



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:30 AM GMT

PDB ID : 3M8P
Title : HIV-1 RT with NNRTI TMC-125
Authors : Harris, S.F.; Villasenor, A.
Deposited on : 2010-03-18
Resolution : 2.67 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

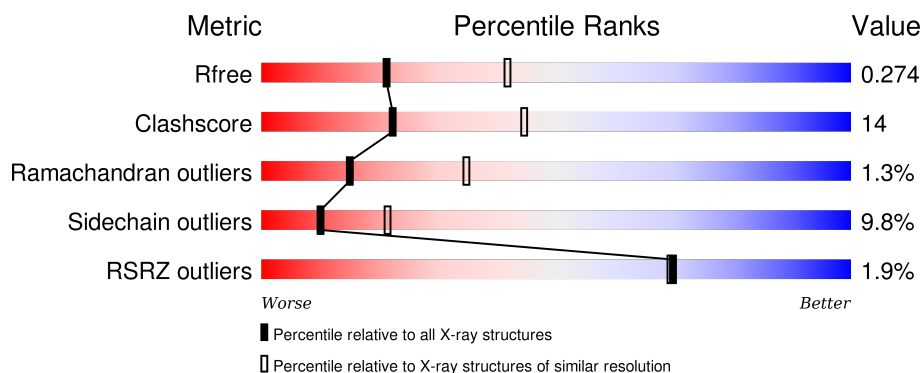
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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	561	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 28%, yellow 28%, yellow 65%, green 65%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 65% 28% 5% </div> </div>
2	B	440	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 25%, yellow 25%, yellow 61%, green 61%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 61% 25% 5% 9% </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8138 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.

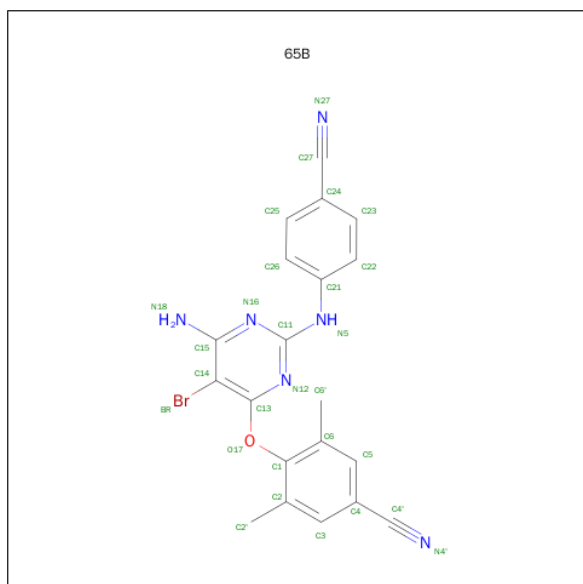
- Molecule 1 is a protein called Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4485	2900	748	829	8			

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3320	2166	545	602	7			

- Molecule 3 is 4-({6-AMINO-5-BROMO-2-[(4-CYANOPHENYL)AMINO]PYRIMIDIN-4-YL}OXY)-3,5-DIMETHYLBENZONITRILE (three-letter code: 65B) (formula: C₂₀H₁₅BrN₆O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			28	1	20	6	1		

