



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 02:19 am GMT

PDB ID : 1HQE
Title : HUMAN IMMUNODEFICIENCY VIRUS TYPE 1
Authors : Ding, J.; Hsiou, Y.; Arnold, E.
Deposited on : 2000-12-15
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

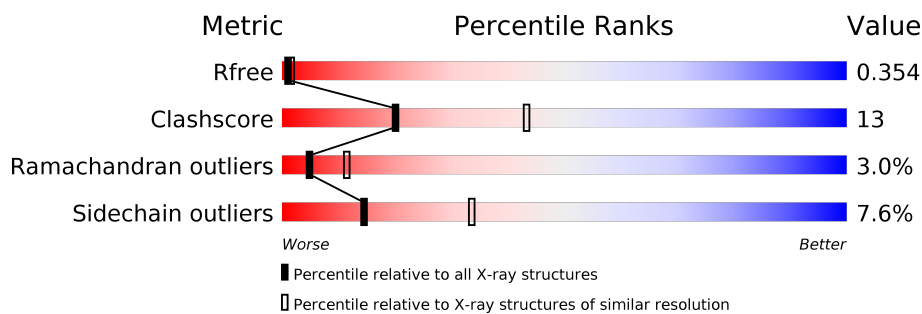
1 Overall quality at a glance

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))
R_{free}	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (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. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	560	
2	B	430	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7832 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 POL POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4349	2820	721	802	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	LYS	ENGINEERED	UNP P03366
A	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 2 is a protein called POL POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	415	Total	C	N	O	S	34	0	0
			3301	2142	547	607	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	103	ASN	LYS	ENGINEERED	UNP P03366
B	280	SER	CYS	ENGINEERED	UNP P03366

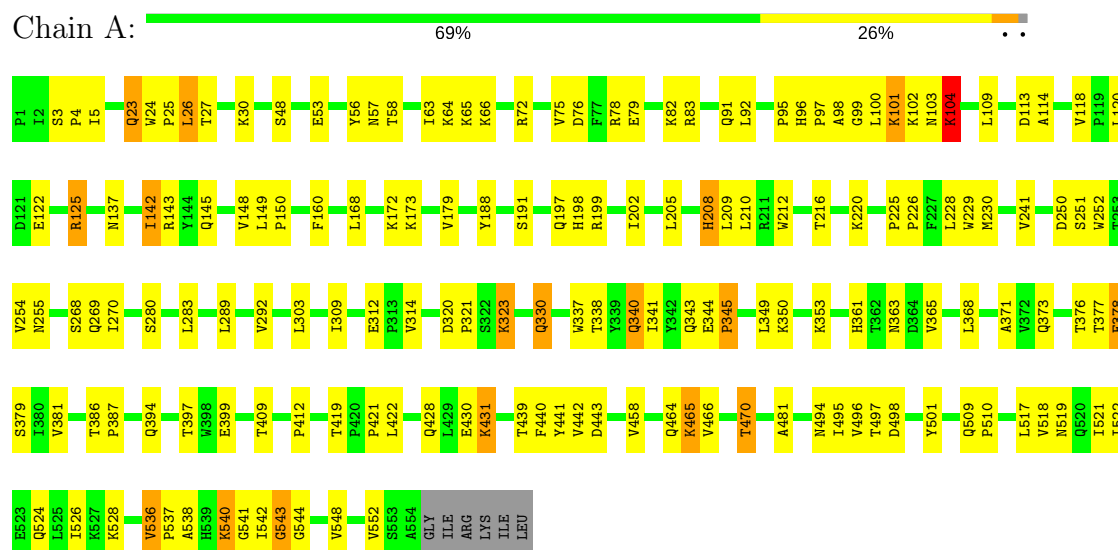
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	78	Total	O	0	0
			78	78		
3	B	104	Total	O	0	0
			104	104		

