Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2014 – 10:10 AM GMT

PDB ID	:	3DM2
Title	:	Crystal structure of HIV-1 K103N mutant reverse transcriptase in complex with GW564511.
Authors	:	Ren, J.; Chamberlain, P.P.; Stammers, D.K.
Deposited on	:	2008-06-30
Resolution	:	3.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html

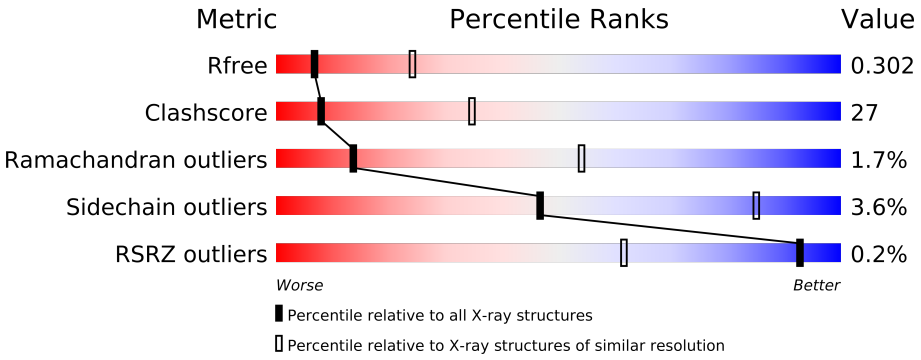
The following versions of software and data (see references) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.10 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}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	560	
2	B	440	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7702 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reverse transcriptase/ribonucleaseH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	532	4354	2820	723	803	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	LYS	ENGINEERED	UNP P04585

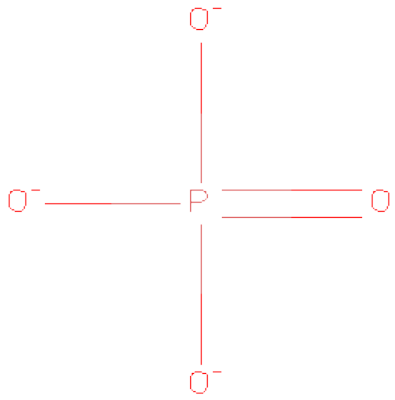
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	400	3302	2146	550	599	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

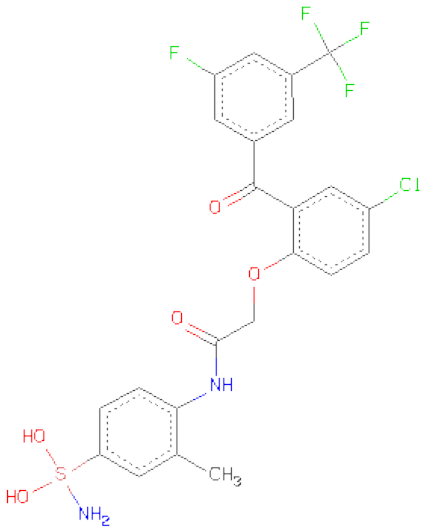
Chain	Residue	Modelled	Actual	Comment	Reference
B	103	ASN	LYS	ENGINEERED	UNP P04585

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



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

- Molecule 4 is N-{4-[AMINO(DIHYDROXY)-LAMBDA 4 -SULFANYL]-2-METHYLPHENYL}-2-(4-CHLORO-2-{[3-FLUORO-5-(TRIFLUOROMETHYL)PHENYL]CARBONYL}PHENOXY)ACETAMIDE (three-letter code: GWE) (formula: $C_{23}H_{19}ClF_4N_2O_5S$).



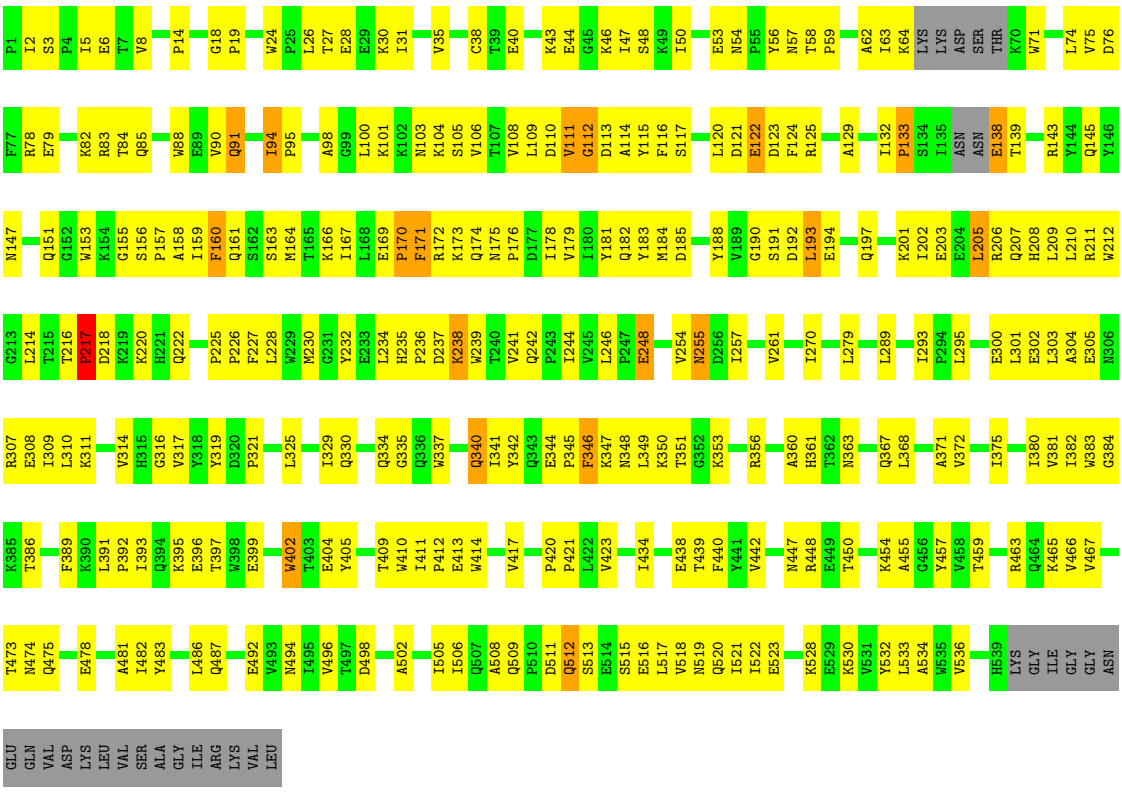
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Cl F N O S 36 23 1 4 2 5 1	0	0

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.

