Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:58 AM GMT

PDB ID	:	3QIP
Title	:	Structure of HIV-1 reverse transcriptase in complex with an RNase H inhibitor and nevirapine
Authors	:	Lansdon, E.B.; Kirschberg, T.A.
Deposited on	:	2011-01-27
Resolution	:	2.09 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:

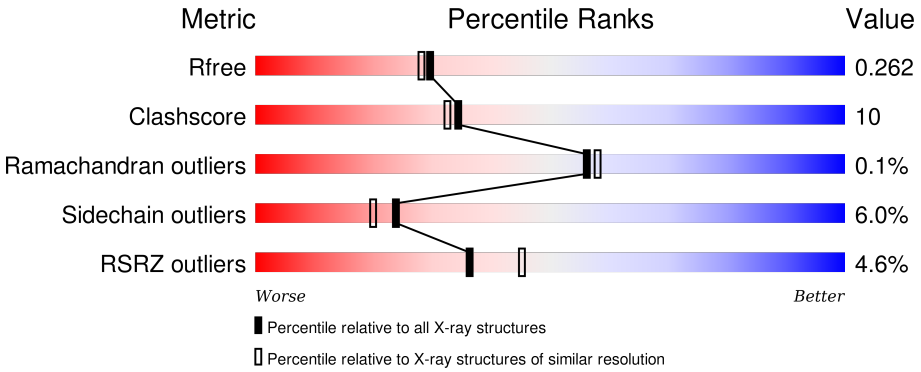
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	4% 75% 21%
2	B	440	5% 70% 19% 9%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8317 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.

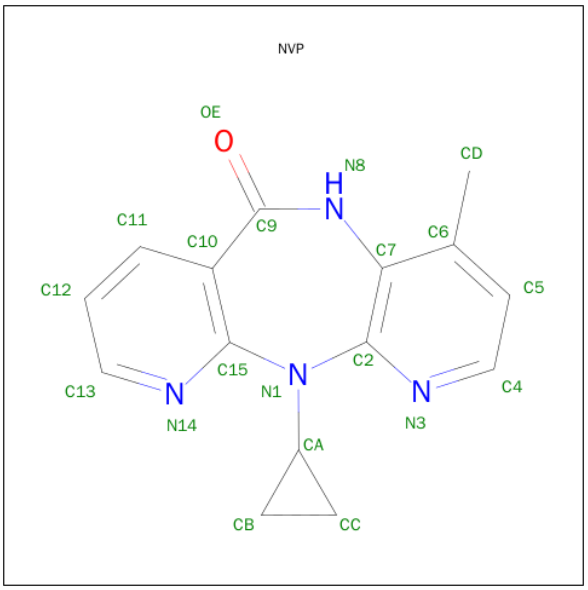
- Molecule 1 is a protein called Reverse HIV-1 reverse transcriptase p66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4508	2915	752	833	8			

- Molecule 2 is a protein called p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			3330	2169	549	606	6			

- Molecule 3 is 11-CYCLOPROPYL-5,11-DIHYDRO-4-METHYL-6H-DIPYRIDO[3,2-B:2',3' -E][1,4]DIAZEPIN-6-ONE (three-letter code: NVP) (formula: $C_{15}H_{14}N_4O$).

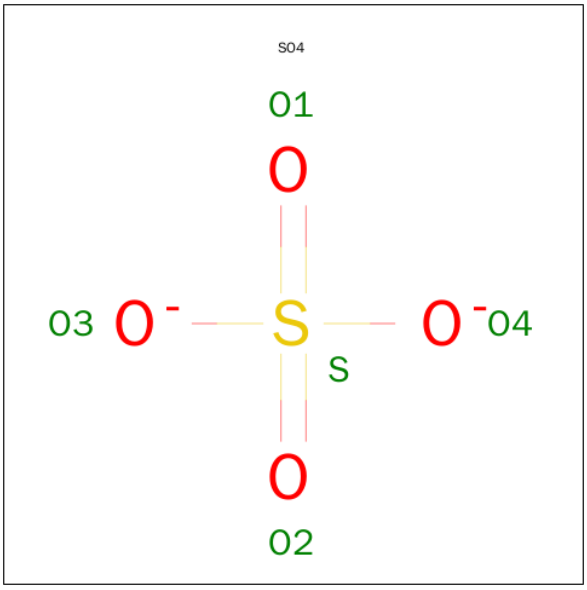


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	15	4	1		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mn 2 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

