Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:46 PM GMT

PDB ID	:	1LWE
Title	:	CRYSTAL STRUCTURE OF M41L/T215Y MUTANT HIV-1 REVERSE TRANSCRIPTASE (RTMN) IN COMPLEX WITH NEVIRAPINE
Authors	:	Ren, J.; Chamberlain, P.P.; Nichols, C.E.; Douglas, L.; Stuart, D.I.; Stammers, D.K.
Deposited on	:	2002-05-31
Resolution	:	2.81 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

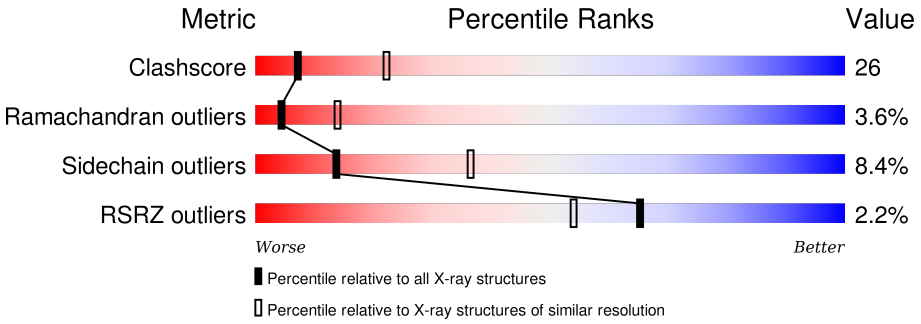
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.81 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	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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	2% 46% 44% 7% .
2	B	440	2% 51% 34% 6% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CSD	A	280	-	-	X	-
3	PO4	A	1301	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7793 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	543	Total	C	N	O	S	0	0	0
			4427	2866	735	819	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	LEU	MET	ENGINEERED	UNP P04585
A	215	TYR	THR	ENGINEERED	UNP P04585
A	280	CSD	CYS	MODIFIED RESIDUE	UNP P04585

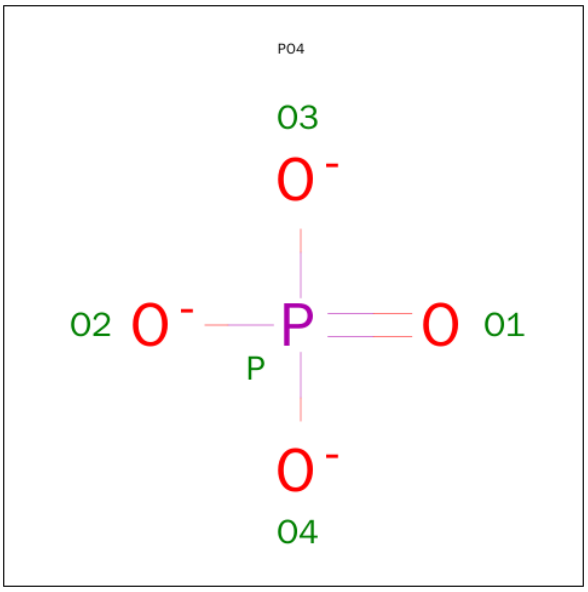
- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3322	2162	552	602	6			

There are 2 discrepancies between the modelled and reference sequences:

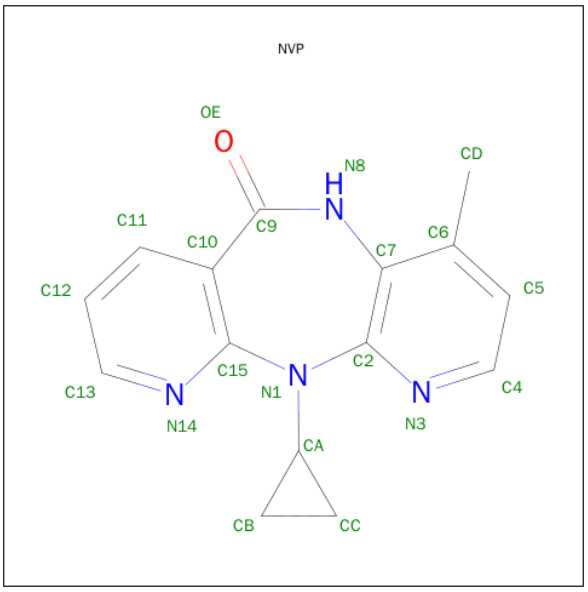
Chain	Residue	Modelled	Actual	Comment	Reference
B	41	LEU	MET	ENGINEERED	UNP P04585
B	215	TYR	THR	ENGINEERED	UNP P04585

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 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
4	A	1	Total C N O 20 15 4 1	0	0

- Molecule 5 is water.

