



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:33 PM UTC

PDB ID : 1DLO / pdb_00001dlo
Title : HUMAN IMMUNODEFICIENCY VIRUS TYPE 1
Authors : Hsiou, Y.; Ding, J.; Das, K.; Hughes, S.; Arnold, E.
Deposited on : 1996-04-17
Resolution : 2.70 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

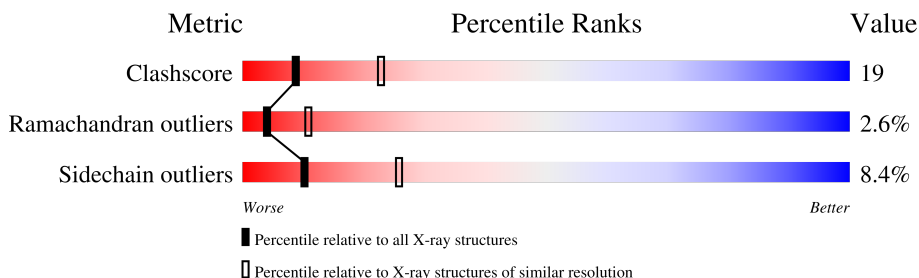
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	556	
2	B	427	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7691 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 HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	0	0
			4370	2835	727	802	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	415	Total	C	N	O	S	0	0	0
			3321	2163	549	604	5			

There is a discrepancy between the modelled and reference sequences:

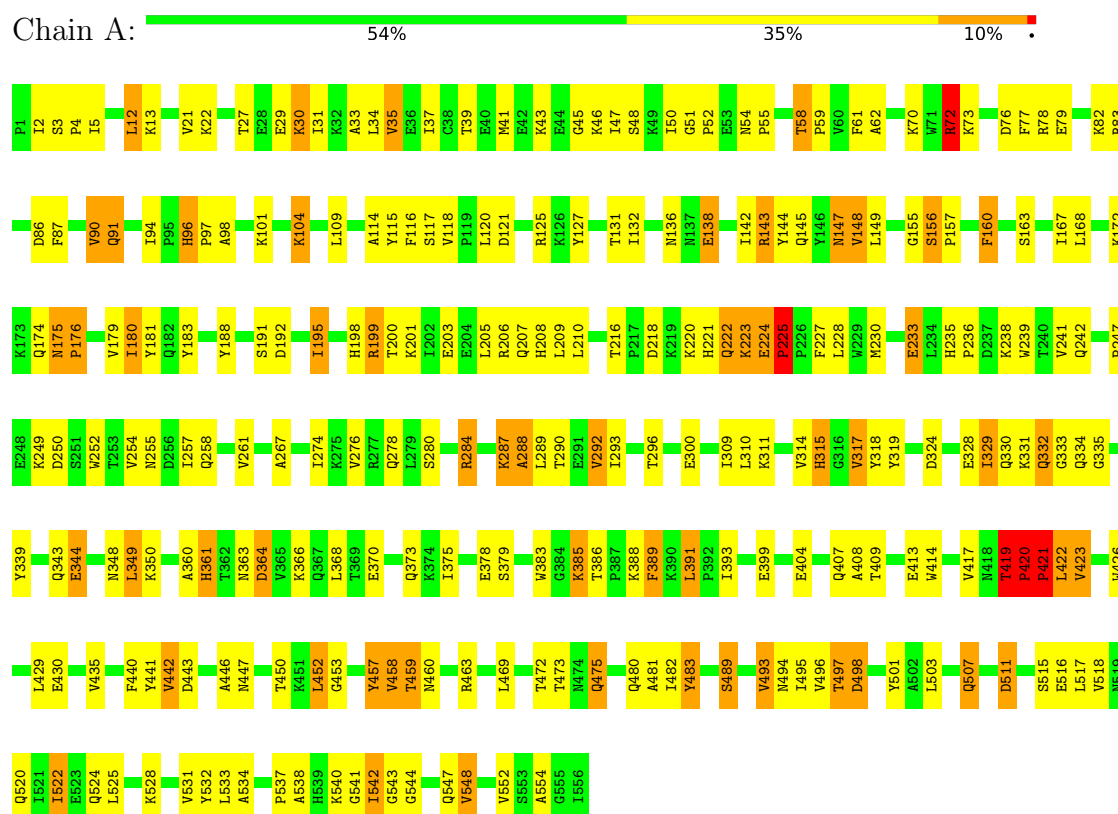
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

3 Residue-property plots

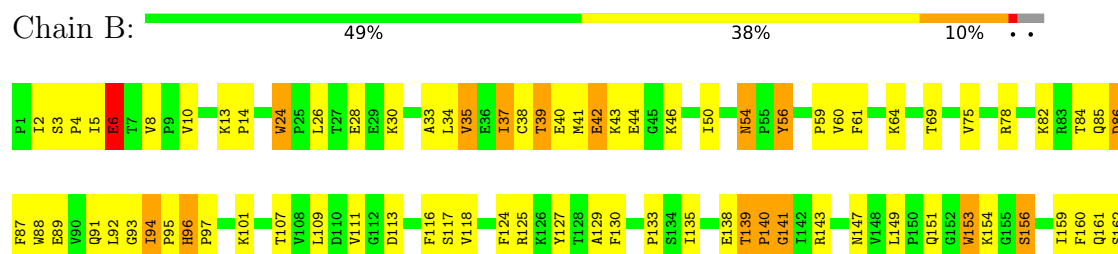
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE



