Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:45 PM GMT

PDB ID	:	1LWC
Title	:	CRYSTAL STRUCTURE OF M184V MUTANT HIV-1 REVERSE TRANSCRIPTASE 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	:	2.62 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:

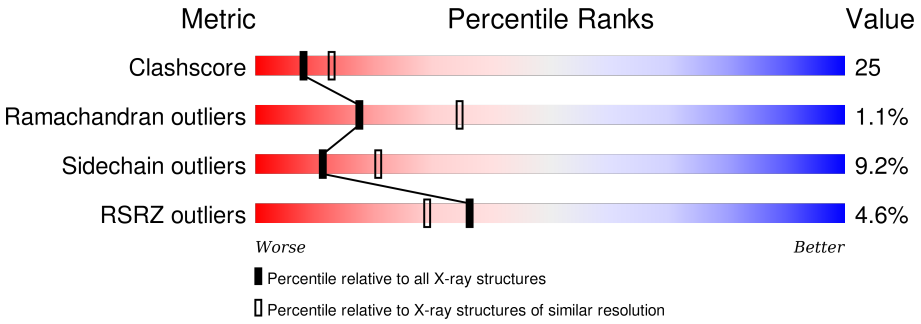
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.62 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	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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% 47% 36% 7% 9%
2	B	440	7% 53% 34% • 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
3	PO4	A	1300	-	-	-	X
3	PO4	A	1301	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7542 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	507	Total	C	N	O	S	0	0	0
			4158	2698	686	767	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	VAL	MET	ENGINEERED	UNP P04585
A	280	CSD	CYS	MODIFIED RESIDUE	UNP P04585

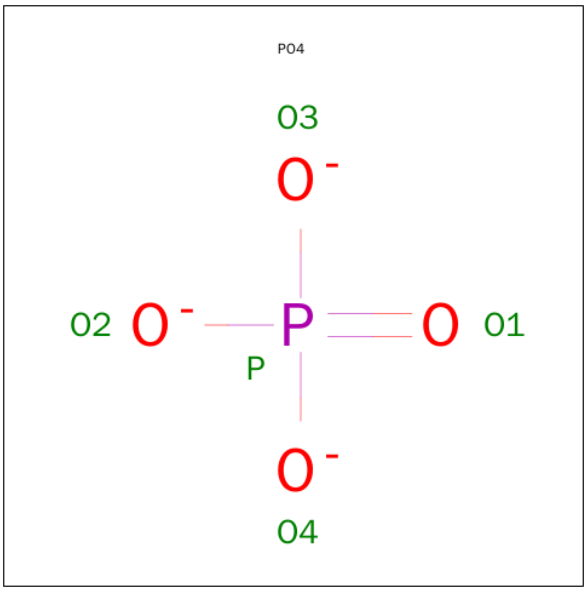
- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			3336	2178	550	602	6			

There is a discrepancy between the modelled and reference sequences:

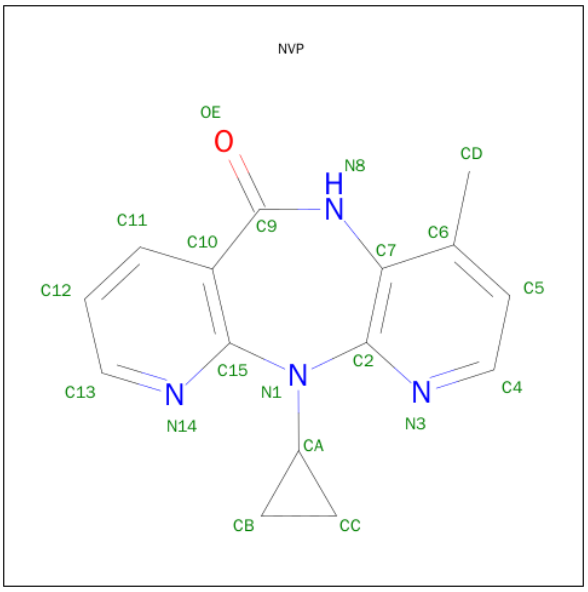
Chain	Residue	Modelled	Actual	Comment	Reference
B	184	VAL	MET	ENGINEERED	UNP P04585

- 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
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.