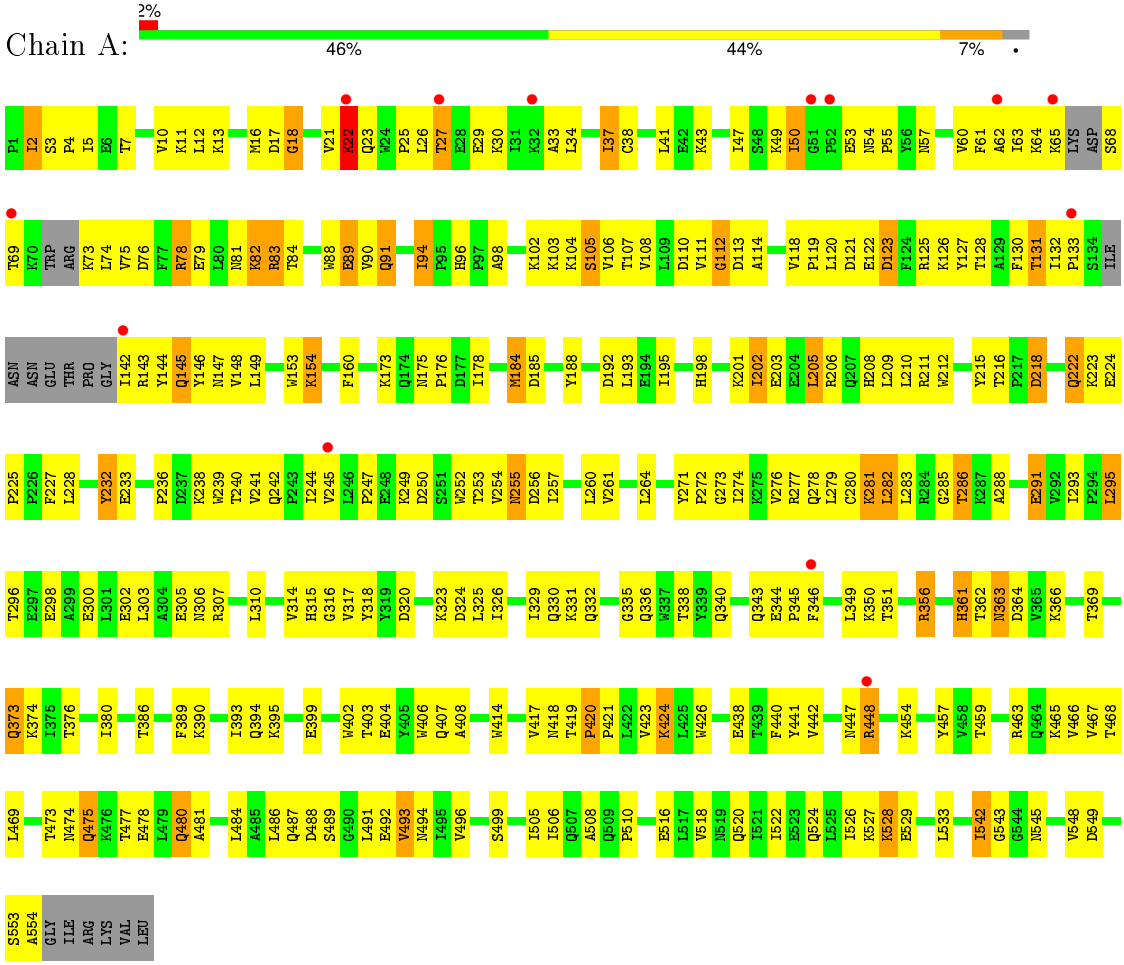
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	12	Total O 12 12	0	0
5	B	7	Total O 7 7	0	0

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.

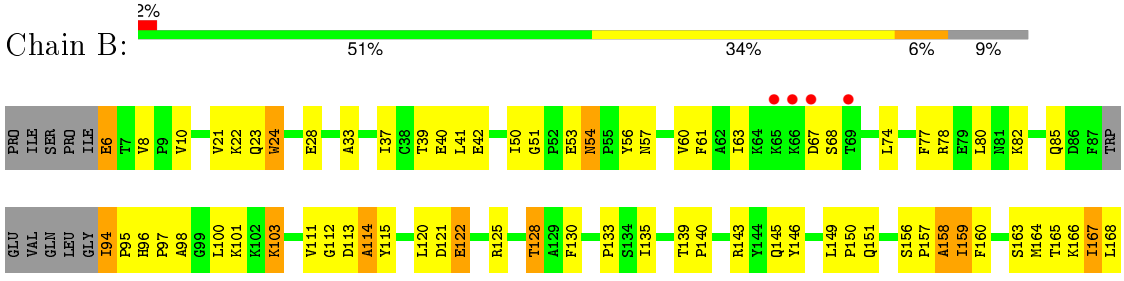
- Molecule 1: HIV-1 REVERSE TRANSCRIPTASE

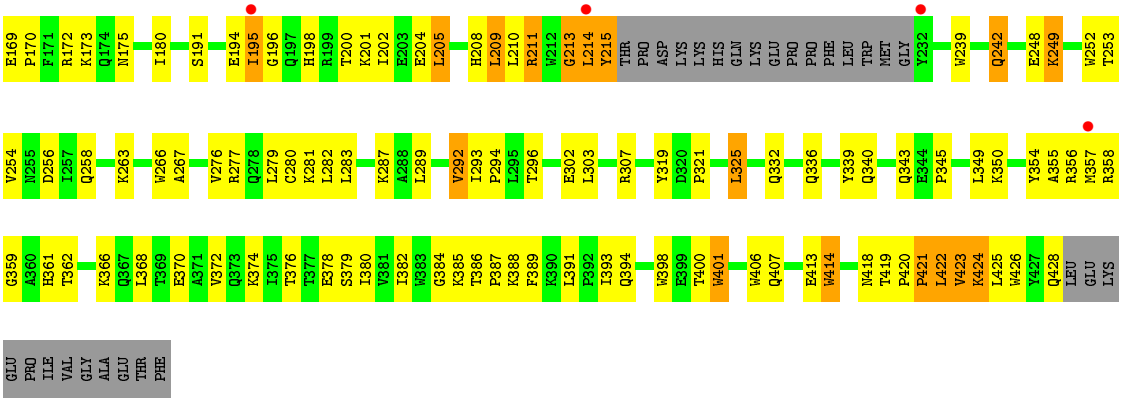
Chain A:



- Molecule 2: HIV-1 REVERSE TRANSCRIPTASE

Chain B:




E169 P170 F171 R172 K173 Q174 N175 I180 S191 E194 I195 G196 Q197 H198 R199 T200 K201 I202 E203 E204 L205 H208 L209 L210 R211 W212 G213 L214 Y215 THR PRO ASP LYS LYS HIS GLN LYS GLU PRO PRO PHE LEU TRP MET GLY Y232 W239 Q242 E248 K249 W252 T253
V254 N255 D256 I257 Q258 K263 W266 A267 V276 R277 Q278 L279 C280 K281 L282 L283 K287 A288 L289 V292 I293 P294 L295 T296 E302 L303 R307 Y319 D320 P321 L325 Q332 Q336 Y339 Q340 Q343 E344 P345 L349 K350 Y354 A355 R356 M357 R358
G359 A360 H361 T362 K366 Q367 L368 T369 E370 A371 V372 Q373 K374 I375 T376 T377 E378 S379 I380 V381 I382 W383 G384 K385 T386 P387 K388 F389 K390 L391 P392 I393 Q394 W398 E399 T400 W401 W406 Q407 E413 W414 N418 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 (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	139.70Å 111.30Å 74.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 2.81 29.99 – 2.81	Depositor EDS
% Data completeness (in resolution range)	93.8 (29.99-2.81) 93.9 (29.99-2.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.213 , 0.302 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	65.9	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 84.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 27228 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7793	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: CSD, PO4, NVP

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	0.54	0/4531	0.74	1/6152 (0.0%)
2	B	0.58	0/3415	0.79	4/4638 (0.1%)
All	All	0.56	0/7946	0.76	5/10790 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	68	SER	N-CA-C	-6.65	93.04	111.00
1	A	193	LEU	CA-CB-CG	6.45	130.12	115.30
2	B	357	MET	N-CA-C	-6.17	94.34	111.00
2	B	213	GLY	N-CA-C	5.57	127.03	113.10
2	B	401	TRP	N-CA-C	5.24	125.15	111.00

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	4427	0	4478	244	0
2	B	3322	0	3353	173	0
3	A	5	0	0	0	0
4	A	20	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	12	0	0	1	0
5	B	7	0	0	0	0
All	All	7793	0	7845	407	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 26.