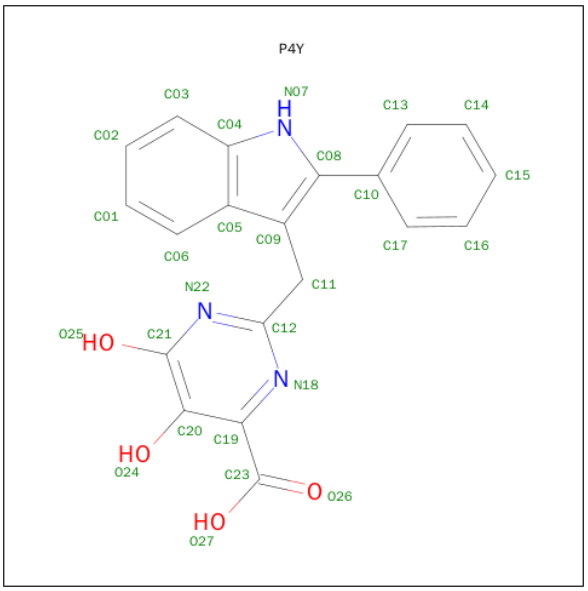


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is 5,6-DIHYDROXY-2-[(2-PHENYL-1H-INDOL-3-YL)METHYL]PYRIMIDINE -4-CARBOXYLIC ACID (three-letter code: P4Y) (formula: $C_{20}H_{15}N_3O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			27	20	3	4		

- Molecule 8 is water.

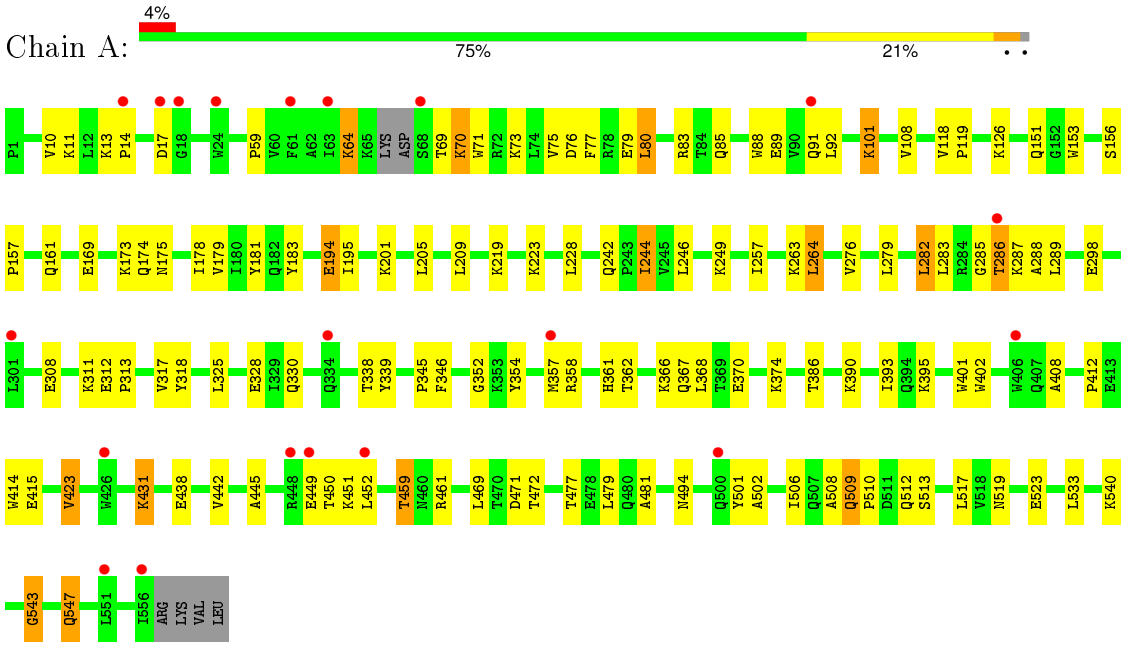
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	248	Total	O	0	0
			248	248		
8	B	170	Total	O	0	0
			170	170		

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.