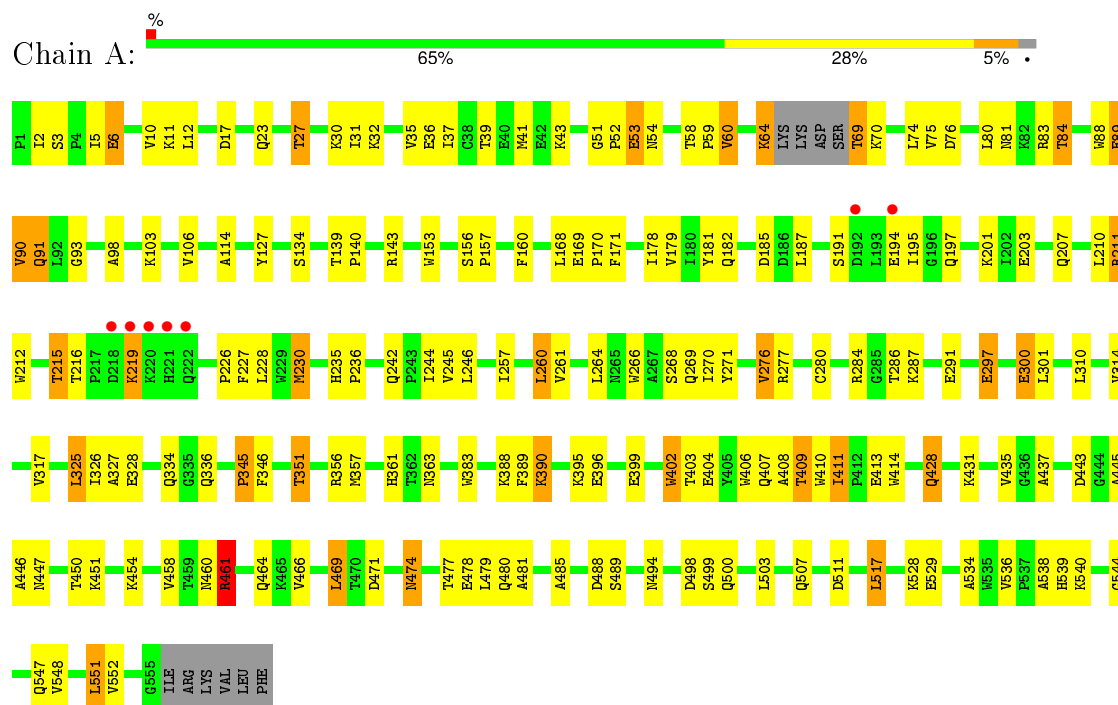
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	169	Total 169	O 169	0	0
4	B	136	Total 136	O 136	0	0

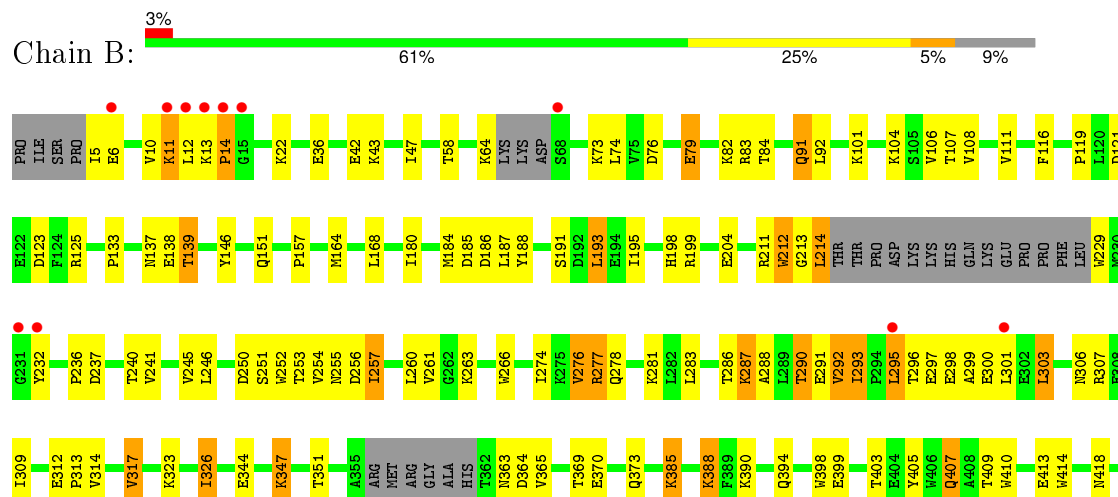
3 Residue-property plots

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: Reverse transcriptase/ribonuclease H



• Molecule 2: p51 RT



L422	423	424	428	LEU	GLU	LYS	GLU	PRO	ILE	VAL	GLY	ALA	GLU	THR	PHE
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.44Å 153.53Å 154.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.01 – 2.67 47.01 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.01-2.67) 99.7 (47.01-2.67)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.209 , 0.283 0.208 , 0.274	Depositor DCC
R_{free} test set	2042 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 40211 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8138	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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.*