All (407) 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:34:LEU:HD21	1:A:62:ALA:HB2	1.39	1.02
1:A:91:GLN:NE2	2:B:140:PRO:HA	1.79	0.97
1:A:91:GLN:HE22	2:B:140:PRO:HA	1.28	0.97
1:A:175:ASN:HB3	1:A:178:ILE:HD13	1.53	0.89
2:B:242:GLN:H	2:B:242:GLN:HE21	1.17	0.87
1:A:13:LYS:HB2	1:A:16:MET:HG3	1.58	0.85
1:A:478:GLU:HG2	1:A:499:SER:HB2	1.59	0.84
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.13	0.83
2:B:125:ARG:O	2:B:128:THR:HG23	1.80	0.81
2:B:332:GLN:HE22	2:B:428:GLN:HA	1.44	0.81
1:A:3:SER:HB3	1:A:5:ILE:HG22	1.61	0.81
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.63	0.80
2:B:356:ARG:HH22	2:B:359:GLY:HA3	1.47	0.79
2:B:139:THR:HG22	2:B:140:PRO:O	1.83	0.79
1:A:76:ASP:OD1	1:A:78:ARG:HG3	1.83	0.78
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.66	0.78
1:A:362:THR:HG22	1:A:363:ASN:H	1.49	0.77
2:B:276:VAL:HA	2:B:302:GLU:OE2	1.84	0.77
1:A:306:ASN:O	1:A:310:LEU:HD13	1.85	0.76
1:A:335:GLY:O	1:A:356:ARG:HA	1.85	0.76
1:A:468:THR:O	1:A:469:LEU:HD23	1.85	0.76
2:B:393:ILE:HG12	2:B:394:GLN:H	1.51	0.75
2:B:242:GLN:H	2:B:242:GLN:NE2	1.85	0.75
2:B:111:VAL:HB	2:B:214:LEU:HD11	1.67	0.74
1:A:424:LYS:HE3	1:A:426:TRP:CE2	2.22	0.74
1:A:34:LEU:HD21	1:A:62:ALA:CB	2.17	0.73
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.23	0.73
2:B:263:LYS:HE3	2:B:426:TRP:CZ3	2.23	0.73
1:A:376:THR:O	1:A:380:ILE:HG12	1.88	0.72
1:A:23:GLN:HE22	1:A:60:VAL:HG12	1.55	0.72
2:B:163:SER:O	2:B:167:ILE:HG22	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ASN:HD21	2:B:201:LYS:HE3	1.55	0.71
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.26	0.71
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.72	0.71
2:B:196:GLY:O	2:B:200:THR:HG23	1.90	0.71
2:B:37:ILE:O	2:B:41:LEU:HD13	1.91	0.71
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.73	0.71
1:A:466:VAL:O	1:A:467:VAL:HG23	1.91	0.70
2:B:160:PHE:HD1	2:B:160:PHE:O	1.74	0.70
1:A:2:ILE:HD12	1:A:2:ILE:H	1.56	0.70
1:A:50:ILE:HG13	1:A:143:ARG:CB	2.21	0.70
1:A:335:GLY:HA3	1:A:356:ARG:HG3	1.75	0.69
2:B:254:VAL:O	2:B:258:GLN:HG3	1.92	0.69
1:A:408:ALA:HB3	2:B:393:ILE:HG13	1.74	0.69
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.28	0.69
1:A:241:VAL:HB	1:A:314:VAL:CG2	2.23	0.68
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.74	0.68
2:B:175:ASN:HD21	2:B:201:LYS:CE	2.05	0.68
1:A:317:VAL:HG12	1:A:318:TYR:N	2.09	0.68
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.74	0.67
1:A:441:TYR:O	1:A:548:VAL:HG11	1.95	0.67
1:A:438:GLU:OE1	1:A:463:ARG:HD3	1.94	0.67
2:B:214:LEU:CD2	2:B:215:TYR:H	2.07	0.67
1:A:91:GLN:NE2	2:B:140:PRO:CA	2.58	0.66
1:A:491:LEU:HD23	1:A:529:GLU:OE1	1.94	0.66
2:B:51:GLY:HA3	2:B:53:GLU:OE1	1.94	0.66
2:B:406:TRP:C	2:B:407:GLN:HG2	2.14	0.66
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.92	0.66
1:A:131:THR:HG23	1:A:143:ARG:HG2	1.77	0.66
2:B:54:ASN:C	2:B:54:ASN:HD22	1.99	0.66
1:A:282:LEU:HD11	1:A:296:THR:HG23	1.78	0.66
1:A:257:ILE:O	1:A:261:VAL:HG23	1.97	0.65
1:A:94:ILE:HD13	1:A:94:ILE:H	1.60	0.65
1:A:241:VAL:HB	1:A:314:VAL:HG23	1.77	0.65
2:B:332:GLN:HE22	2:B:428:GLN:CA	2.10	0.65
1:A:283:LEU:N	1:A:283:LEU:HD12	2.11	0.65
2:B:319:TYR:HE1	2:B:321:PRO:HB3	1.60	0.65
1:A:131:THR:CG2	1:A:143:ARG:HG2	2.26	0.65
2:B:267:ALA:HB2	2:B:426:TRP:CH2	2.32	0.64
1:A:260:LEU:HD23	1:A:279:LEU:HD21	1.79	0.64
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.31	0.64
2:B:366:LYS:O	2:B:370:GLU:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:LEU:O	2:B:372:VAL:HG23	1.97	0.64
2:B:368:LEU:HD21	2:B:391:LEU:HD22	1.79	0.64
2:B:167:ILE:HD11	2:B:209:LEU:CD1	2.27	0.64
1:A:184:MET:CE	1:A:184:MET:HA	2.27	0.64
2:B:94:ILE:HB	2:B:95:PRO:HD2	1.78	0.64
1:A:320:ASP:OD1	1:A:323:LYS:HE3	1.97	0.64
