



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 02:53 PM UTC

PDB ID : 3N2B / pdb_00003n2b
Title : 1.8 Angstrom Resolution Crystal Structure of Diaminopimelate Decarboxylase (lysA) from *Vibrio cholerae*.
Authors : Minasov, G.; Halavaty, A.; Shuvalova, L.; Dubrovskaya, I.; Winsor, J.; Papazisi, L.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2010-05-17
Resolution : 1.80 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

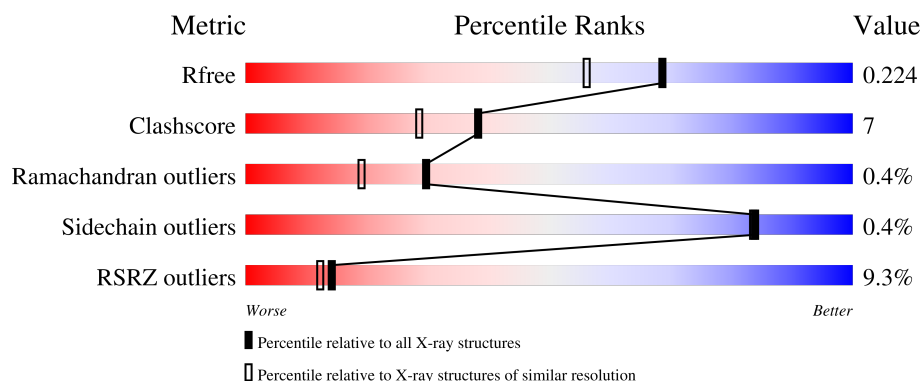
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	441	7% 83% 9% 7%
1	B	441	10% 78% 11% 11%
1	C	441	7% 82% 11% 7%
1	D	441	10% 77% 13% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14009 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 Diaminopimelate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	8	0
			3279	2072	579	618	10			
1	B	392	Total	C	N	O	S	0	7	0
			3123	1982	546	586	9			
1	C	411	Total	C	N	O	S	0	10	0
			3283	2079	574	620	10			
1	D	398	Total	C	N	O	S	0	8	0
			3179	2008	558	603	10			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q9KVL7
A	-22	HIS	-	expression tag	UNP Q9KVL7
A	-21	HIS	-	expression tag	UNP Q9KVL7
A	-20	HIS	-	expression tag	UNP Q9KVL7
A	-19	HIS	-	expression tag	UNP Q9KVL7
A	-18	HIS	-	expression tag	UNP Q9KVL7
A	-17	HIS	-	expression tag	UNP Q9KVL7
A	-16	SER	-	expression tag	UNP Q9KVL7
A	-15	SER	-	expression tag	UNP Q9KVL7
A	-14	GLY	-	expression tag	UNP Q9KVL7
A	-13	VAL	-	expression tag	UNP Q9KVL7
A	-12	ASP	-	expression tag	UNP Q9KVL7
A	-11	LEU	-	expression tag	UNP Q9KVL7
A	-10	GLY	-	expression tag	UNP Q9KVL7
A	-9	THR	-	expression tag	UNP Q9KVL7
A	-8	GLU	-	expression tag	UNP Q9KVL7
A	-7	ASN	-	expression tag	UNP Q9KVL7
A	-6	LEU	-	expression tag	UNP Q9KVL7
A	-5	TYR	-	expression tag	UNP Q9KVL7
A	-4	PHE	-	expression tag	UNP Q9KVL7
A	-3	GLN	-	expression tag	UNP Q9KVL7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9KVL7
A	-1	ASN	-	expression tag	UNP Q9KVL7
A	0	ALA	-	expression tag	UNP Q9KVL7
B	-23	MET	-	expression tag	UNP Q9KVL7
B	-22	HIS	-	expression tag	UNP Q9KVL7
B	-21	HIS	-	expression tag	UNP Q9KVL7
B	-20	HIS	-	expression tag	UNP Q9KVL7
B	-19	HIS	-	expression tag	UNP Q9KVL7
B	-18	HIS	-	expression tag	UNP Q9KVL7
B	-17	HIS	-	expression tag	UNP Q9KVL7
B	-16	SER	-	expression tag	UNP Q9KVL7
B	-15	SER	-	expression tag	UNP Q9KVL7
B	-14	GLY	-	expression tag	UNP Q9KVL7
B	-13	VAL	-	expression tag	UNP Q9KVL7
B	-12	ASP	-	expression tag	UNP Q9KVL7
B	-11	LEU	-	expression tag	UNP Q9KVL7
B	-10	GLY	-	expression tag	UNP Q9KVL7
B	-9	THR	-	expression tag	UNP Q9KVL7
B	-8	GLU	-	expression tag	UNP Q9KVL7
B	-7	ASN	-	expression tag	UNP Q9KVL7
B	-6	LEU	-	expression tag	UNP Q9KVL7
B	-5	TYR	-	expression tag	UNP Q9KVL7
B	-4	PHE	-	expression tag	UNP Q9KVL7
B	-3	GLN	-	expression tag	UNP Q9KVL7
B	-2	SER	-	expression tag	UNP Q9KVL7
B	-1	ASN	-	expression tag	UNP Q9KVL7
B	0	ALA	-	expression tag	UNP Q9KVL7
C	-23	MET	-	expression tag	UNP Q9KVL7
C	-22	HIS	-	expression tag	UNP Q9KVL7
C	-21	HIS	-	expression tag	UNP Q9KVL7
C	-20	HIS	-	expression tag	UNP Q9KVL7
C	-19	HIS	-	expression tag	UNP Q9KVL7
C	-18	HIS	-	expression tag	UNP Q9KVL7
C	-17	HIS	-	expression tag	UNP Q9KVL7
C	-16	SER	-	expression tag	UNP Q9KVL7
C	-15	SER	-	expression tag	UNP Q9KVL7
C	-14	GLY	-	expression tag	UNP Q9KVL7
C	-13	VAL	-	expression tag	UNP Q9KVL7
C	-12	ASP	-	expression tag	UNP Q9KVL7
C	-11	LEU	-	expression tag	UNP Q9KVL7
C	-10	GLY	-	expression tag	UNP Q9KVL7
C	-9	THR	-	expression tag	UNP Q9KVL7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLU	-	expression tag	UNP Q9KVL7
C	-7	ASN	-	expression tag	UNP Q9KVL7
C	-6	LEU	-	expression tag	UNP Q9KVL7
C	-5	TYR	-	expression tag	UNP Q9KVL7
C	-4	PHE	-	expression tag	UNP Q9KVL7
C	-3	GLN	-	expression tag	UNP Q9KVL7
C	-2	SER	-	expression tag	UNP Q9KVL7
C	-1	ASN	-	expression tag	UNP Q9KVL7
C	0	ALA	-	expression tag	UNP Q9KVL7
D	-23	MET	-	expression tag	UNP Q9KVL7
D	-22	HIS	-	expression tag	UNP Q9KVL7
D	-21	HIS	-	expression tag	UNP Q9KVL7
D	-20	HIS	-	expression tag	UNP Q9KVL7
D	-19	HIS	-	expression tag	UNP Q9KVL7
D	-18	HIS	-	expression tag	UNP Q9KVL7
D	-17	HIS	-	expression tag	UNP Q9KVL7
D	-16	SER	-	expression tag	UNP Q9KVL7
D	-15	SER	-	expression tag	UNP Q9KVL7
D	-14	GLY	-	expression tag	UNP Q9KVL7
D	-13	VAL	-	expression tag	UNP Q9KVL7
D	-12	ASP	-	expression tag	UNP Q9KVL7
D	-11	LEU	-	expression tag	UNP Q9KVL7
D	-10	GLY	-	expression tag	UNP Q9KVL7
D	-9	THR	-	expression tag	UNP Q9KVL7
D	-8	GLU	-	expression tag	UNP Q9KVL7
D	-7	ASN	-	expression tag	UNP Q9KVL7
D	-6	LEU	-	expression tag	UNP Q9KVL7
D	-5	TYR	-	expression tag	UNP Q9KVL7
D	-4	PHE	-	expression tag	UNP Q9KVL7
D	-3	GLN	-	expression tag	UNP Q9KVL7
D	-2	SER	-	expression tag	UNP Q9KVL7
D	-1	ASN	-	expression tag	UNP Q9KVL7
D	0	ALA	-	expression tag	UNP Q9KVL7