- Molecule 2: HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE



S163	V245	G316	I393	S163
L246	V317	V318	K395	L246
P247	Y319	Y319	E396	P247
E248	D320	D320	T397	E248
K249	P321	P321	W398	K249
D250			E399	D250
	A327	A327	T400	
V254	Q332	Q332	W401	V254
N255			W402	N255
D256	Q336	Q336	T403	D256
I257	K337	K337	W410	I257
	T338	T338		
L260	Y339	Y339	E413	L260
V261	Q340	Q340	W414	V261
	Q343	Q343	E415	
A267	E344	E344	F416	A267
S268	P345	P345	W417	S268
Q269	F346	F346	N418	Q269
L270	K347	K347	T419	L270
Y271	N348	N348	P420	Y271
	L349	L349	P421	
I274	K350	K350	L422	I274
K275	T351	T351	V423	K275
V276	G352	G352		V276
R277	K353	K353	Y427	R277
Q278	Y354	Y354		Q278
L279	M357	M357		L279
S280				S280
K281				K281
L282				L282
L283				L283
Q213	T286	T286		Q213
L214				L214
T215				T215
T216	L289	L289		T216
P217	T290	T290		P217
D218				D218
LYS	I293	I293		LYS
LYS	P294	P294		LYS
HIS	L295	L295		HIS
GLN	T296	T296		GLN
LYS	E297	E297		LYS
GLU	E298	E298		GLU
PRO	A299	A299		PRO
PRO	E300	E300		PRO
PHE	L301	L301		PHE
LEU	E302	E302		LEU
TRP	L303	L303		TRP
MET	A304	A304		MET
G231	E305	E305		G231
Y232	N306	N306		Y232
E233	R307	R307		E233
L234	E308	E308		L234
H235	I309	I309		H235
P236	L310	L310		P236
D237	K311	K311		D237
K238	E312	E312		K238
W239	F313	F313		W239
	V314	V314		
	H315	H315		

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	235.50Å 70.30Å 93.30Å 90.00° 106.10° 90.00°	Depositor
Resolution (Å)	8.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.249 , 0.336	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7691	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

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	0.86	3/4486 (0.1%)	1.33	64/6119 (1.0%)
2	B	0.93	3/3415 (0.1%)	1.32	48/4652 (1.0%)
All	All	0.89	6/7901 (0.1%)	1.33	112/10771 (1.0%)

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	1
2	B	0	2
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	420	PRO	CA-C	6.70	1.58	1.52
1	A	493	VAL	CA-CB	-6.10	1.49	1.55
2	B	189	VAL	CA-CB	5.67	1.60	1.53
1	A	522	ILE	CA-CB	5.39	1.60	1.54
1	A	386	THR	CA-CB	5.12	1.61	1.52
2	B	393	ILE	CA-CB	5.08	1.61	1.55

