



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:53 PM GMT

PDB ID : 1HQU  
Title : HUMAN IMMUNODEFICIENCY VIRUS TYPE 1  
Authors : Hsiou, Y.; Ding, J.; Arnold, E.  
Deposited on : 2000-12-19  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

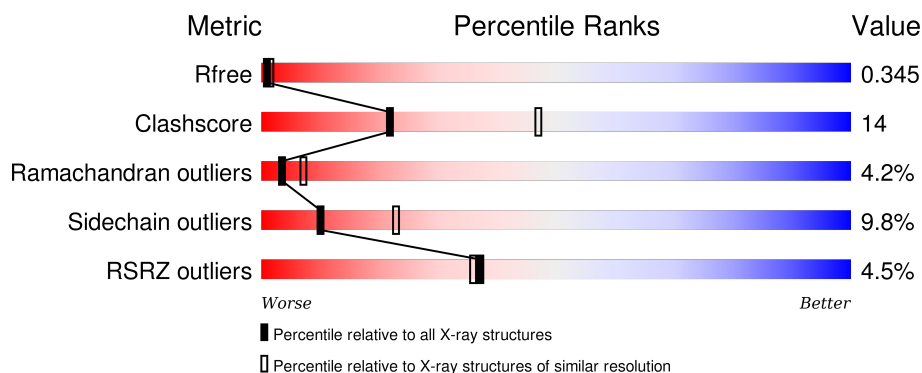
# 1 Overall quality at a glance

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>4%</div> <div>62%</div> <div>33%</div> <div>..</div> </div>
2	B	430	<div> <div>5%</div> <div>67%</div> <div>28%</div> <div>5%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7820 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	556	Total	C	N	O	S	0	0	0
			4377	2826	725	819	7			

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

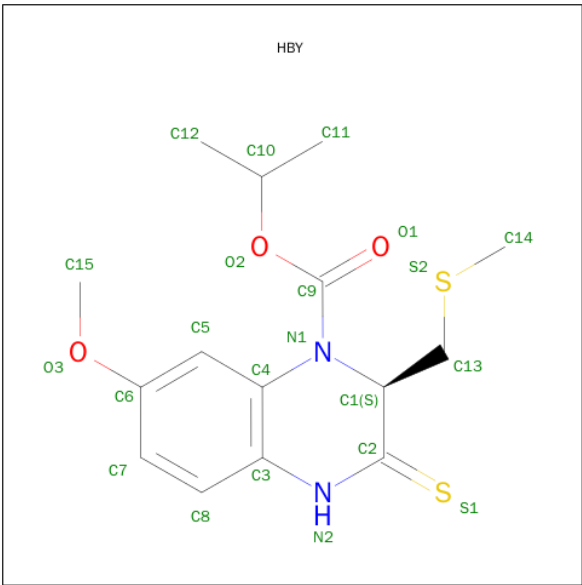
- Molecule 2 is a protein called POL POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	36	0	0
			3421	2224	561	630	6			

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 (S)-4-ISOPROPOXYCARBONYL-6-METHOXY-3-METHYLTHIOMETHYL-3,4-DIHYDROQUINOXALIN-2(1H)-THIONE (three-letter code: HBY) (formula: C<sub>15</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>S<sub>2</sub>).