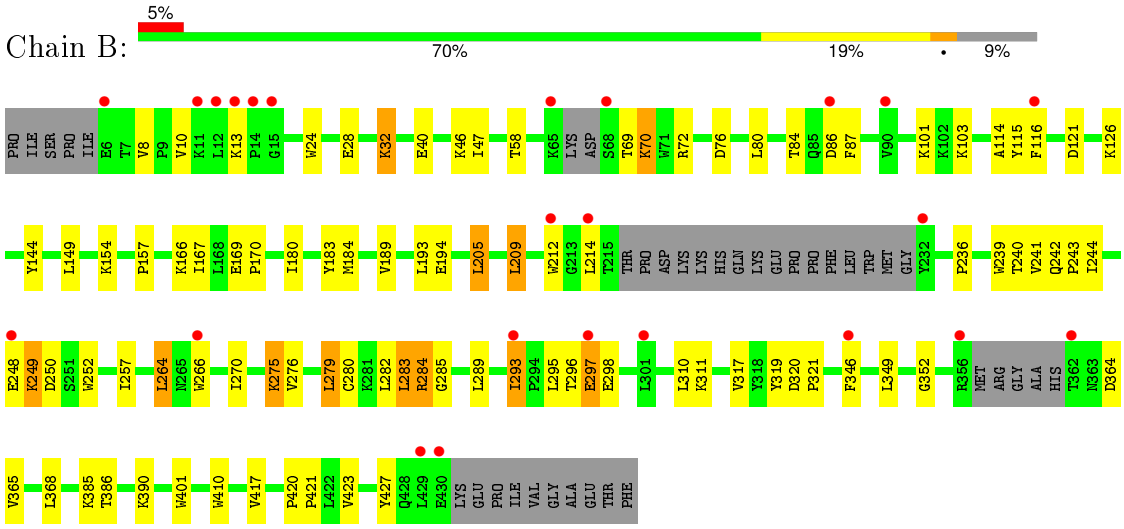
- Molecule 1: Reverse HIV-1 reverse transcriptase p66

Chain A:



- Molecule 2: p51

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	118.90Å 154.88Å 153.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.35 – 2.09 47.35 – 2.09	Depositor EDS
% Data completeness (in resolution range)	91.7 (47.35-2.09) 91.0 (47.35-2.09)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.216 , 0.267 0.214 , 0.262	Depositor DCC
R_{free} test set	4099 reflections (5.70%)	DCC
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 81858 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8317	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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

Bond lengths and bond angles in the following residue types are not validated in this section: P4Y, NVP, SO4, MN, CL

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	0.40	0/4624	0.54	0/6282
2	B	0.39	0/3422	0.54	0/4649
All	All	0.39	0/8046	0.54	0/10931

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	4508	0	4559	90	0
2	B	3330	0	3358	69	0
3	A	20	0	14	1	0
4	A	2	0	0	0	0
5	A	10	0	0	0	0
6	A	1	0	0	1	0
6	B	1	0	0	1	0
7	A	27	0	13	0	0
8	A	248	0	0	6	0
8	B	170	0	0	3	0
All	All	8317	0	7944	159	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 10.