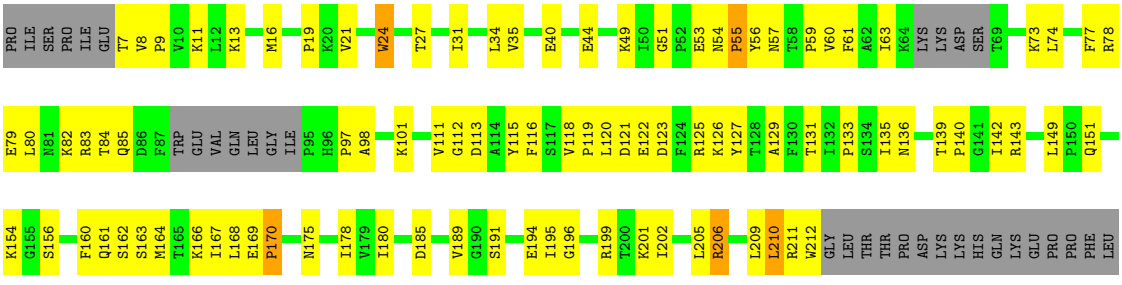
• Molecule 1: Reverse transcriptase/ribonucleaseH

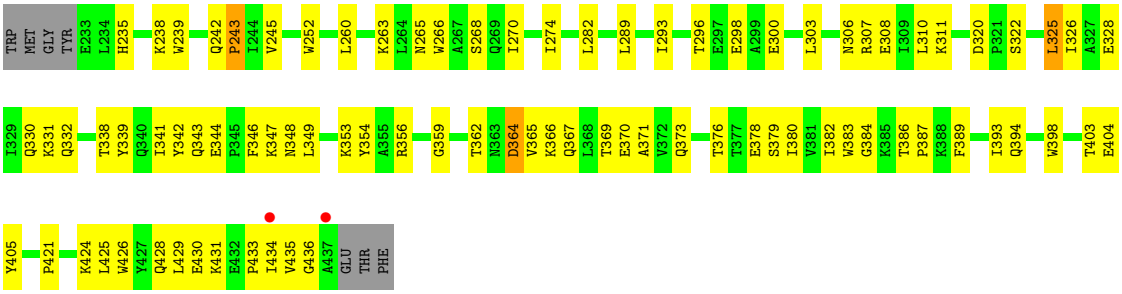
Chain A:



• Molecule 2: p51 RT

Chain B:




TRP MET GLY TYR E233 L234 H235 K238 W239 Q242 P243 I244 V245 W252 L260 K263 L264 N265 W266 A267 S268 Q269 I270 I274 L282 L289 I293 T296 E297 E298 A299 E300 L303 N306 R307 E308 I309 L310 K311 D320 P321 S322 L325 I326 A327 E328
I329 Q330 K331 Q332 T338 Y339 Q340 I341 Y342 Q343 E344 P345 F346 K347 N348 L349 K353 Y354 A355 R356 G359 T362 N363 D364 V365 K366 Q367 L368 T369 E370 A371 V372 Q373 T376 T377 E378 S379 I380 V381 I382 W383 G384 K385 T386 P387 K388 F389 I393 Q394 W398 T403 E404
Y405 P421 K424 L425 W426 Y427 Q428 L429 E430 K431 E432 P433 I434 V435 G436 A437 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	135.91Å 109.21Å 71.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.54 – 3.10 29.54 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.9 (29.54-3.10) 88.0 (29.54-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.307 0.225 , 0.302	Depositor DCC
R_{free} test set	938 reflections (5.11%)	DCC
Wilson B-factor (Å^2)	61.8	Xtriage
Anisotropy	0.690	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 19285 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7702	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GWE, CSD, PO4

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	0.39	0/4461	0.65	0/6064
2	B	0.38	0/3393	0.62	0/4608
All	All	0.39	0/7854	0.63	0/10672