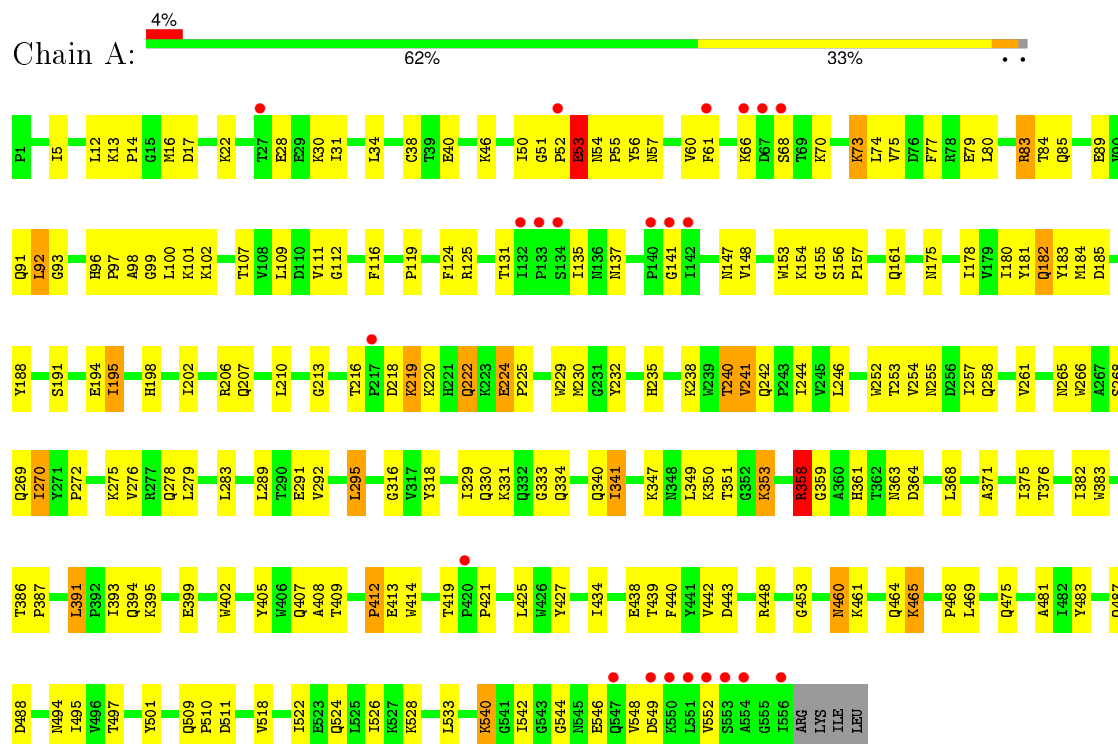


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			22	15	2	3	2		

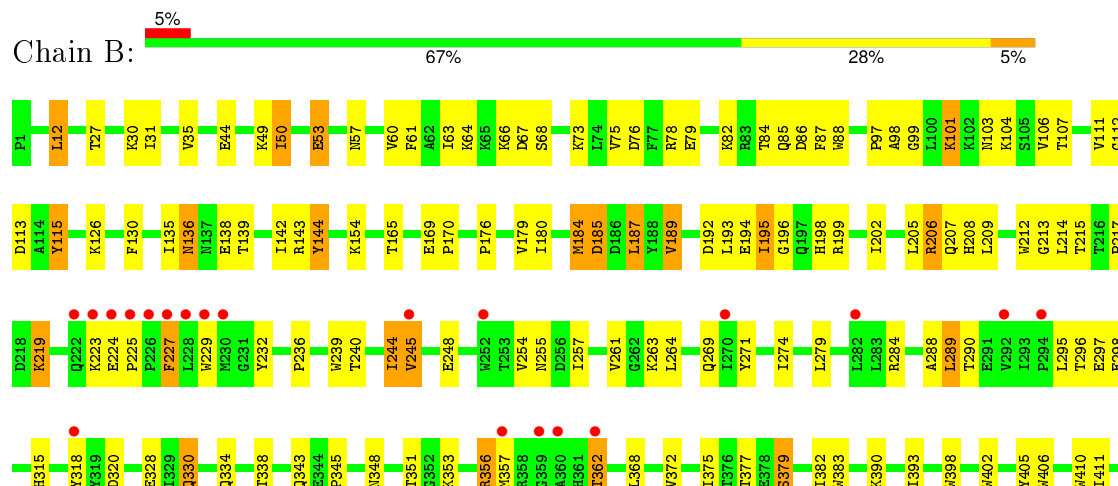
### 3 Residue-property plots

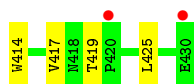
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $RSRZ > 2$ ). 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



#### • Molecule 2: POL POLYPROTEIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.90Å 68.90Å 103.90Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70 32.68 – 2.70	Depositor EDS
% Data completeness (in resolution range)	81.9 (25.00-2.70) 85.3 (32.68-2.70)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.68Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.249 , 0.345 0.258 , 0.345	Depositor DCC
$R_{free}$ test set	1787 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.4	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 71.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 37583 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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

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

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	0/4491	0.76	1/6122 (0.0%)
2	B	0.53	0/3520	0.79	2/4804 (0.0%)
All	All	0.51	0/8011	0.78	3/10926 (0.0%)

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
2	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	227	PHE	N-CA-C	5.06	124.65	111.00
1	A	347	LYS	N-CA-C	-5.04	97.39	111.00
2	B	219	LYS	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	144	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	4377	0	4280	132	0
2	B	3421	0	3339	84	0
3	A	22	0	20	7	0
All	All	7820	0	7639	215	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 14.