All (159) 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:154:LYS:HE2	2:B:184:MET:HE1	1.44	0.99
2:B:154:LYS:HE2	2:B:184:MET:CE	1.98	0.94
1:A:547:GLN:HE21	1:A:547:GLN:H	1.18	0.91
6:B:441:CL:CL	8:B:557:HOH:O	2.25	0.89
1:A:194:GLU:CD	1:A:194:GLU:H	1.71	0.89
1:A:70:LYS:HD3	1:A:71:TRP:H	1.39	0.87
2:B:13:LYS:HD3	2:B:86:ASP:H	1.44	0.80
1:A:438:GLU:OE2	1:A:459:THR:HG21	1.83	0.78
1:A:70:LYS:HD3	1:A:71:TRP:N	1.97	0.78
1:A:509:GLN:HG2	8:A:805:HOH:O	1.83	0.78
1:A:543:GLY:O	1:A:547:GLN:NE2	2.16	0.76
1:A:547:GLN:N	1:A:547:GLN:HE21	1.86	0.72
1:A:308:GLU:HA	1:A:311:LYS:HG3	1.73	0.71
1:A:244:ILE:HD11	1:A:246:LEU:HD21	1.73	0.71
1:A:386:THR:HG21	1:A:412:PRO:HB3	1.73	0.70
1:A:174:GLN:HG3	8:A:776:HOH:O	1.91	0.70
1:A:79:GLU:OE1	1:A:83:ARG:NH1	2.25	0.69
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.74	0.69
1:A:459:THR:CG2	1:A:461:ARG:H	2.05	0.69
2:B:297:GLU:H	2:B:297:GLU:CD	1.96	0.69
1:A:195:ILE:HD12	1:A:195:ILE:H	1.57	0.68
1:A:64:LYS:HE3	1:A:69:THR:HA	1.76	0.68
1:A:451:LYS:HG2	1:A:471:ASP:HA	1.76	0.66
1:A:459:THR:HG22	1:A:461:ARG:H	1.60	0.66
1:A:175:ASN:HB3	1:A:178:ILE:HG12	1.79	0.65
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.33	0.63
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.83	0.61
2:B:284:ARG:CZ	2:B:285:GLY:H	2.14	0.61
2:B:319:TYR:OH	2:B:385:LYS:HE3	2.01	0.60
2:B:244:ILE:HD13	2:B:266:TRP:HZ3	1.66	0.60
1:A:108:VAL:HG11	1:A:223:LYS:HE3	1.83	0.60
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.84	0.60
2:B:166:LYS:HE2	2:B:212:TRP:HH2	1.67	0.60
1:A:362:THR:HG22	1:A:366:LYS:HE2	1.83	0.60
2:B:241:VAL:O	2:B:243:PRO:HD3	2.02	0.59
1:A:283:LEU:O	1:A:286:THR:HB	2.01	0.59
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:THR:HG22	2:B:241:VAL:O	2.03	0.58
1:A:479:LEU:HD21	1:A:501:TYR:CE2	2.39	0.58
1:A:89:GLU:HB3	1:A:92:LEU:HD21	1.86	0.57
1:A:298:GLU:H	1:A:298:GLU:CD	2.08	0.57
2:B:284:ARG:HA	2:B:284:ARG:NE	2.19	0.57
2:B:205:LEU:HD22	2:B:209:LEU:HD22	1.86	0.57
1:A:288:ALA:N	8:A:738:HOH:O	2.38	0.56
2:B:84:THR:HG22	2:B:84:THR:O	2.05	0.56
2:B:257:ILE:HG23	2:B:279:LEU:HD12	1.86	0.56
1:A:431:LYS:NZ	1:A:431:LYS:HB2	2.20	0.56
2:B:72:ARG:NH2	8:B:552:HOH:O	2.38	0.56
2:B:154:LYS:HE2	2:B:184:MET:HE2	1.85	0.56
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.42	0.55
1:A:479:LEU:HD21	1:A:501:TYR:HE2	1.69	0.55
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.88	0.55
2:B:284:ARG:NH2	2:B:285:GLY:H	2.05	0.55
1:A:361:HIS:CE1	1:A:513:SER:HG	2.23	0.54
2:B:47:ILE:HD12	2:B:144:TYR:CG	2.43	0.54
1:A:194:GLU:N	1:A:194:GLU:CD	2.51	0.53
2:B:114:ALA:CB	2:B:214:LEU:HD22	2.38	0.53
2:B:154:LYS:CE	2:B:184:MET:HE1	2.29	0.53
1:A:390:LYS:HE2	1:A:415:GLU:OE1	2.09	0.53
1:A:450:THR:CG2	1:A:452:LEU:HB3	2.39	0.52
1:A:508:ALA:HB3	8:A:603:HOH:O	2.10	0.52
1:A:228:LEU:HD22	1:A:242:GLN:HG2	1.91	0.52
1:A:13:LYS:HB3	1:A:14:PRO:HD2	1.93	0.51
2:B:8:VAL:O	2:B:121:ASP:HB2	2.11	0.51
1:A:263:LYS:HE2	8:A:744:HOH:O	2.09	0.51
1:A:179:VAL:HG12	3:A:561:NVP:HCB2	1.92	0.50
1:A:354:TYR:CD1	1:A:374:LYS:HD3	2.46	0.50
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.94	0.49
2:B:101:LYS:O	2:B:236:PRO:HB2	2.12	0.49
2:B:28:GLU:O	2:B:32:LYS:HD2	2.12	0.49
1:A:17:ASP:O	1:A:83:ARG:HD3	2.13	0.49
2:B:69:THR:O	2:B:70:LYS:HE3	2.12	0.49
2:B:242:GLN:HB2	2:B:352:GLY:HA2	1.94	0.49
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.95	0.49
1:A:354:TYR:HD1	1:A:374:LYS:HD3	1.78	0.49
1:A:257:ILE:HG22	1:A:283:LEU:HD21	1.96	0.48
1:A:401:TRP:HD1	1:A:402:TRP:CD1	2.31	0.48
1:A:509:GLN:N	1:A:510:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:THR:C	2:B:70:LYS:HE3	2.34	0.48
1:A:330:GLN:OE1	1:A:338:THR:HG23	2.13	0.48
1:A:452:LEU:HD12	1:A:469:LEU:O	2.14	0.48
2:B:103:LYS:O	2:B:236:PRO:HG2	2.13	0.48