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4354	0	4391	258	0
2	B	3302	0	3331	169	0
3	A	5	0	0	0	0
3	B	5	0	0	2	0
4	A	36	0	17	4	0
All	All	7702	0	7739	416	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (416) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:195:ILE:HB	2:B:199:ARG:HH12	1.22	1.03
1:A:106:VAL:H	4:A:999:GWE:HNS	1.05	0.98
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.29	0.96
2:B:242:GLN:HE21	2:B:243:PRO:HD2	1.29	0.96
2:B:353:LYS:HE3	2:B:430:GLU:HB3	1.48	0.94
2:B:359:GLY:N	3:B:1300:PO4:O1	2.08	0.87
2:B:235:HIS:HB3	2:B:238:LYS:HE3	1.57	0.84
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.58	0.83
1:A:448:ARG:NH2	1:A:475:GLN:H	1.76	0.83
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.58	0.82
1:A:216:THR:OG1	1:A:217:PRO:HD2	1.80	0.82
2:B:73:LYS:HB3	2:B:73:LYS:NZ	1.95	0.81
2:B:195:ILE:HB	2:B:199:ARG:NH1	1.97	0.79
1:A:448:ARG:HE	1:A:473:THR:HB	1.47	0.78
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.65	0.78
1:A:211:ARG:HG2	1:A:211:ARG:NH1	1.92	0.77
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.67	0.77
1:A:502:ALA:HA	1:A:505:ILE:HD12	1.66	0.77
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.66	0.77
1:A:217:PRO:HB2	1:A:222:GLN:NE2	1.99	0.76
2:B:161:GLN:HA	2:B:161:GLN:HE21	1.49	0.76
2:B:356:ARG:HB2	2:B:367:GLN:HG2	1.66	0.76
2:B:242:GLN:NE2	2:B:243:PRO:HD2	2.01	0.76
1:A:111:VAL:HG23	1:A:160:PHE:HZ	1.49	0.76
2:B:79:GLU:O	2:B:83:ARG:HG3	1.85	0.76
1:A:448:ARG:NE	1:A:474:ASN:H	1.84	0.75
1:A:114:ALA:HA	1:A:117:SER:OG	1.87	0.75
1:A:270:ILE:HG22	1:A:314:VAL:HG11	1.67	0.75
1:A:163:SER:O	1:A:167:ILE:HG13	1.86	0.74
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.27	0.74
2:B:235:HIS:HB2	2:B:238:LYS:HD2	1.67	0.74
2:B:379:SER:OG	2:B:387:PRO:HD3	1.87	0.73
1:A:448:ARG:HH21	1:A:475:GLN:H	1.35	0.73
2:B:235:HIS:HB3	2:B:238:LYS:CE	2.18	0.73
2:B:178:ILE:HG12	2:B:191:SER:HB3	1.71	0.73
1:A:257:ILE:O	1:A:261:VAL:HG23	1.87	0.73
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.23	0.72
1:A:237:ASP:OD1	1:A:238:LYS:HD2	1.88	0.72
1:A:181:TYR:HB2	1:A:188:TYR:HB2	1.71	0.72
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.04	0.71
2:B:235:HIS:CB	2:B:238:LYS:HD2	2.19	0.71
1:A:106:VAL:N	4:A:999:GWE:HNS	1.85	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:515:SER:HB3	1:A:518:VAL:HG23	1.74	0.70
1:A:50:ILE:HG21	1:A:145:GLN:HG2	1.74	0.69
1:A:448:ARG:NE	1:A:473:THR:HB	2.07	0.69
1:A:101:LYS:HE2	1:A:321:PRO:HG3	1.73	0.68
1:A:393:ILE:HB	1:A:423:VAL:HG13	1.75	0.67
1:A:94:ILE:HD11	1:A:230:MET:HG3	1.77	0.67
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.77	0.67
2:B:376:THR:HG23	2:B:386:THR:HG22	1.76	0.66
1:A:447:ASN:HB3	1:A:450:THR:OG1	1.95	0.66
1:A:483:TYR:CE2	1:A:487:GLN:NE2	2.63	0.66
2:B:265:ASN:O	2:B:268:SER:HB3	1.96	0.66
1:A:409:THR:O	2:B:364:ASP:HB2	1.94	0.66
1:A:448:ARG:HE	1:A:473:THR:CB	2.08	0.66
2:B:376:THR:CG2	2:B:386:THR:HG22	2.25	0.66
2:B:31:ILE:O	2:B:35:VAL:HG23	1.96	0.66
2:B:164:MET:HA	2:B:167:ILE:HD11	1.78	0.65
1:A:160:PHE:HD2	1:A:160:PHE:C	1.99	0.65
2:B:116:PHE:HZ	2:B:151:GLN:NE2	1.92	0.65
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.32	0.65
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.79	0.65
2:B:434:ILE:HG22	2:B:435:VAL:HG13	1.78	0.65
2:B:235:HIS:CB	2:B:238:LYS:CD	2.75	0.65
1:A:448:ARG:CZ	1:A:474:ASN:H	2.11	0.64
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.32	0.64
2:B:426:TRP:O	2:B:429:LEU:HB2	1.97	0.64
1:A:74:LEU:HD23	1:A:75:VAL:N	2.12	0.64
1:A:448:ARG:HH11	1:A:448:ARG:HG3	1.63	0.64
1:A:317:VAL:HG23	1:A:349:LEU:HD23	1.78	0.64
1:A:160:PHE:CD2	1:A:160:PHE:C	2.72	0.63
1:A:211:ARG:CG	1:A:211:ARG:HH11	2.07	0.63
2:B:162:SER:O	2:B:166:LYS:HG3	1.99	0.63
2:B:376:THR:O	2:B:380:ILE:HG13	1.99	0.62
1:A:442:VAL:HG22	1:A:496:VAL:O	1.99	0.62
2:B:31:ILE:HD13	2:B:133:PRO:O	1.99	0.62
1:A:116:PHE:CE2	1:A:151:GLN:HG2	2.35	0.62
1:A:246:LEU:O	1:A:307:ARG:NH1	2.26	0.62
2:B:433:PRO:HB3	2:B:436:GLY:O	2.00	0.61
1:A:335:GLY:O	1:A:356:ARG:HA	2.00	0.61
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.81	0.61
1:A:346:PHE:N	1:A:346:PHE:CD2	2.67	0.61
2:B:235:HIS:O	2:B:238:LYS:HG2	2.00	0.60
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.35	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:120:LEU:HD23	1:A:125:ARG:HG2	1.83	0.60
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.37	0.60
2:B:369:THR:O	2:B:373:GLN:HG3	2.00	0.60
1:A:40:GLU:O	1:A:43:LYS:HG2	2.01	0.60
1:A:448:ARG:HE	1:A:473:THR:CA	2.14	0.60
2:B:194:GLU:CD	2:B:196:GLY:H	2.05	0.60
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.82	0.59
1:A:203:GLU:HG3	1:A:207:GLN:HE21	1.66	0.59
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.00	0.59
2:B:425:LEU:O	2:B:429:LEU:HD13	2.02	0.59
1:A:40:GLU:O	1:A:44:GLU:HG3	2.03	0.59
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.84	0.59
