



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:02 PM GMT

PDB ID : 1RT3
Title : AZT DRUG RESISTANT HIV-1 REVERSE TRANSCRIPTASE COM-
PLEXED WITH 1051U91
Authors : Ren, J.; Stammers, D.K.; Stuart, D.I.
Deposited on : 1998-06-29
Resolution : 3.00 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 ⓘ symbol.

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

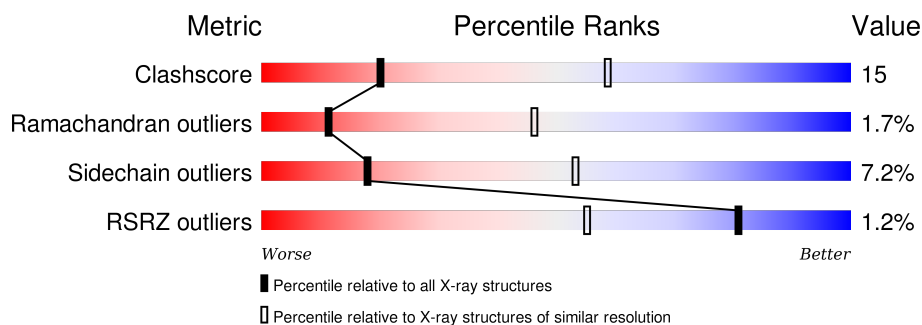
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 $\leq 5\%$. 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></div> <div> <div></div> <div>59%</div> <div>29%</div> <div>5%</div> <div>7%</div> </div> </div>
2	B	440	<div> <div></div> <div> <div></div> <div>57%</div> <div>32%</div> <div>•</div> <div>10%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7599 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 HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			4283	2779	709	787	8			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ASN	ASP	ENGINEERED	UNP P04585
A	70	ARG	LYS	ENGINEERED	UNP P04585
A	215	PHE	THR	ENGINEERED	UNP P04585
A	219	GLN	LYS	ENGINEERED	UNP P04585
A	280	CSD	CYS	MODIFIED RESIDUE	UNP P04585

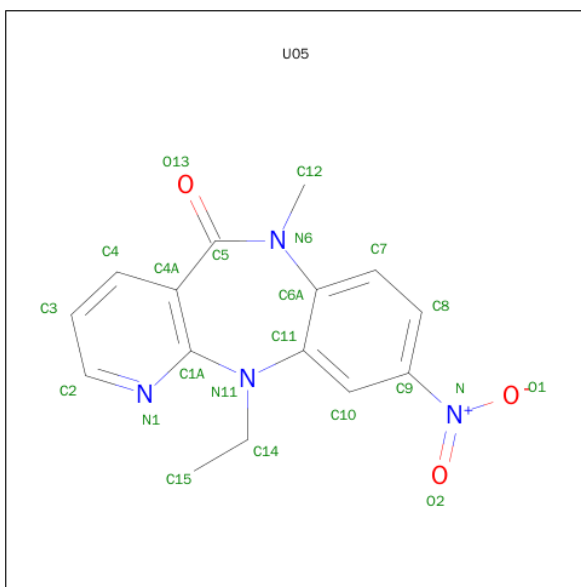
- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	398	Total	C	N	O	S	0	0	0
			3294	2143	547	597	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	ASN	ASP	ENGINEERED	UNP P04585
B	70	ARG	LYS	ENGINEERED	UNP P04585

- Molecule 3 is 6,11-DIHYDRO-11-ETHYL-6-METHYL-9-NITRO-5H-PYRIDO[2,3-B][1,5]BENZODIAZEPIN-5-ONE (three-letter code: U05) (formula: C₁₅H₁₄N₄O₃).