1:A:317:VAL:HG12	1:A:318:TYR:N	2.28	0.47
2:B:296:THR:HB	2:B:298:GLU:OE1	2.14	0.47
1:A:450:THR:HG22	1:A:452:LEU:HB3	1.95	0.47
1:A:219:LYS:HD3	1:A:219:LYS:C	2.34	0.47
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.97	0.47
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.97	0.47
2:B:13:LYS:HD3	2:B:86:ASP:N	2.22	0.47
2:B:284:ARG:NE	2:B:285:GLY:H	2.13	0.47
1:A:285:GLY:O	1:A:287:LYS:HE2	2.15	0.47
2:B:248:GLU:HA	2:B:248:GLU:OE1	2.14	0.47
1:A:459:THR:HG22	1:A:461:ARG:N	2.27	0.47
2:B:266:TRP:CH2	2:B:427:TYR:CZ	3.03	0.46
2:B:257:ILE:HG22	2:B:283:LEU:HD21	1.98	0.46
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.50	0.46
1:A:279:LEU:O	1:A:282:LEU:HB2	2.15	0.46
2:B:266:TRP:CZ2	2:B:427:TYR:CZ	3.04	0.46
1:A:317:VAL:CG1	1:A:318:TYR:N	2.79	0.46
1:A:519:ASN:O	1:A:523:GLU:HG2	2.15	0.46
6:A:566:CL:CL	8:A:742:HOH:O	2.57	0.46
1:A:89:GLU:OE2	1:A:91:GLN:HG3	2.16	0.46
1:A:298:GLU:N	1:A:298:GLU:OE1	2.48	0.46
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.51	0.46
1:A:345:PRO:HA	1:A:346:PHE:HA	1.57	0.45
1:A:101:LYS:N	1:A:101:LYS:HD3	2.31	0.45
2:B:266:TRP:HH2	2:B:427:TYR:CE1	2.35	0.45
2:B:10:VAL:HG13	2:B:87:PHE:CD1	2.52	0.45
2:B:282:LEU:HB3	2:B:293:ILE:HD11	1.97	0.45
2:B:183:TYR:OH	2:B:386:THR:HG23	2.17	0.45
2:B:24:TRP:N	2:B:24:TRP:CD1	2.85	0.45
2:B:244:ILE:CD1	2:B:266:TRP:CZ3	3.01	0.44
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.99	0.44
1:A:459:THR:HG23	1:A:461:ARG:H	1.81	0.44
2:B:317:VAL:HB	8:B:608:HOH:O	2.16	0.44
2:B:252:TRP:NE1	2:B:295:LEU:HD11	2.33	0.44
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.99	0.44
2:B:284:ARG:CA	2:B:284:ARG:NE	2.80	0.44
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LEU:HD23	1:A:276:VAL:HG12	2.00	0.44
1:A:244:ILE:HD11	1:A:246:LEU:CD2	2.45	0.44
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.83	0.43
1:A:368:LEU:HD22	1:A:423:VAL:HG11	2.01	0.43
2:B:46:LYS:HE2	2:B:116:PHE:HB3	1.99	0.43
2:B:390:LYS:HD2	2:B:417:VAL:HG11	2.01	0.43
2:B:115:TYR:HB3	2:B:149:LEU:HB2	2.00	0.42
2:B:58:THR:HG23	2:B:76:ASP:O	2.19	0.42
2:B:214:LEU:N	2:B:214:LEU:HD23	2.34	0.42
1:A:523:GLU:HG2	1:A:523:GLU:H	1.72	0.42
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.55	0.42
2:B:264:LEU:HB3	2:B:276:VAL:CG1	2.50	0.42
2:B:365:VAL:HG11	2:B:401:TRP:HB2	2.01	0.42
2:B:275:LYS:HB3	2:B:275:LYS:HE3	1.88	0.42
1:A:79:GLU:HG3	1:A:83:ARG:HH11	1.82	0.42
2:B:241:VAL:HG21	2:B:311:LYS:O	2.19	0.42
2:B:420:PRO:HA	2:B:421:PRO:HD2	1.92	0.42
1:A:219:LYS:HD3	1:A:219:LYS:O	2.20	0.41
1:A:358:ARG:HD3	1:A:370:GLU:CD	2.41	0.41
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.55	0.41
1:A:118:VAL:HG13	1:A:119:PRO:HD2	2.02	0.41
1:A:479:LEU:CD2	1:A:501:TYR:HE2	2.33	0.41
1:A:393:ILE:HB	1:A:423:VAL:HG13	2.01	0.41
1:A:502:ALA:O	1:A:506:ILE:HG12	2.21	0.41
1:A:173:LYS:HE3	1:A:173:LYS:HB2	1.82	0.41
1:A:80:LEU:HD13	1:A:153:TRP:CD1	2.55	0.41
1:A:445:ALA:O	1:A:477:THR:HG21	2.21	0.41
1:A:312:GLU:HA	1:A:313:PRO:HD3	1.94	0.41
1:A:494:ASN:HB3	2:B:289:LEU:HD12	2.03	0.41
1:A:175:ASN:OD1	1:A:201:LYS:HD2	2.20	0.41
1:A:10:VAL:C	1:A:11:LYS:HG2	2.41	0.41
2:B:420:PRO:HB2	2:B:423:VAL:HG23	2.03	0.41
1:A:75:VAL:HG11	1:A:77:PHE:CZ	2.56	0.41
2:B:157:PRO:HG3	2:B:184:MET:HA	2.03	0.40
2:B:167:ILE:HG12	2:B:212:TRP:CD2	2.56	0.40
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.56	0.40
1:A:11:LYS:O	1:A:85:GLN:HG2	2.22	0.40
1:A:367:GLN:NE2	1:A:512:GLN:NE2	2.69	0.40
2:B:320:ASP:HA	2:B:321:PRO:HD3	1.76	0.40
2:B:166:LYS:HE2	2:B:212:TRP:CH2	2.52	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	550/560 (98%)	532 (97%)	17 (3%)	1 (0%)	52 53
2	B	394/440 (90%)	378 (96%)	16 (4%)	0	100 100
All	All	944/1000 (94%)	910 (96%)	33 (4%)	1 (0%)	56 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	543	GLY