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	C	2	Total Cl 2 2	0	0
2	D	1	Total Cl 1 1	0	0

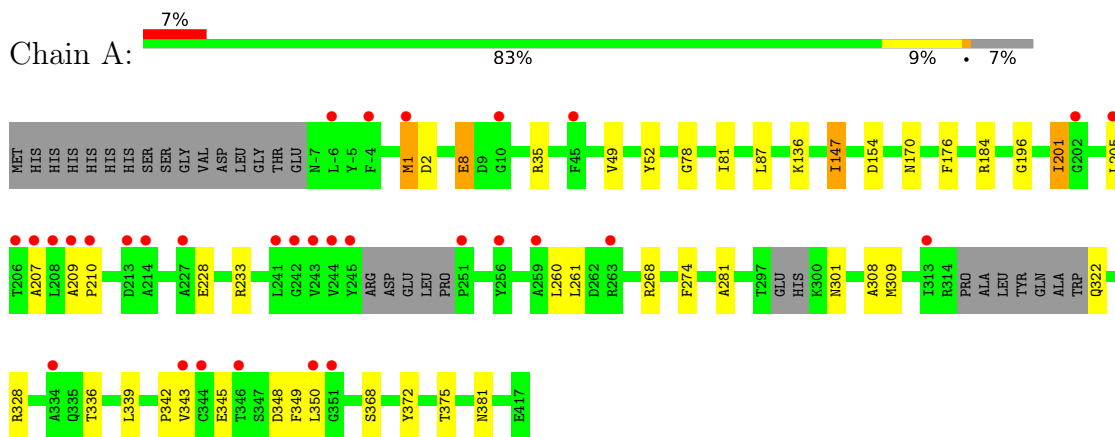
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	324	Total 328	O 328	0	5
3	B	280	Total 284	O 284	0	4
3	C	285	Total 290	O 290	0	7
3	D	232	Total 239	O 239	0	7