1:A:518:VAL:O	1:A:522:ILE:HG13	1.96	0.64
1:A:280:CSD:C	1:A:282:LEU:H	2.11	0.64
2:B:96:HIS:HD2	2:B:97:PRO:HD2	1.61	0.64
2:B:419:THR:HG22	2:B:420:PRO:O	1.97	0.64
1:A:16:MET:HE1	1:A:82:LYS:O	1.98	0.64
2:B:164:MET:O	2:B:167:ILE:HG23	1.97	0.64
2:B:356:ARG:NH2	2:B:359:GLY:HA3	2.11	0.63
1:A:522:ILE:O	1:A:526:ILE:HG13	1.97	0.63
1:A:4:PRO:HG2	1:A:212:TRP:CE3	2.33	0.63
1:A:252:TRP:CD1	1:A:295:LEU:HD13	2.34	0.63
2:B:428:GLN:O	2:B:428:GLN:HG2	1.99	0.63
1:A:120:LEU:HD23	1:A:121:ASP:N	2.13	0.63
1:A:478:GLU:HG2	1:A:499:SER:CB	2.28	0.63
1:A:394:GLN:OE1	1:A:394:GLN:HA	1.99	0.63
2:B:263:LYS:HE3	2:B:426:TRP:CE3	2.34	0.62
2:B:332:GLN:OE1	2:B:424:LYS:HG2	1.99	0.62
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.81	0.62
2:B:424:LYS:HD2	2:B:425:LEU:N	2.14	0.62
2:B:54:ASN:O	2:B:143:ARG:NH2	2.32	0.62
2:B:33:ALA:O	2:B:37:ILE:HG13	1.99	0.62
2:B:242:GLN:N	2:B:242:GLN:HE21	1.94	0.62
1:A:73:LYS:HZ2	1:A:75:VAL:HG23	1.65	0.62
1:A:54:ASN:O	1:A:143:ARG:NH1	2.32	0.62
2:B:172:ARG:HE	2:B:180:ILE:HD12	1.64	0.62
1:A:110:ASP:HB2	1:A:223:LYS:HE3	1.81	0.61
2:B:336:GLN:HE21	2:B:355:ALA:CB	2.13	0.61
1:A:257:ILE:HD12	1:A:293:ILE:HD13	1.82	0.61
1:A:317:VAL:HG12	1:A:318:TYR:H	1.64	0.61
2:B:387:PRO:HG2	2:B:389:PHE:HE1	1.65	0.61
2:B:175:ASN:ND2	2:B:201:LYS:HE3	2.16	0.61
1:A:272:PRO:O	1:A:274:ILE:N	2.34	0.61
2:B:263:LYS:HG3	2:B:426:TRP:CE3	2.36	0.60
1:A:244:ILE:HG13	1:A:245:VAL:N	2.16	0.60
1:A:91:GLN:HE22	2:B:140:PRO:CA	2.07	0.60
2:B:160:PHE:CD1	2:B:160:PHE:O	2.53	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HG13	1:A:143:ARG:HB2	1.82	0.60
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.36	0.60
1:A:362:THR:HG22	1:A:366:LYS:HB3	1.84	0.59
1:A:208:HIS:O	1:A:211:ARG:HB3	2.01	0.59
1:A:545:ASN:O	1:A:549:ASP:HB2	2.02	0.59
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.37	0.59
1:A:325:LEU:C	1:A:326:ILE:HG13	2.23	0.59
2:B:393:ILE:HG12	2:B:394:GLN:N	2.18	0.58
2:B:169:GLU:HB3	2:B:170:PRO:CD	2.33	0.58
1:A:293:ILE:H	1:A:293:ILE:HD12	1.68	0.58
1:A:105:SER:HB2	1:A:198:HIS:CD2	2.38	0.58
2:B:349:LEU:O	2:B:350:LYS:HG3	2.03	0.58
1:A:332:GLN:HG2	1:A:332:GLN:O	2.03	0.58
2:B:115:TYR:CD1	2:B:156:SER:HB3	2.38	0.58
1:A:30:LYS:HB3	1:A:62:ALA:HB3	1.86	0.58
1:A:53:GLU:O	1:A:55:PRO:HD3	2.04	0.58
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.38	0.57
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.33	0.57
2:B:167:ILE:HD11	2:B:209:LEU:HD13	1.85	0.57
1:A:79:GLU:OE1	1:A:79:GLU:HA	2.04	0.57
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.70	0.57
2:B:210:LEU:HD13	2:B:214:LEU:O	2.05	0.57
2:B:332:GLN:NE2	2:B:428:GLN:HA	2.18	0.57
1:A:23:GLN:NE2	1:A:60:VAL:HG12	2.20	0.57
2:B:343:GLN:HG3	2:B:349:LEU:HD11	1.87	0.57
1:A:272:PRO:O	1:A:274:ILE:HG12	2.05	0.57
1:A:50:ILE:HG13	1:A:143:ARG:HB3	1.86	0.57
1:A:122:GLU:OE2	1:A:122:GLU:N	2.32	0.57
2:B:169:GLU:O	2:B:173:LYS:HG2	2.04	0.56
2:B:98:ALA:O	2:B:101:LYS:HG2	2.05	0.56
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.40	0.56
1:A:478:GLU:CG	1:A:499:SER:HB2	2.32	0.56
2:B:356:ARG:NH2	2:B:359:GLY:CA	2.68	0.56
1:A:448:ARG:O	1:A:448:ARG:HG3	2.06	0.56
1:A:30:LYS:O	1:A:33:ALA:HB3	2.06	0.56
1:A:29:GLU:OE2	1:A:30:LYS:HE3	2.06	0.55
2:B:111:VAL:HA	2:B:214:LEU:HD21	1.89	0.55
2:B:165:THR:O	2:B:169:GLU:N	2.40	0.55
1:A:62:ALA:C	1:A:63:ILE:HD12	2.26	0.55
1:A:178:ILE:HD12	1:A:178:ILE:N	2.21	0.55
1:A:277:ARG:NH1	1:A:277:ARG:HG2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.41	0.55
1:A:253:THR:O	1:A:256:ASP:HB2	2.06	0.55
2:B:195:ILE:HG23	2:B:195:ILE:O	2.05	0.55
1:A:23:GLN:HE22	1:A:60:VAL:CG1	2.20	0.55
1:A:553:SER:O	1:A:554:ALA:HB2	2.07	0.54
2:B:242:GLN:NE2	2:B:242:GLN:N	2.53	0.54
2:B:21:VAL:HG12	2:B:22:LYS:N	2.23	0.54