1:A:114:ALA:HB3	1:A:160:PHE:CE1	2.37	0.59
2:B:366:LYS:HE3	2:B:405:TYR:CE2	2.38	0.59
2:B:73:LYS:HB3	2:B:73:LYS:HZ3	1.65	0.58
2:B:175:ASN:HD21	2:B:201:LYS:HE3	1.67	0.58
2:B:235:HIS:HB2	2:B:238:LYS:CD	2.33	0.58
1:A:114:ALA:HB3	1:A:160:PHE:CZ	2.37	0.58
2:B:73:LYS:HZ2	2:B:73:LYS:HB3	1.67	0.58
2:B:163:SER:O	2:B:167:ILE:HG12	2.02	0.58
2:B:332:GLN:NE2	2:B:424:LYS:HE2	2.18	0.58
1:A:405:TYR:O	2:B:331:LYS:HD3	2.04	0.58
2:B:344:GLU:HB2	2:B:347:LYS:HD2	1.85	0.58
1:A:194:GLU:HB2	1:A:197:GLN:HG3	1.83	0.58
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.21	0.58
1:A:46:LYS:CE	1:A:116:PHE:HB3	2.34	0.58
1:A:208:HIS:O	1:A:211:ARG:HB3	2.03	0.58
1:A:206:ARG:O	1:A:210:LEU:HD13	2.03	0.58
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.84	0.58
1:A:171:PHE:HE2	1:A:175:ASN:HB2	1.69	0.57
1:A:164:MET:HG2	1:A:182:GLN:HE21	1.69	0.57
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.39	0.57
2:B:365:VAL:O	2:B:369:THR:HG23	2.04	0.57
2:B:308:GLU:OE1	2:B:311:LYS:HE3	2.05	0.57
1:A:208:HIS:CE1	1:A:212:TRP:HE1	2.22	0.57
1:A:143:ARG:HG2	1:A:143:ARG:HH11	1.69	0.57
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.87	0.57
2:B:78:ARG:O	2:B:82:LYS:HG3	2.05	0.57
2:B:34:LEU:CD2	2:B:73:LYS:HG3	2.34	0.57
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.40	0.57
1:A:138:GLU:OE1	1:A:139:THR:HG23	2.04	0.57
1:A:518:VAL:O	1:A:522:ILE:HG13	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.38	0.57
1:A:380:ILE:O	1:A:384:GLY:HA2	2.04	0.57
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.87	0.56
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.33	0.56
1:A:50:ILE:CG2	1:A:145:GLN:HG2	2.35	0.56
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.06	0.56
2:B:344:GLU:CB	2:B:347:LYS:HD2	2.35	0.56
2:B:354:TYR:OH	2:B:370:GLU:HB3	2.05	0.56
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.86	0.56
1:A:111:VAL:HG22	1:A:185:ASP:O	2.05	0.56
1:A:340:GLN:CB	1:A:351:THR:HG22	2.36	0.56
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.41	0.56
1:A:58:THR:HG23	1:A:76:ASP:O	2.05	0.56
1:A:46:LYS:NZ	1:A:116:PHE:HB3	2.20	0.55
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.70	0.55
1:A:248:GLU:OE1	1:A:248:GLU:HA	2.07	0.55
2:B:160:PHE:CD1	2:B:160:PHE:O	2.60	0.55
1:A:101:LYS:HA	1:A:319:TYR:O	2.06	0.55
1:A:214:LEU:C	1:A:214:LEU:HD23	2.27	0.55
1:A:454:LYS:HA	1:A:467:VAL:O	2.07	0.55
1:A:334:GLN:O	1:A:356:ARG:HD3	2.06	0.55
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.37	0.55
1:A:122:GLU:CD	1:A:122:GLU:H	2.11	0.54
1:A:5:ILE:HD11	1:A:166:LYS:HD2	1.88	0.54
1:A:57:ASN:HA	1:A:129:ALA:O	2.07	0.54
2:B:54:ASN:O	2:B:143:ARG:NH2	2.40	0.54
1:A:88:TRP:CH2	2:B:57:ASN:CB	2.90	0.54
1:A:301:LEU:O	1:A:304:ALA:HB3	2.07	0.54
1:A:206:ARG:HH11	1:A:216:THR:HG21	1.73	0.54
1:A:63:ILE:HD12	1:A:64:LYS:N	2.23	0.54
1:A:175:ASN:CB	1:A:178:ILE:HD12	2.33	0.54
2:B:40:GLU:O	2:B:44:GLU:HG3	2.07	0.54
1:A:28:GLU:HG2	1:A:28:GLU:O	2.08	0.54
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.89	0.54
2:B:328:GLU:O	2:B:339:TYR:HA	2.08	0.53
1:A:346:PHE:N	1:A:346:PHE:HD2	2.07	0.53
1:A:420:PRO:HA	1:A:421:PRO:C	2.27	0.53
2:B:27:THR:O	2:B:31:ILE:HG13	2.09	0.53
2:B:326:ILE:O	2:B:341:ILE:HA	2.09	0.53
2:B:118:VAL:HB	2:B:149:LEU:HG	1.91	0.53
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.08	0.53
2:B:235:HIS:HB3	2:B:238:LYS:CD	2.39	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:112:GLY:C	1:A:114:ALA:H	2.10	0.52
2:B:209:LEU:C	2:B:211:ARG:H	2.13	0.52
2:B:111:VAL:HG22	2:B:185:ASP:O	2.09	0.52
1:A:217:PRO:HB2	1:A:222:GLN:HE21	1.73	0.52
1:A:110:ASP:HB3	1:A:217:PRO:HG3	1.90	0.52
2:B:206:ARG:O	2:B:210:LEU:HB2	2.09	0.52
1:A:241:VAL:HG22	1:A:242:GLN:O	2.09	0.52
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.40	0.52
1:A:492:GLU:OE2	1:A:530:LYS:HD2	2.08	0.52
1:A:90:VAL:HG23	1:A:90:VAL:O	2.10	0.52
1:A:244:ILE:HB	1:A:310:LEU:HD13	1.91	0.52
1:A:57:ASN:HD22	1:A:143:ARG:HH12	1.57	0.52
1:A:31:ILE:O	1:A:35:VAL:HG23	2.10	0.51
1:A:227:PHE:O	1:A:234:LEU:N	2.41	0.51
1:A:317:VAL:HG23	1:A:349:LEU:CD2	2.39	0.51
1:A:516:GLU:O	1:A:519:ASN:HB2	2.09	0.51
1:A:171:PHE:CE2	1:A:175:ASN:HB2	2.44	0.51
2:B:51:GLY:HA3	2:B:53:GLU:OE1	2.10	0.51
2:B:245:VAL:HG23	2:B:431:LYS:HB2	1.93	0.51
1:A:78:ARG:O	1:A:82:LYS:HG3	2.11	0.51
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.92	0.51
1:A:382:ILE:O	2:B:136:ASN:HB2	2.09	0.51
1:A:38:CYS:O	1:A:47:ILE:HD11	2.11	0.51
1:A:216:THR:O	1:A:217:PRO:O	2.29	0.50
1:A:235:HIS:HB2	1:A:238:LYS:O	2.11	0.50
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.26	0.50
2:B:263:LYS:HE2	2:B:425:LEU:HB3	1.93	0.50
1:A:417:VAL:O	1:A:417:VAL:HG13	2.11	0.50
1:A:112:GLY:O	1:A:114:ALA:N	2.33	0.50
2:B:139:THR:HG22	2:B:140:PRO:O	2.11	0.50
2:B:167:ILE:HG22	2:B:212:TRP:CZ2	2.47	0.50
1:A:111:VAL:CG2	1:A:160:PHE:HZ	2.22	0.49
2:B:379:SER:CB	2:B:387:PRO:HD3	2.42	0.49
1:A:440:PHE:CD2	1:A:459:THR:HG22	2.47	0.49