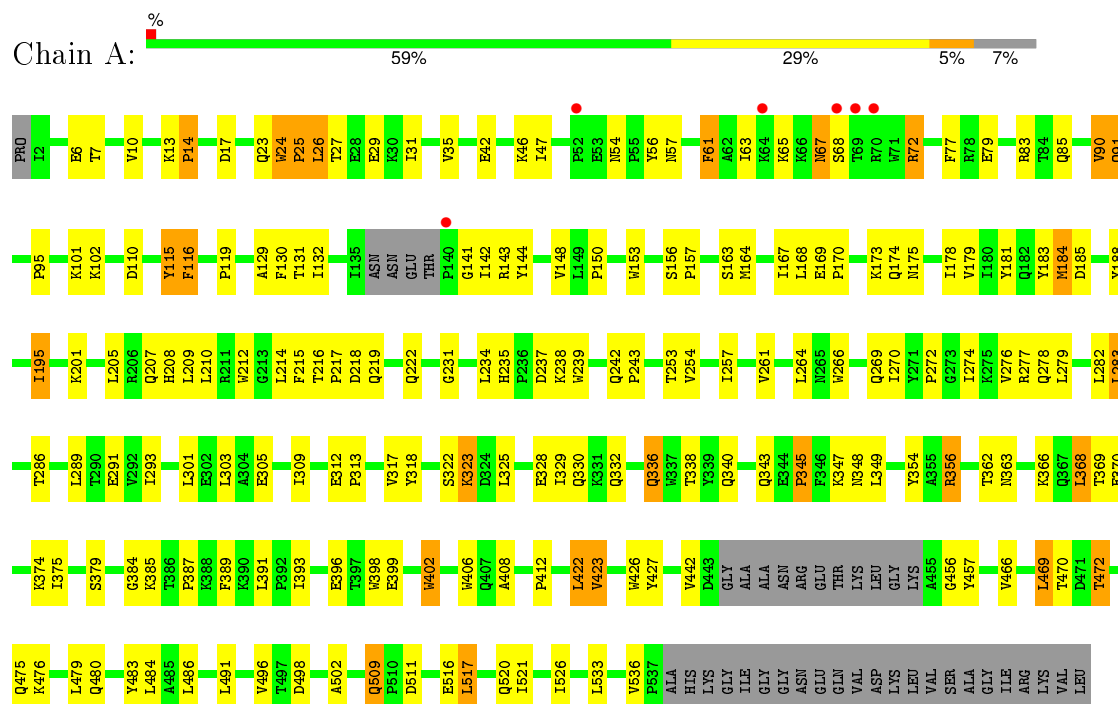


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	22	15	4	3	0	0

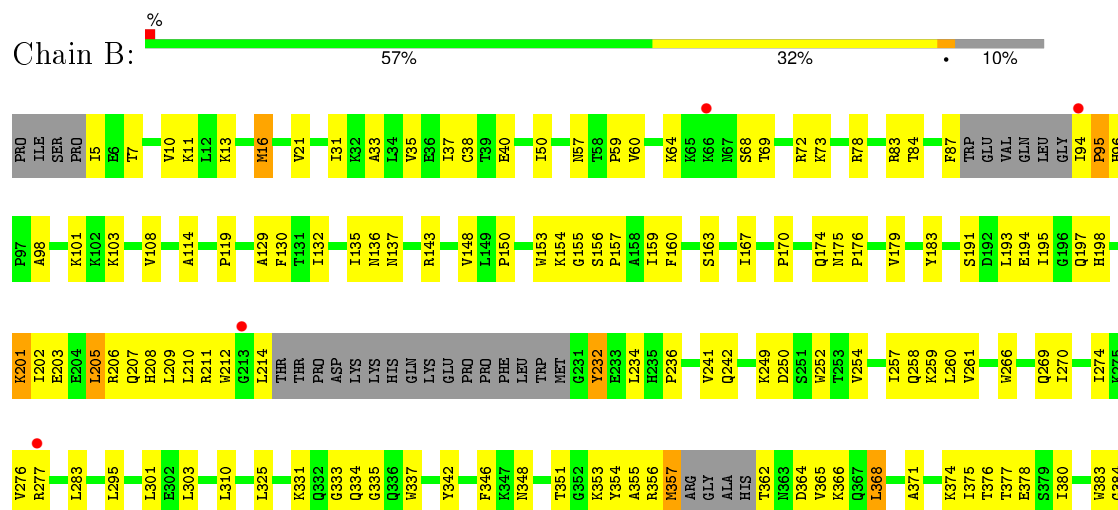
3 Residue-property plots

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: HIV-1 REVERSE TRANSCRIPTASE



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE



K385	T386	P387	K388	F389	I393	Q394	W401	W402	T403	E404	W410	I411	P412	E413	W414	M418	T419	P420	P421	L422	V423	K424	L425	W426	Y427	Q428	LEU	GLU	LYS	GLU	PRO	ILE	VAL	GLY	ALA	GLU	THR	PHE
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	138.90 Å 114.40 Å 65.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00 14.79 – 3.00	Depositor EDS
% Data completeness (in resolution range)	83.3 (25.00-3.00) 83.9 (14.79-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.01 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.264 , 0.335 0.237 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 81.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 17935 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7599	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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, 0.375 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: CSD, U05

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	0.32	0/4389	0.58	0/5965
2	B	0.32	0/3384	0.56	0/4594
All	All	0.32	0/7773	0.57	0/10559

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4283	0	4320	127	0
2	B	3294	0	3329	102	0
3	A	22	0	14	5	0
All	All	7599	0	7663	224	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 15.