2:B:122:GLU:HB3	2:B:125:ARG:NH1	2.22	0.54
1:A:278:GLN:HE22	1:A:281:LYS:NZ	2.06	0.54
2:B:266:TRP:CE3	2:B:422:LEU:HD13	2.43	0.54
1:A:111:VAL:O	1:A:111:VAL:HG23	2.07	0.54
2:B:336:GLN:HE21	2:B:355:ALA:HB1	1.72	0.53
1:A:253:THR:HA	1:A:291:GLU:O	2.09	0.53
2:B:111:VAL:HB	2:B:214:LEU:CD1	2.36	0.53
1:A:120:LEU:HD23	1:A:121:ASP:H	1.74	0.53
1:A:276:VAL:O	1:A:280:CSD:HB3	2.09	0.53
1:A:64:LYS:HG2	1:A:65:LYS:H	1.74	0.53
1:A:175:ASN:OD1	1:A:201:LYS:HE3	2.08	0.53
1:A:280:CSD:C	1:A:282:LEU:N	2.71	0.53
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.43	0.53
2:B:21:VAL:HG12	2:B:22:LYS:H	1.74	0.53
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.89	0.53
1:A:491:LEU:HD23	1:A:529:GLU:CD	2.30	0.53
1:A:22:LYS:HE3	1:A:23:GLN:N	2.24	0.52
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.90	0.52
2:B:422:LEU:O	2:B:424:LYS:N	2.43	0.52
1:A:125:ARG:CG	1:A:146:TYR:O	2.58	0.52
2:B:100:LEU:O	2:B:103:LYS:HB2	2.09	0.52
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.43	0.52
1:A:61:PHE:O	1:A:73:LYS:HG3	2.09	0.52
2:B:422:LEU:O	2:B:425:LEU:N	2.43	0.52
1:A:330:GLN:HB2	1:A:338:THR:OG1	2.09	0.52
2:B:94:ILE:HD13	2:B:94:ILE:N	2.25	0.52
1:A:516:GLU:O	1:A:520:GLN:HG3	2.10	0.51
2:B:168:LEU:O	2:B:172:ARG:HG2	2.10	0.51
1:A:402:TRP:CE3	1:A:403:THR:HG22	2.46	0.51
1:A:84:THR:HB	1:A:154:LYS:HD3	1.92	0.51
1:A:175:ASN:HB3	1:A:178:ILE:CD1	2.34	0.51
2:B:163:SER:HA	2:B:166:LYS:HE2	1.93	0.51
1:A:205:LEU:HD22	1:A:209:LEU:HD11	1.93	0.51
1:A:91:GLN:CD	2:B:140:PRO:HA	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:HG12	1:A:11:LYS:N	2.25	0.51
1:A:244:ILE:HG13	1:A:245:VAL:H	1.75	0.51
1:A:419:THR:HG22	1:A:419:THR:O	2.10	0.51
2:B:56:TYR:O	2:B:57:ASN:HB2	2.11	0.50
2:B:336:GLN:NE2	2:B:355:ALA:HB1	2.25	0.50
1:A:125:ARG:HG3	1:A:146:TYR:O	2.11	0.50
1:A:480:GLN:HA	1:A:480:GLN:OE1	2.10	0.50
1:A:49:LYS:HA	1:A:143:ARG:O	2.11	0.50
1:A:325:LEU:O	1:A:326:ILE:HG13	2.11	0.50
1:A:335:GLY:C	1:A:356:ARG:HA	2.31	0.50
2:B:248:GLU:O	2:B:249:LYS:HD2	2.11	0.50
2:B:113:ASP:O	2:B:115:TYR:N	2.45	0.50
2:B:214:LEU:HD23	2:B:215:TYR:H	1.75	0.50
1:A:49:LYS:HE3	1:A:142:ILE:HG23	1.94	0.50
1:A:81:ASN:C	1:A:83:ARG:H	2.15	0.50
2:B:156:SER:HB2	2:B:157:PRO:CD	2.41	0.50
1:A:73:LYS:NZ	1:A:75:VAL:HG23	2.27	0.50
2:B:194:GLU:C	2:B:196:GLY:H	2.15	0.50
1:A:125:ARG:O	1:A:128:THR:OG1	2.30	0.50
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.94	0.50
1:A:118:VAL:O	1:A:148:VAL:HA	2.12	0.49
1:A:277:ARG:HH11	1:A:277:ARG:HG2	1.76	0.49
1:A:206:ARG:O	1:A:210:LEU:HB2	2.12	0.49
1:A:94:ILE:HD13	1:A:94:ILE:N	2.26	0.49
1:A:281:LYS:O	1:A:281:LYS:HG3	2.12	0.49
1:A:96:HIS:HD2	1:A:98:ALA:H	1.61	0.49
1:A:465:LYS:HG2	1:A:466:VAL:N	2.28	0.49
2:B:112:GLY:O	2:B:115:TYR:HD2	1.95	0.49
1:A:107:THR:HG22	1:A:108:VAL:N	2.27	0.49
1:A:280:CSD:O	1:A:283:LEU:HD13	2.12	0.49
1:A:345:PRO:C	1:A:346:PHE:HD1	2.16	0.49
2:B:319:TYR:CE1	2:B:321:PRO:HB3	2.46	0.49
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.47	0.49
1:A:37:ILE:O	1:A:41:LEU:HB2	2.13	0.49
2:B:356:ARG:HH21	2:B:359:GLY:N	2.12	0.48
1:A:60:VAL:HG23	1:A:75:VAL:HG22	1.94	0.48
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.95	0.48
1:A:395:LYS:HD2	1:A:414:TRP:CZ2	2.47	0.48
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.48	0.48
1:A:362:THR:C	1:A:363:ASN:HD22	2.16	0.48
1:A:484:LEU:O	1:A:487:GLN:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:GLN:HG2	2:B:133:PRO:HD3	1.95	0.48
1:A:90:VAL:O	1:A:91:GLN:C	2.51	0.48
1:A:454:LYS:NZ	1:A:554:ALA:HB3	2.29	0.48
1:A:43:LYS:HB3	1:A:43:LYS:NZ	2.29	0.48
2:B:96:HIS:CD2	2:B:97:PRO:HD2	2.45	0.48
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.96	0.48
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.54	0.48