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.11	0.49
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.93	0.49
1:A:90:VAL:O	1:A:91:GLN:C	2.51	0.49
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.46	0.49
1:A:74:LEU:C	1:A:74:LEU:HD23	2.32	0.49
2:B:366:LYS:HE3	2:B:405:TYR:CD2	2.46	0.49
2:B:142:ILE:HD12	2:B:142:ILE:N	2.27	0.49
1:A:76:ASP:OD2	1:A:78:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:164:MET:HG2	1:A:182:GLN:NE2	2.27	0.49
2:B:122:GLU:HG3	2:B:123:ASP:N	2.26	0.49
1:A:161:GLN:NE2	2:B:140:PRO:HB3	2.26	0.49
1:A:396:GLU:HG3	1:A:397:THR:N	2.28	0.49
1:A:98:ALA:HB2	1:A:350:LYS:HB2	1.94	0.49
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.95	0.49
1:A:206:ARG:HH11	1:A:216:THR:CG2	2.26	0.49
1:A:46:LYS:NZ	1:A:116:PHE:CB	2.76	0.48
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.48	0.48
1:A:101:LYS:HG2	1:A:321:PRO:HD3	1.94	0.48
1:A:335:GLY:HA3	1:A:356:ARG:CD	2.44	0.48
1:A:334:GLN:NE2	1:A:512:GLN:HB3	2.29	0.48
2:B:11:LYS:O	2:B:85:GLN:HB3	2.13	0.48
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.48	0.48
1:A:455:ALA:O	1:A:466:VAL:HA	2.14	0.48
1:A:79:GLU:CD	1:A:83:ARG:HH21	2.16	0.48
1:A:235:HIS:O	1:A:238:LYS:O	2.32	0.48
1:A:103:ASN:ND2	4:A:999:GWE:H5	2.28	0.48
1:A:448:ARG:HE	1:A:474:ASN:H	1.62	0.48
2:B:303:LEU:O	2:B:307:ARG:HG3	2.13	0.47
1:A:392:PRO:O	1:A:423:VAL:HG12	2.14	0.47
1:A:108:VAL:C	1:A:109:LEU:HD12	2.34	0.47
1:A:169:GLU:CG	1:A:173:LYS:HE3	2.43	0.47
1:A:27:THR:O	1:A:31:ILE:HG13	2.15	0.47
1:A:19:PRO:O	1:A:56:TYR:HA	2.15	0.47
1:A:79:GLU:O	1:A:83:ARG:HG3	2.15	0.47
1:A:48:SER:O	1:A:50:ILE:HG23	2.15	0.47
1:A:380:ILE:HD11	1:A:386:THR:HG22	1.97	0.47
2:B:84:THR:HB	2:B:154:LYS:HE2	1.95	0.47
1:A:111:VAL:O	1:A:111:VAL:HG23	2.14	0.47
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.50	0.47
1:A:344:GLU:HG3	1:A:347:LYS:HD2	1.96	0.47
1:A:329:ILE:O	1:A:392:PRO:HD3	2.14	0.47
2:B:421:PRO:O	2:B:425:LEU:HG	2.14	0.47
2:B:126:LYS:HE3	2:B:127:TYR:CE1	2.50	0.47
2:B:112:GLY:HA2	2:B:115:TYR:CE2	2.49	0.47
1:A:63:ILE:C	1:A:63:ILE:HD12	2.34	0.47
1:A:226:PRO:HB3	1:A:235:HIS:ND1	2.29	0.47
2:B:211:ARG:HG3	2:B:212:TRP:CD1	2.50	0.47
1:A:381:VAL:O	2:B:136:ASN:N	2.46	0.46
1:A:183:TYR:CE1	1:A:184:MET:HG3	2.50	0.46
2:B:8:VAL:HG23	2:B:9:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:279:LEU:HG	1:A:302:GLU:OE1	2.16	0.46
2:B:320:ASP:OD1	2:B:322:SER:N	2.48	0.46
2:B:118:VAL:HB	2:B:149:LEU:CD1	2.46	0.46
1:A:295:LEU:HD12	1:A:300:GLU:OE1	2.16	0.46
2:B:7:THR:CG2	2:B:119:PRO:HG2	2.39	0.46
1:A:57:ASN:HB2	1:A:143:ARG:HH22	1.80	0.46
1:A:225:PRO:HA	1:A:226:PRO:C	2.36	0.46
1:A:110:ASP:C	1:A:112:GLY:H	2.18	0.46
2:B:178:ILE:HG12	2:B:191:SER:CB	2.44	0.46
1:A:26:LEU:HD12	1:A:133:PRO:HG3	1.97	0.46
1:A:205:LEU:O	1:A:206:ARG:C	2.53	0.46
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.48	0.46
1:A:478:GLU:O	1:A:482:ILE:HG13	2.16	0.46
1:A:508:ALA:O	1:A:509:GLN:C	2.54	0.46
2:B:31:ILE:HD12	2:B:135:ILE:HG13	1.98	0.46
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.97	0.46
2:B:167:ILE:H	2:B:167:ILE:HG12	1.55	0.46
2:B:49:LYS:HA	2:B:143:ARG:O	2.16	0.46
2:B:206:ARG:O	2:B:210:LEU:N	2.40	0.46
1:A:255:ASN:HD22	1:A:289:LEU:HB3	1.80	0.46
1:A:254:VAL:HB	1:A:289:LEU:HA	1.98	0.46
1:A:208:HIS:CE1	1:A:212:TRP:NE1	2.84	0.45
2:B:57:ASN:HD22	2:B:143:ARG:HH11	1.62	0.45
2:B:282:LEU:HB3	2:B:293:ILE:HG21	1.97	0.45
2:B:24:TRP:HH2	2:B:61:PHE:CD2	2.34	0.45
2:B:209:LEU:C	2:B:211:ARG:N	2.70	0.45
2:B:169:GLU:OE2	2:B:169:GLU:HA	2.17	0.45
2:B:206:ARG:HG2	2:B:206:ARG:NH1	2.31	0.45
2:B:202:ILE:O	2:B:205:LEU:HB3	2.17	0.45
2:B:206:ARG:HH11	2:B:206:ARG:HG2	1.82	0.45
1:A:371:ALA:O	1:A:375:ILE:HG13	2.16	0.45
1:A:2:ILE:HG22	1:A:3:SER:N	2.31	0.45
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.99	0.45
2:B:393:ILE:HG12	2:B:394:GLN:N	2.31	0.45
2:B:425:LEU:HA	2:B:428:GLN:HE21	1.81	0.45
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.98	0.45
1:A:155:GLY:O	1:A:159:ILE:HG13	2.17	0.45
2:B:242:GLN:HE21	2:B:243:PRO:CD	2.14	0.45
1:A:438:GLU:HG2	1:A:459:THR:HB	1.99	0.45
1:A:308:GLU:OE1	1:A:311:LYS:NZ	2.46	0.45
1:A:169:GLU:HG2	1:A:173:LYS:HE3	1.98	0.44
2:B:63:ILE:HD13	2:B:74:LEU:CD2	2.39	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.99	0.44
1:A:498:ASP:HA	1:A:536:VAL:O	2.17	0.44
1:A:176:PRO:C	1:A:178:ILE:H	2.19	0.44
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.46	0.44
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.52	0.44
1:A:8:VAL:O	1:A:121:ASP:HB2	2.17	0.44
2:B:359:GLY:CA	3:B:1300:PO4:O1	2.65	0.44
2:B:265:ASN:O	2:B:268:SER:CB	2.65	0.44
1:A:511:ASP:O	1:A:512:GLN:HB3	2.16	0.44
2:B:139:THR:HG23	2:B:140:PRO:HD2	2.00	0.44
1:A:225:PRO:HG2	4:A:999:GWE:O4	2.17	0.44
1:A:303:LEU:O	1:A:307:ARG:HG3	2.17	0.44
2:B:77:PHE:CD2	2:B:80:LEU:HD23	2.51	0.44
1:A:516:GLU:O	1:A:520:GLN:HG3	2.18	0.44
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.99	0.44