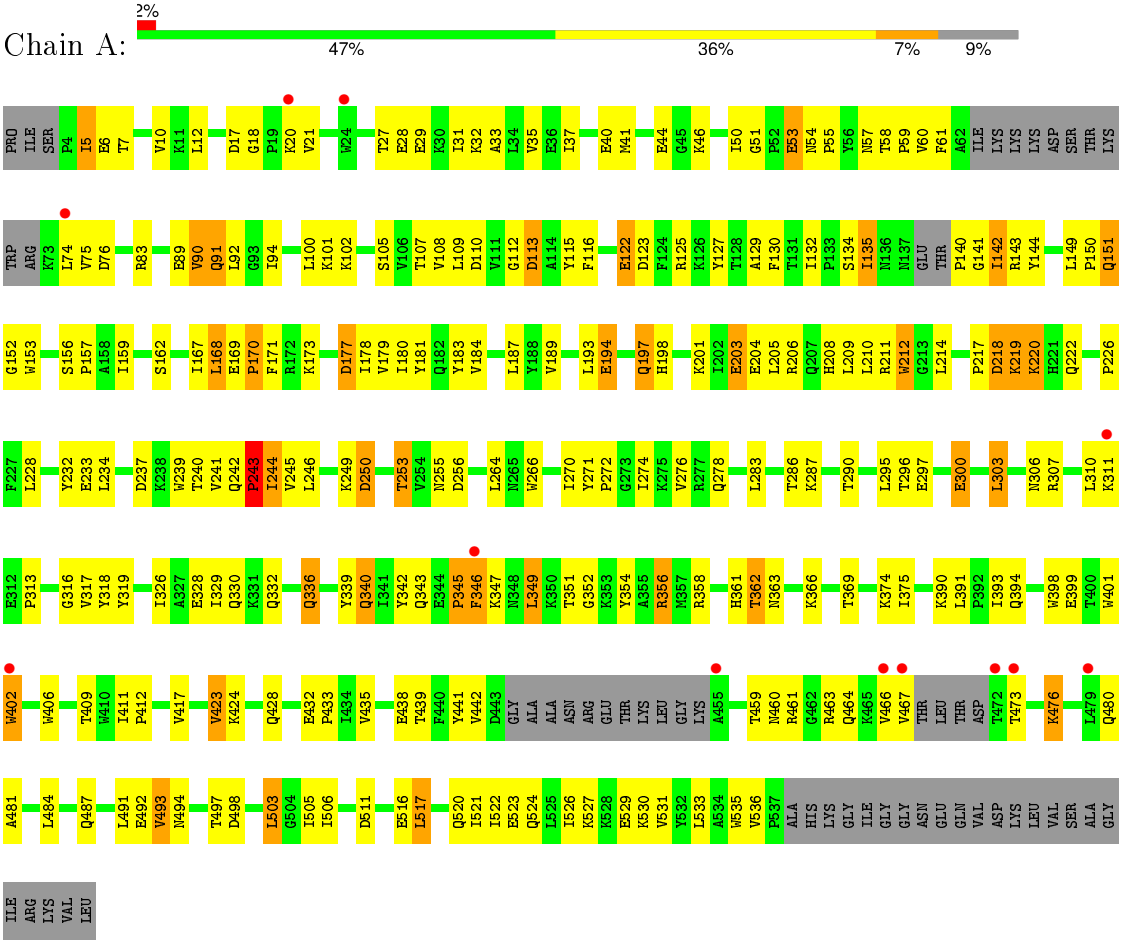
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	9	Total O 9 9	0	0
5	B	9	Total O 9 9	0	0

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.

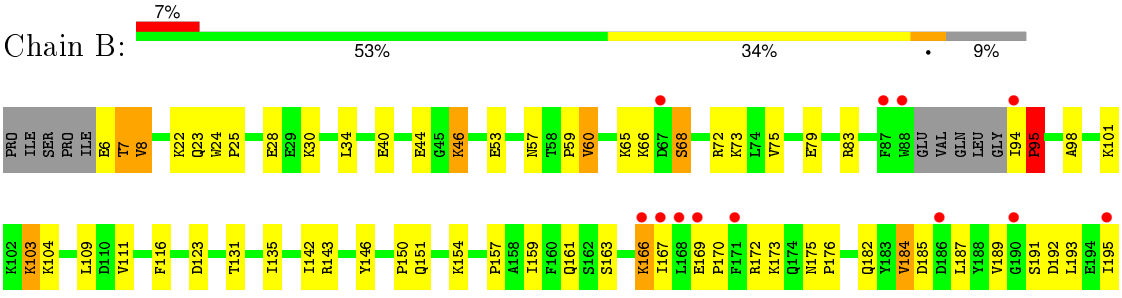
- Molecule 1: HIV-1 REVERSE TRANSCRIPTASE

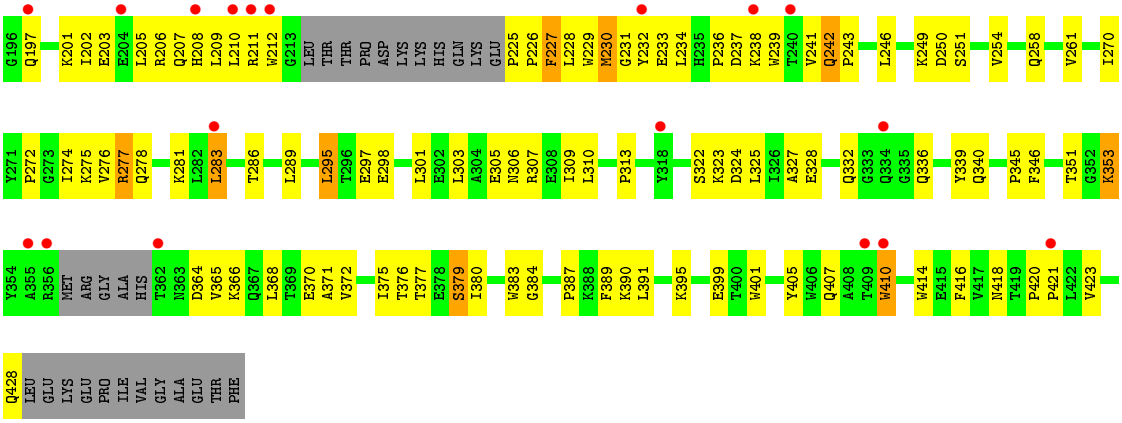
Chain A:



- Molecule 2: HIV-1 REVERSE TRANSCRIPTASE

Chain B:




G196 Q197 K201 I202 E203 E204 L205 R206 Q207 H208 L209 L210 R211 W212 G213 LEU THR THR PRO ASP LYS LYS HIS GLN LYS GLU P225 P226 F227 L228 W229 M230 G231 Y232 E233 L234 H235 P236 D237 K238 W239 T240 V241 Q242 P243 L246 K249 D250 S251 V254 Q258 V261 I270
Y271 P272 G273 I274 K275 V276 R277 Q278 K281 L282 L283 T286 L289 L295 T296 E297 E298 L301 E302 L303 A304 E305 N306 R307 E308 I309 L310 P313 Y318 S322 K323 D324 L325 I326 A327 E328 Q332 G333 Q334 G335 Q336 Y339 Q340 P345 F346 T351 G352 K353
Y354 A355 R356 MET ARG GLY ALA HIS T362 N363 D364 V365 K366 Q367 L368 T369 E370 A371 V372 I375 T376 T377 E378 S379 I380 W383 G384 P387 K388 F389 K390 L391 K395 E399 T400 W401 Y405 W406 Q407 A408 T409 W410 W414 E415 F416 V417 N418 T419 P420 P421 L422 V423
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	140.00Å 115.20Å 65.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 2.62 29.80 – 2.62	Depositor EDS
% Data completeness (in resolution range)	87.2 (29.80-2.62) 87.6 (29.80-2.62)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.215 , 0.279 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	61.5	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 74.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 28462 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7542	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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	0.56	0/4259	0.74	0/5788
2	B	0.53	0/3433	0.76	3/4665 (0.1%)
All	All	0.55	0/7692	0.75	3/10453 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	7	THR	N-CA-C	6.06	127.37	111.00
2	B	232	TYR	N-CA-C	6.05	127.34	111.00
2	B	68	SER	N-CA-C	-5.67	95.69	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	4158	0	4185	207	0
2	B	3336	0	3360	166	0
3	A	10	0	0	3	0
4	A	20	0	14	1	0
5	A	9	0	0	1	0
5	B	9	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7542	0	7559	370	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 25.