1:A:64:LYS:HG2	1:A:65:LYS:N	2.29	0.48
2:B:208:HIS:O	2:B:211:ARG:HG2	2.14	0.48
1:A:465:LYS:NZ	1:A:465:LYS:CB	2.77	0.48
2:B:406:TRP:O	2:B:407:GLN:HG2	2.13	0.48
2:B:10:VAL:HG21	2:B:159:ILE:HD11	1.95	0.48
1:A:373:GLN:HG3	1:A:374:LYS:N	2.28	0.48
1:A:21:VAL:N	1:A:57:ASN:O	2.45	0.48
2:B:202:ILE:O	2:B:205:LEU:N	2.47	0.47
2:B:253:THR:H	2:B:256:ASP:HB2	1.79	0.47
2:B:211:ARG:CZ	2:B:211:ARG:HB2	2.43	0.47
1:A:467:VAL:HG12	1:A:469:LEU:HD21	1.96	0.47
1:A:356:ARG:HG2	1:A:356:ARG:O	2.14	0.47
2:B:277:ARG:HG3	2:B:277:ARG:HH21	1.79	0.47
1:A:202:ILE:HG22	1:A:203:GLU:N	2.30	0.47
2:B:115:TYR:CE1	2:B:156:SER:HB3	2.49	0.47
1:A:12:LEU:HD23	1:A:83:ARG:HB3	1.97	0.47
2:B:303:LEU:HD13	2:B:307:ARG:HH21	1.79	0.47
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.97	0.47
1:A:110:ASP:HB2	1:A:223:LYS:CE	2.43	0.47
1:A:407:GLN:HG2	2:B:393:ILE:HA	1.96	0.47
2:B:214:LEU:HD23	2:B:215:TYR:N	2.30	0.47
1:A:2:ILE:CD1	1:A:2:ILE:H	2.18	0.47
1:A:228:LEU:HA	1:A:232:TYR:O	2.15	0.47
1:A:131:THR:O	1:A:133:PRO:HD3	2.14	0.47
1:A:465:LYS:NZ	1:A:488:ASP:OD1	2.34	0.47
2:B:380:ILE:O	2:B:384:GLY:N	2.47	0.47
1:A:255:ASN:HD22	1:A:255:ASN:HA	1.52	0.47
1:A:249:LYS:HB2	5:A:1002:HOH:O	2.15	0.47
2:B:191:SER:OG	2:B:198:HIS:ND1	2.44	0.46
2:B:51:GLY:CA	2:B:53:GLU:OE1	2.64	0.46
2:B:421:PRO:HG2	2:B:422:LEU:H	1.81	0.46
2:B:158:ALA:O	2:B:160:PHE:N	2.49	0.46
1:A:331:LYS:CE	1:A:364:ASP:OD1	2.63	0.46
1:A:442:VAL:HG12	1:A:457:TYR:CB	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG23	1:A:236:PRO:HB3	1.97	0.46
1:A:89:GLU:OE1	1:A:90:VAL:C	2.53	0.46
1:A:474:ASN:O	1:A:478:GLU:HB2	2.15	0.46
1:A:228:LEU:CD2	1:A:233:GLU:HG2	2.45	0.46
2:B:422:LEU:O	2:B:423:VAL:C	2.53	0.46
2:B:54:ASN:ND2	2:B:56:TYR:H	2.14	0.46
1:A:260:LEU:CD2	1:A:279:LEU:HD21	2.45	0.46
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.86	0.46
1:A:402:TRP:CZ2	2:B:362:THR:HG23	2.51	0.46
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.98	0.46
1:A:279:LEU:HB2	1:A:302:GLU:OE1	2.15	0.46
2:B:214:LEU:HD22	2:B:215:TYR:H	1.77	0.46
1:A:88:TRP:HE3	1:A:88:TRP:HA	1.81	0.46
2:B:325:LEU:HD22	2:B:385:LYS:HE2	1.96	0.45
1:A:317:VAL:CG1	1:A:318:TYR:N	2.78	0.45
1:A:466:VAL:O	1:A:467:VAL:CG2	2.63	0.45
1:A:210:LEU:HD12	1:A:215:TYR:HA	1.98	0.45
1:A:102:LYS:O	1:A:103:LYS:HD3	2.17	0.45
2:B:388:LYS:HE2	2:B:413:GLU:HB3	1.98	0.45
2:B:339:TYR:O	2:B:340:GLN:HG3	2.17	0.45
1:A:486:LEU:O	1:A:528:LYS:NZ	2.48	0.45
1:A:466:VAL:HG12	1:A:467:VAL:N	2.32	0.44
2:B:205:LEU:CD2	2:B:209:LEU:HD22	2.47	0.44
1:A:76:ASP:OD1	1:A:78:ARG:CG	2.59	0.44
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.40	0.44
1:A:118:VAL:HB	1:A:149:LEU:HD22	1.98	0.44
1:A:173:LYS:HB3	1:A:173:LYS:HE2	1.67	0.44
2:B:400:THR:HG22	2:B:401:TRP:CD2	2.52	0.44
2:B:111:VAL:CB	2:B:214:LEU:HD11	2.43	0.44
2:B:368:LEU:HD22	2:B:398:TRP:CZ3	2.53	0.44
1:A:2:ILE:N	1:A:2:ILE:HD12	2.29	0.44
1:A:126:LYS:HA	1:A:145:GLN:OE1	2.18	0.44
1:A:418:ASN:OD1	1:A:420:PRO:HD3	2.18	0.44
1:A:41:LEU:HB3	1:A:47:ILE:HD11	1.99	0.44
1:A:404:GLU:O	1:A:404:GLU:HG3	2.18	0.44
1:A:505:ILE:O	1:A:510:PRO:HD3	2.18	0.44
2:B:122:GLU:HA	2:B:125:ARG:HG3	2.00	0.43
1:A:280:CSD:O	1:A:283:LEU:CD1	2.66	0.43
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.75	0.43
2:B:263:LYS:HG3	2:B:426:TRP:HE3	1.80	0.43
2:B:201:LYS:NZ	2:B:204:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:SER:CB	2:B:387:PRO:HD3	2.49	0.43
1:A:295:LEU:HD23	1:A:300:GLU:OE1	2.17	0.43
1:A:285:GLY:O	1:A:286:THR:C	2.57	0.43
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.53	0.43
1:A:62:ALA:O	1:A:63:ILE:HD12	2.17	0.43
1:A:344:GLU:O	1:A:345:PRO:C	2.55	0.43
2:B:414:TRP:O	2:B:414:TRP:HD1	2.01	0.43
1:A:475:GLN:HG2	1:A:475:GLN:H	1.50	0.43