All (215) 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)
3:A:561:HBX:O2	3:A:561:HBX:C10	1.65	1.41
1:A:240:THR:HG22	1:A:241:VAL:H	1.22	1.04
1:A:460:ASN:H	1:A:460:ASN:HD22	1.05	0.97
1:A:206:ARG:HH22	1:A:219:LYS:NZ	1.67	0.93
1:A:295:LEU:HD12	1:A:295:LEU:H	1.37	0.87
1:A:206:ARG:HH22	1:A:219:LYS:HZ3	1.22	0.84
2:B:255:ASN:HB2	2:B:289:LEU:HD21	1.62	0.82
1:A:57:ASN:HD21	1:A:131:THR:H	1.27	0.81
1:A:125:ARG:NH1	1:A:147:ASN:HD22	1.80	0.80
2:B:143:ARG:HG2	2:B:143:ARG:HH11	1.47	0.78
2:B:154:LYS:HG2	2:B:184:MET:SD	2.26	0.75
1:A:524:GLN:O	1:A:528:LYS:HG2	1.85	0.75
3:A:561:HBX:C10	3:A:561:HBX:C9	2.65	0.74
1:A:518:VAL:O	1:A:522:ILE:HG13	1.86	0.74
1:A:54:ASN:N	1:A:55:PRO:HD2	2.03	0.73
1:A:240:THR:HG22	1:A:241:VAL:N	2.02	0.72
2:B:31:ILE:O	2:B:35:VAL:HG23	1.90	0.71
1:A:460:ASN:N	1:A:460:ASN:HD22	1.85	0.71
1:A:241:VAL:HG21	1:A:266:TRP:HE1	1.55	0.71
2:B:101:LYS:HD3	2:B:382:ILE:HG23	1.71	0.71
1:A:240:THR:CG2	1:A:241:VAL:H	1.98	0.70
2:B:64:LYS:HB3	2:B:68:SER:HA	1.72	0.70
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.40	0.69
1:A:181:TYR:CD2	3:A:561:HBX:H121	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ASN:ND2	1:A:353:LYS:NZ	2.41	0.68
2:B:320:ASP:N	2:B:343:GLN:HE22	1.91	0.68
1:A:460:ASN:H	1:A:460:ASN:ND2	1.80	0.68
2:B:328:GLU:HB3	2:B:390:LYS:HB2	1.75	0.67
1:A:254:VAL:HG13	1:A:283:LEU:HD11	1.75	0.67
1:A:98:ALA:HB2	1:A:350:LYS:HG3	1.77	0.66
1:A:258:GLN:HG2	1:A:283:LEU:HD21	1.76	0.66
1:A:382:ILE:O	2:B:136:ASN:HB2	1.96	0.66
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.77	0.66
2:B:135:ILE:O	2:B:138:GLU:HG2	1.96	0.65
1:A:265:ASN:ND2	1:A:353:LYS:HZ1	1.95	0.65
1:A:439:THR:H	1:A:460:ASN:ND2	1.94	0.65
1:A:57:ASN:ND2	1:A:131:THR:H	1.96	0.64
1:A:438:GLU:HG2	1:A:460:ASN:HD21	1.62	0.64
1:A:419:THR:HG22	1:A:421:PRO:HD2	1.79	0.64
1:A:427:TYR:OH	1:A:509:GLN:HA	1.97	0.63
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.80	0.63
2:B:112:GLY:CA	2:B:185:ASP:HB3	2.28	0.63
1:A:60:VAL:HG13	1:A:75:VAL:HG22	1.81	0.63
2:B:320:ASP:H	2:B:343:GLN:HE22	1.48	0.62
2:B:255:ASN:HB2	2:B:289:LEU:CD2	2.30	0.62
1:A:265:ASN:HD21	1:A:353:LYS:NZ	1.98	0.62
2:B:143:ARG:HG2	2:B:143:ARG:NH1	2.15	0.61
1:A:295:LEU:H	1:A:295:LEU:CD1	2.13	0.61
2:B:111:VAL:HG12	2:B:111:VAL:O	2.00	0.61
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.37	0.60
1:A:442:VAL:CG1	1:A:481:ALA:HB1	2.31	0.60
1:A:549:ASP:HA	1:A:552:VAL:HG22	1.83	0.60
2:B:289:LEU:HD23	2:B:290:THR:H	1.67	0.59
1:A:544:GLY:O	1:A:548:VAL:HG23	2.02	0.59
1:A:13:LYS:O	1:A:16:MET:HB2	2.01	0.59
2:B:12:LEU:H	2:B:12:LEU:HD12	1.69	0.58
2:B:320:ASP:H	2:B:343:GLN:NE2	2.02	0.58
1:A:79:GLU:O	1:A:83:ARG:HD3	2.04	0.58
1:A:183:TYR:CD2	1:A:184:MET:SD	2.97	0.58
2:B:63:ILE:HG22	2:B:64:LYS:N	2.19	0.57
1:A:224:GLU:CD	1:A:224:GLU:H	2.07	0.57
2:B:398:TRP:O	2:B:402:TRP:HD1	1.88	0.56
1:A:483:TYR:O	1:A:487:GLN:HG3	2.05	0.55
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.72	0.55
1:A:73:LYS:HD2	1:A:74:LEU:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LYS:O	1:A:399:GLU:HG2	2.06	0.55
1:A:270:ILE:O	1:A:272:PRO:HD3	2.06	0.55
1:A:341:ILE:O	1:A:349:LEU:HB3	2.07	0.55
1:A:331:LYS:HE2	1:A:333:GLY:HA2	1.88	0.55
1:A:232:TYR:HA	1:A:241:VAL:HG22	1.89	0.55