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: 65B

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	1.32	15/4601 (0.3%)	1.06	8/6252 (0.1%)
2	B	1.32	12/3414 (0.4%)	1.04	6/4640 (0.1%)
All	All	1.32	27/8015 (0.3%)	1.05	14/10892 (0.1%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	THR	CA-CB	7.82	1.73	1.53
1	A	402	TRP	CB-CG	7.63	1.64	1.50
2	B	36	GLU	CG-CD	7.32	1.62	1.51
1	A	478	GLU	CB-CG	7.21	1.65	1.52
2	B	399	GLU	CG-CD	6.60	1.61	1.51
1	A	194	GLU	CG-CD	6.35	1.61	1.51
2	B	139	THR	CB-CG2	6.30	1.73	1.52
1	A	297	GLU	CB-CG	6.28	1.64	1.52
1	A	478	GLU	CG-CD	6.20	1.61	1.51
2	B	407	GLN	CG-CD	6.17	1.65	1.51
2	B	138	GLU	CB-CG	6.05	1.63	1.52
1	A	404	GLU	CG-CD	6.04	1.61	1.51
2	B	204	GLU	CG-CD	5.89	1.60	1.51
2	B	291	GLU	CG-CD	5.88	1.60	1.51
1	A	6	GLU	CG-CD	5.83	1.60	1.51
1	A	534	ALA	CA-CB	-5.82	1.40	1.52
2	B	370	GLU	CB-CG	5.67	1.62	1.52
2	B	104	LYS	CD-CE	5.65	1.65	1.51
1	A	399	GLU	CG-CD	5.47	1.60	1.51
2	B	344	GLU	CB-CG	5.44	1.62	1.52
1	A	390	LYS	CD-CE	5.32	1.64	1.51
1	A	89	GLU	CG-CD	5.29	1.59	1.51
2	B	266	TRP	CB-CG	-5.28	1.40	1.50
1	A	396	GLU	CG-CD	5.16	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	GLU	CG-CD	5.05	1.59	1.51
1	A	69	THR	CA-CB	5.05	1.66	1.53
2	B	79	GLU	CD-OE2	5.00	1.31	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	ARG	NE-CZ-NH2	7.62	124.11	120.30
2	B	123	ASP	CB-CG-OD2	-6.85	112.14	118.30
2	B	199	ARG	NE-CZ-NH2	-6.52	117.04	120.30
2	B	187	LEU	CB-CG-CD1	-6.52	99.92	111.00
1	A	345	PRO	C-N-CA	5.84	136.31	121.70
2	B	125	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	A	345	PRO	CA-C-N	-5.47	105.17	117.20
1	A	346	PHE	CB-CA-C	5.41	121.22	110.40
2	B	164	MET	CG-SD-CE	5.39	108.82	100.20
1	A	182	GLN	N-CA-CB	-5.37	100.94	110.60
1	A	551	LEU	CA-CB-CG	5.30	127.49	115.30
2	B	276	VAL	CB-CA-C	-5.29	101.34	111.40
1	A	345	PRO	O-C-N	5.05	130.78	122.70
1	A	488	ASP	CB-CG-OD2	5.05	122.84	118.30