1:A:224:GLU:HA	1:A:225:PRO:HD3	1.68	0.43
2:B:354:TYR:CD1	2:B:374:LYS:HD2	2.54	0.43
2:B:279:LEU:HA	2:B:279:LEU:HD23	1.81	0.43
1:A:466:VAL:HG12	1:A:467:VAL:H	1.82	0.43
1:A:288:ALA:O	1:A:291:GLU:HB2	2.18	0.43
1:A:98:ALA:HB2	1:A:349:LEU:O	2.19	0.43
2:B:24:TRP:HZ3	2:B:61:PHE:CD2	2.37	0.43
2:B:376:THR:CG2	2:B:386:THR:HG22	2.48	0.43
2:B:156:SER:HB2	2:B:157:PRO:HD3	2.01	0.43
1:A:215:TYR:C	1:A:215:TYR:CD1	2.92	0.43
1:A:264:LEU:CD2	1:A:306:ASN:ND2	2.82	0.43
1:A:424:LYS:HE3	1:A:426:TRP:CD2	2.52	0.42
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.48	0.42
1:A:17:ASP:OD1	1:A:18:GLY:N	2.52	0.42
1:A:112:GLY:C	1:A:114:ALA:H	2.22	0.42
1:A:389:PHE:O	1:A:414:TRP:HA	2.20	0.42
2:B:277:ARG:O	2:B:281:LYS:HG3	2.19	0.42
1:A:74:LEU:O	1:A:74:LEU:HG	2.18	0.42
1:A:417:VAL:O	1:A:417:VAL:HG12	2.19	0.42
1:A:393:ILE:HG12	1:A:394:GLN:N	2.35	0.42
1:A:492:GLU:C	1:A:493:VAL:HG22	2.39	0.42
2:B:78:ARG:O	2:B:82:LYS:HG3	2.19	0.42
2:B:113:ASP:O	2:B:114:ALA:C	2.57	0.42
2:B:205:LEU:HD22	2:B:209:LEU:HD22	2.00	0.42
2:B:194:GLU:HG3	2:B:196:GLY:H	1.85	0.42
1:A:54:ASN:HD21	1:A:126:LYS:HB2	1.85	0.42
1:A:94:ILE:CD1	1:A:94:ILE:N	2.83	0.42
2:B:414:TRP:CD1	2:B:414:TRP:C	2.93	0.42
1:A:26:LEU:HD22	1:A:27:THR:HG22	2.00	0.42
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.35	0.42
1:A:402:TRP:HE3	1:A:403:THR:CG2	2.32	0.42
1:A:228:LEU:HD21	1:A:233:GLU:HG2	2.01	0.42
2:B:376:THR:HG23	2:B:386:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:HG22	1:A:69:THR:O	2.20	0.42
1:A:329:ILE:HG22	1:A:330:GLN:N	2.35	0.42
1:A:178:ILE:N	1:A:178:ILE:CD1	2.83	0.41
2:B:356:ARG:NH2	2:B:359:GLY:N	2.67	0.41
1:A:293:ILE:N	1:A:293:ILE:HD12	2.34	0.41
2:B:54:ASN:C	2:B:54:ASN:ND2	2.70	0.41
1:A:283:LEU:N	1:A:283:LEU:CD1	2.81	0.41
2:B:77:PHE:CD2	2:B:80:LEU:HD23	2.55	0.41
2:B:125:ARG:HD3	2:B:146:TYR:O	2.20	0.41
2:B:253:THR:HA	2:B:292:VAL:HA	2.02	0.41
2:B:60:VAL:HG11	2:B:130:PHE:CD1	2.55	0.41
1:A:350:LYS:HG2	1:A:351:THR:N	2.35	0.41
2:B:113:ASP:HB2	2:B:214:LEU:HG	2.02	0.41
2:B:419:THR:HA	2:B:420:PRO:HD3	1.94	0.41
1:A:298:GLU:OE2	1:A:298:GLU:N	2.35	0.41
1:A:247:PRO:O	1:A:307:ARG:NH2	2.54	0.41
1:A:336:GLN:HG3	1:A:356:ARG:HB2	2.01	0.41
2:B:6:GLU:OE1	2:B:6:GLU:N	2.54	0.41
2:B:254:VAL:HG22	2:B:293:ILE:HD11	2.02	0.41
2:B:293:ILE:HG23	2:B:294:PRO:HD2	2.02	0.41
1:A:122:GLU:HG2	1:A:123:ASP:N	2.35	0.41
2:B:249:LYS:HB2	2:B:252:TRP:CZ2	2.55	0.41
1:A:188:TYR:N	1:A:188:TYR:CD1	2.88	0.41
2:B:354:TYR:CE1	2:B:374:LYS:HD2	2.55	0.41
1:A:324:ASP:O	1:A:343:GLN:HG2	2.20	0.41
2:B:41:LEU:N	2:B:41:LEU:HD12	2.35	0.41
2:B:349:LEU:O	2:B:350:LYS:CG	2.68	0.41
1:A:362:THR:HG22	1:A:363:ASN:N	2.26	0.41
2:B:194:GLU:O	2:B:196:GLY:N	2.48	0.41
1:A:211:ARG:C	1:A:211:ARG:HD3	2.41	0.41
1:A:153:TRP:O	1:A:154:LYS:C	2.60	0.41
2:B:414:TRP:CD1	2:B:414:TRP:O	2.74	0.41
1:A:130:PHE:CE2	1:A:144:TYR:HB2	2.56	0.41
1:A:506:ILE:C	1:A:508:ALA:N	2.73	0.41
1:A:524:GLN:O	1:A:527:LYS:HB2	2.21	0.41
2:B:96:HIS:HE1	2:B:382:ILE:O	2.04	0.40
2:B:39:THR:O	2:B:42:GLU:HB3	2.22	0.40
1:A:542:ILE:HG13	1:A:542:ILE:H	1.67	0.40
1:A:240:THR:HG22	1:A:315:HIS:ND1	2.36	0.40
2:B:163:SER:O	2:B:166:LYS:HB3	2.21	0.40
1:A:363:ASN:ND2	1:A:363:ASN:N	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LYS:NZ	1:A:465:LYS:HB2	2.35	0.40
1:A:447:ASN:OD1	1:A:448:ARG:N	2.54	0.40
1:A:420:PRO:HA	1:A:421:PRO:C	2.41	0.40
1:A:175:ASN:N	1:A:176:PRO:CD	2.84	0.40
2:B:350:LYS:HE3	2:B:382:ILE:CD1	2.51	0.40
1:A:218:ASP:O	1:A:222:GLN:OE1	2.39	0.40
1:A:473:THR:O	1:A:477:THR:HG23	2.21	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	534/560 (95%)	452 (85%)	64 (12%)	18 (3%)	5	15
2	B	395/440 (90%)	337 (85%)	43 (11%)	15 (4%)	4	12
All	All	929/1000 (93%)	789 (85%)	107 (12%)	33 (4%)	4	14