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	VAL	N-CA-C	15.36	126.48	110.36
1	A	91	GLN	N-CA-C	11.40	125.95	110.55
1	A	360	ALA	N-CA-C	-10.78	100.26	113.41
1	A	225	PRO	N-CA-C	10.36	123.33	110.70
1	A	175	ASN	CA-C-N	9.44	129.67	119.28
1	A	175	ASN	C-N-CA	9.44	129.67	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ASN	N-CA-C	-8.58	96.80	109.15
2	B	198	HIS	N-CA-C	-8.45	102.78	113.43
1	A	147	ASN	N-CA-C	-8.44	103.58	114.04
1	A	361	HIS	N-CA-C	-8.43	97.75	110.14
1	A	457	TYR	N-CA-C	8.41	121.25	109.31
1	A	224	GLU	CA-C-N	8.14	128.77	120.38
1	A	224	GLU	C-N-CA	8.14	128.77	120.38
2	B	54	ASN	CA-C-N	7.83	127.55	119.56
2	B	54	ASN	C-N-CA	7.83	127.55	119.56
1	A	30	LYS	N-CA-C	-7.70	102.01	111.40
2	B	8	VAL	CB-CA-C	-7.68	103.80	110.94
1	A	388	LYS	N-CA-C	-7.55	98.27	110.20
2	B	382	ILE	N-CA-C	7.41	117.53	110.42
1	A	442	VAL	N-CA-C	7.32	119.53	109.80
2	B	305	GLU	N-CA-C	-7.22	103.34	111.14
1	A	176	PRO	N-CA-C	7.17	123.33	113.65
2	B	209	LEU	N-CA-C	-7.08	103.64	111.36
2	B	87	PHE	N-CA-C	7.02	119.90	110.35
2	B	6	GLU	N-CA-C	-6.93	97.96	109.46
1	A	155	GLY	N-CA-C	6.67	122.31	113.37
1	A	12	LEU	N-CA-C	-6.67	101.92	110.53
1	A	498	ASP	N-CA-C	-6.59	104.47	113.30
2	B	86	ASP	N-CA-C	-6.57	99.19	109.25
1	A	364	ASP	N-CA-C	6.57	118.32	111.03
1	A	344	GLU	N-CA-C	-6.54	101.83	110.07
2	B	92	LEU	N-CA-C	-6.51	104.18	111.28
1	A	96	HIS	CA-C-N	6.49	126.17	119.56
1	A	96	HIS	C-N-CA	6.49	126.17	119.56
2	B	247	PRO	N-CA-C	6.49	120.80	111.13
2	B	401	TRP	N-CA-C	6.39	122.67	114.56
1	A	368	LEU	N-CA-C	-6.38	104.02	110.97
2	B	303	LEU	N-CA-C	6.33	118.70	111.11
1	A	143	ARG	N-CA-C	6.27	119.73	109.76
2	B	363	ASN	N-CA-C	-6.25	97.62	108.69
1	A	419	THR	CA-C-N	6.25	126.82	120.38
1	A	419	THR	C-N-CA	6.25	126.82	120.38
1	A	225	PRO	CA-C-N	-6.18	112.12	119.84
1	A	225	PRO	C-N-CA	-6.18	112.12	119.84
1	A	138	GLU	N-CA-C	-6.13	105.65	113.01
2	B	96	HIS	N-CA-C	6.13	123.35	109.81
1	A	156	SER	CA-C-N	-6.09	112.64	118.97
1	A	156	SER	C-N-CA	-6.09	112.64	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	419	THR	CA-C-N	6.09	126.66	120.38
2	B	419	THR	C-N-CA	6.09	126.66	120.38
2	B	298	GLU	N-CA-C	-6.07	104.01	112.45
1	A	242	GLN	N-CA-C	-6.04	102.44	109.93
1	A	70	LYS	N-CA-C	6.03	118.34	108.52
2	B	43	LYS	N-CA-C	-5.98	104.76	111.28
1	A	148	VAL	N-CA-CB	-5.98	105.52	112.34
2	B	294	PRO	N-CA-C	5.96	119.85	110.50
2	B	371	ALA	N-CA-C	-5.93	104.16	111.40
2	B	271	TYR	CB-CA-C	-5.89	105.14	110.44
2	B	269	GLN	N-CA-C	-5.88	104.95	111.36
1	A	13	LYS	N-CA-C	-5.88	102.37	109.83
2	B	235	HIS	CA-C-N	5.87	127.17	119.84
2	B	235	HIS	C-N-CA	5.87	127.17	119.84
1	A	86	ASP	N-CA-C	-5.85	101.82	110.48
2	B	200	THR	N-CA-C	-5.83	103.75	111.96
2	B	338	THR	N-CA-C	-5.78	100.63	109.41
1	A	101	LYS	N-CA-C	-5.76	100.74	109.85
1	A	278	GLN	N-CA-C	5.74	117.62	111.36
1	A	51	GLY	CA-C-N	5.73	127.01	119.84
1	A	51	GLY	C-N-CA	5.73	127.01	119.84
1	A	391	LEU	N-CA-C	5.71	118.76	110.14
1	A	22	LYS	N-CA-C	5.71	119.22	110.20
1	A	195	ILE	N-CA-C	5.70	121.19	109.34
1	A	292	VAL	N-CA-C	5.64	117.44	108.87
2	B	417	VAL	N-CA-C	5.61	121.01	109.34
2	B	423	VAL	N-CA-C	-5.61	104.86	110.30
1	A	200	THR	N-CA-C	-5.61	105.09	111.14
1	A	160	PHE	N-CA-C	-5.59	105.18	111.28
2	B	204	GLU	N-CA-C	-5.57	105.36	111.82
1	A	349	LEU	N-CA-C	-5.54	104.64	111.40
1	A	72	ARG	N-CA-C	5.52	118.26	109.65
2	B	237	ASP	N-CA-C	-5.48	104.83	112.45
2	B	54	ASN	N-CA-C	-5.45	96.82	108.93
1	A	421	PRO	CA-N-CD	-5.44	104.39	112.00
2	B	286	THR	N-CA-C	-5.42	102.31	110.06
1	A	46	LYS	N-CA-C	-5.37	105.51	111.36
2	B	139	THR	CB-CA-C	-5.36	105.62	110.44
2	B	39	THR	N-CA-C	-5.35	105.53	111.36
2	B	245	VAL	N-CA-C	5.35	115.60	108.11
2	B	415	GLU	N-CA-C	-5.34	101.24	109.52
1	A	296	THR	N-CA-C	-5.34	102.85	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	213	GLY	N-CA-C	5.34	121.86	114.92
1	A	489	SER	N-CA-C	5.32	116.61	108.42
2	B	380	ILE	N-CA-C	-5.31	105.32	110.42
2	B	389	PHE	N-CA-C	5.30	118.86	109.96
1	A	58	THR	CA-C-N	5.26	125.56	119.93
1	A	58	THR	C-N-CA	5.26	125.56	119.93
1	A	348	ASN	N-CA-C	5.26	118.12	109.76
1	A	389	PHE	N-CA-C	5.25	118.62	110.17
1	A	267	ALA	N-CA-C	5.21	117.70	111.71
2	B	351	THR	N-CA-C	-5.21	100.81	108.99
1	A	483	TYR	N-CA-C	-5.20	105.52	111.14
1	A	404	GLU	N-CA-C	5.18	119.75	113.38
1	A	87	PHE	N-CA-C	-5.16	101.91	109.81
2	B	118	VAL	N-CA-C	5.14	112.95	107.76
1	A	35	VAL	N-CA-C	-5.13	105.41	111.00
2	B	344	GLU	CA-C-N	5.09	126.20	119.84
2	B	344	GLU	C-N-CA	5.09	126.20	119.84
1	A	329	ILE	N-CA-C	5.08	115.80	108.48
2	B	388	LYS	N-CA-C	-5.07	100.47	108.73
1	A	284	ARG	N-CA-C	-5.04	105.87	111.36
2	B	56	TYR	N-CA-C	5.03	117.17	110.53
2	B	233	GLU	N-CA-C	5.03	118.00	109.76

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	501	TYR	Sidechain
2	B	127	TYR	Sidechain
2	B	183	TYR	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	4370	0	4315	165	0
2	B	3321	0	3293	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7691	0	7608	286	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 19.

