Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:53 PM 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

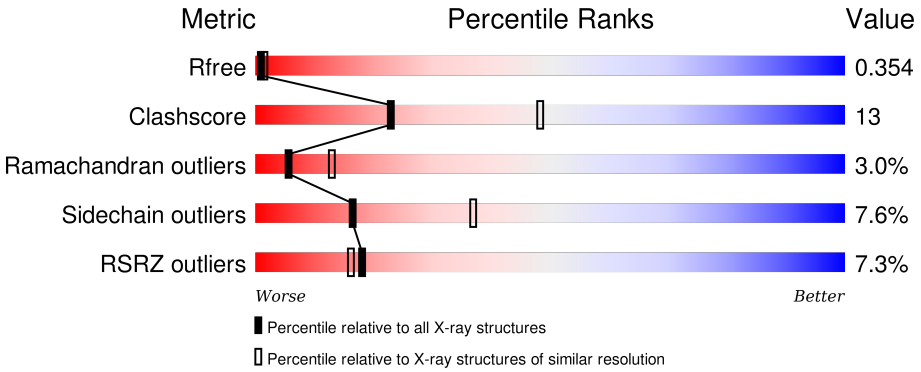
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 <=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	560	8% 69% 26%
2	B	430	6% 60% 33%

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.

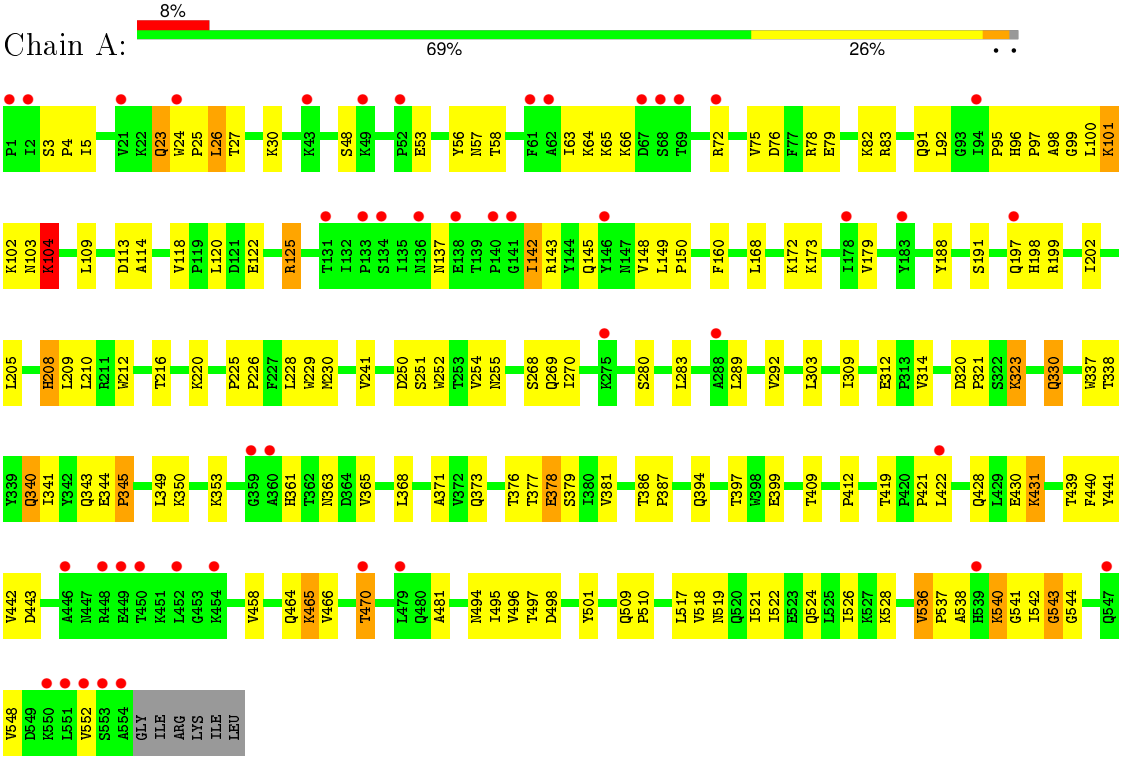
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	78	Total	O	0	0
			78	78		
3	B	104	Total	O	0	0
			104	104		

3 Residue-property plots (i)

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 (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.