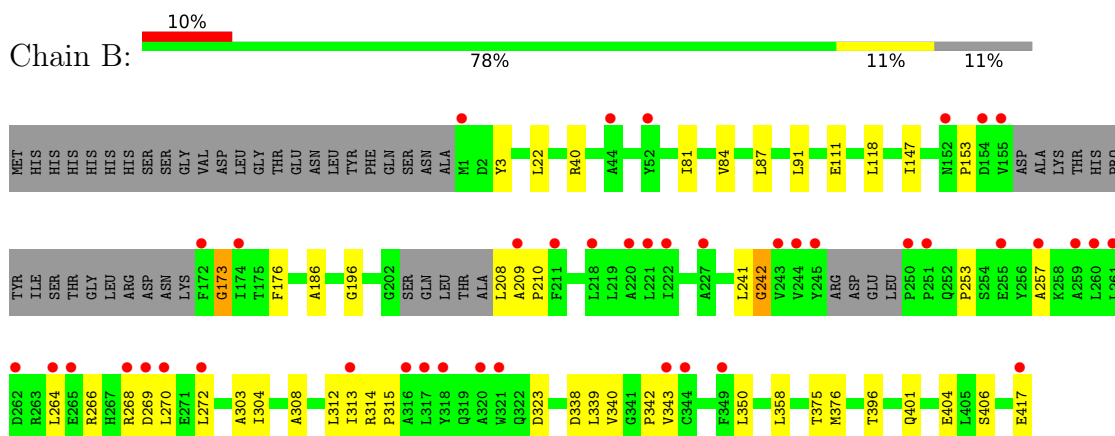
3 Residue-property plots [i](#)

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.

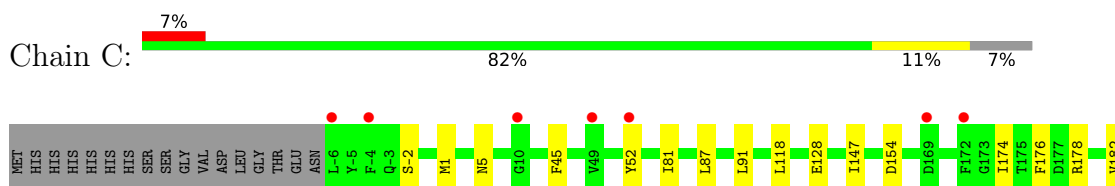
• Molecule 1: Diaminopimelate decarboxylase

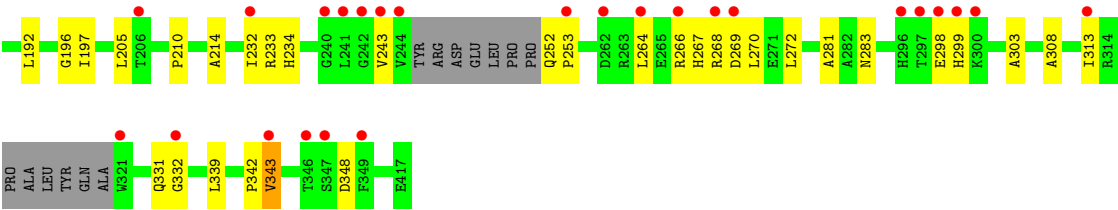


• Molecule 1: Diaminopimelate decarboxylase

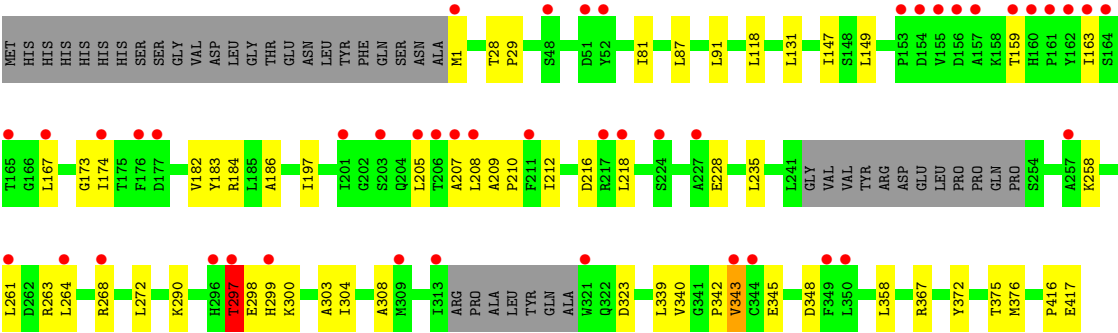
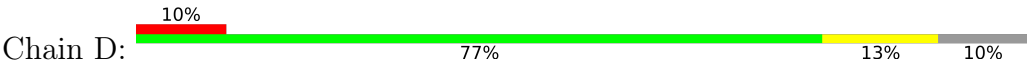