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	GLY
1	A	528	LYS
1	A	542	ILE
2	B	195	ILE
2	B	423	VAL
1	A	112	GLY
1	A	356	ARG
2	B	67	ASP
2	B	114	ALA
2	B	159	ILE
2	B	361	HIS

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Mol	Chain	Res	Type
1	A	361	HIS
1	A	420	PRO
2	B	122	GLU
2	B	358	ARG
1	A	18	GLY
1	A	22	LYS
1	A	154	LYS
1	A	286	THR
2	B	85	GLN
2	B	121	ASP
1	A	91	GLN
1	A	127	TYR
2	B	103	LYS
2	B	158	ALA
2	B	213	GLY
1	A	50	ILE
1	A	123	ASP
2	B	422	LEU
2	B	421	PRO
1	A	37	ILE
1	A	25	PRO
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	484/499 (97%)	436 (90%)	48 (10%)	10	27
2	B	365/400 (91%)	342 (94%)	23 (6%)	22	52
All	All	849/899 (94%)	778 (92%)	71 (8%)	14	36

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE

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Mol	Chain	Res	Type
1	A	22	LYS
1	A	27	THR
1	A	68	SER
1	A	78	ARG
1	A	82	LYS
1	A	83	ARG
1	A	89	GLU
1	A	94	ILE
1	A	105	SER
1	A	113	ASP
1	A	131	THR
1	A	145	GLN
1	A	147	ASN
1	A	184	MET
1	A	185	ASP
1	A	195	ILE
1	A	202	ILE
1	A	205	LEU
1	A	216	THR
1	A	218	ASP
1	A	222	GLN
1	A	232	TYR
1	A	238	LYS
1	A	242	GLN
1	A	250	ASP
1	A	255	ASN
1	A	281	LYS
1	A	282	LEU
1	A	291	GLU
1	A	295	LEU
1	A	305	GLU
1	A	340	GLN
1	A	361	HIS
1	A	363	ASN
1	A	369	THR
1	A	373	GLN
1	A	386	THR
1	A	399	GLU
1	A	423	VAL
1	A	424	LYS
1	A	448	ARG
1	A	459	THR

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Mol	Chain	Res	Type
1	A	475	GLN
1	A	480	GLN
1	A	493	VAL
1	A	496	VAL
1	A	533	LEU
2	B	6	GLU
2	B	8	VAL
2	B	24	TRP
2	B	40	GLU
2	B	54	ASN
2	B	94	ILE
2	B	128	THR
2	B	151	GLN
2	B	167	ILE
2	B	205	LEU
2	B	209	LEU
2	B	211	ARG
2	B	214	LEU
2	B	215	TYR
2	B	242	GLN
2	B	249	LYS
2	B	280	CYS
2	B	287	LYS
2	B	292	VAL
2	B	325	LEU
2	B	345	PRO
2	B	414	TRP
2	B	424	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	54	ASN
1	A	91	GLN
1	A	96	HIS
1	A	145	GLN
1	A	174	GLN
1	A	208	HIS
1	A	221	HIS
1	A	242	GLN
1	A	255	ASN

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Mol	Chain	Res	Type
1	A	278	GLN
1	A	306	ASN
1	A	336	GLN
1	A	340	GLN
1	A	363	ASN
1	A	428	GLN
1	A	475	GLN
1	A	545	ASN
2	B	54	ASN
2	B	57	ASN
2	B	96	HIS
2	B	175	ASN
2	B	197	GLN
2	B	207	GLN
2	B	242	GLN
2	B	278	GLN
2	B	332	GLN
2	B	336	GLN
2	B	394	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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	0.94	0	3,8,10	4.51	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(^{o})	Ideal(^{o})
1	A	280	CSD	OD1-SG-CB	7.52	117.94	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.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	5	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are 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	PO4	A	1301	-	4,4,4	1.13	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NVP	A	999	-	18,23,23	1.40	5 (27%)	18,34,34	1.27	2 (11%)

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	PO4	A	1301	-	-	0/0/0/0	0/0/0/0
4	NVP	A	999	-	-	0/0/6/6	0/2/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	NVP	CA-N1	-2.23	1.45	1.49
4	A	999	NVP	C4-N3	2.02	1.36	1.32
4	A	999	NVP	C12-C11	2.23	1.41	1.36
4	A	999	NVP	C13-N14	2.43	1.37	1.32
4	A	999	NVP	C10-C15	2.80	1.43	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	999	NVP	CB-CA-N1	-2.89	115.28	118.25
4	A	999	NVP	C11-C10-C15	2.19	119.04	117.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	542/560 (96%)	-0.45	13 (2%) 62 50	27, 67, 115, 149	0
2	B	401/440 (91%)	-0.47	8 (1%) 68 58	31, 63, 114, 145	0
All	All	943/1000 (94%)	-0.46	21 (2%) 65 54	27, 65, 115, 149	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	232	TYR	5.0
2	B	69	THR	4.5
2	B	214	LEU	3.2
1	A	65	LYS	3.2
2	B	67	ASP	3.2
1	A	51	GLY	3.1
1	A	133	PRO	3.0
1	A	27	THR	2.8
1	A	245	VAL	2.8
1	A	22	LYS	2.7
2	B	65	LYS	2.7
1	A	448	ARG	2.7
1	A	32	LYS	2.6
1	A	142	ILE	2.6
2	B	357	MET	2.5
1	A	62	ALA	2.5
1	A	52	PRO	2.4
2	B	195	ILE	2.3
1	A	69	THR	2.3
2	B	66	LYS	2.3
1	A	346	PHE	2.1

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, 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
1	CSD	A	280	8/9	0.95	0.10	-	50,57,71,71	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, 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
3	PO4	A	1301	5/5	0.86	0.23	2.37	119,122,128,130	0
4	NVP	A	999	20/20	0.97	0.14	0.14	35,47,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.