All (370) 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:142:ILE:HD13	1:A:142:ILE:H	1.18	1.05
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.35	1.04
2:B:207:GLN:HB3	2:B:211:ARG:HD2	1.42	1.02
1:A:28:GLU:OE1	1:A:135:ILE:HG22	1.62	0.99
2:B:30:LYS:HE3	5:B:1016:HOH:O	1.65	0.96
2:B:184:VAL:HG12	2:B:185:ASP:H	1.32	0.95
2:B:66:LYS:HD2	2:B:407:GLN:HE22	1.32	0.94
2:B:195:ILE:HD11	2:B:233:GLU:OE1	1.69	0.93
1:A:206:ARG:NH1	1:A:218:ASP:HA	1.86	0.91
2:B:166:LYS:HA	2:B:166:LYS:HE3	1.53	0.90
1:A:362:THR:HG22	1:A:366:LYS:HD3	1.53	0.90
1:A:132:ILE:HB	1:A:142:ILE:HG12	1.54	0.88
2:B:295:LEU:HD12	2:B:295:LEU:H	1.39	0.88
2:B:207:GLN:HB3	2:B:211:ARG:CD	2.04	0.87
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.56	0.87
2:B:66:LYS:HG2	2:B:230:MET:HG2	1.57	0.85
2:B:277:ARG:HG2	2:B:278:GLN:N	1.91	0.85
2:B:173:LYS:HA	2:B:176:PRO:HG3	1.60	0.83
1:A:142:ILE:HD13	1:A:142:ILE:N	1.94	0.83
2:B:295:LEU:HD12	2:B:295:LEU:N	1.92	0.82
1:A:206:ARG:HH12	1:A:218:ASP:HA	1.42	0.81
1:A:28:GLU:O	1:A:32:LYS:HG3	1.81	0.81
2:B:184:VAL:HG12	2:B:185:ASP:N	1.95	0.80
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.62	0.80
2:B:306:ASN:HA	2:B:309:ILE:HD12	1.63	0.80
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.18	0.79
2:B:40:GLU:O	2:B:44:GLU:HG3	1.81	0.79
1:A:194:GLU:HG3	1:A:197:GLN:HB2	1.66	0.78
2:B:295:LEU:H	2:B:295:LEU:CD1	1.95	0.78
2:B:72:ARG:HH11	2:B:72:ARG:HG3	1.48	0.77
1:A:438:GLU:HB2	1:A:461:ARG:NH1	1.99	0.76
1:A:220:LYS:NZ	1:A:220:LYS:HB2	2.00	0.76
1:A:27:THR:HG22	1:A:29:GLU:H	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:HG22	1:A:256:ASP:H	1.51	0.75
2:B:420:PRO:O	2:B:423:VAL:HG12	1.85	0.75
1:A:476:LYS:HD2	1:A:476:LYS:O	1.87	0.74
2:B:151:GLN:HB3	2:B:185:ASP:OD1	1.87	0.73
2:B:169:GLU:N	2:B:170:PRO:HD2	2.03	0.73
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.87	0.71
2:B:175:ASN:N	2:B:176:PRO:HD3	2.06	0.70
1:A:228:LEU:HD22	1:A:242:GLN:HB3	1.73	0.70
2:B:207:GLN:O	2:B:211:ARG:N	2.22	0.69
2:B:275:LYS:HZ3	2:B:277:ARG:NH1	1.90	0.69
1:A:503:LEU:CD1	1:A:535:TRP:HB2	2.18	0.69
1:A:92:LEU:HD12	1:A:92:LEU:H	1.56	0.69
2:B:275:LYS:NZ	2:B:277:ARG:NH1	2.41	0.69
1:A:244:ILE:HD13	1:A:244:ILE:C	2.13	0.69
1:A:91:GLN:HG3	1:A:91:GLN:O	1.91	0.69
2:B:332:GLN:HB3	2:B:428:GLN:HE22	1.57	0.69
2:B:66:LYS:HD2	2:B:407:GLN:NE2	2.08	0.68
1:A:100:LEU:O	1:A:318:TYR:HB3	1.94	0.68
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.76	0.68
1:A:208:HIS:O	1:A:212:TRP:HE3	1.77	0.68
1:A:249:LYS:NZ	1:A:256:ASP:CG	2.48	0.68
2:B:395:LYS:HD2	2:B:416:PHE:CE1	2.28	0.67
1:A:244:ILE:HD13	1:A:244:ILE:O	1.94	0.67
1:A:503:LEU:HD13	1:A:535:TRP:CB	2.20	0.67
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.76	0.67
2:B:227:PHE:CD2	2:B:231:GLY:HA2	2.30	0.67
2:B:195:ILE:HD11	2:B:233:GLU:CD	2.16	0.67
2:B:172:ARG:O	2:B:176:PRO:HG3	1.94	0.67
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.31	0.66
2:B:203:GLU:HG3	2:B:207:GLN:HE22	1.61	0.65
1:A:264:LEU:HD13	1:A:276:VAL:HG12	1.78	0.65
1:A:409:THR:O	2:B:364:ASP:HB2	1.97	0.65
2:B:154:LYS:O	2:B:157:PRO:HD2	1.97	0.64
2:B:207:GLN:CB	2:B:211:ARG:HD2	2.24	0.64
2:B:65:LYS:HB2	2:B:68:SER:HB3	1.79	0.64
1:A:461:ARG:NH1	3:A:1300:PO4:O4	2.31	0.64
1:A:253:THR:HG23	1:A:255:ASN:H	1.63	0.63
1:A:150:PRO:HG2	1:A:153:TRP:HB2	1.79	0.63
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.80	0.63
1:A:142:ILE:H	1:A:142:ILE:CD1	1.84	0.63
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:GLN:HA	1:A:524:GLN:OE1	1.99	0.63
1:A:239:TRP:NE1	1:A:316:GLY:HA3	2.14	0.62
1:A:220:LYS:HZ3	1:A:220:LYS:HB2	1.65	0.62
2:B:163:SER:O	2:B:167:ILE:HG22	1.99	0.62
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.82	0.62
2:B:229:TRP:CE3	2:B:229:TRP:HA	2.33	0.62
1:A:210:LEU:C	1:A:212:TRP:H	2.01	0.62
1:A:58:THR:HG23	1:A:76:ASP:O	2.00	0.61
1:A:134:SER:HB2	1:A:140:PRO:O	2.00	0.61
1:A:362:THR:HG22	1:A:366:LYS:CD	2.28	0.61
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.30	0.61
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.83	0.61
1:A:193:LEU:HB3	1:A:197:GLN:HB3	1.82	0.61
1:A:369:THR:OG1	1:A:398:TRP:CZ3	2.55	0.60
1:A:463:ARG:HG2	1:A:464:GLN:N	2.16	0.59
1:A:228:LEU:HD23	1:A:233:GLU:HA	1.85	0.59
1:A:102:LYS:HG3	1:A:237:ASP:HA	1.85	0.59
1:A:112:GLY:O	1:A:113:ASP:HB2	2.01	0.59
2:B:184:VAL:CG1	2:B:185:ASP:H	2.09	0.58