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	4485	0	4530	132	0
2	B	3320	0	3341	90	0
3	A	28	0	15	4	0
4	A	169	0	0	19	0
4	B	136	0	0	9	0
All	All	8138	0	7886	217	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 (217) 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:80:LEU:O	1:A:84:THR:HG22	1.39	1.18
1:A:409:THR:HG21	4:A:695:HOH:O	1.63	0.98
1:A:27:THR:HG21	4:A:722:HOH:O	1.64	0.96
1:A:428:GLN:HE22	1:A:431:LYS:HZ3	0.97	0.96
1:A:428:GLN:NE2	1:A:431:LYS:HZ3	1.63	0.94
1:A:428:GLN:NE2	1:A:431:LYS:NZ	2.20	0.89
1:A:428:GLN:HE22	1:A:431:LYS:NZ	1.75	0.83
1:A:31:ILE:O	1:A:35:VAL:HG23	1.78	0.83
2:B:326:ILE:HD11	2:B:390:LYS:HG3	1.59	0.83
2:B:283:LEU:HA	2:B:287:LYS:HZ1	1.44	0.83
1:A:406:TRP:HZ3	4:A:708:HOH:O	1.61	0.82
1:A:268:SER:O	1:A:351:THR:HG22	1.81	0.81
2:B:240:THR:HG22	4:B:485:HOH:O	1.84	0.78
2:B:257:ILE:HG22	2:B:283:LEU:HD11	1.65	0.77
2:B:214:LEU:O	4:B:557:HOH:O	2.02	0.77
2:B:211:ARG:O	2:B:212:TRP:HB2	1.84	0.76
1:A:51:GLY:CA	1:A:53:GLU:OE1	2.34	0.75
2:B:91:GLN:O	2:B:92:LEU:HD12	1.85	0.75
3:A:562:65B:H22	3:A:562:65B:N12	2.00	0.74
2:B:283:LEU:HA	2:B:287:LYS:NZ	2.02	0.74
1:A:80:LEU:O	1:A:84:THR:CG2	2.28	0.73
2:B:296:THR:HG22	2:B:297:GLU:N	2.03	0.73
1:A:215:THR:HG23	4:A:703:HOH:O	1.90	0.72
1:A:469:LEU:HD21	1:A:480:GLN:HG2	1.71	0.72
1:A:106:VAL:HG22	1:A:227:PHE:CE2	2.24	0.72
1:A:411:ILE:HD11	1:A:414:TRP:CD1	2.25	0.71
1:A:37:ILE:HG22	1:A:41:MET:CE	2.20	0.71
1:A:51:GLY:HA3	1:A:53:GLU:OE1	1.91	0.71
2:B:365:VAL:O	2:B:369:THR:HG23	1.91	0.70
1:A:27:THR:HG22	1:A:30:LYS:HG3	1.74	0.70
1:A:23:GLN:OE1	1:A:60:VAL:HG23	1.94	0.68
2:B:347:LYS:O	4:B:553:HOH:O	2.11	0.67
1:A:37:ILE:HG22	1:A:41:MET:HE2	1.76	0.66
1:A:178:ILE:CD1	1:A:191:SER:HB3	2.24	0.66
2:B:186:ASP:OD2	4:B:560:HOH:O	2.14	0.66
2:B:191:SER:OG	2:B:198:HIS:ND1	2.24	0.66
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.59	0.66
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:VAL:HG13	2:B:290:THR:OG1	1.96	0.65
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.78	0.65
2:B:314:VAL:HB	2:B:317:VAL:CG2	2.26	0.65
2:B:296:THR:CG2	2:B:297:GLU:N	2.59	0.65
2:B:418:ASN:HB2	4:B:523:HOH:O	1.96	0.64
1:A:106:VAL:HG22	1:A:227:PHE:CZ	2.31	0.64
2:B:91:GLN:C	2:B:92:LEU:HD12	2.18	0.64
1:A:246:LEU:HD23	1:A:246:LEU:N	2.12	0.64
1:A:178:ILE:HD12	1:A:191:SER:HB3	1.79	0.63
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.33	0.63
2:B:214:LEU:C	4:B:557:HOH:O	2.37	0.62
2:B:191:SER:HG	2:B:198:HIS:HD1	1.44	0.62
1:A:428:GLN:HB2	4:A:650:HOH:O	2.01	0.61
2:B:317:VAL:HG12	2:B:347:LYS:HB3	1.82	0.61
2:B:211:ARG:O	2:B:212:TRP:CB	2.46	0.61
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.82	0.61
1:A:300:GLU:HG3	4:A:725:HOH:O	2.00	0.60
1:A:39:THR:HG22	1:A:43:LYS:HD3	1.83	0.60
2:B:312:GLU:HG3	2:B:313:PRO:HD2	1.84	0.60
1:A:27:THR:O	1:A:31:ILE:HG13	2.01	0.60
1:A:32:LYS:NZ	1:A:36:GLU:OE1	2.34	0.60
1:A:460:ASN:HD22	2:B:288:ALA:HB2	1.67	0.60
1:A:27:THR:CG2	1:A:30:LYS:HG3	2.32	0.60
1:A:261:VAL:HG13	1:A:276:VAL:HG21	1.84	0.60
1:A:58:THR:HG23	4:A:586:HOH:O	2.01	0.60
1:A:406:TRP:CZ3	4:A:708:HOH:O	2.43	0.59
1:A:461:ARG:NE	4:A:702:HOH:O	2.33	0.59
2:B:84:THR:O	2:B:84:THR:HG22	2.02	0.59
1:A:325:LEU:C	1:A:326:ILE:HD12	2.22	0.59
1:A:458:VAL:HG12	2:B:286:THR:HG21	1.84	0.59
1:A:261:VAL:HG13	1:A:276:VAL:CG2	2.33	0.58
2:B:253:THR:HG23	2:B:256:ASP:OD2	2.03	0.58
2:B:306:ASN:HA	2:B:309:ILE:HD12	1.87	0.57
