



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:59 PM GMT

PDB ID : 1DLO
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 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/ValidationPDFNotes.html>

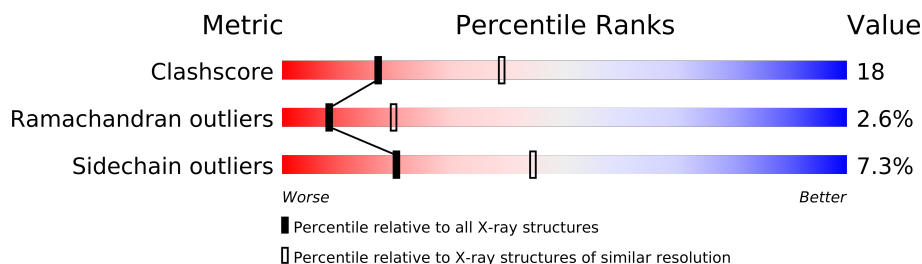
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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	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:

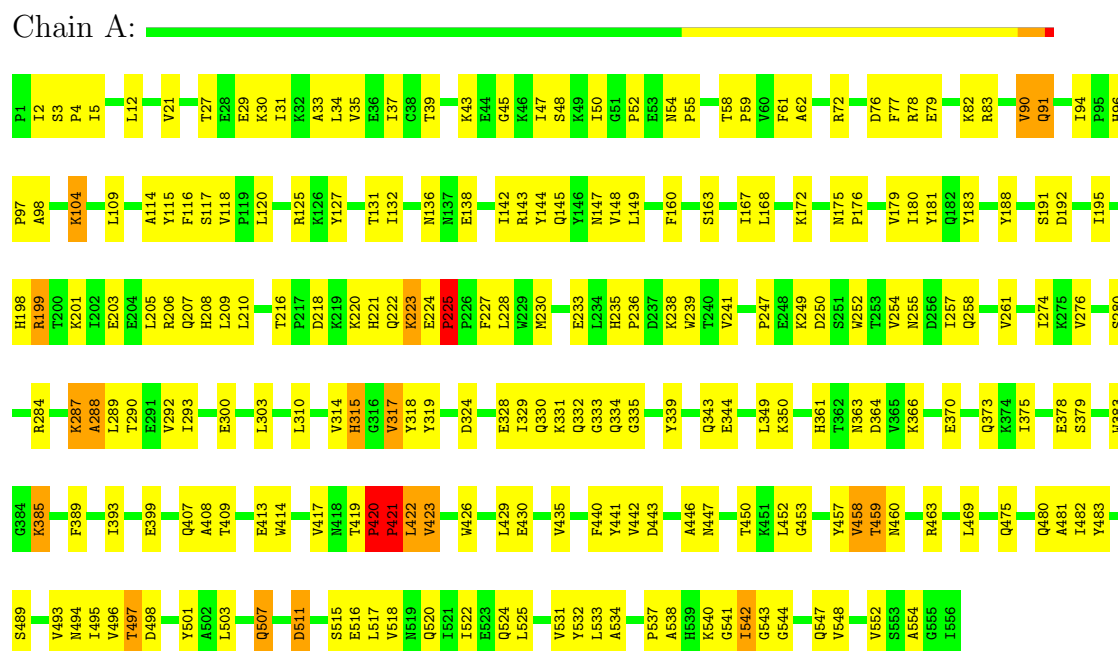
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED	UNP P03366

3 Residue-property plots

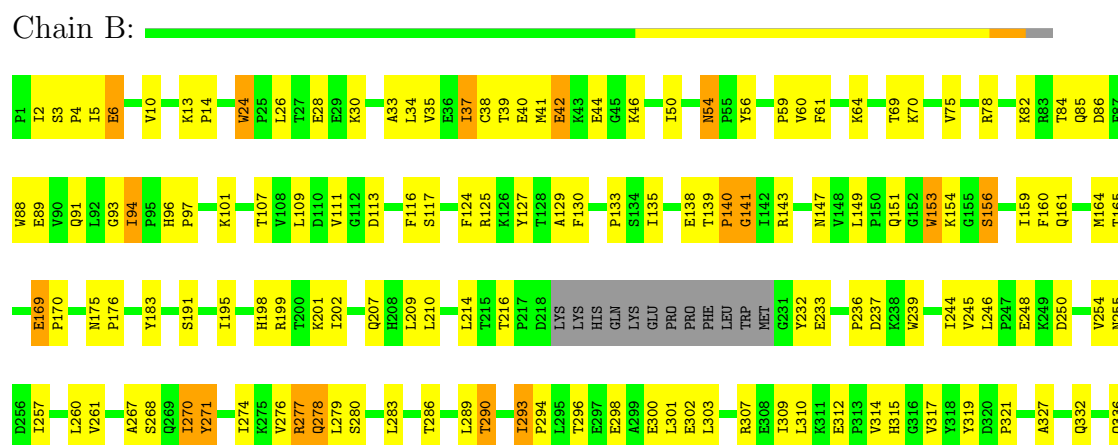
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE