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.38	0.58
2:B:332:GLN:HB2	2:B:336:GLN:O	2.03	0.58
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.83	0.58
1:A:306:ASN:O	1:A:310:LEU:HG	2.03	0.58
2:B:175:ASN:ND2	2:B:201:LYS:HD3	2.19	0.58
1:A:197:GLN:HE21	1:A:197:GLN:CA	2.17	0.57
2:B:116:PHE:CE1	2:B:151:GLN:HG3	2.40	0.57
2:B:94:ILE:N	2:B:95:PRO:CD	2.67	0.57
2:B:169:GLU:N	2:B:170:PRO:CD	2.68	0.57
2:B:227:PHE:HD2	2:B:231:GLY:HA2	1.68	0.57
2:B:275:LYS:HE2	2:B:277:ARG:HH11	1.69	0.56
1:A:249:LYS:HZ3	1:A:256:ASP:CG	2.08	0.56
1:A:393:ILE:HD12	1:A:423:VAL:CG2	2.35	0.56
2:B:379:SER:OG	2:B:387:PRO:HG3	2.04	0.56
2:B:297:GLU:O	2:B:301:LEU:HG	2.06	0.56
1:A:523:GLU:O	1:A:527:LYS:HG2	2.05	0.56
1:A:497:THR:O	1:A:535:TRP:HA	2.06	0.56
2:B:254:VAL:O	2:B:258:GLN:HG3	2.05	0.56
2:B:270:ILE:O	2:B:272:PRO:HD3	2.05	0.56
1:A:283:LEU:O	1:A:286:THR:HG23	2.06	0.56
1:A:363:ASN:ND2	1:A:401:TRP:CZ3	2.72	0.56
1:A:493:VAL:HG23	1:A:531:VAL:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:ARG:HG2	2:B:278:GLN:H	1.68	0.56
1:A:33:ALA:O	1:A:37:ILE:HG13	2.06	0.56
1:A:167:ILE:O	1:A:170:PRO:HD2	2.05	0.55
2:B:366:LYS:O	2:B:370:GLU:HG3	2.06	0.55
2:B:295:LEU:CD1	2:B:295:LEU:N	2.59	0.55
1:A:250:ASP:N	1:A:250:ASP:OD2	2.38	0.55
2:B:173:LYS:C	2:B:176:PRO:HD3	2.27	0.54
1:A:369:THR:OG1	1:A:398:TRP:HZ3	1.89	0.54
2:B:72:ARG:HH11	2:B:72:ARG:CG	2.20	0.54
2:B:8:VAL:HG11	2:B:159:ILE:HG23	1.88	0.54
2:B:323:LYS:HE3	5:B:1018:HOH:O	2.05	0.54
1:A:264:LEU:HD22	1:A:274:ILE:HG23	1.90	0.54
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.88	0.54
2:B:328:GLU:HG2	2:B:390:LYS:HD2	1.88	0.54
2:B:66:LYS:HG2	2:B:230:MET:CG	2.33	0.54
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.72	0.54
1:A:522:ILE:O	1:A:526:ILE:HG13	2.08	0.54
1:A:460:ASN:ND2	3:A:1301:PO4:O4	2.30	0.54
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.89	0.54
1:A:35:VAL:HG22	1:A:132:ILE:HG21	1.88	0.53
1:A:399:GLU:HG3	1:A:402:TRP:CZ3	2.43	0.53
2:B:372:VAL:HA	2:B:389:PHE:CE2	2.44	0.53
2:B:173:LYS:HA	2:B:176:PRO:CG	2.35	0.53
1:A:94:ILE:HG13	1:A:94:ILE:O	2.08	0.53
1:A:505:ILE:HG22	1:A:506:ILE:N	2.22	0.53
1:A:197:GLN:NE2	1:A:197:GLN:CA	2.71	0.53
1:A:122:GLU:HG3	1:A:123:ASP:N	2.23	0.53
2:B:169:GLU:HG2	2:B:170:PRO:HD3	1.90	0.53
1:A:398:TRP:CH2	1:A:411:ILE:HD12	2.44	0.53
1:A:358:ARG:O	1:A:366:LYS:NZ	2.41	0.53
1:A:177:ASP:OD1	1:A:177:ASP:N	2.38	0.53
2:B:53:GLU:OE1	2:B:53:GLU:N	2.40	0.53
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.39	0.53
2:B:332:GLN:HB3	2:B:428:GLN:NE2	2.24	0.53
1:A:233:GLU:HB3	1:A:240:THR:HG23	1.90	0.52
2:B:241:VAL:HG11	2:B:313:PRO:HG3	1.91	0.52
2:B:28:GLU:HA	2:B:135:ILE:HD11	1.91	0.52
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.45	0.52
1:A:129:ALA:HA	1:A:144:TYR:O	2.09	0.52
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.91	0.52
2:B:201:LYS:HA	2:B:201:LYS:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LYS:O	1:A:313:PRO:HD3	2.09	0.52
2:B:242:GLN:OE1	2:B:353:LYS:HE2	2.10	0.52
2:B:207:GLN:O	2:B:211:ARG:HB2	2.09	0.52
2:B:184:VAL:CG1	2:B:185:ASP:N	2.67	0.52
1:A:170:PRO:O	1:A:173:LYS:N	2.43	0.52
1:A:461:ARG:NH2	3:A:1301:PO4:O1	2.43	0.52
2:B:94:ILE:O	2:B:95:PRO:O	2.28	0.52
1:A:209:LEU:O	1:A:214:LEU:HB2	2.10	0.52
1:A:498:ASP:HA	1:A:536:VAL:O	2.09	0.52
1:A:74:LEU:HD23	1:A:75:VAL:N	2.25	0.52
1:A:332:GLN:HB3	1:A:336:GLN:HB3	1.92	0.52
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.92	0.52
1:A:31:ILE:O	1:A:35:VAL:HG23	2.09	0.51
2:B:305:GLU:O	2:B:309:ILE:HG13	2.10	0.51
1:A:53:GLU:O	1:A:55:PRO:HD3	2.09	0.51
1:A:197:GLN:NE2	1:A:197:GLN:HA	2.25	0.51
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.92	0.51
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.90	0.51
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.55	0.51
1:A:58:THR:CG2	1:A:76:ASP:O	2.58	0.51
2:B:109:LEU:HA	2:B:227:PHE:HA	1.93	0.51
1:A:17:ASP:O	1:A:83:ARG:HD3	2.10	0.51
2:B:173:LYS:O	2:B:176:PRO:HD3	2.11	0.51
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.46	0.51
1:A:109:LEU:HD22	1:A:205:LEU:HD23	1.93	0.51
2:B:372:VAL:HA	2:B:389:PHE:HE2	1.75	0.51
2:B:208:HIS:O	2:B:212:TRP:HB2	2.11	0.50
2:B:278:GLN:CD	2:B:298:GLU:HB3	2.32	0.50
2:B:104:LYS:HG3	2:B:192:ASP:OD2	2.11	0.50
2:B:366:LYS:HA	2:B:405:TYR:CD1	2.46	0.50