2:B:276:VAL:HG12	2:B:276:VAL:O	2.03	0.57
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.39	0.57
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.85	0.57
1:A:409:THR:CG2	4:A:695:HOH:O	2.38	0.57
2:B:323:LYS:O	2:B:385:LYS:NZ	2.37	0.57
2:B:296:THR:HG22	2:B:298:GLU:H	1.68	0.57
1:A:489:SER:HB3	1:A:528:LYS:HZ1	1.70	0.56
1:A:169:GLU:N	1:A:170:PRO:HD2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:VAL:HG13	2:B:283:LEU:HD21	1.87	0.56
2:B:296:THR:HB	2:B:299:ALA:CB	2.36	0.56
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.41	0.55
1:A:460:ASN:ND2	2:B:288:ALA:HB2	2.20	0.55
1:A:461:ARG:HG3	1:A:461:ARG:HH21	1.72	0.55
2:B:317:VAL:CG1	2:B:347:LYS:HB3	2.36	0.54
1:A:428:GLN:O	1:A:428:GLN:HG3	2.08	0.54
2:B:12:LEU:O	2:B:14:PRO:CD	2.55	0.54
1:A:406:TRP:NE1	4:A:720:HOH:O	2.34	0.53
2:B:314:VAL:HB	2:B:317:VAL:HG21	1.90	0.53
2:B:314:VAL:HB	2:B:317:VAL:HG22	1.90	0.53
1:A:203:GLU:OE2	1:A:219:LYS:HG2	2.09	0.53
1:A:37:ILE:HG22	1:A:41:MET:HE1	1.89	0.53
2:B:295:LEU:HD13	2:B:300:GLU:OE1	2.09	0.53
1:A:244:ILE:HG22	1:A:246:LEU:HD21	1.91	0.52
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.43	0.52
1:A:466:VAL:HG21	1:A:551:LEU:HD13	1.90	0.52
2:B:12:LEU:O	2:B:14:PRO:HD2	2.09	0.52
2:B:111:VAL:HG22	2:B:185:ASP:O	2.10	0.52
2:B:58:THR:HG23	2:B:76:ASP:O	2.10	0.52
1:A:27:THR:HG22	1:A:30:LYS:CG	2.40	0.51
1:A:485:ALA:O	1:A:489:SER:HB2	2.10	0.51
1:A:98:ALA:HB1	1:A:383:TRP:HZ2	1.75	0.51
2:B:252:TRP:CH2	2:B:260:LEU:HD22	2.45	0.51
1:A:178:ILE:HD11	1:A:191:SER:HB3	1.92	0.51
1:A:544:GLY:O	1:A:548:VAL:HG23	2.11	0.51
1:A:64:LYS:NZ	1:A:69:THR:O	2.42	0.51
2:B:101:LYS:O	2:B:236:PRO:HB2	2.11	0.51
1:A:402:TRP:CE2	1:A:403:THR:HG22	2.46	0.51
2:B:64:LYS:C	2:B:407:GLN:HE22	2.15	0.50
2:B:43:LYS:HD2	4:B:532:HOH:O	2.11	0.50
1:A:411:ILE:HD11	1:A:414:TRP:CG	2.45	0.50
1:A:286:THR:N	4:A:726:HOH:O	2.45	0.50
1:A:93:GLY:HA3	2:B:137:ASN:ND2	2.26	0.50
1:A:134:SER:OG	1:A:139:THR:O	2.21	0.50
1:A:230:MET:HE3	4:A:578:HOH:O	2.11	0.50
2:B:82:LYS:HD2	2:B:413:GLU:OE2	2.12	0.50
2:B:300:GLU:HG3	4:B:566:HOH:O	2.12	0.50
2:B:254:VAL:HG13	2:B:283:LEU:CD2	2.42	0.49
1:A:51:GLY:C	1:A:53:GLU:OE1	2.51	0.49
1:A:466:VAL:CG2	1:A:551:LEU:HD13	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LEU:HG	1:A:507:GLN:HG3	1.94	0.49
2:B:274:ILE:HD13	2:B:309:ILE:CD1	2.43	0.49
1:A:75:VAL:HG12	1:A:76:ASP:N	2.28	0.49
2:B:246:LEU:HD12	2:B:307:ARG:HG3	1.95	0.49
1:A:178:ILE:HD12	1:A:191:SER:CB	2.43	0.48
2:B:296:THR:HB	2:B:299:ALA:HB3	1.94	0.48
1:A:443:ASP:O	1:A:481:ALA:HB2	2.14	0.48
1:A:244:ILE:HG22	1:A:246:LEU:CD2	2.44	0.48
1:A:81:ASN:HA	1:A:84:THR:HG23	1.94	0.48
1:A:460:ASN:HD21	1:A:461:ARG:NH2	2.11	0.48
1:A:406:TRP:CD1	4:A:720:HOH:O	2.66	0.48
2:B:296:THR:HG22	2:B:298:GLU:N	2.28	0.48
1:A:181:TYR:HB2	3:A:562:65B:BR	2.70	0.47
4:A:590:HOH:O	2:B:394:GLN:HG3	2.13	0.47
1:A:169:GLU:N	1:A:170:PRO:CD	2.77	0.47
1:A:211:ARG:HG3	4:A:643:HOH:O	2.14	0.47
1:A:271:TYR:CE1	1:A:314:VAL:HG23	2.50	0.47
2:B:326:ILE:HD12	2:B:388:LYS:O	2.14	0.47
3:A:562:65B:C22	3:A:562:65B:N12	2.67	0.47
2:B:157:PRO:HG3	2:B:184:MET:HA	1.95	0.47
2:B:276:VAL:CG1	2:B:276:VAL:O	2.62	0.47
1:A:266:TRP:O	1:A:269:GLN:HG3	2.15	0.47
1:A:171:PHE:CD1	1:A:171:PHE:C	2.89	0.46
2:B:79:GLU:OE1	2:B:83:ARG:NH1	2.48	0.46
1:A:156:SER:N	1:A:157:PRO:CD	2.79	0.46
2:B:250:ASP:CG	2:B:251:SER:N	2.68	0.46
1:A:260:LEU:HD22	1:A:264:LEU:HG	1.98	0.46