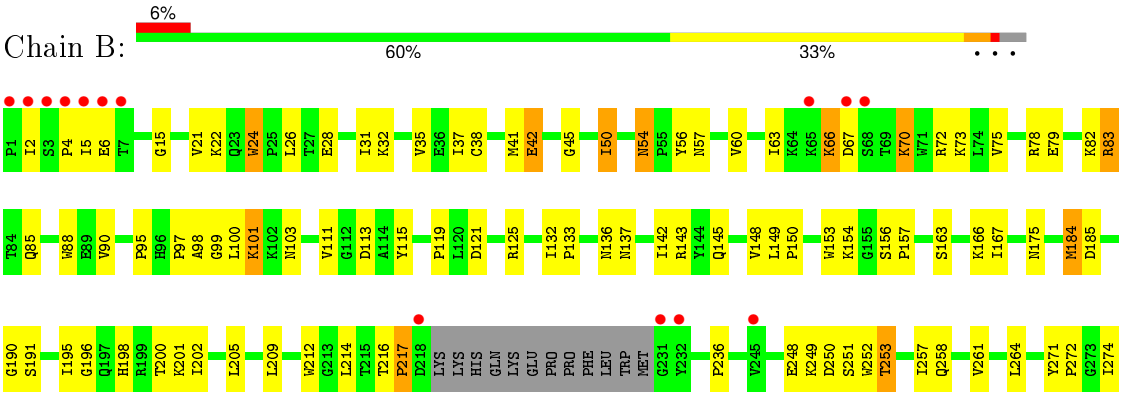
- Molecule 1: POL POLYPROTEIN

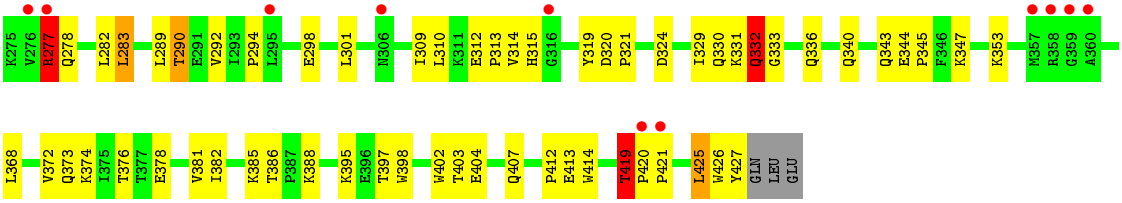
Chain A:



- Molecule 2: POL POLYPROTEIN

Chain B:




K275 V276 R277 Q278 L282 L283 L289 T290 E291 V292 I293 P294 L295 E298 L301 N306 I309 L310 K311 E312 P313 V314 H315 G316 Y319 D320 P321 D324 I329 Q330 K331 Q332 G333 Q336 Q340 Q343 E344 P345 F346 K347 K353 N357 R358 G359 A360
L368 V372 Q373 K374 I375 T376 T377 E378 V381 I382 K385 T386 P387 K388 K395 E396 T397 W398 W402 T403 E404 Q407 P412 E413 W414 T419 P420 P421 L425 W426 Y427 GLN LEU GLU

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	1512 reflections (4.37%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 37612 reflections (0.003%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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 (i)