All (286) 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)
2:B:260:LEU:HD21	2:B:303:LEU:HD21	1.58	0.86
1:A:420:PRO:HB3	1:A:421:PRO:HD2	1.57	0.85
1:A:420:PRO:CB	1:A:421:PRO:HD2	2.06	0.85
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.57	0.83
2:B:255:ASN:HB2	2:B:289:LEU:HB3	1.61	0.80
2:B:348:ASN:HD22	2:B:351:THR:HG22	1.45	0.80
1:A:435:VAL:HA	2:B:290:THR:HG21	1.64	0.80
2:B:198:HIS:O	2:B:202:ILE:HG12	1.84	0.78
1:A:228:LEU:HD23	1:A:233:GLU:HG3	1.66	0.77
1:A:543:GLY:HA2	2:B:283:LEU:O	1.84	0.77
2:B:250:ASP:OD2	2:B:303:LEU:HD13	1.84	0.76
1:A:442:VAL:HG13	1:A:481:ALA:HB1	1.69	0.75
1:A:50:ILE:HG21	1:A:145:GLN:HE21	1.51	0.74
2:B:209:LEU:HD22	2:B:214:LEU:HD12	1.68	0.74
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.71	0.72
1:A:34:LEU:HB3	1:A:132:ILE:HD12	1.72	0.71
1:A:199:ARG:O	1:A:199:ARG:HD3	1.91	0.71
1:A:276:VAL:HG12	1:A:280:SER:OG	1.92	0.69
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.74	0.68
2:B:195:ILE:HG12	2:B:199:ARG:NE	2.07	0.68
2:B:109:LEU:HD22	2:B:216:THR:HG21	1.75	0.68
1:A:206:ARG:HH22	1:A:218:ASP:HA	1.60	0.67
2:B:195:ILE:HG12	2:B:199:ARG:HE	1.59	0.67
1:A:532:TYR:CE1	1:A:534:ALA:HB2	2.31	0.66
1:A:116:PHE:O	1:A:148:VAL:HG21	1.95	0.66
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.32	0.65
1:A:457:TYR:O	1:A:458:VAL:HG23	1.98	0.64
1:A:109:LEU:HD22	1:A:216:THR:HG21	1.80	0.63
1:A:223:LYS:HD2	1:A:227:PHE:HZ	1.64	0.62
2:B:89:GLU:O	2:B:91:GLN:HG2	1.99	0.62
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.80	0.62
1:A:257:ILE:HD12	1:A:293:ILE:HD12	1.81	0.62
2:B:140:PRO:O	2:B:141:GLY:O	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.81	0.61
1:A:199:ARG:HE	1:A:220:LYS:HE2	1.64	0.61
2:B:209:LEU:HB3	2:B:214:LEU:HB2	1.81	0.61
2:B:348:ASN:ND2	2:B:351:THR:HG22	2.15	0.61
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.00	0.61
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.35	0.61
2:B:191:SER:OG	2:B:198:HIS:CD2	2.54	0.60
2:B:40:GLU:O	2:B:44:GLU:HG3	2.01	0.60
1:A:541:GLY:O	2:B:280:SER:HB3	2.02	0.60
1:A:41:MET:HE2	1:A:72:ARG:HH12	1.65	0.60
2:B:298:GLU:O	2:B:301:LEU:HB3	2.02	0.60
2:B:420:PRO:HB2	2:B:421:PRO:CD	2.32	0.60
1:A:426:TRP:HE1	1:A:511:ASP:HB2	1.67	0.59
1:A:518:VAL:O	1:A:522:ILE:HG12	2.02	0.59
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.83	0.59
2:B:28:GLU:HG3	2:B:135:ILE:CD1	2.33	0.59
1:A:168:LEU:HD13	1:A:180:ILE:HG21	1.85	0.58
1:A:41:MET:HE2	1:A:72:ARG:NH1	2.17	0.58
2:B:395:LYS:O	2:B:399:GLU:HG3	2.03	0.58
2:B:363:ASN:O	2:B:367:GLN:HG3	2.03	0.58
1:A:331:LYS:HG2	1:A:332:GLN:N	2.17	0.58
2:B:24:TRP:HH2	2:B:61:PHE:CD1	2.22	0.58
1:A:235:HIS:HB2	1:A:238:LYS:O	2.03	0.58
2:B:207:GLN:OE1	2:B:210:LEU:HD23	2.04	0.58
1:A:203:GLU:O	1:A:207:GLN:HB2	2.03	0.57
2:B:254:VAL:HA	2:B:257:ILE:HD12	1.86	0.57
2:B:244:ILE:HB	2:B:310:LEU:HD22	1.86	0.57
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.05	0.57
2:B:420:PRO:HB2	2:B:421:PRO:HD2	1.86	0.57
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.86	0.57
1:A:441:TYR:O	1:A:548:VAL:HG21	2.04	0.57
1:A:252:TRP:O	1:A:292:VAL:HG13	2.05	0.57
1:A:495:ILE:H	1:A:495:ILE:HD12	1.70	0.57
1:A:495:ILE:HG22	1:A:496:VAL:N	2.20	0.57
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.87	0.57
2:B:107:THR:HA	2:B:232:TYR:O	2.04	0.57