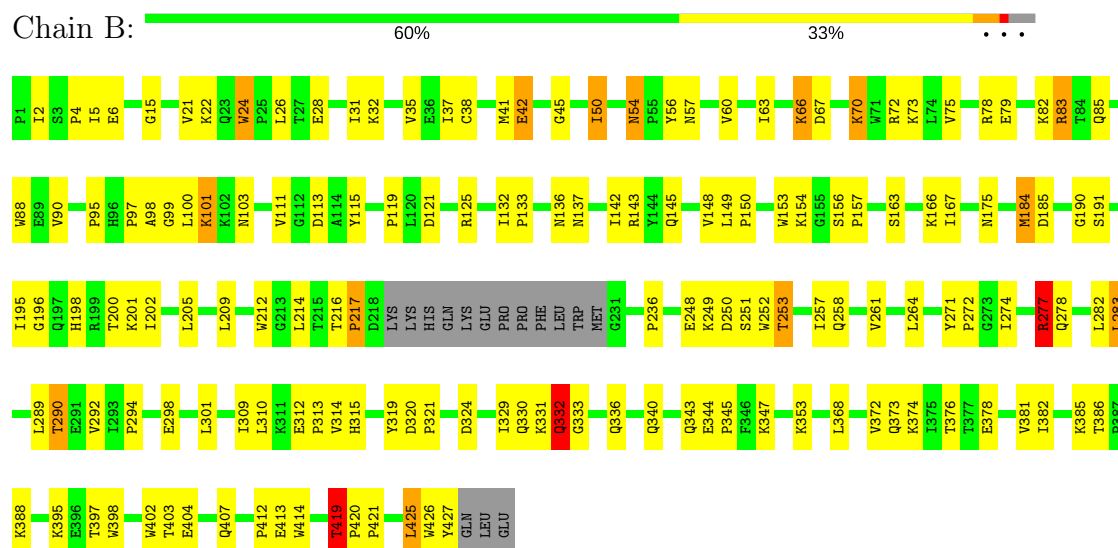
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

• Molecule 1: POL POLYPROTEIN



• Molecule 2: POL POLYPROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	236.10Å 70.40Å 93.40Å 90.00° 106.20° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70 28.34 – 2.70	Depositor EDS
% Data completeness (in resolution range)	88.4 (25.00-2.70) 88.4 (28.34-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.68Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.250 , 0.331 0.304 , 0.354	Depositor DCC
R_{free} test set	1513 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	7832	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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

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	0.49	0/4467	0.76	1/6098 (0.0%)
2	B	0.52	0/3394	0.82	5/4626 (0.1%)
All	All	0.50	0/7861	0.79	6/10724 (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	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	ILE	N-CA-C	5.85	126.80	111.00
2	B	196	GLY	N-CA-C	-5.64	99.00	113.10
1	A	538	ALA	N-CA-C	5.58	126.07	111.00
2	B	419	THR	N-CA-C	5.49	125.82	111.00
2	B	425	LEU	N-CA-C	5.23	125.12	111.00
2	B	277	ARG	N-CA-C	5.19	125.02	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	TYR	Sidechain
1	A	501	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	4349	0	4251	103	2
2	B	3301	0	3228	104	1
3	A	78	0	0	7	0
3	B	104	0	0	7	1
All	All	7832	0	7479	203	2

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 13.