- Molecule 2: HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE



W144	W145	F416	V417	P420	P421	V427	W337	T338	V339	Q340	Q343	E344	P345	F346	K347	N348	L349	A350	G351	G352	K353	Y354	M357	T362	N363	D364	V365	A366	Q367	L368	T369	Q373	K374	T375	T376	T377	E378	V381	K385	T386	F389	T393	Q394	K395	E396	T397	W398	E399	T400	W401	W402	T403	E404	Y405	W410	F412
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4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section will therefore be 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.	Xtrriage
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	0.69	0/4486	0.87	5/6119 (0.1%)
2	B	0.72	0/3415	0.90	1/4652 (0.0%)
All	All	0.70	0/7901	0.89	6/10771 (0.1%)

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	VAL	N-CA-C	5.73	126.48	111.00
1	A	91	GLN	N-CA-C	5.54	125.95	111.00
1	A	136	ASN	N-CA-C	-5.26	96.80	111.00
2	B	54	ASN	N-CA-C	-5.25	96.82	111.00
1	A	120	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	421	PRO	CA-N-CD	-5.08	104.39	111.50

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4370	0	4315	151	0
2	B	3321	0	3293	135	0
All	All	7691	0	7608	270	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (270) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:199:ARG:HD3	1:A:199:ARG:O	1.91	0.71
1:A:34:LEU:HB3	1:A:132:ILE:HD12	1.72	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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:348:ASN:ND2	2:B:351:THR:HG22	2.15	0.61
2:B:209:LEU:HB3	2:B:214:LEU:HB2	1.81	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
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
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
2:B:207:GLN:OE1	2:B:210:LEU:HD23	2.04	0.58
1:A:235:HIS:HB2	1:A:238:LYS:O	2.03	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:319:TYR:OH	2:B:385:LYS:HE2	2.05	0.57
2:B:244:ILE:HB	2:B:310:LEU:HD22	1.86	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:495:ILE:HD12	1:A:495:ILE:H	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
1:A:252:TRP:O	1:A:292:VAL:HG13	2.05	0.57
2:B:107:THR:HA	2:B:232:TYR:O	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:493:VAL:HG22	1:A:494:ASN:N	2.21	0.56
2:B:354:TYR:CE1	2:B:374:LYS:HD2	2.40	0.56
1:A:366:LYS:O	1:A:370:GLU:HG3	2.05	0.56
1:A:132:ILE:HB	1:A:142:ILE:HB	1.88	0.56
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:276:VAL:HG12	1:A:280:SER:HG	1.72	0.55
2:B:260:LEU:HD23	2:B:279:LEU:HD13	1.89	0.54
1:A:458:VAL:HG12	2:B:286:THR:HG21	1.88	0.54
2:B:396:GLU:O	2:B:400:THR:HG23	2.07	0.54
2:B:64:LYS:HE2	2:B:69:THR:H	1.73	0.54
1:A:131:THR:HG23	1:A:143:ARG:HG2	1.88	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:495:ILE:N	1:A:495:ILE:HD12	2.24	0.53
1:A:319:TYR:HE1	1:A:343:GLN:NE2	2.07	0.53
1:A:344:GLU:HA	1:A:344:GLU:OE1	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:407:GLN:NE2	2:B:417:VAL:O	2.43	0.52
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.91	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
2:B:139:THR:O	2:B:141:GLY:N	2.44	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:26:LEU:HD12	2:B:133:PRO:CG	2.40	0.51
1:A:27:THR:O	1:A:31:ILE:HG13	2.11	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
2:B:101:LYS:O	2:B:236:PRO:HB2	2.11	0.51
2:B:160:PHE:CD2	2:B:160:PHE:O	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
2:B:191:SER:OG	2:B:198:HIS:HD2	1.94	0.50
1:A:442:VAL:CG1	1:A:443:ASP:N	2.75	0.50
1:A:59:PRO:HB2	1:A:76:ASP:HB3	1.94	0.50
2:B:257:ILE:O	2:B:261:VAL:HG23	2.11	0.49
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.94	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
2:B:314:VAL:HG12	2:B:315:HIS:N	2.28	0.49
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.43	0.49
1:A:35:VAL:O	1:A:39:THR:HG23	2.11	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
2:B:296:THR:HB	2:B:298:GLU:HG2	1.95	0.48
1:A:191:SER:OG	1:A:198:HIS:HD2	1.97	0.48
1:A:3:SER:OG	1:A:5:ILE:HG22	2.13	0.48
2:B:2:ILE:HA	2:B:117:SER:O	2.13	0.48
2:B:357:MET:CB	2:B:367:GLN:NE2	2.76	0.48
1:A:379:SER:HA	1:A:383:TRP:CE3	2.49	0.48
1:A:435:VAL:HG13	2:B:290:THR:HG21	1.95	0.48
2:B:85:GLN:O	2:B:85:GLN:HG3	2.14	0.48