• Molecule 1: Diaminopimelate decarboxylase





● Molecule 1: Diaminopimelate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.39Å 80.33Å 118.69Å 105.31° 93.62° 90.52°	Depositor
Resolution (Å)	29.94 – 1.80 29.94 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.94-1.80) 97.5 (29.94-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.183 , 0.219 0.188 , 0.224	Depositor DCC
R_{free} test set	7289 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14009	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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

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

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	0.71	0/3340	0.87	6/4521 (0.1%)
1	B	0.69	0/3185	0.85	4/4317 (0.1%)
1	C	0.68	0/3352	0.85	1/4543 (0.0%)
1	D	0.66	0/3239	0.85	4/4388 (0.1%)
All	All	0.69	0/13116	0.85	15/17769 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	281	ALA	N-CA-C	5.88	120.73	113.50
1	B	358	LEU	N-CA-C	5.79	118.98	109.72
1	D	358	LEU	N-CA-C	5.55	118.77	109.95
1	A	2	ASP	N-CA-C	5.51	115.81	108.38
1	B	196	GLY	N-CA-C	5.49	119.30	111.12
1	A	196	GLY	N-CA-C	5.47	119.28	111.12
1	A	201	ILE	N-CA-C	5.34	120.44	109.34
1	B	338	ASP	N-CA-C	-5.30	100.59	109.24
1	B	173	GLY	N-CA-C	5.29	125.72	113.18
1	D	173	GLY	N-CA-C	5.13	121.60	112.22
1	A	78	GLY	N-CA-C	-5.13	104.48	112.58
1	D	297	THR	CA-C-N	5.06	130.81	121.70
1	D	297	THR	C-N-CA	5.06	130.81	121.70
1	A	281	ALA	N-CA-C	5.05	119.57	113.41
1	A	147	ILE	N-CA-C	5.00	117.01	108.86

There are no chirality outliers.

There are no planarity outliers.

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	3279	0	3261	40	0
1	B	3123	0	3101	35	0
1	C	3283	0	3260	42	0
1	D	3179	0	3152	62	0
2	A	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	A	328	0	0	2	0
3	B	284	0	0	5	0
3	C	290	0	0	2	0
3	D	239	0	0	3	0
All	All	14009	0	12774	177	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 7.