All (224) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.57	0.85
1:A:90:VAL:HG12	1:A:91:GLN:H	1.41	0.83
1:A:181:TYR:HD2	3:A:999:U05:H141	1.46	0.79
1:A:469:LEU:HD22	1:A:469:LEU:H	1.50	0.76
1:A:264:LEU:HD23	1:A:276:VAL:HG12	1.68	0.76
1:A:277:ARG:NH1	1:A:336:GLN:HE22	1.84	0.75
1:A:354:TYR:HD1	1:A:374:LYS:HD2	1.53	0.73
2:B:193:LEU:HD23	2:B:197:GLN:HG3	1.71	0.71
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.55	0.70
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.73	0.69
1:A:90:VAL:HG12	1:A:91:GLN:N	2.08	0.69
2:B:119:PRO:HA	2:B:148:VAL:HA	1.75	0.68
2:B:242:GLN:HE21	2:B:353:LYS:HE3	1.58	0.68
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.74	0.68
1:A:181:TYR:HD2	3:A:999:U05:H10	1.59	0.67
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.77	0.66
1:A:181:TYR:CD2	3:A:999:U05:H10	2.30	0.66
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.78	0.66
2:B:203:GLU:HG3	2:B:207:GLN:HE22	1.60	0.66
2:B:38:CYS:SG	2:B:73:LYS:HE2	2.37	0.65
1:A:279:LEU:HA	1:A:282:LEU:HD23	1.80	0.63
1:A:90:VAL:CG1	1:A:91:GLN:H	2.08	0.63
1:A:456:GLY:HA3	1:A:466:VAL:HG22	1.79	0.63
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.82	0.62
2:B:242:GLN:NE2	2:B:353:LYS:HE3	2.14	0.62
2:B:13:LYS:HE3	2:B:84:THR:O	2.00	0.61
2:B:362:THR:HA	2:B:366:LYS:HD3	1.80	0.61
1:A:181:TYR:CD2	3:A:999:U05:H141	2.33	0.61
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.81	0.61
1:A:195:ILE:H	1:A:195:ILE:HD12	1.66	0.60
2:B:362:THR:HG22	2:B:366:LYS:HD3	1.83	0.59
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.83	0.59
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.85	0.59
2:B:154:LYS:O	2:B:157:PRO:HD2	2.02	0.59
1:A:235:HIS:HB2	1:A:238:LYS:O	2.03	0.59
2:B:37:ILE:O	2:B:40:GLU:HG2	2.03	0.58
2:B:420:PRO:O	2:B:423:VAL:HG12	2.03	0.58
1:A:132:ILE:HB	1:A:142:ILE:HD11	1.86	0.58
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.85	0.58
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.84	0.58
1:A:115:TYR:CE2	1:A:156:SER:HB3	2.38	0.58
2:B:254:VAL:O	2:B:258:GLN:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:LYS:HA	2:B:201:LYS:HE3	1.86	0.57
1:A:366:LYS:O	1:A:370:GLU:HG3	2.04	0.57
1:A:427:TYR:OH	1:A:509:GLN:HA	2.05	0.57
2:B:193:LEU:HB3	2:B:197:GLN:HB3	1.88	0.56
2:B:354:TYR:CZ	2:B:357:MET:SD	2.99	0.56
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.03	0.56
1:A:498:ASP:HA	1:A:536:VAL:O	2.06	0.55
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.88	0.55
1:A:131:THR:OG1	1:A:143:ARG:HD2	2.07	0.55
1:A:132:ILE:HB	1:A:142:ILE:CD1	2.37	0.55
1:A:207:GLN:HA	1:A:210:LEU:HB2	1.88	0.55
2:B:64:LYS:HE2	2:B:68:SER:O	2.07	0.54