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	494/500 (99%)	464 (94%)	30 (6%)	23 19
2	B	367/400 (92%)	345 (94%)	22 (6%)	24 20
All	All	861/900 (96%)	809 (94%)	52 (6%)	24 20

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LYS
1	A	70	LYS
1	A	73	LYS
1	A	80	LEU
1	A	101	LYS

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Mol	Chain	Res	Type
1	A	126	LYS
1	A	151	GLN
1	A	161	GLN
1	A	169	GLU
1	A	194	GLU
1	A	205	LEU
1	A	209	LEU
1	A	244	ILE
1	A	249	LYS
1	A	264	LEU
1	A	282	LEU
1	A	286	THR
1	A	289	LEU
1	A	325	LEU
1	A	357	MET
1	A	423	VAL
1	A	431	LYS
1	A	449	GLU
1	A	459	THR
1	A	472	THR
1	A	509	GLN
1	A	517	LEU
1	A	533	LEU
1	A	540	LYS
1	A	547	GLN
2	B	32	LYS
2	B	40	GLU
2	B	70	LYS
2	B	80	LEU
2	B	126	LYS
2	B	193	LEU
2	B	194	GLU
2	B	205	LEU
2	B	209	LEU
2	B	249	LYS
2	B	250	ASP
2	B	264	LEU
2	B	275	LYS
2	B	279	LEU
2	B	280	CYS
2	B	283	LEU
2	B	284	ARG