1:A:175:ASN:N	1:A:176:PRO:HD3	2.28	0.48
2:B:271:TYR:CD1	2:B:271:TYR:N	2.82	0.48
1:A:2:ILE:HD11	1:A:45:GLY:O	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	Distance(Å)	Clash(Å)
1:A:94:ILE:O	1:A:94:ILE:HG13	2.14	0.47
1:A:239:TRP:HZ2	1:A:349:LEU:O	1.96	0.47
1:A:163:SER:O	1:A:167:ILE:HG13	2.14	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: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
1:A:47:ILE:HD12	1:A:144:TYR:CD1	2.50	0.47
2:B:37:ILE:HG22	2:B:41:MET:HE3	1.96	0.47
2:B:343:GLN:HG3	2:B:349:LEU:HD11	1.95	0.47
2:B:30:LYS:O	2:B:34:LEU:HD12	2.15	0.47
2:B:54:ASN:ND2	2:B:129:ALA:HB2	2.29	0.47
2:B:89:GLU:O	2:B:91:GLN:N	2.48	0.47
2:B:35:VAL:O	2:B:39:THR:HG23	2.15	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:228:LEU:CD2	1:A:233:GLU:HG3	2.42	0.46
1:A:222:GLN:O	1:A:224:GLU:N	2.49	0.46
1:A:532:TYR:HE1	1:A:534:ALA:HB2	1.79	0.46
1:A:241:VAL:CG2	1:A:314:VAL:HB	2.46	0.46
2:B:195:ILE:HG23	2:B:199:ARG:HH21	1.81	0.46
1:A:426:TRP:NE1	1:A:511:ASP:HB2	2.31	0.46
1:A:247:PRO:HB2	1:A:249:LYS:HE3	1.98	0.46
2:B:124:PHE:CE2	2:B:153:TRP:CZ2	3.04	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:429:LEU:HD23	1:A:531:VAL:HB	1.98	0.45
1:A:181:TYR:CE2	2:B:138:GLU:HA	2.52	0.45
2:B:33:ALA:O	2:B:37:ILE:HG13	2.17	0.45
1:A:167:ILE:O	1:A:208:HIS:NE2	2.49	0.45
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.52	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:458:VAL:O	1:A:458:VAL:HG12	2.15	0.44
2:B:283:LEU:HD23	2:B:283:LEU:HA	1.79	0.44
2:B:124:PHE:CZ	2:B:153:TRP:CZ2	3.04	0.44
2:B:169:GLU:HG2	2:B:170:PRO:N	2.32	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: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: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
2:B:94:ILE:H	2:B:94:ILE:HD13	1.82	0.43
1:A:79:GLU:HG3	1:A:83:ARG:HE	1.83	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:376:THR:CG2	2:B:386:THR:HG22	2.47	0.43
2:B:270:ILE:HG22	2:B:271:TYR:CD1	2.53	0.43
2:B:362:THR:HA	2:B:367:GLN:HE21	1.83	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
1:A:78:ARG:HD3	1:A:258:GLN:NE2	2.33	0.43
1:A:181:TYR:HB2	1:A:188:TYR:HB3	2.00	0.43
2:B:111:VAL:CG1	2:B:111:VAL:O	2.67	0.43
2:B:160:PHE:HE2	2:B:164:MET:HE2	1.84	0.42
1:A:205:LEU:O	1:A:209:LEU:HG	2.19	0.42
2:B:96:HIS:HE1	2:B:381:VAL:O	2.01	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
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:116:PHE:CZ	2:B:151:GLN:HG3	2.54	0.42
2:B:93:GLY:HA2	2:B:161:GLN:OE1	2.20	0.42
2:B:337:TRP:CZ3	2:B:368:LEU:HD13	2.54	0.42
1:A:78:ARG:O	1:A:82:LYS:HG3	2.18	0.42
1:A:540:LYS:HZ3	2:B:276:VAL:HG11	1.85	0.42
2:B:24:TRP:NE1	2:B:59:PRO:HB3	2.34	0.42
1:A:33:ALA:O	1:A:37:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:389:PHE:O	2:B:415:GLU:N	2.52	0.42
2:B:309:ILE:HD12	2:B:312:GLU:OE2	2.20	0.42
2:B:246:LEU:HD21	2:B:310:LEU:HD11	2.02	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
1:A:2:ILE:HA	1:A:117:SER:O	2.20	0.42
2:B:107:THR:OG1	2:B:198:HIS:HE1	2.03	0.41
1:A:118:VAL:O	1:A:148:VAL:HG22	2.20	0.41
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.55	0.41
1:A:220:LYS:HE3	1:A:222:GLN:HG3	2.03	0.41
2:B:195:ILE:HG13	2:B:233:GLU:OE1	2.21	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.90	0.41
2:B:344:GLU:HA	2:B:345:PRO:HD2	1.87	0.41
1:A:537:PRO:HG2	1:A:542:ILE:HD11	2.01	0.41
1:A:482:ILE:HD11	1:A:497:THR:HG21	2.02	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:373:GLN:NE2	2:B:397:THR:HG23	2.35	0.41
1:A:21:VAL:HB	1:A:59:PRO:HD3	2.02	0.41
1:A:142:ILE:N	1:A:142:ILE:HD13	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:HG2	1:A:138:GLU:O	2.21	0.41
1:A:274:ILE:HD11	1:A:310:LEU:HD21	2.03	0.41
2:B:149:LEU:HD13	2:B:156:SER:HA	2.02	0.41
2:B:149:LEU:HD21	2:B:159:ILE:HD12	2.02	0.40
1:A:54:ASN:HA	1:A:55:PRO:HD3	1.83	0.40
2:B:270:ILE:HG22	2:B:271:TYR:N	2.35	0.40
1:A:181:TYR:CZ	2:B:138:GLU:HB2	2.57	0.40
2:B:357:MET:CB	2:B:367:GLN:CD	2.90	0.40
1:A:525:LEU:HD23	1:A:531:VAL:HG21	2.03	0.40
1:A:287:LYS:O	1:A:288:ALA:C	2.60	0.40
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	554/556 (100%)	490 (88%)	50 (9%)	14 (2%)	9	21
2	B	411/427 (96%)	353 (86%)	47 (11%)	11 (3%)	8	19
All	All	965/983 (98%)	843 (87%)	97 (10%)	25 (3%)	8	20