1:A:270:ILE:O	1:A:272:PRO:HD3	2.07	0.54
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.90	0.54
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.43	0.53
1:A:77:PHE:CE2	1:A:150:PRO:HB3	2.43	0.53
2:B:94:ILE:N	2:B:95:PRO:CD	2.71	0.53
1:A:422:LEU:HD12	1:A:422:LEU:H	1.74	0.53
1:A:17:ASP:O	1:A:83:ARG:HD3	2.08	0.53
2:B:16:MET:CE	2:B:83:ARG:HA	2.39	0.53
2:B:401:TRP:O	2:B:404:GLU:HB2	2.07	0.53
1:A:61:PHE:N	1:A:61:PHE:CD1	2.77	0.53
1:A:469:LEU:HD23	1:A:472:THR:HG21	1.90	0.53
2:B:266:TRP:O	2:B:269:GLN:HG2	2.09	0.53
2:B:103:LYS:O	2:B:236:PRO:HG2	2.09	0.53
2:B:31:ILE:O	2:B:35:VAL:HG23	2.09	0.53
1:A:42:GLU:HA	1:A:47:ILE:O	2.09	0.53
2:B:211:ARG:HG2	2:B:212:TRP:CZ3	2.43	0.52
1:A:384:GLY:HA3	2:B:135:ILE:HD12	1.90	0.52
1:A:282:LEU:HD12	1:A:293:ILE:CG2	2.40	0.52
1:A:95:PRO:HB3	2:B:136:ASN:O	2.10	0.52
1:A:379:SER:CB	1:A:387:PRO:HD3	2.39	0.52
1:A:26:LEU:HD12	1:A:26:LEU:N	2.25	0.52
1:A:27:THR:HG22	1:A:29:GLU:H	1.75	0.52
2:B:103:LYS:HE2	2:B:179:VAL:HG21	1.91	0.51
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.45	0.51
1:A:46:LYS:HD3	1:A:116:PHE:CD2	2.45	0.51
1:A:354:TYR:CD1	1:A:374:LYS:HD2	2.39	0.51
2:B:84:THR:HB	2:B:154:LYS:HE2	1.91	0.51
2:B:163:SER:O	2:B:167:ILE:HG13	2.10	0.51
2:B:193:LEU:HD23	2:B:197:GLN:CG	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:HG22	1:A:29:GLU:N	2.25	0.51
1:A:368:LEU:HD21	1:A:391:LEU:HD22	1.92	0.51
2:B:259:LYS:HE3	2:B:425:LEU:HD11	1.93	0.51
1:A:239:TRP:HZ2	1:A:349:LEU:O	1.94	0.50
1:A:174:GLN:HG3	1:A:175:ASN:ND2	2.27	0.50
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.93	0.50
1:A:31:ILE:O	1:A:35:VAL:HG23	2.12	0.50
1:A:266:TRP:O	1:A:269:GLN:HG2	2.12	0.49
1:A:90:VAL:CG1	1:A:91:GLN:N	2.73	0.49
2:B:16:MET:HE3	2:B:83:ARG:HA	1.94	0.49
1:A:178:ILE:HG22	1:A:179:VAL:N	2.27	0.49
1:A:26:LEU:HD12	1:A:26:LEU:H	1.78	0.49
2:B:10:VAL:HG21	2:B:159:ILE:HD11	1.95	0.48
2:B:295:LEU:HD12	2:B:295:LEU:H	1.77	0.48
2:B:393:ILE:HG12	2:B:394:GLN:N	2.27	0.48
1:A:475:GLN:O	1:A:479:LEU:HD13	2.14	0.48
1:A:369:THR:HG1	1:A:398:TRP:HH2	1.60	0.48
1:A:23:GLN:NE2	1:A:24:TRP:O	2.46	0.48
2:B:57:ASN:HA	2:B:129:ALA:O	2.13	0.48
2:B:355:ALA:O	2:B:357:MET:SD	2.72	0.48
2:B:371:ALA:O	2:B:375:ILE:HG13	2.14	0.47
1:A:115:TYR:HE2	1:A:156:SER:HB3	1.78	0.47
1:A:208:HIS:O	1:A:212:TRP:HD1	1.97	0.47
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.95	0.47
1:A:27:THR:O	1:A:31:ILE:HG13	2.14	0.47
1:A:323:LYS:O	1:A:343:GLN:NE2	2.48	0.47
1:A:442:VAL:HG22	1:A:496:VAL:O	2.15	0.47
2:B:50:ILE:HG13	2:B:143:ARG:HB3	1.97	0.47
1:A:317:VAL:HG12	1:A:318:TYR:O	2.15	0.47
1:A:516:GLU:O	1:A:520:GLN:HG3	2.15	0.46