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
2:B:70:LYS:HD3	2:B:70:LYS:H	1.60	0.65
1:A:544:GLY:O	1:A:548:VAL:HG23	1.96	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:70:LYS:N	2:B:70:LYS:HD3	2.12	0.63
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.33	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:344:GLU:O	2:B:347:LYS:HB2	2.03	0.58
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.04	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
2:B:157:PRO:HG3	2:B:184:MET:HA	1.87	0.57
1:A:343:GLN:HG2	1:A:349:LEU:HD11	1.86	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
2:B:373:GLN:NE2	2:B:407:GLN:H	2.03	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
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
2:B:42:GLU:HB3	3:B:472:HOH:O	2.06	0.56
1:A:517:LEU:O	1:A:521:ILE:HG13	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:HD22	2:B:137:ASN:N	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:313:PRO:HG2	3:B:506:HOH:O	2.10	0.50
2:B:21:VAL:HG12	2:B:22:LYS:N	2.26	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
2:B:314:VAL:CG1	2:B:315:HIS:H	2.19	0.49
1:A:97:PRO:C	1:A:99:GLY:H	2.14	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
2:B:163:SER:O	2:B:166:LYS:HB2	2.14	0.48
2:B:54:ASN:HD21	2:B:56:TYR:HB2	1.79	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:37:ILE:O	2:B:41:MET:HG3	2.14	0.48
2:B:251:SER:HB3	2:B:294:PRO:HA	1.95	0.48
2:B:78:ARG:O	2:B:82:LYS:HG3	2.14	0.47
1:A:208:HIS:HE1	1:A:212:TRP:HE1	1.61	0.47
2:B:153:TRP:O	2:B:184:MET:SD	2.72	0.47
2:B:205:LEU:O	2:B:209:LEU:HG	2.15	0.47
1:A:363:ASN:OD1	1:A:365:VAL:HG22	2.14	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
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.14	0.45
1:A:198:HIS:O	1:A:202:ILE:HG12	2.16	0.45
1:A:439:THR:HG21	2:B:289:LEU:H	1.82	0.45
1:A:509:GLN:N	1:A:510:PRO:HD3	2.31	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
2:B:66:LYS:CG	2:B:67:ASP:H	2.30	0.45
2:B:119:PRO:HA	2:B:148:VAL:HA	1.97	0.45
1:A:24:TRP:HA	1:A:25:PRO:HD2	1.77	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
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
1:A:241:VAL:HG23	1:A:314:VAL:O	2.17	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:N	1:A:495:ILE:HD12	2.33	0.44
2:B:60:VAL:CG1	2:B:75:VAL:HG22	2.36	0.44
1:A:168:LEU:O	1:A:172:LYS:HG3	2.18	0.44
2:B:385:LYS:HG2	2:B:386:THR:N	2.32	0.43
1:A:53:GLU:CD	1:A:53:GLU:N	2.71	0.43
1:A:344:GLU:HB3	1:A:345:PRO:HD2	2.00	0.43
1:A:337:TRP:O	1:A:353:LYS:HA	2.18	0.43
1:A:120:LEU:O	1:A:125:ARG:NE	2.51	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:78:ARG:NH1	2:B:412:PRO:O	2.51	0.43
2:B:209:LEU:HB3	2:B:214:LEU:HB2	2.01	0.43
1:A:441:TYR:CD1	1:A:441:TYR:N	2.86	0.43
1:A:441:TYR:HD1	1:A:441:TYR:N	2.15	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: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:103:ASN:O	1:A:104:LYS:C	2.57	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
2:B:101:LYS:HE3	2:B:382:ILE:HA	2.02	0.42
1:A:280:SER:HA	1:A:283:LEU:HD12	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:330:GLN:NE2	2:B:340:GLN:OE1	2.46	0.42
2:B:310:LEU:HD23	2:B:310:LEU:HA	1.85	0.42
2:B:32:LYS:HD2	3:B:480:HOH:O	2.19	0.42
2:B:329:ILE:HG22	2:B:330:GLN:N	2.34	0.42
1:A:228:LEU:HD23	3:A:570:HOH:O	2.20	0.42
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.82	0.41
1:A:122:GLU:HB2	3:A:604:HOH:O	2.19	0.41
2:B:79:GLU:HG3	2:B:83:ARG:HH11	1.84	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:66:LYS:HG2	2:B:67:ASP:N	2.36	0.41
2:B:121:ASP:O	2:B:125:ARG:HG3	2.20	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:ND2	2:B:137:ASN:N	2.67	0.41
2:B:272:PRO:C	2:B:274:ILE:H	2.24	0.41
1:A:440:PHE:CD1	1:A:440:PHE:N	2.87	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
2:B:97:PRO:C	2:B:99:GLY:H	2.24	0.41
2:B:336:GLN:HG2	2:B:353:LYS:HD3	2.03	0.41
2:B:332:GLN:NE2	2:B:426:TRP:HB2	2.36	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:54:ASN:C	2:B:54:ASN:HD22	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ILE:CG2	1:A:496:VAL:N	2.84	0.41
1:A:5:ILE:H	1:A:5:ILE:HG13	1.58	0.41
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
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
2:B:150:PRO:HB2	2:B:153:TRP:HB2	2.02	0.40
1:A:91:GLN:O	1:A:92:LEU:HB3	2.21	0.40
1:A:379:SER:OG	1:A:387:PRO:HD3	2.22	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%)	7 19
2	B	411/430 (96%)	345 (84%)	50 (12%)	16 (4%)	4 8
All	All	963/990 (97%)	833 (86%)	101 (10%)	29 (3%)	5 13

