	2.3
1	B	237	CYS	2.3
1	A	250	GLY	2.3
1	B	250	GLY	2.3
1	B	58	THR	2.3
1	A	110	SER	2.3
1	B	62	SER	2.3
1	A	121	VAL	2.3
1	A	270	TYR	2.3
1	B	357	VAL	2.3
1	B	42	THR	2.3
1	B	238	GLN	2.3
1	A	103	CYS	2.3
1	B	59	ILE	2.3
1	B	260	ALA	2.3
1	B	291	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	217	MET	2.3
1	A	413	PRO	2.3
1	A	248	ILE	2.3
1	B	133	GLY	2.3
1	B	204	THR	2.3
1	A	369	TYR	2.3
1	B	293	ALA	2.3
1	A	372	PHE	2.3
1	B	182	PHE	2.3
1	B	386	PHE	2.3
1	A	79	ASP	2.3
1	B	319	LYS	2.3
1	A	266	SER	2.2
1	B	12	SER	2.2
1	B	283	PHE	2.2
1	B	6	GLU	2.2
1	B	8	LEU	2.2
1	A	157	ALA	2.2
1	A	194	SER	2.2
1	B	169	VAL	2.2
1	A	403	TYR	2.2
1	B	282	GLY	2.2
1	A	47	ASP	2.2
1	B	145	ASN	2.2
1	B	121	VAL	2.2
1	A	77	PHE	2.2
1	A	46	PRO	2.2
1	A	253	GLN	2.2
1	A	448	ALA	2.2
1	A	104	VAL	2.2
1	B	279	GLY	2.2
1	B	72	PHE	2.2
1	B	288	TYR	2.2
1	A	31	PRO	2.2
1	B	191	LEU	2.2
1	B	365	ASN	2.2
1	A	285	CYS	2.2
1	B	311	ALA	2.2
1	B	135	LEU	2.1
1	B	153	LEU	2.1
1	B	395	LEU	2.1
1	B	444	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	336	ALA	2.1
1	B	84	SER	2.1
1	A	379	ASP	2.1
1	A	158	ALA	2.1
1	A	159	GLY	2.1
1	B	236	GLY	2.1
1	A	90	CYS	2.1
1	B	52	ILE	2.1
1	B	73	ILE	2.1
1	B	47	ASP	2.1
1	B	114	TYR	2.1
1	A	28	LEU	2.1
1	B	50	GLN	2.1
1	B	361	GLY	2.1
1	B	98	SER	2.1
1	B	199	VAL	2.1
1	B	215	PHE	2.1
1	B	137	SER	2.1
1	B	434	SER	2.1
1	B	189	VAL	2.1
1	A	252	TRP	2.1
1	B	394	ASP	2.1
1	B	227	PHE	2.0
1	B	28	LEU	2.0
1	B	235	PRO	2.0
1	B	388	SER	2.0
1	A	63	ASN	2.0
1	A	240	ASN	2.0
1	A	416	GLY	2.0
1	A	42	THR	2.0
1	B	368	GLN	2.0
1	B	387	ASP	2.0
1	B	161	ALA	2.0
1	B	208	PRO	2.0
1	B	184	GLY	2.0
1	B	203	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	B	970	1/1	0.52	0.15	-2.39	21,21,21,21	0
2	CA	A	960	1/1	0.90	0.09	-3.04	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.