1:A:257:ILE:O	1:A:261:VAL:HG23	2.14	0.46
1:A:183:TYR:HB3	1:A:188:TYR:CE2	2.50	0.46
1:A:54:ASN:ND2	1:A:129:ALA:HB2	2.31	0.46
2:B:132:ILE:N	2:B:132:ILE:HD12	2.31	0.46
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.50	0.46
1:A:163:SER:O	1:A:167:ILE:HG13	2.15	0.46
1:A:63:ILE:O	1:A:72:ARG:N	2.49	0.46
1:A:332:GLN:HB2	1:A:338:THR:HG23	1.97	0.46
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.63	0.46
1:A:235:HIS:HB2	1:A:238:LYS:HG3	1.97	0.46
1:A:170:PRO:O	1:A:173:LYS:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:HD12	1:A:293:ILE:HG22	1.97	0.46
1:A:234:LEU:HD23	3:A:999:U05:C5	2.47	0.45
1:A:426:TRP:CE3	1:A:526:ILE:HD13	2.52	0.45
1:A:13:LYS:HG3	1:A:85:GLN:HA	1.97	0.45
1:A:253:THR:HG22	1:A:289:LEU:O	2.17	0.45
1:A:167:ILE:HG23	1:A:212:TRP:CD1	2.52	0.45
1:A:102:LYS:HG3	1:A:237:ASP:HA	1.98	0.45
1:A:79:GLU:OE1	1:A:79:GLU:HA	2.16	0.45
1:A:278:GLN:O	1:A:282:LEU:HD22	2.17	0.45
2:B:167:ILE:O	2:B:208:HIS:HE1	2.00	0.45
2:B:241:VAL:HG13	2:B:351:THR:OG1	2.17	0.45
2:B:94:ILE:N	2:B:95:PRO:HD3	2.32	0.45
2:B:103:LYS:HE2	2:B:179:VAL:CG2	2.46	0.45
2:B:335:GLY:HA3	2:B:356:ARG:HE	1.81	0.45
2:B:183:TYR:OH	2:B:386:THR:HG23	2.17	0.45
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.52	0.45
2:B:362:THR:HA	2:B:366:LYS:CD	2.46	0.45
2:B:170:PRO:HG2	2:B:208:HIS:NE2	2.32	0.45
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.52	0.44
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.17	0.44
1:A:205:LEU:O	1:A:205:LEU:HD22	2.17	0.44
2:B:205:LEU:O	2:B:209:LEU:HG	2.18	0.44
1:A:254:VAL:HG23	1:A:291:GLU:O	2.18	0.44
2:B:150:PRO:HG2	2:B:153:TRP:HB2	1.99	0.44
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.82	0.44
1:A:24:TRP:O	1:A:24:TRP:CD1	2.70	0.44
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.99	0.44
1:A:317:VAL:HG12	1:A:318:TYR:N	2.33	0.44
2:B:98:ALA:O	2:B:101:LYS:HG2	2.18	0.44
2:B:270:ILE:HG12	2:B:346:PHE:HB3	2.00	0.44
1:A:102:LYS:HD2	1:A:237:ASP:HB2	2.00	0.44
1:A:24:TRP:HA	1:A:25:PRO:HD2	1.70	0.43
1:A:347:LYS:HD3	1:A:347:LYS:HA	1.71	0.43
1:A:231:GLY:O	1:A:242:GLN:HG2	2.17	0.43
1:A:366:LYS:NZ	1:A:370:GLU:OE2	2.51	0.43
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.54	0.43
2:B:33:ALA:O	2:B:37:ILE:HG13	2.18	0.43
2:B:208:HIS:O	2:B:211:ARG:HB3	2.19	0.43
2:B:295:LEU:HD12	2:B:295:LEU:N	2.34	0.43
2:B:380:ILE:O	2:B:384:GLY:HA2	2.18	0.43
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:LEU:HD23	2:B:368:LEU:HA	1.77	0.43
1:A:389:PHE:CE2	1:A:412:PRO:HG2	2.53	0.43
2:B:13:LYS:HB2	2:B:16:MET:HG3	2.01	0.43
1:A:54:ASN:HB3	1:A:143:ARG:HH21	1.84	0.43
1:A:54:ASN:HD21	1:A:129:ALA:HB2	1.83	0.43