All (203) 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:465:LYS:HG2	3:A:620:HOH:O	0.93	1.10
2:B:57:ASN:HD22	2:B:143:ARG:HH21	1.05	0.97
1:A:142:ILE:H	1:A:142:ILE:HD13	1.27	0.96
2:B:332:GLN:HE22	2:B:427:TYR:H	1.12	0.96
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.54	0.87
2:B:314:VAL:HG12	2:B:315:HIS:H	1.39	0.87
2:B:57:ASN:HD22	2:B:143:ARG:NH2	1.80	0.79
2:B:253:THR:O	2:B:257:ILE:HD12	1.87	0.75
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.23	0.74
1:A:465:LYS:O	1:A:466:VAL:HG23	1.88	0.73
2:B:101:LYS:NZ	2:B:101:LYS:H	1.85	0.73
1:A:101:LYS:HD3	1:A:102:LYS:H	1.53	0.73
2:B:373:GLN:HE22	2:B:407:GLN:H	1.35	0.72
2:B:332:GLN:NE2	2:B:427:TYR:H	1.87	0.69
2:B:50:ILE:HD12	2:B:143:ARG:HB3	1.75	0.68
1:A:442:VAL:CG1	1:A:481:ALA:HB1	2.25	0.67
1:A:330:GLN:HE22	1:A:340:GLN:NE2	1.93	0.67
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.30	0.66
2:B:314:VAL:HG12	2:B:315:HIS:N	2.09	0.66
2:B:163:SER:O	2:B:167:ILE:HG13	1.95	0.66
1:A:544:GLY:O	1:A:548:VAL:HG23	1.96	0.65
2:B:70:LYS:HD3	2:B:70:LYS:H	1.60	0.65
2:B:101:LYS:H	2:B:101:LYS:HZ2	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:HG12	1:A:443:ASP:N	2.12	0.64
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.33	0.63
2:B:70:LYS:N	2:B:70:LYS:HD3	2.12	0.63
2:B:57:ASN:ND2	2:B:143:ARG:HH21	1.88	0.63
1:A:101:LYS:HD3	1:A:102:LYS:N	2.13	0.62
1:A:3:SER:OG	1:A:4:PRO:HD2	2.00	0.62
2:B:31:ILE:O	2:B:35:VAL:HG23	2.00	0.62
1:A:536:VAL:HG12	1:A:537:PRO:HD2	1.82	0.61
1:A:79:GLU:HG3	1:A:83:ARG:HE	1.65	0.60
2:B:100:LEU:HG	2:B:381:VAL:HG13	1.84	0.59
2:B:332:GLN:HE22	2:B:427:TYR:N	1.93	0.58
1:A:199:ARG:HH22	1:A:220:LYS:HD2	1.68	0.58
1:A:464:GLN:O	1:A:465:LYS:HB2	2.02	0.58
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.04	0.58
2:B:344:GLU:O	2:B:347:LYS:HB2	2.03	0.58
1:A:78:ARG:O	1:A:82:LYS:HG3	2.03	0.57
1:A:26:LEU:HD12	1:A:26:LEU:H	1.69	0.57
1:A:343:GLN:HG2	1:A:349:LEU:HD11	1.86	0.57
2:B:157:PRO:HG3	2:B:184:MET:HA	1.87	0.57
2:B:277:ARG:HB3	2:B:278:GLN:HE21	1.70	0.57
1:A:96:HIS:ND1	1:A:97:PRO:HD2	2.19	0.56
1:A:378:GLU:O	1:A:378:GLU:HG2	2.04	0.56
1:A:540:LYS:O	1:A:542:ILE:N	2.35	0.56
2:B:373:GLN:NE2	2:B:407:GLN:H	2.03	0.56
1:A:254:VAL:HB	1:A:289:LEU:HA	1.86	0.56
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.46	0.56