1:A:461:ARG:CD	4:A:702:HOH:O	2.63	0.46
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.50	0.46
1:A:257:ILE:O	1:A:261:VAL:HG23	2.15	0.46
1:A:168:LEU:O	1:A:169:GLU:C	2.54	0.46
1:A:445:ALA:O	1:A:477:THR:HG21	2.16	0.46
1:A:168:LEU:C	1:A:170:PRO:HD2	2.37	0.45
1:A:10:VAL:HG12	1:A:11:LYS:N	2.31	0.45
1:A:246:LEU:HD11	1:A:310:LEU:CD1	2.45	0.45
2:B:286:THR:O	2:B:286:THR:HG22	2.17	0.45
1:A:10:VAL:HG12	1:A:11:LYS:H	1.81	0.45
1:A:287:LYS:HG3	1:A:291:GLU:OE1	2.17	0.45
1:A:69:THR:HG22	1:A:70:LYS:H	1.81	0.45
1:A:402:TRP:CE2	1:A:403:THR:CG2	3.00	0.45
1:A:286:THR:C	1:A:287:LYS:HD2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:LEU:HD13	2:B:180:ILE:HG21	1.99	0.44
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.18	0.44
3:A:562:65B:C13	3:A:562:65B:H6'3	2.48	0.44
2:B:211:ARG:HD2	2:B:211:ARG:N	2.32	0.44
2:B:292:VAL:CG2	2:B:293:ILE:N	2.80	0.44
1:A:437:ALA:HB3	1:A:494:ASN:ND2	2.32	0.44
1:A:210:LEU:C	1:A:212:TRP:H	2.20	0.44
1:A:270:ILE:HA	1:A:351:THR:HB	2.00	0.44
1:A:139:THR:HB	1:A:140:PRO:HD2	2.00	0.44
2:B:303:LEU:HD22	2:B:307:ARG:NH1	2.32	0.44
1:A:500:GLN:OE1	2:B:422:LEU:HD12	2.18	0.44
1:A:297:GLU:O	1:A:301:LEU:HD13	2.18	0.44
2:B:283:LEU:HD23	2:B:287:LYS:HZ3	1.83	0.43
1:A:538:ALA:HB1	1:A:539:HIS:CD2	2.53	0.43
1:A:407:GLN:HG3	4:A:708:HOH:O	2.18	0.43
2:B:274:ILE:HD13	2:B:309:ILE:HD13	2.00	0.43
2:B:373:GLN:NE2	4:B:552:HOH:O	2.50	0.43
2:B:213:GLY:O	2:B:214:LEU:HG	2.18	0.43
2:B:405:TYR:O	2:B:407:GLN:HG2	2.18	0.43
1:A:211:ARG:HD2	4:A:638:HOH:O	2.18	0.43
2:B:180:ILE:HD13	2:B:180:ILE:HG21	1.75	0.43
1:A:226:PRO:HB3	1:A:235:HIS:CD2	2.53	0.43
2:B:10:VAL:HG12	2:B:11:LYS:N	2.33	0.43
2:B:108:VAL:HG22	2:B:188:TYR:CD1	2.53	0.43
1:A:53:GLU:OE2	1:A:54:ASN:N	2.51	0.43
1:A:328:GLU:HG2	1:A:390:LYS:HB2	2.01	0.43
2:B:303:LEU:HD22	2:B:307:ARG:HH12	1.84	0.43
2:B:106:VAL:HG12	2:B:107:THR:N	2.32	0.43
2:B:278:GLN:O	2:B:281:LYS:HB2	2.18	0.43
2:B:195:ILE:HA	2:B:195:ILE:HD12	1.68	0.42
1:A:461:ARG:CG	1:A:461:ARG:HH21	2.32	0.42
1:A:17:ASP:O	1:A:83:ARG:NH1	2.43	0.42
2:B:191:SER:HB2	2:B:193:LEU:HD22	2.01	0.42
1:A:446:ALA:HB3	1:A:474:ASN:HD22	1.85	0.42
2:B:250:ASP:CG	2:B:251:SER:H	2.23	0.42
2:B:5:ILE:HG22	2:B:119:PRO:HD2	2.01	0.42
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.55	0.42
1:A:103:LYS:O	1:A:236:PRO:HB3	2.19	0.42
1:A:437:ALA:HB3	1:A:494:ASN:HD21	1.84	0.42
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.54	0.42
1:A:210:LEU:C	1:A:212:TRP:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:O	1:A:143:ARG:NH2	2.53	0.42
1:A:479:LEU:HD23	1:A:517:LEU:HD13	2.01	0.42
2:B:108:VAL:HG22	2:B:188:TYR:CE1	2.55	0.41
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.20	0.41
2:B:241:VAL:HG12	2:B:351:THR:H	1.85	0.41
1:A:228:LEU:HD22	1:A:242:GLN:HG2	2.03	0.41
1:A:90:VAL:HG12	1:A:91:GLN:N	2.35	0.41
1:A:498:ASP:HA	1:A:536:VAL:O	2.21	0.41
1:A:59:PRO:O	1:A:75:VAL:HG13	2.20	0.41
1:A:277:ARG:HB2	1:A:336:GLN:HE21	1.84	0.41
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.56	0.40
2:B:116:PHE:CE1	2:B:151:GLN:HG3	2.56	0.40
1:A:327:ALA:O	1:A:389:PHE:HA	2.22	0.40
2:B:261:VAL:HG13	2:B:276:VAL:HG11	2.03	0.40
1:A:2:ILE:O	1:A:3:SER:C	2.60	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	547/561 (98%)	509 (93%)	34 (6%)	4 (1%)	26	53
2	B	393/440 (89%)	364 (93%)	21 (5%)	8 (2%)	9	22
All	All	940/1001 (94%)	873 (93%)	55 (6%)	12 (1%)	15	35