1:A:398:TRP:CZ3	1:A:411:ILE:HD12	2.46	0.50
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.91	0.50
1:A:151:GLN:NE2	1:A:152:GLY:N	2.60	0.50
1:A:210:LEU:C	1:A:212:TRP:N	2.64	0.50
2:B:66:LYS:HE3	2:B:230:MET:HG2	1.94	0.50
2:B:241:VAL:O	2:B:243:PRO:HD3	2.11	0.50
1:A:391:LEU:C	1:A:417:VAL:HG12	2.32	0.50
2:B:79:GLU:HA	2:B:79:GLU:OE1	2.12	0.50
1:A:249:LYS:NZ	1:A:256:ASP:OD1	2.45	0.49
1:A:107:THR:HG22	1:A:109:LEU:CD1	2.43	0.49
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LEU:O	1:A:529:GLU:HB2	2.12	0.49
2:B:28:GLU:CA	2:B:135:ILE:HD11	2.42	0.49
1:A:467:VAL:CG2	1:A:484:LEU:HD11	2.42	0.49
1:A:361:HIS:O	1:A:362:THR:HG23	2.13	0.49
2:B:94:ILE:O	2:B:95:PRO:C	2.51	0.49
2:B:234:LEU:HD21	2:B:377:THR:CG2	2.43	0.49
1:A:362:THR:CG2	1:A:366:LYS:HZ3	2.25	0.49
2:B:281:LYS:C	2:B:283:LEU:H	2.16	0.49
2:B:380:ILE:O	2:B:384:GLY:HA2	2.12	0.49
2:B:205:LEU:O	2:B:205:LEU:HD23	2.13	0.49
1:A:40:GLU:O	1:A:44:GLU:HG3	2.13	0.49
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.48	0.49
1:A:244:ILE:HD12	1:A:310:LEU:HD13	1.93	0.49
2:B:322:SER:O	2:B:323:LYS:HD2	2.12	0.49
1:A:203:GLU:OE2	1:A:206:ARG:NH1	2.45	0.49
1:A:246:LEU:HD12	1:A:307:ARG:HA	1.95	0.49
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.13	0.49
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.47	0.49
1:A:343:GLN:HG3	1:A:349:LEU:CD1	2.43	0.48
2:B:207:GLN:O	2:B:211:ARG:CB	2.61	0.48
2:B:340:GLN:HG3	2:B:351:THR:HG22	1.95	0.48
2:B:175:ASN:N	2:B:176:PRO:CD	2.77	0.48
1:A:481:ALA:O	1:A:484:LEU:HB2	2.13	0.48
2:B:203:GLU:O	2:B:207:GLN:NE2	2.47	0.48
1:A:241:VAL:HB	1:A:266:TRP:HE1	1.78	0.48
2:B:46:LYS:HE2	2:B:116:PHE:CD2	2.48	0.48
1:A:232:TYR:HA	1:A:241:VAL:HA	1.95	0.48
2:B:229:TRP:HE3	2:B:229:TRP:HA	1.78	0.47
1:A:346:PHE:N	1:A:346:PHE:CD1	2.82	0.47
2:B:246:LEU:HB2	2:B:307:ARG:NH1	2.28	0.47
2:B:66:LYS:HD3	2:B:407:GLN:OE1	2.14	0.47
1:A:115:TYR:HB3	1:A:149:LEU:O	2.13	0.47
1:A:244:ILE:CD1	1:A:244:ILE:C	2.79	0.47
1:A:516:GLU:O	1:A:520:GLN:HG3	2.14	0.47
2:B:275:LYS:CE	2:B:277:ARG:HH11	2.25	0.47
1:A:208:HIS:O	1:A:212:TRP:CE3	2.62	0.47
2:B:57:ASN:ND2	2:B:143:ARG:NH1	2.57	0.47
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.49	0.47
1:A:201:LYS:O	1:A:204:GLU:HB2	2.15	0.47
1:A:246:LEU:HD13	1:A:303:LEU:CD2	2.45	0.47
1:A:219:LYS:HE2	1:A:219:LYS:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.70	0.47
1:A:60:VAL:O	1:A:61:PHE:CD2	2.68	0.46
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.50	0.46
2:B:339:TYR:CD1	2:B:375:ILE:HD11	2.50	0.46
1:A:5:ILE:HD12	1:A:6:GLU:N	2.30	0.46
1:A:278:GLN:HA	1:A:278:GLN:NE2	2.31	0.46
1:A:319:TYR:HA	1:A:349:LEU:HD21	1.98	0.46
2:B:228:LEU:HD23	2:B:228:LEU:HA	1.80	0.46
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.98	0.46
1:A:296:THR:HG23	5:A:1009:HOH:O	2.15	0.46
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.50	0.46
1:A:27:THR:HG22	1:A:29:GLU:N	2.25	0.46
2:B:34:LEU:CD2	2:B:73:LYS:HG3	2.46	0.46
2:B:189:VAL:HG11	2:B:202:ILE:HD13	1.97	0.46
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.49	0.46
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.81	0.46
1:A:467:VAL:HG21	1:A:484:LEU:HD11	1.96	0.46
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.46	0.45
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.31	0.45
2:B:345:PRO:O	2:B:346:PHE:HB2	2.15	0.45
2:B:277:ARG:O	2:B:281:LYS:HG3	2.16	0.45
1:A:105:SER:HB2	1:A:198:HIS:CG	2.51	0.45
1:A:270:ILE:O	1:A:272:PRO:HD3	2.16	0.45
1:A:362:THR:HG21	1:A:366:LYS:HZ3	1.81	0.45
1:A:466:VAL:HG12	1:A:466:VAL:O	2.16	0.45
2:B:98:ALA:O	2:B:101:LYS:HE3	2.15	0.45
2:B:249:LYS:HD3	2:B:251:SER:O	2.16	0.45
1:A:218:ASP:O	1:A:222:GLN:HG3	2.16	0.45
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.52	0.45
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.51	0.45
1:A:362:THR:CG2	1:A:366:LYS:NZ	2.80	0.45
2:B:230:MET:HE2	2:B:230:MET:HA	1.98	0.45
2:B:327:ALA:O	2:B:389:PHE:HA	2.17	0.45
2:B:208:HIS:ND1	2:B:208:HIS:O	2.50	0.45
2:B:336:GLN:HE21	2:B:336:GLN:HB2	1.54	0.45
2:B:72:ARG:NH1	2:B:72:ARG:HG3	2.22	0.45
1:A:210:LEU:O	1:A:212:TRP:N	2.50	0.45
2:B:46:LYS:CE	2:B:116:PHE:HB3	2.47	0.44
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.43	0.44
2:B:175:ASN:H	2:B:176:PRO:HD3	1.82	0.44
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:TRP:CG	2:B:25:PRO:HD2	2.53	0.44