1:A:419:THR:O	1:A:422:LEU:HD23	2.04	0.56
2:B:354:TYR:CD1	2:B:374:LYS:HD2	2.41	0.56
1:A:366:LYS:O	1:A:370:GLU:HG3	2.05	0.56
2:B:354:TYR:CE1	2:B:374:LYS:HD2	2.40	0.56
1:A:132:ILE:HB	1:A:142:ILE:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:THR:O	2:B:300:GLU:HG2	2.05	0.56
1:A:225:PRO:HB3	1:A:236:PRO:HD3	1.88	0.56
2:B:41:MET:HG3	2:B:46:LYS:HD2	1.87	0.56
2:B:24:TRP:CH2	2:B:61:PHE:CD1	2.93	0.55
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.42	0.55
1:A:98:ALA:HB1	1:A:349:LEU:HB3	1.88	0.55
1:A:493:VAL:HG22	1:A:494:ASN:N	2.21	0.55
1:A:458:VAL:HG12	2:B:286:THR:HG21	1.88	0.54
2:B:260:LEU:HD23	2:B:279:LEU:HD13	1.89	0.54
2:B:396:GLU:O	2:B:400:THR:HG23	2.07	0.54
1:A:131:THR:HG23	1:A:143:ARG:HG2	1.88	0.54
2:B:64:LYS:HE2	2:B:69:THR:H	1.73	0.54
1:A:435:VAL:CA	2:B:290:THR:HG21	2.36	0.54
2:B:393:ILE:HG21	2:B:398:TRP:HB2	1.89	0.54
1:A:417:VAL:O	1:A:417:VAL:HG13	2.08	0.54
1:A:115:TYR:O	1:A:149:LEU:HB2	2.07	0.54
2:B:64:LYS:HE2	2:B:69:THR:N	2.23	0.54
1:A:261:VAL:HG13	1:A:276:VAL:CG1	2.37	0.54
1:A:125:ARG:HB3	1:A:145:GLN:OE1	2.08	0.54
1:A:319:TYR:HE1	1:A:343:GLN:NE2	2.07	0.53
1:A:495:ILE:HD12	1:A:495:ILE:N	2.24	0.53
1:A:344:GLU:OE1	1:A:344:GLU:HA	2.07	0.53
1:A:503:LEU:O	1:A:507:GLN:HB2	2.07	0.53
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.91	0.53
1:A:333:GLY:O	1:A:335:GLY:N	2.42	0.53
1:A:520:GLN:O	1:A:524:GLN:HG2	2.09	0.53
1:A:317:VAL:HG13	1:A:318:TYR:N	2.22	0.52
2:B:96:HIS:CE1	2:B:381:VAL:O	2.63	0.52
2:B:332:GLN:O	2:B:336:GLN:HB3	2.08	0.52
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.91	0.52
1:A:407:GLN:NE2	2:B:417:VAL:O	2.43	0.52
2:B:376:THR:HG23	2:B:386:THR:HG22	1.92	0.52
1:A:480:GLN:O	1:A:483:TYR:HB3	2.10	0.52
1:A:90:VAL:HG23	1:A:91:GLN:N	2.25	0.52
2:B:293:ILE:HG23	2:B:294:PRO:HD2	1.92	0.51
1:A:27:THR:O	1:A:31:ILE:HG13	2.11	0.51
2:B:26:LEU:HD12	2:B:133:PRO:CG	2.40	0.51
2:B:139:THR:O	2:B:141:GLY:N	2.44	0.51
2:B:338:THR:HA	2:B:353:LYS:HA	1.90	0.51
1:A:223:LYS:HD2	1:A:227:PHE:CZ	2.44	0.51
1:A:389:PHE:O	1:A:414:TRP:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:LYS:O	2:B:236:PRO:HB2	2.11	0.51
2:B:160:PHE:O	2:B:160:PHE:CD2	2.63	0.51
1:A:440:PHE:CZ	1:A:489:SER:HB2	2.46	0.51
2:B:278:GLN:HB2	2:B:302:GLU:OE1	2.11	0.51
1:A:183:TYR:CD2	1:A:230:MET:SD	3.04	0.50
1:A:350:LYS:HE2	1:A:378:GLU:OE2	2.11	0.50
2:B:111:VAL:HG12	2:B:111:VAL:O	2.11	0.50
1:A:319:TYR:OH	1:A:385:LYS:HD3	2.12	0.50
2:B:3:SER:O	2:B:5:ILE:HG13	2.11	0.50
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.77	0.50
1:A:59:PRO:HB2	1:A:76:ASP:HB3	1.94	0.50
1:A:442:VAL:CG1	1:A:443:ASP:N	2.75	0.50
2:B:191:SER:OG	2:B:198:HIS:HD2	1.94	0.50
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.94	0.49
2:B:257:ILE:O	2:B:261:VAL:HG23	2.11	0.49
1:A:27:THR:OG1	1:A:30:LYS:HG3	2.12	0.49
2:B:271:TYR:HD1	2:B:271:TYR:H	1.59	0.49
2:B:175:ASN:OD1	2:B:201:LYS:NZ	2.44	0.49
1:A:459:THR:HG23	1:A:463:ARG:HB3	1.94	0.49
1:A:61:PHE:CE1	1:A:290:THR:HG23	2.48	0.49
1:A:35:VAL:O	1:A:39:THR:HG23	2.11	0.49
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.43	0.49
1:A:446:ALA:HA	1:A:453:GLY:HA3	1.95	0.49
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.95	0.48
1:A:3:SER:OG	1:A:5:ILE:HG22	2.13	0.48
1:A:191:SER:OG	1:A:198:HIS:HD2	1.97	0.48
2:B:296:THR:HB	2:B:298:GLU:HG2	1.95	0.48