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.88	0.55
1:A:522:ILE:O	1:A:526:ILE:HG13	2.07	0.54
2:B:375:ILE:N	2:B:375:ILE:HD13	2.21	0.54
1:A:17:ASP:O	1:A:83:ARG:HG2	2.07	0.54
1:A:91:GLN:C	1:A:93:GLY:H	2.11	0.54
2:B:49:LYS:HA	2:B:143:ARG:O	2.08	0.54
1:A:38:CYS:C	1:A:40:GLU:H	2.11	0.54
1:A:119:PRO:HA	1:A:148:VAL:HA	1.91	0.53
2:B:170:PRO:HB2	2:B:208:HIS:NE2	2.24	0.53
3:A:561:HBY:S2	3:A:561:HBY:C9	2.97	0.53
1:A:363:ASN:HD21	1:A:425:LEU:HD21	1.74	0.53
2:B:257:ILE:O	2:B:261:VAL:HG23	2.09	0.53
1:A:206:ARG:HH22	1:A:219:LYS:HZ2	1.52	0.53
1:A:368:LEU:O	1:A:371:ALA:HB3	2.09	0.52
2:B:111:VAL:HG21	2:B:187:LEU:HB2	1.91	0.52
2:B:213:GLY:C	2:B:215:THR:H	2.12	0.52
2:B:206:ARG:NH1	2:B:217:PRO:HG2	2.26	0.51
1:A:295:LEU:HD12	1:A:295:LEU:N	2.16	0.51
1:A:511:ASP:HA	1:A:522:ILE:HD13	1.92	0.51
1:A:265:ASN:HD21	1:A:353:LYS:HZ2	1.57	0.51
1:A:254:VAL:HG13	1:A:283:LEU:CD1	2.40	0.51
2:B:187:LEU:HD23	2:B:189:VAL:HG22	1.92	0.51
1:A:494:ASN:N	1:A:494:ASN:HD22	2.09	0.51
1:A:460:ASN:N	1:A:460:ASN:ND2	2.48	0.51
1:A:99:GLY:HA2	1:A:383:TRP:HE1	1.76	0.51
1:A:408:ALA:O	2:B:393:ILE:HG13	2.11	0.50
1:A:341:ILE:HD12	1:A:350:LYS:O	2.10	0.50
2:B:206:ARG:HH11	2:B:206:ARG:HB3	1.75	0.50
1:A:253:THR:O	1:A:257:ILE:HG13	2.12	0.50
1:A:391:LEU:HD11	1:A:414:TRP:HB2	1.93	0.50
2:B:356:ARG:HE	2:B:357:MET:H	1.58	0.50
2:B:63:ILE:HD12	2:B:406:TRP:HB3	1.94	0.50
2:B:417:VAL:HG12	2:B:419:THR:H	1.75	0.50
2:B:103:ASN:OD1	2:B:104:LYS:N	2.45	0.50
1:A:46:LYS:HD2	1:A:116:PHE:O	2.12	0.50
2:B:112:GLY:HA2	2:B:185:ASP:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:HIS:O	2:B:202:ILE:HG12	2.12	0.49
2:B:379:SER:O	2:B:383:TRP:N	2.44	0.49
1:A:276:VAL:O	1:A:276:VAL:HG12	2.12	0.49
1:A:257:ILE:O	1:A:261:VAL:HG23	2.12	0.49
1:A:116:PHE:O	1:A:148:VAL:HG11	2.13	0.49
1:A:487:GLN:HG2	1:A:524:GLN:NE2	2.27	0.48
1:A:509:GLN:N	1:A:510:PRO:HD3	2.28	0.48
1:A:269:GLN:O	1:A:351:THR:N	2.39	0.48
1:A:255:ASN:HD22	1:A:289:LEU:HB2	1.79	0.48
1:A:464:GLN:O	1:A:465:LYS:HB2	2.13	0.48
1:A:31:ILE:HA	1:A:34:LEU:HD12	1.95	0.48
1:A:50:ILE:HG13	1:A:51:GLY:N	2.28	0.48
2:B:185:ASP:N	2:B:185:ASP:OD1	2.47	0.48
1:A:100:LEU:HB3	3:A:561:HBY:N2	2.29	0.47
2:B:224:GLU:HB3	2:B:225:PRO:HD2	1.95	0.47
2:B:271:TYR:HB2	2:B:274:ILE:HD11	1.97	0.47
2:B:53:GLU:HG3	2:B:53:GLU:H	1.41	0.47
2:B:12:LEU:N	2:B:12:LEU:HD12	2.30	0.46
1:A:265:ASN:ND2	1:A:353:LYS:HZ2	2.13	0.46
1:A:191:SER:OG	1:A:198:HIS:CD2	2.69	0.46
2:B:101:LYS:O	2:B:236:PRO:HB2	2.16	0.46
1:A:102:LYS:HG3	1:A:318:TYR:HB2	1.97	0.46
1:A:53:GLU:HB3	1:A:54:ASN:H	1.56	0.46
2:B:142:ILE:HD12	2:B:142:ILE:H	1.80	0.46
1:A:358:ARG:HD2	1:A:358:ARG:N	2.30	0.46
2:B:106:VAL:HG12	2:B:107:THR:N	2.29	0.46
2:B:49:LYS:HA	2:B:144:TYR:HA	1.98	0.46
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.97	0.45
2:B:84:THR:OG1	2:B:85:GLN:N	2.49	0.45
2:B:79:GLU:O	2:B:82:LYS:HB2	2.17	0.45
1:A:207:GLN:HE22	1:A:210:LEU:HD23	1.81	0.45
1:A:495:ILE:O	1:A:533:LEU:HD12	2.15	0.45
2:B:97:PRO:O	2:B:99:GLY:N	2.49	0.45
1:A:330:GLN:NE2	1:A:340:GLN:HE22	2.15	0.45
1:A:253:THR:HA	1:A:292:VAL:HA	1.99	0.45
2:B:254:VAL:HG21	2:B:288:ALA:O	2.17	0.45
1:A:191:SER:HG	1:A:198:HIS:CD2	2.34	0.45
1:A:350:LYS:HD2	1:A:351:THR:N	2.31	0.45
1:A:12:LEU:HD22	1:A:83:ARG:HB3	1.98	0.45