2:B:275:LYS:CE	2:B:277:ARG:NH1	2.79	0.44
1:A:363:ASN:HA	1:A:511:ASP:CG	2.37	0.44
1:A:149:LEU:HD21	1:A:159:ILE:HG21	2.00	0.44
1:A:296:THR:HG22	1:A:297:GLU:N	2.33	0.44
1:A:340:GLN:HA	1:A:351:THR:HA	1.99	0.44
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.87	0.44
1:A:228:LEU:HA	1:A:232:TYR:O	2.17	0.44
1:A:398:TRP:CH2	1:A:411:ILE:CD1	3.00	0.44
1:A:354:TYR:CZ	1:A:356:ARG:HB3	2.52	0.44
1:A:328:GLU:O	1:A:339:TYR:HA	2.17	0.44
2:B:368:LEU:O	2:B:371:ALA:HB3	2.17	0.44
2:B:109:LEU:N	2:B:109:LEU:HD12	2.32	0.44
2:B:207:GLN:HB3	2:B:211:ARG:NE	2.31	0.44
2:B:72:ARG:NH1	2:B:72:ARG:CG	2.78	0.44
1:A:363:ASN:HB2	1:A:511:ASP:OD2	2.17	0.43
1:A:492:GLU:HA	1:A:530:LYS:O	2.17	0.43
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.53	0.43
2:B:173:LYS:CA	2:B:176:PRO:HG3	2.40	0.43
1:A:339:TYR:CD1	1:A:339:TYR:C	2.91	0.43
1:A:517:LEU:HA	1:A:517:LEU:HD23	1.83	0.43
1:A:54:ASN:HA	1:A:55:PRO:HD2	1.94	0.43
1:A:46:LYS:NZ	1:A:116:PHE:HB3	2.33	0.43
1:A:108:VAL:HG13	1:A:108:VAL:O	2.18	0.43
1:A:226:PRO:HA	1:A:234:LEU:O	2.18	0.43
1:A:170:PRO:O	1:A:171:PHE:C	2.57	0.43
2:B:372:VAL:HG13	2:B:389:PHE:CZ	2.54	0.43
2:B:276:VAL:HG12	2:B:276:VAL:O	2.17	0.43
1:A:28:GLU:CD	1:A:135:ILE:HG22	2.33	0.43
1:A:527:LYS:HD2	1:A:527:LYS:HA	1.76	0.43
1:A:438:GLU:CG	1:A:461:ARG:HD2	2.49	0.43
1:A:326:ILE:HB	1:A:342:TYR:CE1	2.53	0.43
1:A:417:VAL:O	1:A:417:VAL:HG13	2.19	0.43
2:B:34:LEU:HD21	2:B:73:LYS:HG3	2.00	0.43
1:A:110:ASP:O	1:A:217:PRO:HD3	2.19	0.43
1:A:432:GLU:HB2	1:A:433:PRO:HD2	2.00	0.43
1:A:50:ILE:HD12	1:A:54:ASN:CB	2.49	0.42
1:A:271:TYR:OH	1:A:313:PRO:HA	2.19	0.42
1:A:244:ILE:HD11	1:A:246:LEU:HD23	2.00	0.42
2:B:275:LYS:HE2	2:B:275:LYS:HB3	1.86	0.42
2:B:206:ARG:HD2	2:B:225:PRO:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:O	1:A:91:GLN:C	2.57	0.42
1:A:51:GLY:C	1:A:53:GLU:H	2.23	0.42
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.84	0.42
2:B:237:ASP:OD2	2:B:238:LYS:HG3	2.18	0.42
1:A:115:TYR:N	1:A:115:TYR:CD2	2.87	0.42
1:A:54:ASN:OD1	1:A:54:ASN:C	2.58	0.42
2:B:205:LEU:CD2	2:B:209:LEU:HG	2.50	0.42
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.02	0.42
2:B:270:ILE:O	2:B:272:PRO:CD	2.68	0.42
1:A:197:GLN:C	1:A:197:GLN:HE21	2.23	0.42
2:B:142:ILE:HD12	2:B:142:ILE:H	1.85	0.42
2:B:79:GLU:O	2:B:83:ARG:HG3	2.19	0.41
2:B:376:THR:HB	2:B:410:TRP:CH2	2.54	0.41
2:B:103:LYS:HG2	2:B:191:SER:N	2.35	0.41
1:A:132:ILE:O	1:A:141:GLY:CA	2.69	0.41
1:A:132:ILE:O	1:A:141:GLY:HA3	2.20	0.41
1:A:438:GLU:OE1	1:A:459:THR:CB	2.68	0.41
2:B:242:GLN:CD	2:B:353:LYS:HG2	2.41	0.41
2:B:324:ASP:N	5:B:1018:HOH:O	2.50	0.41
2:B:211:ARG:O	2:B:212:TRP:CD1	2.73	0.41
1:A:402:TRP:C	1:A:402:TRP:CD1	2.94	0.41
2:B:189:VAL:HG11	2:B:202:ILE:CD1	2.51	0.41
1:A:345:PRO:C	1:A:347:LYS:H	2.24	0.41
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.94	0.41
1:A:57:ASN:OD1	1:A:130:PHE:HA	2.20	0.41
1:A:245:VAL:O	1:A:245:VAL:HG13	2.20	0.41
1:A:101:LYS:O	4:A:999:NVP:H13	2.21	0.41
2:B:66:LYS:HE3	2:B:230:MET:CG	2.51	0.41
2:B:389:PHE:HB3	2:B:391:LEU:HD21	2.03	0.41
2:B:275:LYS:NZ	2:B:277:ARG:CZ	2.82	0.41
2:B:103:LYS:O	2:B:236:PRO:HG2	2.21	0.41
1:A:283:LEU:C	1:A:286:THR:HG23	2.41	0.41
1:A:54:ASN:O	1:A:143:ARG:NH2	2.54	0.41
2:B:234:LEU:HD21	2:B:377:THR:HG21	2.02	0.41
2:B:24:TRP:CE2	2:B:399:GLU:HB3	2.56	0.41
1:A:58:THR:HA	1:A:59:PRO:HD3	1.87	0.41
2:B:193:LEU:HB3	2:B:197:GLN:HB2	2.03	0.41
1:A:220:LYS:HZ2	1:A:220:LYS:HB2	1.80	0.40
1:A:168:LEU:O	1:A:169:GLU:C	2.59	0.40
1:A:18:GLY:HA3	1:A:127:TYR:CD1	2.55	0.40
1:A:242:GLN:HA	1:A:243:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:HD2	1:A:237:ASP:HB2	2.02	0.40
1:A:37:ILE:O	1:A:41:MET:HG3	2.21	0.40
1:A:178:ILE:HG22	1:A:179:VAL:N	2.36	0.40
1:A:10:VAL:HG11	1:A:153:TRP:CH2	2.57	0.40
1:A:295:LEU:HD12	1:A:300:GLU:HG3	2.04	0.40
1:A:521:ILE:O	1:A:524:GLN:HB2	2.21	0.40
1:A:122:GLU:HA	1:A:125:ARG:HD2	2.03	0.40
1:A:439:THR:O	1:A:459:THR:HA	2.21	0.40
1:A:239:TRP:CD1	1:A:316:GLY:C	2.95	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	496/560 (89%)	451 (91%)	37 (8%)	8 (2%)	12	23
2	B	394/440 (90%)	348 (88%)	44 (11%)	2 (0%)	34	58
All	All	890/1000 (89%)	799 (90%)	81 (9%)	10 (1%)	17	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	PRO
2	B	95	PRO
1	A	91	GLN
1	A	184	VAL
1	A	211	ARG
1	A	170	PRO
2	B	184	VAL
1	A	346	PHE
1	A	243	PRO