1:A:171:PHE:O	1:A:172:ARG:C	2.55	0.44
1:A:115:TYR:HE1	1:A:185:ASP:OD2	2.01	0.44
1:A:389:PHE:HB3	1:A:391:LEU:HD21	2.00	0.44
1:A:74:LEU:C	1:A:74:LEU:CD2	2.86	0.44
1:A:335:GLY:HA3	1:A:356:ARG:HD2	1.99	0.44
1:A:143:ARG:HG2	1:A:143:ARG:NH1	2.31	0.44
2:B:169:GLU:O	2:B:170:PRO:C	2.55	0.44
1:A:342:TYR:HB3	1:A:348:ASN:HA	2.00	0.44
1:A:114:ALA:O	1:A:117:SER:HB2	2.18	0.44
1:A:205:LEU:HD22	1:A:209:LEU:HD11	1.99	0.44
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.52	0.44
1:A:228:LEU:HA	1:A:232:TYR:O	2.18	0.44
1:A:88:TRP:CH2	2:B:57:ASN:HB2	2.52	0.44
1:A:492:GLU:HA	1:A:530:LYS:O	2.18	0.44
2:B:274:ILE:HD11	2:B:310:LEU:HD21	2.00	0.44
1:A:90:VAL:HG12	1:A:158:ALA:HA	2.00	0.44
1:A:439:THR:O	1:A:459:THR:HA	2.17	0.44
1:A:482:ILE:O	1:A:486:LEU:HG	2.19	0.43
2:B:168:LEU:HA	2:B:168:LEU:HD23	1.88	0.43
2:B:57:ASN:HD21	2:B:131:THR:N	2.16	0.43
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.18	0.43
1:A:440:PHE:CG	1:A:459:THR:HG22	2.53	0.43
1:A:478:GLU:O	1:A:481:ALA:HB3	2.18	0.43
2:B:343:GLN:HG3	2:B:349:LEU:HD11	2.00	0.43
1:A:170:PRO:O	1:A:173:LYS:HB2	2.18	0.43
1:A:171:PHE:CD2	1:A:171:PHE:C	2.91	0.43
1:A:171:PHE:C	1:A:171:PHE:HD2	2.22	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:337:TRP:O	1:A:353:LYS:HA	2.18	0.43
2:B:332:GLN:HE21	2:B:332:GLN:HA	1.82	0.43
2:B:160:PHE:O	2:B:160:PHE:HD1	2.00	0.43
1:A:305:GLU:O	1:A:309:ILE:HG13	2.19	0.43
1:A:46:LYS:HE2	1:A:116:PHE:HB3	1.99	0.43
2:B:325:LEU:HA	2:B:325:LEU:HD12	1.88	0.43
1:A:410:TRP:CD1	2:B:362:THR:O	2.72	0.43
1:A:515:SER:CB	1:A:518:VAL:HG23	2.47	0.43
2:B:24:TRP:CH2	2:B:61:PHE:CD2	3.07	0.43
1:A:111:VAL:HG23	1:A:160:PHE:CZ	2.41	0.43
1:A:100:LEU:CD2	1:A:181:TYR:HE1	2.31	0.43
1:A:457:TYR:CE1	1:A:463:ARG:HD2	2.54	0.43
1:A:486:LEU:O	1:A:528:LYS:NZ	2.49	0.43
1:A:448:ARG:NH2	1:A:474:ASN:N	2.66	0.42
1:A:125:ARG:HD3	1:A:147:ASN:HA	2.02	0.42
1:A:88:TRP:CH2	2:B:57:ASN:HB3	2.53	0.42
2:B:298:GLU:CD	2:B:298:GLU:H	2.22	0.42
2:B:120:LEU:O	2:B:121:ASP:C	2.58	0.42
1:A:112:GLY:C	1:A:114:ALA:N	2.71	0.42
2:B:57:ASN:HA	2:B:129:ALA:O	2.19	0.42
1:A:399:GLU:OE2	1:A:402:TRP:HZ3	2.03	0.42
1:A:171:PHE:HE2	1:A:175:ASN:CB	2.32	0.42
1:A:171:PHE:O	1:A:174:GLN:N	2.53	0.42
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.49	0.42
1:A:84:THR:HG21	1:A:153:TRP:CZ2	2.54	0.42
2:B:235:HIS:CD2	2:B:238:LYS:NZ	2.88	0.42
1:A:448:ARG:HE	1:A:473:THR:HA	1.84	0.42
1:A:94:ILE:HA	1:A:95:PRO:HD3	1.82	0.42
1:A:30:LYS:HE2	1:A:71:TRP:CH2	2.53	0.42
1:A:519:ASN:O	1:A:523:GLU:HG2	2.19	0.42
1:A:54:ASN:OD1	1:A:56:TYR:N	2.51	0.42
1:A:95:PRO:HA	2:B:136:ASN:OD1	2.19	0.42
1:A:448:ARG:CG	1:A:448:ARG:HH11	2.30	0.42
2:B:175:ASN:ND2	2:B:201:LYS:HE3	2.32	0.42
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.55	0.42
2:B:209:LEU:O	2:B:211:ARG:N	2.53	0.42
1:A:465:LYS:CG	1:A:466:VAL:N	2.83	0.41
1:A:465:LYS:HG2	1:A:466:VAL:N	2.34	0.41
1:A:235:HIS:HA	1:A:236:PRO:HD3	1.91	0.41
1:A:110:ASP:C	1:A:112:GLY:N	2.73	0.41
2:B:380:ILE:O	2:B:384:GLY:N	2.46	0.41
2:B:404:GLU:HB2	2:B:405:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:332:GLN:NE2	2:B:332:GLN:HA	2.35	0.41
2:B:354:TYR:CD2	2:B:371:ALA:HB2	2.55	0.41
1:A:63:ILE:O	1:A:71:TRP:HE3	2.03	0.41
2:B:53:GLU:O	2:B:55:PRO:HD3	2.20	0.41
1:A:293:ILE:HD12	1:A:293:ILE:N	2.35	0.41
1:A:169:GLU:O	1:A:173:LYS:HG3	2.21	0.41
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.51	0.41
2:B:115:TYR:CD1	2:B:156:SER:HB3	2.56	0.41
2:B:19:PRO:O	2:B:56:TYR:HB3	2.21	0.41
1:A:170:PRO:O	1:A:174:GLN:HG3	2.20	0.41
1:A:457:TYR:HE1	1:A:463:ARG:HD2	1.85	0.41
2:B:378:GLU:O	2:B:382:ILE:HG13	2.21	0.41
2:B:60:VAL:HG22	2:B:61:PHE:N	2.35	0.41
2:B:98:ALA:O	2:B:101:LYS:HG2	2.20	0.41
1:A:502:ALA:O	1:A:506:ILE:HG13	2.20	0.41
2:B:245:VAL:CG2	2:B:431:LYS:HB2	2.50	0.41
1:A:360:ALA:O	1:A:513:SER:HB2	2.21	0.41
2:B:235:HIS:O	2:B:238:LYS:CG	2.68	0.41
2:B:63:ILE:CD1	2:B:74:LEU:HD22	2.46	0.41
1:A:192:ASP:O	1:A:193:LEU:O	2.39	0.41
2:B:111:VAL:HG23	2:B:111:VAL:O	2.20	0.41
1:A:325:LEU:HA	1:A:325:LEU:HD12	1.89	0.41
1:A:121:ASP:O	1:A:124:PHE:N	2.49	0.41
2:B:121:ASP:O	2:B:125:ARG:HG3	2.21	0.41
2:B:116:PHE:CZ	2:B:151:GLN:NE2	2.81	0.40
2:B:169:GLU:CB	2:B:170:PRO:HD3	2.51	0.40
2:B:342:TYR:C	2:B:342:TYR:CD1	2.94	0.40
1:A:218:ASP:C	1:A:220:LYS:N	2.72	0.40
1:A:412:PRO:O	1:A:413:GLU:C	2.60	0.40
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.57	0.40
1:A:101:LYS:HE2	1:A:321:PRO:CG	2.48	0.40
1:A:116:PHE:CZ	1:A:151:GLN:HG2	2.56	0.40
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.87	0.40
1:A:201:LYS:O	1:A:202:ILE:C	2.57	0.40
2:B:235:HIS:CB	2:B:238:LYS:CE	2.95	0.40
2:B:332:GLN:HG3	2:B:338:THR:HG23	2.04	0.40
1:A:105:SER:O	1:A:190:GLY:HA2	2.22	0.40
1:A:179:VAL:O	1:A:179:VAL:HG23	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	525/560 (94%)	463 (88%)	49 (9%)	13 (2%)	9 42
2	B	392/440 (89%)	361 (92%)	28 (7%)	3 (1%)	27 74
All	All	917/1000 (92%)	824 (90%)	77 (8%)	16 (2%)	14 54