All (177) 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:233[B]:ARG:NH2	1:A:233[B]:ARG:HG2	1.58	1.05
1:A:233[B]:ARG:HH21	1:A:233[B]:ARG:CG	1.74	0.99
1:A:233[B]:ARG:HG2	1:A:233[B]:ARG:HH21	0.84	0.98
1:A:343:VAL:HG13	1:A:381:ASN:OD1	1.64	0.97
1:A:308:ALA:HB1	1:A:343:VAL:HG23	1.50	0.93
1:C:264:LEU:HD13	1:C:272:LEU:HD11	1.50	0.92
1:B:304:ILE:HD13	1:B:340:VAL:CG2	2.02	0.90
1:A:343:VAL:HG12	1:A:345:GLU:HG2	1.58	0.85
1:C:91[B]:LEU:HD11	1:C:118:LEU:CD1	2.09	0.82
1:D:268[B]:ARG:NE	1:D:268[B]:ARG:H	1.80	0.80
1:A:308:ALA:HB1	1:A:343:VAL:CG2	2.13	0.79
1:D:268[B]:ARG:H	1:D:268[B]:ARG:HE	1.31	0.79
1:A:8[B]:GLU:O	1:A:8[B]:GLU:CD	2.27	0.78
1:D:298:GLU:HB2	1:D:299:HIS:HA	1.65	0.77
1:B:304:ILE:HD13	1:B:340:VAL:HG23	1.66	0.76
1:A:1:MET:HA	1:A:1:MET:HE2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91[A]:LEU:HD11	1:B:118:LEU:HD13	1.67	0.76
1:C:264:LEU:CD1	1:C:272:LEU:HD11	2.14	0.76
1:A:308:ALA:HB2	1:A:342:PRO:HD2	1.67	0.75
1:C:91[B]:LEU:HD11	1:C:118:LEU:HD13	1.68	0.75
1:D:304:ILE:HD13	1:D:340:VAL:CG2	2.17	0.75
1:C:264:LEU:HD13	1:C:272:LEU:HD21	1.67	0.75
1:D:218:LEU:HD21	1:D:235:LEU:HD11	1.69	0.74
1:B:147:ILE:HD11	1:B:186:ALA:HB1	1.72	0.71
1:D:343:VAL:HG22	1:D:348:ASP:OD2	1.91	0.71
1:A:8[B]:GLU:OE2	1:A:8[B]:GLU:C	2.34	0.71
1:D:304:ILE:HD13	1:D:340:VAL:HG23	1.74	0.69
1:D:297:THR:HB	1:D:298:GLU:HA	1.73	0.69
1:B:268:ARG:CB	1:B:269:ASP:HA	2.23	0.69
1:B:396:THR:HG23	3:B:520:HOH:O	1.91	0.69
1:D:297:THR:HG22	1:D:298:GLU:O	1.91	0.69
1:C:331[B]:GLN:OE1	1:C:332:GLY:N	2.26	0.68
1:B:268:ARG:HB3	1:B:269:ASP:HA	1.79	0.64
1:D:208:LEU:HD21	1:D:212:ILE:HD11	1.80	0.64
1:D:147:ILE:HD11	1:D:186:ALA:HB1	1.78	0.64
1:A:8[B]:GLU:CD	1:A:8[B]:GLU:C	2.64	0.64
1:C:264:LEU:CD1	1:C:272:LEU:HD21	2.27	0.64
1:D:174:ILE:HD13	1:D:182:VAL:HG21	1.79	0.64
1:C:91[B]:LEU:HD11	1:C:118:LEU:HD11	1.81	0.62
1:A:268:ARG:HG2	1:A:268:ARG:O	1.99	0.62
1:B:91[A]:LEU:HD11	1:B:118:LEU:CD1	2.29	0.61
1:B:304:ILE:CD1	1:B:340:VAL:HG23	2.31	0.61
1:D:91:LEU:HD11	1:D:118:LEU:CD1	2.31	0.61
1:A:349:PHE:C	1:A:350:LEU:HD12	2.26	0.60
1:D:208:LEU:HD23	1:D:208:LEU:O	2.01	0.60
1:D:290:LYS:HE3	3:D:524:HOH:O	2.01	0.60
1:C:264:LEU:HD13	1:C:272:LEU:CD1	2.26	0.60
1:B:304:ILE:CD1	1:B:340:VAL:CG2	2.77	0.60
1:C:308:ALA:HB2	1:C:342:PRO:HD2	1.84	0.59
1:C:1:MET:HE3	1:C:283:ASN:OD1	2.03	0.58
1:B:264:LEU:CD1	1:B:272:LEU:HD21	2.33	0.58
1:D:81:ILE:HD13	1:D:87:LEU:HB2	1.85	0.58
1:D:261:LEU:HD23	1:D:261:LEU:O	2.03	0.58
1:B:3:TYR:OH	1:B:40[A]:ARG:NH1	2.36	0.58
1:A:233[B]:ARG:NH2	1:A:233[B]:ARG:CG	2.43	0.58
1:C:174:ILE:CD1	1:C:182:VAL:HG11	2.34	0.58
1:C:268:ARG:HB3	1:C:269:ASP:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:NH2	1:B:417:GLU:OE1	2.37	0.57
1:B:253:PRO:HB2	1:B:257:ALA:HB3	1.85	0.57
1:A:308:ALA:CB	1:A:343:VAL:HG23	2.30	0.57
1:C:147[A]:ILE:HD13	1:C:192:LEU:HD13	1.86	0.57
1:B:314:ARG:HB2	1:B:315:PRO:HD3	1.88	0.56
1:C:128:GLU:OE2	1:C:178:ARG:NH2	2.33	0.55
1:C:52:TYR:CE2	1:C:272:LEU:HG	2.40	0.55
1:D:297:THR:HB	1:D:298:GLU:CA	2.35	0.55
1:C:303:ALA:HB3	1:C:339:LEU:HD13	1.88	0.55
1:A:201:ILE:HD11	1:A:260:LEU:HD22	1.89	0.55
1:D:303:ALA:HB3	1:D:339:LEU:HD13	1.89	0.54
1:D:208:LEU:HD23	1:D:208:LEU:C	2.32	0.54
1:C:174:ILE:HD13	1:C:182:VAL:HG11	1.90	0.54
1:C:343:VAL:HG22	1:C:348:ASP:OD2	2.07	0.53
1:A:147:ILE:C	1:A:147:ILE:HD12	2.34	0.53
1:A:343:VAL:N	1:A:348:ASP:OD2	2.42	0.53
1:D:304:ILE:CD1	1:D:340:VAL:HG23	2.38	0.53
1:C:196:GLY:HA2	1:C:232:ILE:HG23	1.92	0.52
1:D:159:THR:HG22	3:D:465:HOH:O	2.08	0.52
1:C:264:LEU:HD13	1:C:272:LEU:CD2	2.37	0.52
1:B:208:LEU:O	1:B:208:LEU:HD23	2.10	0.52
1:D:308:ALA:HB2	1:D:342:PRO:HD2	1.92	0.52
1:C:268:ARG:HA	1:C:270:LEU:H	1.75	0.52
1:D:339:LEU:HD22	1:D:339:LEU:N	2.25	0.52
1:D:91:LEU:HD11	1:D:118:LEU:HD11	1.93	0.51
1:D:163:ILE:O	1:D:167:LEU:HD13	2.10	0.51
1:D:208:LEU:HD21	1:D:212:ILE:CD1	2.39	0.51
1:A:81:ILE:HD13	1:A:87:LEU:HB2	1.92	0.51
1:C:266:ARG:HG3	1:C:267:HIS:N	2.26	0.51
1:A:309:MET:HG2	1:A:343:VAL:HG21	1.93	0.50
1:B:241:LEU:HB3	1:B:242:GLY:HA3	1.93	0.50
1:D:184:ARG:NE	1:D:228:GLU:OE2	2.38	0.50