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
2	B	13	LYS
1	A	471	ASP

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Mol	Chain	Res	Type
2	B	14	PRO
2	B	22	LYS
2	B	277	ARG
2	B	347	LYS
1	A	52	PRO
1	A	413	GLU
2	B	121	ASP
2	B	212	TRP
2	B	133	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	491/501 (98%)	440 (90%)	51 (10%)	9	18
2	B	365/400 (91%)	332 (91%)	33 (9%)	12	25
All	All	856/901 (95%)	772 (90%)	84 (10%)	10	21

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	GLU
1	A	27	THR
1	A	53	GLU
1	A	60	VAL
1	A	64	LYS
1	A	74	LEU
1	A	84	THR
1	A	89	GLU
1	A	91	GLN
1	A	179	VAL
1	A	185	ASP
1	A	187	LEU
1	A	195	ILE

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Mol	Chain	Res	Type
1	A	197	GLN
1	A	201	LYS
1	A	207	GLN
1	A	211	ARG
1	A	215	THR
1	A	216	THR
1	A	219	LYS
1	A	230	MET
1	A	245	VAL
1	A	260	LEU
1	A	276	VAL
1	A	280	CYS
1	A	284	ARG
1	A	300	GLU
1	A	317	VAL
1	A	325	LEU
1	A	334	GLN
1	A	345	PRO
1	A	351	THR
1	A	356	ARG
1	A	357	MET
1	A	361	HIS
1	A	388	LYS
1	A	411	ILE
1	A	428	GLN
1	A	451	LYS
1	A	454	LYS
1	A	461	ARG
1	A	464	GLN
1	A	469	LEU
1	A	474	ASN
1	A	499	SER
1	A	517	LEU
1	A	529	GLU
1	A	540	LYS
1	A	547	GLN
1	A	552	VAL
2	B	6	GLU
2	B	11	LYS
2	B	42	GLU
2	B	73	LYS
2	B	74	LEU