2:B:24:TRP:N	2:B:24:TRP:CD1	2.73	0.56
1:A:517:LEU:O	1:A:521:ILE:HG13	2.06	0.56
2:B:42:GLU:HB3	3:B:472:HOH:O	2.06	0.56
1:A:518:VAL:O	1:A:522:ILE:HG12	2.07	0.55
2:B:309:ILE:HG22	2:B:309:ILE:O	2.07	0.55
1:A:98:ALA:HB1	1:A:349:LEU:HB3	1.88	0.54
2:B:137:ASN:N	2:B:137:ASN:HD22	2.05	0.54
2:B:312:GLU:OE2	2:B:313:PRO:HD2	2.08	0.54
1:A:341:ILE:HD12	1:A:350:LYS:HB3	1.90	0.54
2:B:38:CYS:O	2:B:42:GLU:HB2	2.08	0.53
1:A:95:PRO:HB3	2:B:136:ASN:O	2.08	0.53
1:A:376:THR:HG23	1:A:386:THR:HG22	1.91	0.53
1:A:142:ILE:N	1:A:142:ILE:HD13	2.11	0.53
2:B:50:ILE:HG12	2:B:145:GLN:HE21	1.73	0.53
2:B:101:LYS:O	2:B:236:PRO:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PRO:HG2	1:A:226:PRO:HD3	1.91	0.52
1:A:57:ASN:HD22	1:A:143:ARG:NH2	2.08	0.52
1:A:465:LYS:O	1:A:466:VAL:CG2	2.57	0.51
2:B:374:LYS:O	2:B:378:GLU:HB2	2.10	0.51
2:B:264:LEU:HD13	2:B:274:ILE:HD11	1.92	0.51
1:A:97:PRO:O	1:A:100:LEU:HB2	2.11	0.50
2:B:21:VAL:HG12	2:B:22:LYS:N	2.26	0.50
2:B:313:PRO:HG2	3:B:506:HOH:O	2.10	0.50
1:A:118:VAL:HG21	1:A:160:PHE:HD1	1.76	0.50
2:B:103:ASN:H	2:B:103:ASN:HD22	1.60	0.50
2:B:72:ARG:NH2	3:B:449:HOH:O	2.43	0.50
1:A:439:THR:HG22	1:A:494:ASN:HB2	1.93	0.50
2:B:149:LEU:HB3	2:B:156:SER:HB3	1.94	0.50
1:A:27:THR:OG1	1:A:30:LYS:HB2	2.13	0.49
1:A:268:SER:C	1:A:270:ILE:H	2.16	0.49
1:A:97:PRO:C	1:A:99:GLY:H	2.14	0.49
2:B:314:VAL:CG1	2:B:315:HIS:H	2.19	0.49
1:A:419:THR:HG22	1:A:421:PRO:HD2	1.94	0.48
1:A:142:ILE:H	1:A:142:ILE:CD1	2.08	0.48
1:A:56:TYR:O	1:A:143:ARG:NH2	2.43	0.48
1:A:309:ILE:O	1:A:312:GLU:HB3	2.12	0.48
1:A:498:ASP:HA	1:A:536:VAL:O	2.13	0.48
2:B:376:THR:CG2	2:B:386:THR:HG22	2.44	0.48
2:B:198:HIS:O	2:B:202:ILE:HG12	2.13	0.48
1:A:522:ILE:O	1:A:526:ILE:HG13	2.13	0.48
2:B:331:LYS:O	2:B:333:GLY:N	2.47	0.48
1:A:430:GLU:HA	1:A:431:LYS:HZ1	1.78	0.48
1:A:543:GLY:H	2:B:283:LEU:HD12	1.77	0.48
2:B:163:SER:O	2:B:166:LYS:HB2	2.14	0.48
2:B:37:ILE:O	2:B:41:MET:HG3	2.14	0.48
2:B:54:ASN:HD21	2:B:56:TYR:HB2	1.79	0.48
2:B:251:SER:HB3	2:B:294:PRO:HA	1.95	0.48
1:A:208:HIS:HE1	1:A:212:TRP:HE1	1.61	0.47
2:B:78:ARG:O	2:B:82:LYS:HG3	2.14	0.47
2:B:153:TRP:O	2:B:184:MET:SD	2.72	0.47
1:A:363:ASN:OD1	1:A:365:VAL:HG22	2.14	0.47
2:B:205:LEU:O	2:B:209:LEU:HG	2.15	0.47
1:A:442:VAL:CG1	1:A:443:ASP:N	2.76	0.47