2:B:2:ILE:HA	2:B:117:SER:O	2.13	0.48
1:A:379:SER:HA	1:A:383:TRP:CE3	2.49	0.48
2:B:357:MET:CB	2:B:367:GLN:NE2	2.76	0.48
1:A:435:VAL:HG13	2:B:290:THR:HG21	1.95	0.48
1:A:37:ILE:HG22	1:A:41:MET:HE3	1.96	0.48
1:A:175:ASN:N	1:A:176:PRO:HD3	2.28	0.48
2:B:85:GLN:O	2:B:85:GLN:HG3	2.14	0.48
2:B:41:MET:HE3	2:B:41:MET:HB2	1.70	0.48
2:B:314:VAL:HG12	2:B:315:HIS:N	2.28	0.48
1:A:41:MET:HE1	1:A:73:LYS:HE2	1.95	0.48
2:B:271:TYR:N	2:B:271:TYR:CD1	2.82	0.48
1:A:2:ILE:HD11	1:A:45:GLY:O	2.14	0.47
1:A:94:ILE:O	1:A:94:ILE:HG13	2.14	0.47
2:B:54:ASN:HD21	2:B:129:ALA:HB2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:SER:O	1:A:167:ILE:HG13	2.14	0.47
1:A:239:TRP:HZ2	1:A:349:LEU:O	1.96	0.47
1:A:319:TYR:CE1	1:A:343:GLN:NE2	2.82	0.47
1:A:109:LEU:HD22	1:A:216:THR:CG2	2.43	0.47
1:A:324:ASP:O	1:A:343:GLN:HG2	2.15	0.47
1:A:47:ILE:HD12	1:A:144:TYR:CD1	2.50	0.47
1:A:361:HIS:HD2	1:A:518:VAL:HG11	1.80	0.47
2:B:267:ALA:O	2:B:270:ILE:N	2.47	0.47
2:B:30:LYS:O	2:B:34:LEU:HD12	2.15	0.47
2:B:343:GLN:HG3	2:B:349:LEU:HD11	1.95	0.47
1:A:540:LYS:HZ2	2:B:276:VAL:HG11	1.79	0.47
2:B:54:ASN:ND2	2:B:129:ALA:HB2	2.29	0.47
2:B:35:VAL:O	2:B:39:THR:HG23	2.15	0.47
2:B:89:GLU:O	2:B:91:GLN:N	2.48	0.47
1:A:430:GLU:HG2	1:A:531:VAL:O	2.15	0.46
1:A:50:ILE:HG21	1:A:145:GLN:NE2	2.24	0.46
1:A:254:VAL:HB	1:A:289:LEU:HA	1.98	0.46
1:A:460:ASN:HA	2:B:286:THR:O	2.16	0.46
2:B:420:PRO:CB	2:B:421:PRO:CD	2.93	0.46
1:A:222:GLN:O	1:A:224:GLU:N	2.49	0.46
1:A:228:LEU:CD2	1:A:233:GLU:HG3	2.42	0.46
1:A:241:VAL:CG2	1:A:314:VAL:HB	2.46	0.46
1:A:532:TYR:HE1	1:A:534:ALA:HB2	1.79	0.46
1:A:247:PRO:HB2	1:A:249:LYS:HE3	1.98	0.46
1:A:426:TRP:NE1	1:A:511:ASP:HB2	2.31	0.46
2:B:124:PHE:CE2	2:B:153:TRP:CZ2	3.04	0.46
2:B:195:ILE:HG23	2:B:199:ARG:HH21	1.81	0.46
2:B:254:VAL:HB	2:B:289:LEU:HA	1.98	0.46
1:A:225:PRO:O	1:A:227:PHE:N	2.49	0.45
2:B:78:ARG:O	2:B:82:LYS:HG3	2.16	0.45
2:B:56:TYR:O	2:B:143:ARG:NH2	2.49	0.45
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.38	0.45
2:B:125:ARG:HD3	2:B:147:ASN:HA	1.99	0.45
2:B:293:ILE:HG23	2:B:294:PRO:CD	2.47	0.45
1:A:181:TYR:CE2	2:B:138:GLU:HA	2.52	0.45
1:A:429:LEU:HD23	1:A:531:VAL:HB	1.98	0.45
2:B:357:MET:CB	2:B:367:GLN:CD	2.90	0.45
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.52	0.45
1:A:167:ILE:O	1:A:208:HIS:NE2	2.49	0.45
1:A:276:VAL:HG12	1:A:280:SER:HG	1.78	0.45
1:A:287:LYS:O	1:A:288:ALA:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:ALA:O	2:B:37:ILE:HG13	2.17	0.45
2:B:5:ILE:HG22	2:B:6:GLU:O	2.17	0.45
2:B:13:LYS:HB3	2:B:14:PRO:HD2	1.99	0.45
1:A:515:SER:OG	1:A:518:VAL:HG23	2.17	0.45
1:A:221:HIS:HB3	1:A:227:PHE:CD1	2.52	0.45
1:A:309:ILE:C	1:A:311:LYS:H	2.25	0.45
1:A:458:VAL:HG12	1:A:458:VAL:O	2.15	0.44
2:B:124:PHE:CZ	2:B:153:TRP:CZ2	3.04	0.44
2:B:283:LEU:HA	2:B:283:LEU:HD23	1.79	0.44
1:A:172:LYS:HE2	1:A:180:ILE:HB	2.00	0.44
1:A:542:ILE:CG2	2:B:283:LEU:HD13	2.47	0.44
1:A:255:ASN:HD22	1:A:289:LEU:HD13	1.83	0.44
1:A:328:GLU:O	1:A:339:TYR:HA	2.18	0.44
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.99	0.44
2:B:38:CYS:O	2:B:42:GLU:HB2	2.17	0.44
1:A:120:LEU:O	1:A:121:ASP:C	2.60	0.44
1:A:495:ILE:CG2	1:A:496:VAL:N	2.81	0.44
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.82	0.44
1:A:41:MET:HE1	1:A:73:LYS:NZ	2.33	0.44
1:A:174:GLN:C	1:A:176:PRO:HD3	2.43	0.44