1:B:264:LEU:HD11	1:B:272:LEU:HD21	1.92	0.50
1:B:81:ILE:HD13	1:B:87:LEU:HB2	1.94	0.50
1:B:308:ALA:HB2	1:B:342:PRO:HD2	1.94	0.50
1:D:264:LEU:HD11	1:D:272:LEU:HD21	1.94	0.50
1:C:45:PHE:HA	1:C:243:VAL:HG21	1.94	0.49
1:A:81:ILE:CD1	1:A:87:LEU:HB2	2.42	0.49
1:D:131:LEU:HD11	1:D:147:ILE:HD13	1.95	0.49
1:A:49[B]:VAL:HG11	1:A:274:PHE:CE2	2.49	0.48
1:A:49[A]:VAL:HG13	1:A:261:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:ASP:OD1	1:D:263:ARG:HD3	2.13	0.48
1:D:212:ILE:HG23	1:D:263:ARG:HD2	1.94	0.48
1:B:303:ALA:HB3	1:B:339:LEU:HD13	1.95	0.48
1:D:209:ALA:HB3	1:D:210:PRO:HD3	1.94	0.48
1:B:264:LEU:HD12	1:B:272:LEU:HD11	1.96	0.47
1:D:209:ALA:HB3	1:D:210:PRO:CD	2.44	0.47
1:D:375:THR:HG23	1:D:376:MET:HG3	1.96	0.47
1:D:298:GLU:HB2	1:D:299:HIS:CA	2.41	0.47
1:B:209:ALA:N	1:B:210:PRO:HD2	2.29	0.47
1:C:154:ASP:HB2	1:C:176:PHE:CG	2.50	0.47
1:D:197:ILE:HG23	1:D:235:LEU:CD1	2.44	0.47
1:D:208:LEU:CD2	1:D:212:ILE:CD1	2.92	0.47
1:B:84:VAL:HB	1:B:111:GLU:HG2	1.96	0.47
1:D:149:LEU:HD12	1:D:183:TYR:CD1	2.49	0.47
1:B:342:PRO:O	3:B:957:HOH:O	2.20	0.47
1:C:-2:SER:HA	1:C:5:ASN:ND2	2.29	0.47
1:A:350:LEU:HD12	1:A:350:LEU:N	2.30	0.46
1:A:339:LEU:HD12	1:A:339:LEU:N	2.30	0.46
1:D:264:LEU:CD1	1:D:272:LEU:HD21	2.45	0.46
1:B:268:ARG:HA	1:B:270:LEU:H	1.80	0.46
1:A:154:ASP:HB2	1:A:176:PHE:CG	2.51	0.45
1:A:328:ARG:CZ	1:C:331[B]:GLN:HG2	2.46	0.45
1:C:197:ILE:HB	1:C:232:ILE:HD13	1.98	0.45
1:A:209:ALA:HB3	1:A:210:PRO:CD	2.46	0.45
1:D:218:LEU:HD21	1:D:235:LEU:CD1	2.43	0.45
1:B:404[A]:GLU:OE2	1:B:406[A]:SER:OG	2.30	0.45
1:C:81:ILE:CD1	1:C:87:LEU:HB2	2.47	0.45
1:C:52:TYR:OH	1:C:267:HIS:O	2.29	0.44
1:C:234:HIS:CE1	3:C:441:HOH:O	2.69	0.44
1:D:304:ILE:CD1	1:D:340:VAL:CG2	2.90	0.44
1:A:301:ASN:HB2	1:A:336:THR:O	2.17	0.44
1:D:261:LEU:HD23	1:D:261:LEU:C	2.43	0.44
1:A:184:ARG:NE	1:A:228:GLU:OE1	2.34	0.44
1:D:205:LEU:HD12	1:D:205:LEU:N	2.32	0.44
1:D:372:TYR:HA	1:D:375:THR:CG2	2.47	0.44
1:D:91:LEU:HD11	1:D:118:LEU:HD13	1.98	0.44
1:D:323:ASP:HB3	1:D:367:ARG:HD3	1.98	0.44
1:B:323:ASP:OD1	3:B:951:HOH:O	2.21	0.43
1:A:343:VAL:CG1	1:A:345:GLU:HG2	2.38	0.43
1:A:268:ARG:O	1:A:268:ARG:CG	2.66	0.43
1:B:22:LEU:HD21	1:B:396:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ARG:H	1:B:266:ARG:CD	2.32	0.43
1:D:290:LYS:CE	3:D:524:HOH:O	2.65	0.43
1:B:312:LEU:HD23	1:B:350:LEU:HD22	2.01	0.43
1:C:313:ILE:O	1:C:313:ILE:HG23	2.19	0.42
1:D:343:VAL:CG2	1:D:348:ASP:OD2	2.63	0.42
1:D:197:ILE:HG23	1:D:235:LEU:HD12	2.01	0.42
1:C:268:ARG:HA	1:C:270:LEU:N	2.33	0.42
1:C:339:LEU:N	1:C:339:LEU:HD22	2.35	0.42
1:B:313:ILE:HG22	3:B:949:HOH:O	2.20	0.42
1:C:205:LEU:HD22	1:C:210:PRO:HB2	2.01	0.42
1:C:233:ARG:O	1:C:270:LEU:HA	2.20	0.42
1:B:153:PRO:HA	1:B:176:PHE:HE1	1.85	0.41
1:B:401[A]:GLN:CD	3:B:543:HOH:O	2.62	0.41
1:D:345:GLU:HB2	1:D:348:ASP:HB2	2.01	0.41
1:D:416:PRO:O	1:D:417:GLU:HB2	2.20	0.41
3:C:515:HOH:O	1:D:297:THR:HG22	2.19	0.41
1:A:207:ALA:HB1	3:A:576[B]:HOH:O	2.20	0.41
1:C:252:GLN:HB2	1:C:253:PRO:HD3	2.03	0.41
1:A:322:GLN:HG2	1:A:368[B]:SER:OG	2.21	0.41
1:D:208:LEU:C	1:D:208:LEU:CD2	2.94	0.41
1:A:372:TYR:HA	1:A:375:THR:CG2	2.50	0.41
1:D:174:ILE:HD11	1:D:182:VAL:HG11	2.02	0.41
1:D:207:ALA:HB3	1:D:210:PRO:CG	2.51	0.41
1:D:268[A]:ARG:HA	1:D:268[A]:ARG:HD3	1.80	0.41
1:A:136:LYS:NZ	3:A:897:HOH:O	2.52	0.41
1:D:297:THR:HB	1:D:300:LYS:H	1.86	0.41
1:A:49[A]:VAL:HG12	1:A:52:TYR:HB3	2.02	0.40
1:A:209:ALA:HB3	1:A:210:PRO:HD3	2.01	0.40
1:D:28:THR:HA	1:D:29:PRO:C	2.46	0.40
1:D:131:LEU:HD11	1:D:147:ILE:CD1	2.51	0.40
1:C:298:GLU:HA	1:C:299:HIS:HA	1.85	0.40
1:D:264:LEU:CD1	1:D:272:LEU:HD11	2.52	0.40
1:D:372:TYR:HA	1:D:375:THR:HG22	2.03	0.40
1:B:375:THR:HG23	1:B:376:MET:HG3	2.03	0.40
1:C:205:LEU:HD11	1:C:214:ALA:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/441 (93%)	404 (98%)	6 (2%)	1 (0%)	43	31
1	B	391/441 (89%)	374 (96%)	14 (4%)	3 (1%)	16	6
1	C	415/441 (94%)	404 (97%)	10 (2%)	1 (0%)	43	31
1	D	400/441 (91%)	384 (96%)	14 (4%)	2 (0%)	24	14
All	All	1617/1764 (92%)	1566 (97%)	44 (3%)	7 (0%)	30	19