2:B:297:GLU:HG3	2:B:298:GLU:H	1.80	0.45
1:A:391:LEU:HD13	1:A:393:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ILE:HG22	1:A:181:TYR:N	2.32	0.44
2:B:78:ARG:NH1	2:B:411:ILE:HG22	2.33	0.44
1:A:109:LEU:HD23	1:A:216:THR:HG21	2.00	0.44
1:A:112:GLY:HA2	1:A:185:ASP:OD2	2.17	0.44
1:A:382:ILE:HG23	2:B:136:ASN:OD1	2.18	0.44
1:A:153:TRP:CZ3	1:A:155:GLY:HA3	2.52	0.44
1:A:153:TRP:CG	1:A:154:LYS:N	2.86	0.44
2:B:368:LEU:O	2:B:372:VAL:HG23	2.18	0.44
1:A:439:THR:H	1:A:460:ASN:HD21	1.63	0.44
1:A:235:HIS:HE1	1:A:242:GLN:HE22	1.64	0.44
1:A:468:PRO:O	1:A:469:LEU:HD23	2.18	0.44
1:A:107:THR:HG21	1:A:202:ILE:HG21	1.99	0.44
2:B:27:THR:HB	2:B:30:LYS:HG3	1.99	0.44
1:A:218:ASP:HB2	1:A:222:GLN:HB2	1.99	0.44
2:B:338:THR:HG22	2:B:353:LYS:HG2	2.00	0.44
2:B:261:VAL:HA	2:B:264:LEU:HD12	2.00	0.43
2:B:61:PHE:HE1	2:B:76:ASP:HB2	1.82	0.43
1:A:412:PRO:HB2	1:A:413:GLU:H	1.65	0.43
2:B:289:LEU:O	2:B:290:THR:OG1	2.31	0.43
1:A:161:GLN:HA	1:A:182:GLN:OE1	2.18	0.43
2:B:12:LEU:HB3	2:B:84:THR:HG22	2.00	0.43
1:A:77:PHE:HB3	1:A:80:LEU:HB3	2.00	0.43
1:A:331:LYS:HG2	1:A:333:GLY:H	1.84	0.43
2:B:180:ILE:O	2:B:180:ILE:HG22	2.19	0.43
1:A:89:GLU:O	1:A:92:LEU:HG	2.18	0.43
1:A:395:LYS:HA	1:A:414:TRP:HH2	1.84	0.43
1:A:181:TYR:CE2	3:A:561:HBY:H121	2.53	0.43
2:B:103:ASN:O	2:B:236:PRO:HG2	2.19	0.43
2:B:296:THR:HB	2:B:297:GLU:H	1.61	0.42
2:B:12:LEU:H	2:B:12:LEU:CD1	2.28	0.42
1:A:434:ILE:HB	1:A:494:ASN:HD21	1.84	0.42
2:B:263:LYS:HG3	2:B:425:LEU:HD22	2.00	0.42
1:A:97:PRO:HG2	1:A:232:TYR:CD1	2.55	0.42
1:A:96:HIS:N	2:B:136:ASN:HD21	2.17	0.42
1:A:84:THR:OG1	1:A:154:LYS:HD3	2.20	0.42
2:B:195:ILE:HG23	2:B:196:GLY:H	1.84	0.42
1:A:440:PHE:O	1:A:442:VAL:HG23	2.20	0.42
2:B:255:ASN:CB	2:B:289:LEU:HD21	2.41	0.42
1:A:195:ILE:H	1:A:195:ILE:HD13	1.84	0.42
1:A:229:TRP:CD2	1:A:230:MET:HG2	2.54	0.42
1:A:28:GLU:C	1:A:30:LYS:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:LEU:HD23	2:B:290:THR:N	2.35	0.42
1:A:453:GLY:N	1:A:469:LEU:O	2.52	0.42
2:B:115:TYR:CD2	2:B:115:TYR:N	2.87	0.42
1:A:68:SER:O	1:A:70:LYS:N	2.48	0.41
1:A:442:VAL:HG12	1:A:443:ASP:N	2.35	0.41
1:A:375:ILE:O	1:A:376:THR:C	2.59	0.41
2:B:330:GLN:HB3	2:B:330:GLN:HE21	1.59	0.41
1:A:240:THR:CG2	1:A:241:VAL:N	2.71	0.41
1:A:125:ARG:NH1	1:A:147:ASN:ND2	2.58	0.41
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.56	0.41
1:A:206:ARG:NH2	1:A:219:LYS:HZ3	2.03	0.41
1:A:80:LEU:O	1:A:84:THR:HG23	2.20	0.41
1:A:28:GLU:HB3	1:A:30:LYS:H	1.86	0.41
2:B:205:LEU:O	2:B:209:LEU:HG	2.20	0.41
2:B:377:THR:HG23	2:B:410:TRP:HZ2	1.86	0.41
2:B:60:VAL:HG11	2:B:130:PHE:CD1	2.56	0.41
2:B:184:MET:HB3	2:B:185:ASP:H	1.60	0.41
1:A:244:ILE:O	1:A:244:ILE:HG23	2.21	0.41
1:A:188:TYR:CD2	3:A:561:HBY:H10	2.56	0.40
2:B:63:ILE:CG2	2:B:64:LYS:N	2.84	0.40
2:B:50:ILE:HD11	2:B:144:TYR:C	2.41	0.40
2:B:101:LYS:HB3	2:B:382:ILE:HG12	2.01	0.40
2:B:244:ILE:HG22	2:B:245:VAL:N	2.35	0.40
2:B:199:ARG:HH12	2:B:229:TRP:CB	2.33	0.40
2:B:348:ASN:HD22	2:B:351:THR:CG2	2.35	0.40
1:A:386:THR:HA	1:A:387:PRO:HD3	1.85	0.40
1:A:238:LYS:HA	1:A:316:GLY:O	2.21	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	554/560 (99%)	462 (83%)	68 (12%)	24 (4%)	3	7
2	B	428/430 (100%)	340 (79%)	71 (17%)	17 (4%)	4	8
All	All	982/990 (99%)	802 (82%)	139 (14%)	41 (4%)	3	7