1:A:109:LEU:HB3	1:A:216:THR:HG21	1.97	0.47
1:A:495:ILE:HG22	1:A:496:VAL:N	2.30	0.46
1:A:199:ARG:HH12	1:A:220:LYS:HZ3	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:330:GLN:OE1	2:B:340:GLN:NE2	2.33	0.46
2:B:38:CYS:O	2:B:42:GLU:N	2.48	0.46
1:A:338:THR:HG22	1:A:353:LYS:HB3	1.97	0.46
1:A:350:LYS:HA	3:A:616:HOH:O	2.16	0.45
1:A:118:VAL:O	1:A:148:VAL:HG22	2.17	0.45
1:A:198:HIS:O	1:A:202:ILE:HG12	2.16	0.45
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.14	0.45
1:A:509:GLN:N	1:A:510:PRO:HD3	2.31	0.45
1:A:439:THR:HG21	2:B:289:LEU:H	1.82	0.45
2:B:388:LYS:NZ	2:B:413:GLU:HG3	2.31	0.45
1:A:377:THR:O	1:A:381:VAL:HG23	2.17	0.45
2:B:26:LEU:HD12	2:B:133:PRO:HG3	1.98	0.45
1:A:24:TRP:HA	1:A:25:PRO:HD2	1.77	0.45
2:B:119:PRO:HA	2:B:148:VAL:HA	1.97	0.45
2:B:66:LYS:CG	2:B:67:ASP:H	2.30	0.45
1:A:191:SER:OG	1:A:198:HIS:CD2	2.70	0.45
2:B:184:MET:HB3	2:B:185:ASP:H	1.62	0.44
2:B:419:THR:HG22	2:B:421:PRO:HD2	1.98	0.44
1:A:241:VAL:HG23	1:A:314:VAL:O	2.17	0.44
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.76	0.44
2:B:419:THR:HA	2:B:420:PRO:HD2	1.90	0.44
2:B:216:THR:HA	2:B:217:PRO:HD2	1.68	0.44
1:A:373:GLN:NE2	2:B:397:THR:HG23	2.32	0.44
1:A:58:THR:HG23	1:A:76:ASP:O	2.18	0.44
2:B:258:GLN:HG2	2:B:283:LEU:HD21	2.00	0.44
1:A:495:ILE:HD12	1:A:495:ILE:N	2.33	0.44
1:A:168:LEU:O	1:A:172:LYS:HG3	2.18	0.44
2:B:60:VAL:CG1	2:B:75:VAL:HG22	2.36	0.44
1:A:344:GLU:HB3	1:A:345:PRO:HD2	2.00	0.43
1:A:53:GLU:CD	1:A:53:GLU:N	2.71	0.43
2:B:385:LYS:HG2	2:B:386:THR:N	2.32	0.43
1:A:120:LEU:O	1:A:125:ARG:NE	2.51	0.43
1:A:337:TRP:O	1:A:353:LYS:HA	2.18	0.43
1:A:524:GLN:O	1:A:528:LYS:HG2	2.18	0.43
2:B:154:LYS:O	2:B:157:PRO:HD2	2.19	0.43
1:A:519:ASN:H	1:A:519:ASN:HD22	1.65	0.43
1:A:101:LYS:CD	1:A:102:LYS:H	2.26	0.43
2:B:209:LEU:HB3	2:B:214:LEU:HB2	2.01	0.43
2:B:78:ARG:NH1	2:B:412:PRO:O	2.51	0.43
1:A:441:TYR:HD1	1:A:441:TYR:N	2.15	0.43
1:A:441:TYR:CD1	1:A:441:TYR:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:HG22	1:A:64:LYS:N	2.33	0.43
2:B:319:TYR:O	2:B:321:PRO:HD3	2.19	0.43
1:A:118:VAL:O	1:A:148:VAL:CG2	2.66	0.43
2:B:298:GLU:HG2	2:B:298:GLU:H	1.60	0.43
1:A:103:ASN:O	1:A:104:LYS:C	2.57	0.42
1:A:97:PRO:C	1:A:99:GLY:N	2.72	0.42
2:B:5:ILE:HG22	2:B:5:ILE:O	2.19	0.42