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	133	PRO
1	A	193	LEU
1	A	217	PRO
1	A	112	GLY
1	A	113	ASP
1	A	170	PRO
1	A	345	PRO
2	B	170	PRO
2	B	210	LEU
1	A	85	GLN
1	A	361	HIS
1	A	14	PRO
1	A	512	GLN
1	A	111	VAL
2	B	97	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	476/499 (95%)	454 (95%)	22 (5%)	37 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	363/400 (91%)	355 (98%)	8 (2%)	64 92
All	All	839/899 (93%)	809 (96%)	30 (4%)	47 85

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	24	TRP
1	A	53	GLU
1	A	94	ILE
1	A	122	GLU
1	A	123	ASP
1	A	138	GLU
1	A	160	PHE
1	A	171	PHE
1	A	191	SER
1	A	205	LEU
1	A	217	PRO
1	A	238	LYS
1	A	248	GLU
1	A	255	ASN
1	A	340	GLN
1	A	346	PHE
1	A	368	LEU
1	A	402	TRP
1	A	404	GLU
1	A	517	LEU
1	A	533	LEU
2	B	24	TRP
2	B	55	PRO
2	B	113	ASP
2	B	206	ARG
2	B	243	PRO
2	B	300	GLU
2	B	325	LEU
2	B	364	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN