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Mol	Chain	Res	Type
2	B	91	GLN
2	B	139	THR
2	B	193	LEU
2	B	214	LEU
2	B	229	TRP
2	B	232	TYR
2	B	237	ASP
2	B	245	VAL
2	B	255	ASN
2	B	257	ILE
2	B	263	LYS
2	B	277	ARG
2	B	287	LYS
2	B	290	THR
2	B	292	VAL
2	B	293	ILE
2	B	295	LEU
2	B	301	LEU
2	B	303	LEU
2	B	317	VAL
2	B	326	ILE
2	B	385	LYS
2	B	388	LYS
2	B	403	THR
2	B	409	THR
2	B	410	TRP
2	B	414	TRP
2	B	424	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	198	HIS
1	A	278	GLN
1	A	336	GLN
1	A	428	GLN
1	A	474	ASN
1	A	520	GLN
1	A	539	HIS
2	B	147	ASN
2	B	151	GLN

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Mol	Chain	Res	Type
2	B	182	GLN
2	B	255	ASN
2	B	278	GLN
2	B	394	GLN
2	B	407	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	65B	A	562	-	30,30,30	1.47	4 (13%)	38,42,42	2.60	18 (47%)

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	65B	A	562	-	-	0/12/12/12	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	562	65B	C13-C14	-3.86	1.33	1.38
3	A	562	65B	C3-C2	-2.56	1.35	1.39
3	A	562	65B	C15-N16	-2.52	1.31	1.35
3	A	562	65B	C11-N5	2.62	1.40	1.36

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	562	65B	C14-C13-N12	-5.06	118.60	124.00
3	A	562	65B	C14-C15-N18	-4.84	118.71	122.87
3	A	562	65B	N16-C11-N12	-4.52	119.26	126.22
3	A	562	65B	BR-C14-C13	-4.00	114.74	121.48
3	A	562	65B	C5-C4-C4'	-3.59	114.97	119.51
3	A	562	65B	C6'-C6-C1	-3.29	115.75	120.89
3	A	562	65B	C4-C5-C6	-3.29	115.97	120.96
3	A	562	65B	C2'-C2-C1	-3.21	115.88	120.89
3	A	562	65B	C25-C26-C21	-2.68	117.27	120.28
3	A	562	65B	C21-N5-C11	-2.31	123.08	129.19
3	A	562	65B	C4-C3-C2	-2.05	117.85	120.96
3	A	562	65B	C3-C4-C4'	2.22	122.32	119.51
3	A	562	65B	C3-C2-C1	2.53	121.55	117.78
3	A	562	65B	C5-C6-C1	2.58	121.62	117.78
3	A	562	65B	C11-N16-C15	3.14	122.41	116.91
3	A	562	65B	C11-N12-C13	3.74	120.75	115.31
3	A	562	65B	O17-C13-N12	3.91	127.49	119.45
3	A	562	65B	N18-C15-N16	4.24	123.10	116.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	562	65B	4	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	551/561 (98%)	0.01	7 (1%) 79 79	25, 49, 75, 103	0
2	B	401/440 (91%)	0.02	11 (2%) 58 57	26, 46, 82, 95	0
All	All	952/1001 (95%)	0.02	18 (1%) 70 69	25, 48, 79, 103	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	GLN	5.9
1	A	219	LYS	5.2
1	A	221	HIS	4.9
2	B	13	LYS	4.5
1	A	220	LYS	4.2
2	B	15	GLY	4.1
2	B	12	LEU	3.6
1	A	218	ASP	3.3
2	B	232	TYR	3.2
2	B	6	GLU	2.8
2	B	11	LYS	2.7
2	B	301	LEU	2.6
2	B	231	GLY	2.6
1	A	194	GLU	2.5
2	B	14	PRO	2.5
2	B	68	SER	2.4
1	A	192	ASP	2.2
2	B	295	LEU	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, 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	65B	A	562	28/28	0.98	0.17	-0.13	24,33,40,45	1

6.5 Other polymers [i](#)

There are no such residues in this entry.