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Mol	Chain	Res	Type
2	B	293	ILE
2	B	297	GLU
2	B	310	LEU
2	B	368	LEU
2	B	410	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	547	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

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	NVP	A	561	-	18,23,23	0.92	0	18,34,34	1.00	0
5	SO4	A	564	-	4,4,4	0.19	0	6,6,6	0.50	0
5	SO4	A	565	-	4,4,4	0.28	0	6,6,6	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	P4Y	A	900	4	24,30,30	1.10	1 (4%)	24,43,43	1.41	4 (16%)

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	NVP	A	561	-	-	0/0/6/6	0/2/4/4
5	SO4	A	564	-	-	0/0/0/0	0/0/0/0
5	SO4	A	565	-	-	0/0/0/0	0/0/0/0
7	P4Y	A	900	4	-	0/8/12/12	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	900	P4Y	O25-C21	2.13	1.38	1.28

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	900	P4Y	C02-C03-C04	-2.01	116.84	120.06
7	A	900	P4Y	C10-C08-C09	2.91	134.63	129.57
7	A	900	P4Y	C11-C09-C08	3.30	132.71	127.34
7	A	900	P4Y	C08-N07-C04	3.41	110.86	103.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	561	NVP	1	0

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%)	0.16	20 (3%)	46	55	31, 48, 74, 98	0
2	B	402/440 (91%)	0.29	24 (5%)	25	33	31, 47, 75, 96	0
All	All	956/1000 (95%)	0.21	44 (4%)	36	45	31, 48, 75, 98	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	LEU	7.1
1	A	449	GLU	6.7
2	B	346	PHE	5.5
1	A	24	TRP	5.1
2	B	14	PRO	4.9
1	A	452	LEU	4.0
1	A	448	ARG	3.9
1	A	286	THR	3.7
1	A	18	GLY	3.5
1	A	301	LEU	3.4
2	B	11	LYS	3.3
2	B	12	LEU	3.3
1	A	61	PHE	3.3
1	A	426	TRP	3.2
1	A	551	LEU	3.0
2	B	68	SER	2.9
2	B	13	LYS	2.9
2	B	430	GLU	2.8
2	B	297	GLU	2.6
2	B	232	TYR	2.6
2	B	248	GLU	2.5
1	A	14	PRO	2.5
1	A	357	MET	2.5
1	A	91	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	406	TRP	2.4
2	B	15	GLY	2.4
2	B	429	LEU	2.3
1	A	500	GLN	2.3
2	B	65	LYS	2.3
2	B	301	LEU	2.3
2	B	116	PHE	2.2
2	B	6	GLU	2.2
1	A	63	ILE	2.2
2	B	86	ASP	2.2
1	A	68	SER	2.2
2	B	266	TRP	2.2
1	A	17	ASP	2.1
2	B	362	THR	2.1
1	A	334	GLN	2.1
2	B	212	TRP	2.1
2	B	90	VAL	2.1
1	A	556	ILE	2.0
2	B	293	ILE	2.0
2	B	356	ARG	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^{th} 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
4	MN	A	563	1/1	0.98	0.14	1.30	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NVP	A	561	20/20	0.97	0.14	0.96	25,33,36,41	0
5	SO4	A	564	5/5	0.94	0.12	0.75	48,51,57,58	0
7	P4Y	A	900	27/27	0.81	0.27	0.58	56,80,90,92	0
5	SO4	A	565	5/5	0.95	0.10	-0.32	59,59,65,75	0
4	MN	A	562	1/1	0.97	0.13	-	51,51,51,51	0
6	CL	A	566	1/1	0.97	0.19	-	75,75,75,75	0
6	CL	B	441	1/1	0.91	0.14	-	67,67,67,67	0

6.5 Other polymers

There are no such residues in this entry.