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 (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	452/500 (90%)	420 (93%)	32 (7%)	18 41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	347/392 (88%)	318 (92%)	29 (8%)	14 30
All	All	799/892 (90%)	738 (92%)	61 (8%)	16 37

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

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 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

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, 95^{th} 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	554/560 (98%)	0.56	45 (8%)	15	12	22, 69, 100, 100	0
2	B	408/430 (94%)	0.39	25 (6%)	25	23	8, 58, 100, 100	0
All	All	962/990 (97%)	0.49	70 (7%)	18	16	8, 65, 100, 100	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	231	GLY	7.7
2	B	4	PRO	6.4
2	B	2	ILE	6.3
2	B	1	PRO	6.1
2	B	67	ASP	5.4
1	A	552	VAL	5.4
1	A	551	LEU	5.3
2	B	5	ILE	4.4
1	A	131	THR	4.3
1	A	554	ALA	4.3
1	A	1	PRO	4.3
1	A	72	ARG	4.3
2	B	3	SER	4.1
2	B	360	ALA	4.1
2	B	276	VAL	3.9
1	A	470	THR	3.9
1	A	138	GLU	3.7
1	A	452	LEU	3.7
1	A	197	GLN	3.6
1	A	68	SER	3.4
1	A	539	HIS	3.4
2	B	359	GLY	3.4
1	A	133	PRO	3.3
1	A	134	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	550	LYS	3.1
2	B	420	PRO	3.1
2	B	245	VAL	3.1
2	B	6	GLU	3.1
1	A	69	THR	2.9
1	A	2	ILE	2.9
1	A	454	LYS	2.8
1	A	52	PRO	2.8
2	B	218	ASP	2.7
2	B	277	ARG	2.7
1	A	21	VAL	2.7
1	A	140	PRO	2.7
1	A	67	ASP	2.6
2	B	421	PRO	2.6
2	B	232	TYR	2.6
1	A	49	LYS	2.5
1	A	360	ALA	2.5
1	A	553	SER	2.5
2	B	316	GLY	2.5
1	A	136	ASN	2.5
1	A	359	GLY	2.4
2	B	358	ARG	2.4
2	B	306	ASN	2.4
1	A	288	ALA	2.4
1	A	479	LEU	2.4
1	A	178	ILE	2.4
1	A	183	TYR	2.3
1	A	146	TYR	2.3
1	A	62	ALA	2.3
1	A	450	THR	2.3
1	A	449	GLU	2.2
1	A	422	LEU	2.2
1	A	275	LYS	2.2
2	B	7	THR	2.2
2	B	68	SER	2.2
1	A	61	PHE	2.1
2	B	295	LEU	2.1
2	B	357	MET	2.1
2	B	65	LYS	2.1
1	A	24	TRP	2.1
1	A	448	ARG	2.1
1	A	446	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	547	GLN	2.0
1	A	43	LYS	2.0
1	A	94	ILE	2.0
1	A	141	GLY	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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.