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
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%)	425 (93%)	33 (7%)	21	45
2	B	353/389 (91%)	327 (93%)	26 (7%)	20	43
All	All	811/885 (92%)	752 (93%)	59 (7%)	20	44

All (59) 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	199	ARG
1	A	210	LEU
1	A	225	PRO
1	A	250	ASP
1	A	284	ARG
1	A	287	LYS
1	A	300	GLU
1	A	303	LEU
1	A	315	HIS
1	A	317	VAL
1	A	330	GLN
1	A	363	ASN
1	A	364	ASP
1	A	385	LYS
1	A	399	GLU
1	A	409	THR
1	A	420	PRO
1	A	422	LEU
1	A	423	VAL
1	A	452	LEU
1	A	459	THR
1	A	475	GLN
1	A	497	THR
1	A	507	GLN

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Mol	Chain	Res	Type
1	A	511	ASP
1	A	516	GLU
1	A	533	LEU
1	A	552	VAL
2	B	6	GLU
2	B	10	VAL
2	B	24	TRP
2	B	42	GLU
2	B	70	LYS
2	B	86	ASP
2	B	94	ILE
2	B	113	ASP
2	B	156	SER
2	B	165	THR
2	B	169	GLU
2	B	176	PRO
2	B	237	ASP
2	B	245	VAL
2	B	248	GLU
2	B	268	SER
2	B	271	TYR
2	B	274	ILE
2	B	290	THR
2	B	293	ILE
2	B	307	ARG
2	B	321	PRO
2	B	394	GLN
2	B	405	TYR
2	B	413	GLU
2	B	414	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
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	306	ASN
1	A	330	GLN

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Mol	Chain	Res	Type
1	A	340	GLN
1	A	361	HIS
1	A	373	GLN
1	A	407	GLN
1	A	474	ASN
1	A	475	GLN
2	B	54	ASN
2	B	57	ASN
2	B	96	HIS
2	B	145	GLN
2	B	147	ASN
2	B	198	HIS
2	B	255	ASN
2	B	278	GLN
2	B	348	ASN
2	B	373	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.