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	LYS
1	A	195	ILE
1	A	361	HIS
1	A	412	PRO
2	B	98	ALA
2	B	219	LYS
2	B	227	PHE
1	A	14	PRO
1	A	53	GLU
1	A	85	GLN
1	A	219	LYS
1	A	241	VAL
1	A	465	LYS
2	B	315	HIS
1	A	92	LEU
1	A	213	GLY
2	B	66	LYS
2	B	223	LYS
2	B	245	VAL
2	B	284	ARG
2	B	334	GLN
2	B	362	THR
1	A	240	THR
1	A	358	ARG
1	A	448	ARG
1	A	540	LYS
1	A	542	ILE
1	A	135	ILE
1	A	220	LYS
2	B	212	TRP
2	B	136	ASN
2	B	176	PRO
2	B	214	LEU
2	B	195	ILE
1	A	225	PRO

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Mol	Chain	Res	Type
1	A	52	PRO
1	A	141	GLY
2	B	244	ILE
1	A	359	GLY
1	A	5	ILE
2	B	345	PRO

### 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	459/500 (92%)	419 (91%)	40 (9%)	13	29
2	B	360/392 (92%)	320 (89%)	40 (11%)	8	17
All	All	819/892 (92%)	739 (90%)	80 (10%)	10	23