1:A:57:ASN:OD1	1:A:143:ARG:NH1	2.51	0.43
1:A:150:PRO:HB2	1:A:153:TRP:HB2	1.99	0.43
2:B:375:ILE:HD12	2:B:389:PHE:HE2	1.83	0.43
1:A:283:LEU:O	1:A:286:THR:HG23	2.18	0.43
1:A:195:ILE:HD12	1:A:195:ILE:N	2.32	0.43
1:A:110:ASP:H	1:A:217:PRO:HG3	1.84	0.43
1:A:305:GLU:O	1:A:309:ILE:HG13	2.18	0.43
1:A:24:TRP:O	1:A:24:TRP:HD1	2.02	0.43
2:B:206:ARG:O	2:B:210:LEU:HD23	2.19	0.43
1:A:17:ASP:OD1	1:A:56:TYR:HE1	2.01	0.43
2:B:175:ASN:N	2:B:176:PRO:HD3	2.34	0.43
2:B:94:ILE:HG13	2:B:94:ILE:O	2.19	0.42
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.49	0.42
1:A:264:LEU:O	1:A:274:ILE:HG21	2.19	0.42
2:B:87:PHE:CE2	2:B:155:GLY:HA2	2.54	0.42
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.84	0.42
2:B:31:ILE:HD12	2:B:135:ILE:HD11	2.01	0.42
2:B:422:LEU:HB3	2:B:426:TRP:CH2	2.55	0.42
2:B:170:PRO:O	2:B:174:GLN:HB2	2.20	0.42
1:A:479:LEU:HD12	1:A:502:ALA:HB2	2.02	0.42
1:A:24:TRP:CD1	1:A:24:TRP:C	2.93	0.42
1:A:325:LEU:HD12	1:A:385:LYS:HG3	2.02	0.42
2:B:374:LYS:O	2:B:378:GLU:HG3	2.19	0.42
1:A:119:PRO:HA	1:A:148:VAL:HA	2.02	0.41
1:A:67:ASN:HD22	1:A:67:ASN:C	2.24	0.41
2:B:333:GLY:O	2:B:334:GLN:HG2	2.21	0.41
2:B:234:LEU:HD21	2:B:377:THR:CG2	2.49	0.41
2:B:342:TYR:CB	2:B:348:ASN:HA	2.50	0.41
2:B:95:PRO:O	2:B:96:HIS:HB2	2.20	0.41
2:B:78:ARG:NH1	2:B:412:PRO:O	2.54	0.41
2:B:198:HIS:O	2:B:202:ILE:HG12	2.19	0.41
1:A:253:THR:O	1:A:257:ILE:HG13	2.19	0.41
1:A:219:GLN:HA	1:A:222:GLN:NE2	2.35	0.41
2:B:108:VAL:HB	2:B:232:TYR:HB3	2.03	0.41
1:A:483:TYR:CZ	1:A:520:GLN:HB3	2.55	0.41
2:B:234:LEU:HD12	2:B:234:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:HB3	1:A:185:ASP:H	1.68	0.41
1:A:293:ILE:HD12	1:A:293:ILE:N	2.35	0.41
1:A:168:LEU:HD21	1:A:209:LEU:HD21	2.03	0.41
2:B:269:GLN:HB3	2:B:269:GLN:HE21	1.67	0.41
2:B:150:PRO:HG2	2:B:153:TRP:CB	2.50	0.41
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.94	0.41
1:A:328:GLU:HG2	1:A:330:GLN:NE2	2.36	0.41
2:B:249:LYS:HG3	2:B:252:TRP:CE2	2.56	0.41
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.56	0.41
1:A:257:ILE:HD13	1:A:282:LEU:HB3	2.03	0.40
2:B:365:VAL:HG11	2:B:401:TRP:CB	2.49	0.40
1:A:10:VAL:HG11	1:A:153:TRP:CH2	2.54	0.40
2:B:257:ILE:O	2:B:261:VAL:HG23	2.21	0.40
2:B:425:LEU:HD23	2:B:425:LEU:O	2.21	0.40
1:A:178:ILE:HD11	1:A:201:LYS:HD2	2.03	0.40
1:A:183:TYR:HB3	1:A:188:TYR:HE2	1.85	0.40
1:A:101:LYS:N	1:A:101:LYS:HD2	2.36	0.40
2:B:376:THR:HB	2:B:410:TRP:CH2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	514/560 (92%)	471 (92%)	32 (6%)	11 (2%)	9	40
2	B	390/440 (89%)	363 (93%)	23 (6%)	4 (1%)	19	61
All	All	904/1000 (90%)	834 (92%)	55 (6%)	15 (2%)	11	46