1:A:315:HIS:ND1	1:A:315:HIS:N	2.66	0.43
2:B:327:ALA:HA	2:B:340:GLN:O	2.18	0.43
1:A:79:GLU:HG3	1:A:83:ARG:HE	1.83	0.43
2:B:94:ILE:HD13	2:B:94:ILE:H	1.82	0.43
1:A:450:THR:C	1:A:452:LEU:H	2.26	0.43
1:A:361:HIS:CD2	1:A:518:VAL:HG11	2.53	0.43
2:B:41:MET:HG2	2:B:46:LYS:HB2	2.01	0.43
2:B:270:ILE:HG22	2:B:271:TYR:CD1	2.53	0.43
2:B:376:THR:CG2	2:B:386:THR:HG22	2.47	0.43
1:A:78:ARG:HD3	1:A:258:GLN:NE2	2.33	0.43
1:A:241:VAL:HG23	1:A:314:VAL:HB	1.99	0.43
2:B:317:VAL:HG12	2:B:347:LYS:HB3	2.00	0.43
2:B:362:THR:HA	2:B:367:GLN:HE21	1.83	0.43
1:A:181:TYR:HB2	1:A:188:TYR:HB3	2.00	0.43
1:A:473:THR:C	1:A:475:GLN:N	2.77	0.43
2:B:111:VAL:O	2:B:111:VAL:CG1	2.67	0.43
1:A:205:LEU:O	1:A:209:LEU:HG	2.19	0.42
1:A:116:PHE:C	1:A:148:VAL:HG21	2.43	0.42
1:A:79:GLU:HG3	1:A:83:ARG:HH21	1.84	0.42
1:A:544:GLY:O	1:A:547:GLN:N	2.51	0.42
2:B:96:HIS:HE1	2:B:381:VAL:O	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:GLN:CA	1:A:517:LEU:HD21	2.50	0.42
1:A:498:ASP:HB2	1:A:538:ALA:HB2	2.00	0.42
2:B:93:GLY:HA2	2:B:161:GLN:OE1	2.20	0.42
2:B:116:PHE:CZ	2:B:151:GLN:HG3	2.54	0.42
1:A:78:ARG:O	1:A:82:LYS:HG3	2.18	0.42
2:B:160:PHE:HE2	2:B:164:MET:HE2	1.84	0.42
2:B:337:TRP:CZ3	2:B:368:LEU:HD13	2.54	0.42
1:A:33:ALA:O	1:A:37:ILE:HG13	2.19	0.42
1:A:391:LEU:C	1:A:417:VAL:HG12	2.45	0.42
2:B:24:TRP:NE1	2:B:59:PRO:HB3	2.34	0.42
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.49	0.42
2:B:26:LEU:HD12	2:B:133:PRO:CD	2.49	0.42
2:B:309:ILE:HD12	2:B:312:GLU:OE2	2.20	0.42
2:B:389:PHE:O	2:B:415:GLU:N	2.52	0.42
1:A:2:ILE:HD11	1:A:45:GLY:C	2.45	0.42
1:A:175:ASN:HD21	1:A:201:LYS:NZ	2.18	0.42
2:B:50:ILE:CD1	2:B:54:ASN:HD22	2.33	0.42
2:B:161:GLN:O	2:B:162:SER:C	2.62	0.42
2:B:246:LEU:HD21	2:B:310:LEU:HD11	2.02	0.42
1:A:2:ILE:HA	1:A:117:SER:O	2.20	0.42
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.55	0.41
1:A:118:VAL:O	1:A:148:VAL:HG22	2.20	0.41
2:B:107:THR:OG1	2:B:198:HIS:HE1	2.03	0.41
1:A:220:LYS:HE3	1:A:222:GLN:HG3	2.03	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.90	0.41
2:B:195:ILE:HG13	2:B:233:GLU:OE1	2.21	0.41
2:B:344:GLU:HA	2:B:345:PRO:HD2	1.87	0.41
1:A:482:ILE:HD11	1:A:497:THR:HG21	2.02	0.41
1:A:537:PRO:HG2	1:A:542:ILE:HD11	2.01	0.41
2:B:169:GLU:HG2	2:B:170:PRO:N	2.32	0.41
1:A:373:GLN:NE2	2:B:397:THR:HG23	2.35	0.41
2:B:94:ILE:O	2:B:95:PRO:C	2.63	0.41
2:B:277:ARG:HG2	2:B:278:GLN:NE2	2.35	0.41
2:B:410:TRP:O	2:B:410:TRP:CE3	2.74	0.41
1:A:21:VAL:HB	1:A:59:PRO:HD3	2.02	0.41
1:A:142:ILE:HD13	1:A:142:ILE:N	2.36	0.41
1:A:317:VAL:CG1	1:A:318:TYR:N	2.84	0.41
2:B:84:THR:HB	2:B:154:LYS:HE2	2.02	0.41
1:A:138:GLU:O	1:A:138:GLU:HG2	2.21	0.41
1:A:274:ILE:HD11	1:A:310:LEU:HD21	2.03	0.41
1:A:156:SER:O	1:A:157:PRO:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:LEU:HD13	2:B:156:SER:HA	2.02	0.41
1:A:54:ASN:HA	1:A:55:PRO:HD3	1.83	0.40
2:B:149:LEU:HD21	2:B:159:ILE:HD12	2.02	0.40
1:A:181:TYR:CZ	2:B:138:GLU:HB2	2.57	0.40
2:B:270:ILE:HG22	2:B:271:TYR:N	2.35	0.40
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.57	0.40
1:A:525:LEU:HD23	1:A:531:VAL:HG21	2.03	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	554/556 (100%)	490 (88%)	50 (9%)	14 (2%)	4	11
2	B	411/427 (96%)	353 (86%)	47 (11%)	11 (3%)	4	10
All	All	965/983 (98%)	843 (87%)	97 (10%)	25 (3%)	4	11