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	53	GLU
1	A	56	TYR
1	A	61	PHE
1	A	73	LYS
1	A	83	ARG
1	A	101	LYS
1	A	111	VAL
1	A	137	ASN
1	A	175	ASN
1	A	178	ILE
1	A	182	GLN
1	A	194	GLU
1	A	222	GLN
1	A	224	GLU
1	A	246	LEU
1	A	252	TRP

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Mol	Chain	Res	Type
1	A	268	SER
1	A	270	ILE
1	A	275	LYS
1	A	278	GLN
1	A	279	LEU
1	A	291	GLU
1	A	295	LEU
1	A	329	ILE
1	A	334	GLN
1	A	341	ILE
1	A	353	LYS
1	A	358	ARG
1	A	364	ASP
1	A	391	LEU
1	A	394	GLN
1	A	402	TRP
1	A	409	THR
1	A	460	ASN
1	A	461	LYS
1	A	488	ASP
1	A	497	THR
1	A	540	LYS
1	A	546	GLU
2	B	12	LEU
2	B	44	GLU
2	B	50	ILE
2	B	53	GLU
2	B	67	ASP
2	B	73	LYS
2	B	75	VAL
2	B	86	ASP
2	B	87	PHE
2	B	101	LYS
2	B	113	ASP
2	B	115	TYR
2	B	126	LYS
2	B	139	THR
2	B	165	THR
2	B	169	GLU
2	B	179	VAL
2	B	184	MET
2	B	185	ASP

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Mol	Chain	Res	Type
2	B	187	LEU
2	B	189	VAL
2	B	193	LEU
2	B	194	GLU
2	B	206	ARG
2	B	207	GLN
2	B	232	TYR
2	B	239	TRP
2	B	240	THR
2	B	248	GLU
2	B	269	GLN
2	B	279	LEU
2	B	289	LEU
2	B	295	LEU
2	B	318	TYR
2	B	330	GLN
2	B	356	ARG
2	B	362	THR
2	B	379	SER
2	B	405	TYR
2	B	414	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	81	ASN
1	A	103	ASN
1	A	137	ASN
1	A	147	ASN
1	A	161	GLN
1	A	175	ASN
1	A	207	GLN
1	A	242	GLN
1	A	255	ASN
1	A	265	ASN
1	A	269	GLN
1	A	278	GLN
1	A	306	ASN
1	A	330	GLN
1	A	334	GLN
1	A	340	GLN