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	343	VAL
1	C	343	VAL
1	D	343	VAL
1	A	205	LEU
1	D	297	THR
1	B	242	GLY
1	B	173	GLY

5.3.2 Protein sidechains [i](#)

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	350/368 (95%)	346 (99%)	4 (1%)	65	60
1	B	332/368 (90%)	332 (100%)	0	100	100
1	C	351/368 (95%)	351 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	339/368 (92%)	337 (99%)	2 (1%)	78	77
All	All	1372/1472 (93%)	1366 (100%)	6 (0%)	84	83

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8[A]	GLU
1	A	8[B]	GLU
1	A	170	ASN
1	D	1	MET
1	D	258	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	170	ASN
1	A	187	HIS
1	B	5	ASN
1	B	16	GLN
1	B	25	GLN
1	B	124	ASN
1	B	187	HIS
1	B	191	ASN
1	B	195	HIS
1	B	231	HIS
1	B	234	HIS
1	B	252	GLN
1	B	319	GLN
1	B	322	GLN
1	C	152	ASN
1	C	191	ASN
1	C	195	HIS
1	C	234	HIS
1	D	41	HIS
1	D	191	ASN
1	D	301	ASN
1	D	331	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](#)

Of 4 ligands modelled in this entry, 4 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 [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	411/441 (93%)	0.49	31 (7%) 20 18	12, 34, 60, 76	8 (1%)
1	B	392/441 (88%)	0.59	42 (10%) 11 9	12, 35, 78, 89	7 (1%)
1	C	411/441 (93%)	0.49	32 (7%) 19 17	12, 37, 58, 70	10 (2%)
1	D	398/441 (90%)	0.65	45 (11%) 10 8	12, 36, 68, 86	8 (2%)
All	All	1612/1764 (91%)	0.55	150 (9%) 14 12	12, 36, 66, 89	33 (2%)