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ILE
1	A	223	LYS
1	A	225	PRO
1	A	334	GLN
1	A	420	PRO
1	A	421	PRO
1	A	458	VAL
1	A	542	ILE
2	B	88	TRP
2	B	140	PRO
2	B	141	GLY

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Mol	Chain	Res	Type
2	B	153	TRP
1	A	104	LYS
1	A	288	ALA
2	B	420	PRO
1	A	52	PRO
1	A	554	ALA
2	B	37	ILE
2	B	277	ARG
2	B	278	GLN
1	A	4	PRO
1	A	413	GLU
2	B	97	PRO
2	B	4	PRO
2	B	270	ILE

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	458/496 (92%)	418 (91%)	40 (9%)	9	24
2	B	353/389 (91%)	325 (92%)	28 (8%)	11	28
All	All	811/885 (92%)	743 (92%)	68 (8%)	10	26

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	43	LYS
1	A	48	SER
1	A	72	ARG
1	A	179	VAL
1	A	180	ILE
1	A	199	ARG
1	A	210	LEU
1	A	222	GLN

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Mol	Chain	Res	Type
1	A	225	PRO
1	A	233	GLU
1	A	250	ASP
1	A	284	ARG
1	A	287	LYS
1	A	300	GLU
1	A	315	HIS
1	A	317	VAL
1	A	330	GLN
1	A	332	GLN
1	A	363	ASN
1	A	364	ASP
1	A	385	LYS
1	A	399	GLU
1	A	409	THR
1	A	419	THR
1	A	420	PRO
1	A	422	LEU
1	A	423	VAL
1	A	452	LEU
1	A	459	THR
1	A	472	THR
1	A	475	GLN
1	A	497	THR
1	A	507	GLN
1	A	511	ASP
1	A	516	GLU
1	A	528	LYS
1	A	533	LEU
1	A	548	VAL
1	A	552	VAL
2	B	6	GLU
2	B	10	VAL
2	B	24	TRP
2	B	35	VAL
2	B	42	GLU
2	B	86	ASP
2	B	94	ILE
2	B	113	ASP
2	B	156	SER
2	B	165	THR
2	B	169	GLU

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Mol	Chain	Res	Type
2	B	176	PRO
2	B	237	ASP
2	B	245	VAL
2	B	248	GLU
2	B	257	ILE
2	B	268	SER
2	B	271	TYR
2	B	274	ILE
2	B	275	LYS
2	B	282	LEU
2	B	290	THR
2	B	293	ILE
2	B	302	GLU
2	B	307	ARG
2	B	321	PRO
2	B	394	GLN
2	B	413	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	57	ASN
1	A	145	GLN
1	A	175	ASN
1	A	198	HIS
1	A	255	ASN
1	A	258	GLN
1	A	269	GLN
1	A	306	ASN
1	A	330	GLN
1	A	340	GLN
1	A	367	GLN
1	A	373	GLN
1	A	474	ASN
1	A	475	GLN
1	A	507	GLN
1	A	519	ASN
1	A	524	GLN
2	B	54	ASN
2	B	96	HIS
2	B	145	GLN

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Mol	Chain	Res	Type
2	B	147	ASN
2	B	198	HIS
2	B	255	ASN
2	B	278	GLN
2	B	348	ASN
2	B	373	GLN
2	B	418	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.