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Mol	Chain	Res	Type
1	A	348	ASN
1	A	394	GLN
1	A	460	ASN
1	A	494	ASN
1	A	545	ASN
2	B	57	ASN
2	B	145	GLN
2	B	147	ASN
2	B	151	GLN
2	B	198	HIS
2	B	269	GLN
2	B	343	GLN
2	B	348	ASN
2	B	394	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HBV	A	561	-	21,23,23	8.15	18 (85%)	24,32,32	3.18	6 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HBV	A	561	-	-	1/13/29/29	0/1/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	561	HBV	C13-C1	2.79	1.58	1.53
3	A	561	HBV	C5-C4	3.79	1.46	1.39
3	A	561	HBV	C3-N2	4.27	1.46	1.39
3	A	561	HBV	C4-N1	4.30	1.48	1.42
3	A	561	HBV	C5-C6	4.38	1.46	1.38
3	A	561	HBV	O3-C15	4.51	1.56	1.42
3	A	561	HBV	C2-N2	6.04	1.44	1.36
3	A	561	HBV	C8-C3	7.28	1.52	1.39
3	A	561	HBV	O2-C10	7.37	1.65	1.47
3	A	561	HBV	O2-C9	7.92	1.50	1.34
3	A	561	HBV	C8-C7	8.05	1.53	1.38
3	A	561	HBV	C7-C6	8.46	1.55	1.38
3	A	561	HBV	C13-S2	8.67	1.90	1.80
3	A	561	HBV	O3-C6	9.32	1.58	1.37
3	A	561	HBV	C2-S1	10.72	1.82	1.66
3	A	561	HBV	O1-C9	10.75	1.37	1.21
3	A	561	HBV	C3-C4	15.63	1.57	1.40
3	A	561	HBV	C9-N1	17.61	1.64	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	561	HBV	C3-N2-C2	-8.01	117.12	124.70
3	A	561	HBV	C14-S2-C13	-6.08	91.32	101.21
3	A	561	HBV	C4-N1-C1	-5.07	106.31	115.62
3	A	561	HBV	O2-C9-O1	-2.83	118.87	124.69
3	A	561	HBV	O1-C9-N1	-2.57	119.11	124.13
3	A	561	HBV	O2-C9-N1	9.24	122.00	110.67

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	561	HBY	C10-O2-C9-N1

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	561	HBY	7	0

## 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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	556/560 (99%)	0.04	22 (3%) 42 41	6, 66, 99, 100	0
2	B	425/430 (98%)	0.01	22 (5%) 31 30	6, 54, 99, 100	0
All	All	981/990 (99%)	0.03	44 (4%) 37 36	6, 62, 99, 100	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	GLY	7.6
2	B	226	PRO	6.0
1	A	553	SER	4.8
2	B	227	PHE	4.8
1	A	554	ALA	4.8
1	A	547	GLN	4.6
2	B	225	PRO	4.5
1	A	67	ASP	4.4
1	A	68	SER	4.3
2	B	224	GLU	4.2
2	B	228	LEU	4.1
2	B	292	VAL	4.1
1	A	217	PRO	3.9
1	A	142	ILE	3.8
1	A	133	PRO	3.7
2	B	359	GLY	3.7
2	B	222	GLN	3.6
2	B	230	MET	3.6
1	A	550	LYS	3.4
1	A	556	ILE	3.2
2	B	430	GLU	3.2
1	A	549	ASP	3.1
1	A	551	LEU	3.1
2	B	360	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	245	VAL	3.0
2	B	294	PRO	2.9
1	A	420	PRO	2.8
2	B	229	TRP	2.8
1	A	132	ILE	2.7
1	A	552	VAL	2.7
2	B	282	LEU	2.7
1	A	61	PHE	2.7
2	B	223	LYS	2.5
1	A	27	THR	2.5
2	B	252	TRP	2.4
2	B	420	PRO	2.4
2	B	270	ILE	2.4
1	A	52	PRO	2.3
2	B	357	MET	2.3
1	A	66	LYS	2.2
1	A	134	SER	2.1
2	B	318	TYR	2.0
2	B	362	THR	2.0
1	A	140	PRO	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	HBY	A	561	22/22	0.95	0.19	0.61	21,43,57,63	0

## 6.5 Other polymers

There are no such residues in this entry.