1:A:205:LEU:O	1:A:209:LEU:HG	2.19	0.42
2:B:257:ILE:O	2:B:261:VAL:HG23	2.19	0.42
2:B:345:PRO:C	2:B:347:LYS:H	2.23	0.42
1:A:280:SER:HA	1:A:283:LEU:HD12	2.02	0.42
2:B:101:LYS:HE3	2:B:382:ILE:HA	2.02	0.42
1:A:199:ARG:HH12	1:A:220:LYS:NZ	2.18	0.42
2:B:190:GLY:HA2	3:B:450:HOH:O	2.18	0.42
1:A:229:TRP:O	1:A:230:MET:HB2	2.19	0.42
2:B:191:SER:OG	2:B:198:HIS:HD2	2.02	0.42
2:B:310:LEU:HD23	2:B:310:LEU:HA	1.85	0.42
2:B:330:GLN:NE2	2:B:340:GLN:OE1	2.46	0.42
2:B:32:LYS:HD2	3:B:480:HOH:O	2.19	0.42
1:A:228:LEU:HD23	3:A:570:HOH:O	2.20	0.42
2:B:329:ILE:HG22	2:B:330:GLN:N	2.34	0.42
1:A:122:GLU:HB2	3:A:604:HOH:O	2.19	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.82	0.41
1:A:252:TRP:O	1:A:292:VAL:HG13	2.19	0.41
2:B:45:GLY:HA2	3:B:484:HOH:O	2.20	0.41
2:B:79:GLU:HG3	2:B:83:ARG:HH11	1.84	0.41
2:B:121:ASP:O	2:B:125:ARG:HG3	2.20	0.41
2:B:66:LYS:HG2	2:B:67:ASP:N	2.36	0.41
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.77	0.41
2:B:320:ASP:H	2:B:343:GLN:HE22	1.67	0.41
2:B:137:ASN:N	2:B:137:ASN:ND2	2.67	0.41
2:B:272:PRO:C	2:B:274:ILE:H	2.24	0.41
1:A:320:ASP:HA	1:A:321:PRO:HD2	1.84	0.41
1:A:394:GLN:HB2	1:A:397:THR:OG1	2.20	0.41
1:A:440:PHE:CD1	1:A:440:PHE:N	2.87	0.41
2:B:336:GLN:HG2	2:B:353:LYS:HD3	2.03	0.41
2:B:97:PRO:C	2:B:99:GLY:H	2.24	0.41
1:A:320:ASP:OD2	1:A:323:LYS:HG3	2.21	0.41
1:A:368:LEU:O	1:A:371:ALA:HB3	2.21	0.41
2:B:332:GLN:NE2	2:B:426:TRP:HB2	2.36	0.41
1:A:5:ILE:H	1:A:5:ILE:HG13	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:ASP:N	3:B:491:HOH:O	2.42	0.41
1:A:23:GLN:H	1:A:23:GLN:CD	2.24	0.41
1:A:495:ILE:CG2	1:A:496:VAL:N	2.84	0.41
2:B:54:ASN:C	2:B:54:ASN:HD22	2.24	0.41
2:B:28:GLU:O	2:B:32:LYS:HB2	2.21	0.41
2:B:368:LEU:O	2:B:372:VAL:HG23	2.21	0.41
1:A:330:GLN:NE2	1:A:340:GLN:HE22	2.20	0.40
1:A:379:SER:OG	1:A:387:PRO:HD3	2.22	0.40
1:A:91:GLN:O	1:A:92:LEU:HB3	2.21	0.40
2:B:150:PRO:HB2	2:B:153:TRP:HB2	2.02	0.40
2:B:252:TRP:O	2:B:253:THR:O	2.39	0.40
2:B:398:TRP:O	2:B:402:TRP:HD1	2.04	0.40
1:A:548:VAL:HG11	3:A:566:HOH:O	2.20	0.40
2:B:66:LYS:CG	2:B:67:ASP:N	2.84	0.40
1:A:466:VAL:N	3:A:620:HOH:O	2.53	0.40
1:A:517:LEU:HG	3:A:617:HOH:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASP:CB	3:B:498:HOH:O[4_647]	1.80	0.40
1:A:251:SER:OG	2:B:15:GLY:O[4_647]	1.83	0.37