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Mol	Chain	Res	Type
1	A	345	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	456/499 (91%)	405 (89%)	51 (11%)	7 12
2	B	367/400 (92%)	342 (93%)	25 (7%)	20 38
All	All	823/899 (92%)	747 (91%)	76 (9%)	11 21

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	7	THR
1	A	20	LYS
1	A	21	VAL
1	A	53	GLU
1	A	89	GLU
1	A	90	VAL
1	A	113	ASP
1	A	122	GLU
1	A	135	ILE
1	A	142	ILE
1	A	151	GLN
1	A	162	SER
1	A	168	LEU
1	A	177	ASP
1	A	194	GLU
1	A	197	GLN
1	A	203	GLU
1	A	212	TRP
1	A	218	ASP
1	A	219	LYS
1	A	220	LYS

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Mol	Chain	Res	Type
1	A	243	PRO
1	A	244	ILE
1	A	250	ASP
1	A	253	THR
1	A	287	LYS
1	A	290	THR
1	A	300	GLU
1	A	303	LEU
1	A	317	VAL
1	A	336	GLN
1	A	340	GLN
1	A	349	LEU
1	A	356	ARG
1	A	362	THR
1	A	374	LYS
1	A	394	GLN
1	A	402	TRP
1	A	423	VAL
1	A	424	LYS
1	A	428	GLN
1	A	435	VAL
1	A	473	THR
1	A	476	LYS
1	A	480	GLN
1	A	487	GLN
1	A	493	VAL
1	A	503	LEU
1	A	517	LEU
1	A	533	LEU
2	B	6	GLU
2	B	7	THR
2	B	8	VAL
2	B	22	LYS
2	B	46	LYS
2	B	60	VAL
2	B	95	PRO
2	B	103	LYS
2	B	123	ASP
2	B	166	LYS
2	B	210	LEU
2	B	226	PRO
2	B	227	PHE