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	343	VAL	6.1
1	C	298	GLU	5.4
1	A	251	PRO	5.3
1	A	245	TYR	4.4
1	A	343	VAL	4.2
1	D	268[A]	ARG	4.2
1	A	10	GLY	4.1
1	D	155	VAL	4.1
1	B	318	TYR	4.1
1	B	155	VAL	4.1
1	C	346	THR	4.1
1	D	321	TRP	4.0
1	B	227	ALA	4.0
1	D	167	LEU	3.9
1	C	269	ASP	3.8
1	A	227	ALA	3.7
1	A	-6	LEU	3.6
1	B	1	MET	3.6
1	A	205	LEU	3.5
1	D	52	TYR	3.5
1	A	346	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	205	LEU	3.5
1	D	349	PHE	3.4
1	B	245	TYR	3.4
1	C	321	TRP	3.4
1	B	317	LEU	3.4
1	C	241	LEU	3.4
1	D	297	THR	3.4
1	D	344	CYS	3.3
1	B	320	ALA	3.3
1	C	-6	LEU	3.3
1	A	209	ALA	3.2
1	C	343	VAL	3.2
1	A	206	THR	3.2
1	D	159	THR	3.2
1	C	242	GLY	3.2
1	A	334	ALA	3.2
1	C	297	THR	3.1
1	C	313	ILE	3.1
1	D	163	ILE	3.1
1	D	165	THR	3.1
1	B	269	ASP	3.1
1	B	244	VAL	3.1
1	B	261	LEU	3.1
1	D	261	LEU	3.1
1	D	177	ASP	3.1
1	D	157	ALA	3.0
1	A	350	LEU	3.0
1	A	244	VAL	3.0
1	B	172	PHE	3.0
1	D	161	PRO	3.0
1	B	343	VAL	3.0
1	B	417	GLU	2.9
1	C	10	GLY	2.9
1	B	211	PHE	2.9
1	B	220	ALA	2.9
1	D	350	LEU	2.9
1	B	152	ASN	2.9
1	B	251	PRO	2.9
1	D	217	ARG	2.9
1	D	156	ASP	2.9
1	D	1	MET	2.9
1	C	244	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	256	TYR	2.8
1	D	162	TYR	2.8
1	B	264	LEU	2.8
1	D	208	LEU	2.8
1	B	250	PRO	2.8
1	A	259	ALA	2.8
1	B	344	CYS	2.8
1	B	218	LEU	2.8
1	D	164	SER	2.8
1	D	257	ALA	2.8
1	D	218	LEU	2.8
1	C	169	ASP	2.8
1	B	268	ARG	2.7
1	C	264	LEU	2.7
1	B	349	PHE	2.7
1	C	349	PHE	2.7
1	C	296	HIS	2.7
1	D	296	HIS	2.7
1	A	207	ALA	2.6
1	A	242	GLY	2.6
1	C	232	ILE	2.6
1	A	213	ASP	2.6
1	D	211	PHE	2.6
1	C	253	PRO	2.6
1	C	-4	PHE	2.6
1	C	300	LYS	2.6
1	B	209	ALA	2.6
1	C	243	VAL	2.6
1	C	52	TYR	2.5
1	D	207	ALA	2.5
1	A	1	MET	2.5
1	D	176	PHE	2.5
1	C	268	ARG	2.5
1	B	222	ILE	2.5
1	A	263	ARG	2.4
1	B	52	TYR	2.4
1	A	208	LEU	2.4
1	C	299	HIS	2.4
1	D	154	ASP	2.4
1	C	240	GLY	2.4
1	C	262	ASP	2.4
1	B	316	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	202	GLY	2.4
1	D	48	SER	2.4
1	A	344	CYS	2.4
1	A	241	LEU	2.3
1	D	227	ALA	2.3
1	B	313	ILE	2.3
1	D	174	ILE	2.3
1	A	313	ILE	2.3
1	D	299	HIS	2.3
1	D	309	MET	2.3
1	B	255	GLU	2.2
1	B	259	ALA	2.2
1	C	347	SER	2.2
1	D	203	SER	2.2
1	B	154	ASP	2.2
1	B	265	GLU	2.2
1	A	351	GLY	2.2
1	B	262	ASP	2.2
1	B	174	ILE	2.2
1	D	201	ILE	2.2
1	C	266	ARG	2.2
1	B	221	LEU	2.2
1	B	270	LEU	2.2
1	B	272	LEU	2.2
1	A	214	ALA	2.2
1	D	206	THR	2.2
1	D	51	ASP	2.2
1	D	153	PRO	2.2
1	C	172	PHE	2.1
1	C	206	THR	2.1
1	B	260	LEU	2.1
1	B	44	ALA	2.1
1	B	321	TRP	2.1
1	A	-4	PHE	2.1
1	D	313	ILE	2.1
1	D	224	SER	2.1
1	C	332	GLY	2.1
1	B	243	VAL	2.1
1	D	264	LEU	2.0
1	B	257	ALA	2.0
1	A	45	PHE	2.0
1	D	160	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	210	PRO	2.0
1	A	243	VAL	2.0
1	C	49	VAL	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(Å ²)	Q<0.9
2	CL	C	419	1/1	0.97	0.07	43,43,43,43	0
2	CL	C	418	1/1	0.98	0.07	38,38,38,38	0
2	CL	A	418	1/1	0.98	0.09	44,44,44,44	0
2	CL	D	418	1/1	0.99	0.08	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.