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	552/560 (99%)	488 (88%)	51 (9%)	13 (2%)	6	16
2	B	411/430 (96%)	345 (84%)	50 (12%)	16 (4%)	3	7
All	All	963/990 (97%)	833 (86%)	101 (10%)	29 (3%)	5	11

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	458	VAL
1	A	541	GLY
2	B	66	LYS
2	B	88	TRP
2	B	90	VAL
2	B	95	PRO
2	B	253	THR
2	B	277	ARG
2	B	332	GLN
1	A	345	PRO
2	B	2	ILE
2	B	425	LEU
1	A	104	LYS
1	A	125	ARG
1	A	137	ASN
1	A	412	PRO
1	A	470	THR
2	B	98	ALA
2	B	217	PRO
1	A	66	LYS
1	A	465	LYS
2	B	4	PRO
2	B	290	THR
2	B	292	VAL
2	B	395	LYS
2	B	419	THR
1	A	269	GLN
1	A	543	GLY
1	A	552	VAL

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	452/500 (90%)	420 (93%)	32 (7%)	16	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	347/392 (88%)	318 (92%)	29 (8%)	12	27
All	All	799/892 (90%)	738 (92%)	61 (8%)	14	33

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	26	LEU
1	A	48	SER
1	A	65	LYS
1	A	72	ARG
1	A	75	VAL
1	A	101	LYS
1	A	104	LYS
1	A	113	ASP
1	A	142	ILE
1	A	145	GLN
1	A	173	LYS
1	A	179	VAL
1	A	197	GLN
1	A	208	HIS
1	A	210	LEU
1	A	255	ASN
1	A	303	LEU
1	A	323	LYS
1	A	330	GLN
1	A	340	GLN
1	A	361	HIS
1	A	378	GLU
1	A	399	GLU
1	A	409	THR
1	A	422	LEU
1	A	428	GLN
1	A	431	LYS
1	A	470	THR
1	A	497	THR
1	A	536	VAL
1	A	540	LYS
2	B	6	GLU
2	B	24	TRP
2	B	42	GLU
2	B	50	ILE

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Mol	Chain	Res	Type
2	B	54	ASN
2	B	70	LYS
2	B	73	LYS
2	B	83	ARG
2	B	85	GLN
2	B	101	LYS
2	B	111	VAL
2	B	113	ASP
2	B	142	ILE
2	B	184	MET
2	B	195	ILE
2	B	200	THR
2	B	212	TRP
2	B	248	GLU
2	B	249	LYS
2	B	271	TYR
2	B	282	LEU
2	B	283	LEU
2	B	290	THR
2	B	301	LEU
2	B	324	ASP
2	B	332	GLN
2	B	404	GLU
2	B	414	TRP
2	B	419	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	57	ASN
1	A	145	GLN
1	A	198	HIS
1	A	222	GLN
1	A	306	ASN
1	A	330	GLN
1	A	340	GLN
1	A	373	GLN
1	A	428	GLN
1	A	471	ASN
1	A	475	GLN
1	A	519	ASN

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Mol	Chain	Res	Type
2	B	54	ASN
2	B	57	ASN
2	B	85	GLN
2	B	96	HIS
2	B	103	ASN
2	B	137	ASN
2	B	145	GLN
2	B	147	ASN
2	B	198	HIS
2	B	332	GLN
2	B	334	GLN
2	B	373	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.