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	472	THR
1	A	195	ILE
1	A	313	PRO
2	B	95	PRO
2	B	195	ILE
2	B	277	ARG
1	A	14	PRO
1	A	356	ARG
1	A	243	PRO
1	A	345	PRO
1	A	402	TRP
1	A	25	PRO
2	B	69	THR
1	A	141	GLY

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	470/499 (94%)	428 (91%)	42 (9%)	12	42
2	B	363/400 (91%)	345 (95%)	18 (5%)	30	70
All	All	833/899 (93%)	773 (93%)	60 (7%)	18	53

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	7	THR
1	A	14	PRO
1	A	24	TRP
1	A	26	LEU
1	A	61	PHE
1	A	65	LYS
1	A	67	ASN
1	A	68	SER

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Mol	Chain	Res	Type
1	A	72	ARG
1	A	91	GLN
1	A	115	TYR
1	A	116	PHE
1	A	164	MET
1	A	184	MET
1	A	215	PHE
1	A	216	THR
1	A	218	ASP
1	A	283	LEU
1	A	301	LEU
1	A	303	LEU
1	A	312	GLU
1	A	322	SER
1	A	323	LYS
1	A	336	GLN
1	A	340	GLN
1	A	345	PRO
1	A	348	ASN
1	A	356	ARG
1	A	362	THR
1	A	368	LEU
1	A	396	GLU
1	A	422	LEU
1	A	423	VAL
1	A	469	LEU
1	A	470	THR
1	A	476	LYS
1	A	480	GLN
1	A	491	LEU
1	A	509	GLN
1	A	517	LEU
1	A	533	LEU
2	B	5	ILE
2	B	11	LYS
2	B	16	MET
2	B	72	ARG
2	B	137	ASN
2	B	194	GLU
2	B	201	LYS
2	B	205	LEU
2	B	232	TYR

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Mol	Chain	Res	Type
2	B	250	ASP
2	B	283	LEU
2	B	301	LEU
2	B	303	LEU
2	B	357	MET
2	B	368	LEU
2	B	403	THR
2	B	413	GLU
2	B	414	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	174	GLN
1	A	242	GLN
1	A	255	ASN
1	A	336	GLN
1	A	507	GLN
1	A	520	GLN
2	B	57	ASN
2	B	207	GLN
2	B	242	GLN
2	B	269	GLN
2	B	278	GLN
2	B	428	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](#)

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
1	CSD	A	280	1	3,7,8	0.64	0	3,8,10	2.32	1 (33%)

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
1	CSD	A	280	1	-	1/2/6/8	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	280	CSD	OD1-SG-CB	3.60	111.41	105.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

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	U05	A	999	-	16,24,24	0.81	0	15,35,35	1.02	0

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	U05	A	999	-	-	0/4/6/6	0/2/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	U05	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	520/560 (92%)	-0.29	6 (1%)	81 55	6, 49, 106, 147	0
2	B	398/440 (90%)	-0.45	5 (1%)	79 53	11, 42, 92, 128	0
All	All	918/1000 (91%)	-0.36	11 (1%)	81 55	6, 47, 101, 147	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	THR	3.7
1	A	140	PRO	3.5
1	A	52	PRO	3.1
1	A	68	SER	3.1
1	A	64	LYS	2.6
1	A	70	ARG	2.5
2	B	66	LYS	2.4
2	B	213	GLY	2.2
2	B	277	ARG	2.0
2	B	94	ILE	2.0
2	B	428	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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 ²)	Q<0.9
1	CSD	A	280	8/9	0.96	0.09	-	34,45,52,60	0

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, 95th 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(\AA^2)	Q<0.9
3	U05	A	999	22/22	0.96	0.17	0.04	12,34,85,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.