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Mol	Chain	Res	Type
2	B	230	MET
2	B	242	GLN
2	B	250	ASP
2	B	277	ARG
2	B	283	LEU
2	B	286	THR
2	B	295	LEU
2	B	303	LEU
2	B	353	LYS
2	B	379	SER
2	B	410	TRP
2	B	414	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	182	GLN
1	A	197	GLN
1	A	207	GLN
1	A	222	GLN
1	A	278	GLN
1	A	407	GLN
1	A	475	GLN
1	A	487	GLN
1	A	507	GLN
1	A	509	GLN
1	A	512	GLN
1	A	520	GLN
2	B	57	ASN
2	B	137	ASN
2	B	147	ASN
2	B	161	GLN
2	B	182	GLN
2	B	207	GLN
2	B	269	GLN
2	B	278	GLN
2	B	332	GLN
2	B	336	GLN
2	B	428	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	0.91	0	3,8,10	4.81	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	8.15	118.98	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)

3 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	1300	-	4,4,4	1.15	0	6,6,6	0.27	0
3	PO4	A	1301	-	4,4,4	1.17	0	6,6,6	0.28	0
4	NVP	A	999	-	18,23,23	1.12	1 (5%)	18,34,34	1.08	1 (5%)

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	1300	-	-	0/0/0/0	0/0/0/0
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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	NVP	C5-C4	2.15	1.43	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	999	NVP	CB-CA-N1	-2.24	115.94	118.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1300	PO4	1	0
3	A	1301	PO4	2	0
4	A	999	NVP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	506/560 (90%)	-0.20	12 (2%)	62	56	31, 71, 110, 137	0
2	B	402/440 (91%)	0.21	30 (7%)	17	12	35, 77, 128, 148	0
All	All	908/1000 (90%)	-0.02	42 (4%)	36	29	31, 74, 119, 148	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	195	ILE	7.3
2	B	211	ARG	5.6
2	B	212	TRP	5.4
1	A	467	VAL	4.7
1	A	402	TRP	4.5
2	B	240	THR	4.4
2	B	67	ASP	4.3
2	B	190	GLY	4.2
2	B	334	GLN	4.1
2	B	88	TRP	4.1
2	B	210	LEU	4.0
2	B	167	ILE	4.0
2	B	94	ILE	3.9
2	B	410	TRP	3.4
1	A	472	THR	3.2
2	B	421	PRO	3.0
1	A	74	LEU	3.0
2	B	356	ARG	3.0
2	B	238	LYS	2.8
2	B	204	GLU	2.8
1	A	346	PHE	2.7
1	A	466	VAL	2.7
2	B	171	PHE	2.7
2	B	283	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	186	ASP	2.6
2	B	87	PHE	2.6
1	A	473	THR	2.6
2	B	166	LYS	2.5
1	A	24	TRP	2.5
1	A	455	ALA	2.5
2	B	197	GLN	2.4
2	B	232	TYR	2.4
2	B	362	THR	2.3
2	B	355	ALA	2.3
2	B	168	LEU	2.3
2	B	318	TYR	2.2
1	A	311	LYS	2.2
1	A	479	LEU	2.2
2	B	169	GLU	2.2
2	B	208	HIS	2.1
2	B	409	THR	2.1
1	A	20	LYS	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	0.96	0.12	-	52,68,100,103	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	1300	5/5	0.80	0.23	2.91	139,146,149,149	0
3	PO4	A	1301	5/5	0.89	0.15	0.81	134,141,147,149	0
4	NVP	A	999	20/20	0.98	0.16	0.42	30,50,56,62	0

6.5 Other polymers (i)

There are no such residues in this entry.