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Mol	Chain	Res	Type
1	A	161	GLN
1	A	182	GLN
1	A	207	GLN
1	A	208	HIS
1	A	255	ASN
1	A	278	GLN
1	A	334	GLN
1	A	336	GLN
1	A	407	GLN
1	A	428	GLN
1	A	487	GLN
1	A	500	GLN
1	A	519	ASN
2	B	57	ASN
2	B	151	GLN
2	B	161	GLN
2	B	174	GLN
2	B	175	ASN
2	B	182	GLN
2	B	197	GLN
2	B	235	HIS
2	B	242	GLN
2	B	332	GLN
2	B	394	GLN
2	B	428	GLN

5.3.3 RNA

There are no RNA chains 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	7,7,8	6.67	2 (28%)	6,8,10	4.96	4 (66%)

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	-	0/3/6/8	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	O-C	17.36	1.23	1.11
1	A	280	CSD	CA-C	2.70	1.53	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	CSD	CA-CB-SG	8.68	123.20	110.82
1	A	280	CSD	C-CA-N	-5.52	108.31	113.83
1	A	280	CSD	OD2-SG-CB	4.76	116.58	97.42
1	A	280	CSD	OD2-SG-OD1	4.38	116.67	109.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	1301	-	4,4,4	0.87	0	6,6,6	0.31	0
4	GWE	A	999	-	37,38,38	2.68	10 (27%)	57,57,57	1.96	12 (21%)
3	PO4	B	1300	-	4,4,4	0.96	0	6,6,6	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	1301	-	-	0/0/0/0	0/0/0/0
4	GWE	A	999	-	-	0/29/29/29	0/3/3/3
3	PO4	B	1300	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	GWE	C17-C18	6.97	1.53	1.40
4	A	999	GWE	C2-C1	6.11	1.52	1.40
4	A	999	GWE	C5-C6	6.02	1.50	1.38
4	A	999	GWE	C21-C22	5.77	1.49	1.38
4	A	999	GWE	C3-C4	5.66	1.48	1.38
4	A	999	GWE	C19-C20	5.03	1.50	1.39
4	A	999	GWE	C9-C8	2.38	1.43	1.39
4	A	999	GWE	C9-C10	2.33	1.41	1.37
4	A	999	GWE	C11-C10	2.29	1.41	1.37
4	A	999	GWE	C13-C8	2.01	1.42	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	999	GWE	C20-S1-N2	8.95	109.92	109.75
4	A	999	GWE	O5-S1-C20	5.60	110.38	106.91
4	A	999	GWE	O4-S1-C20	3.56	109.11	106.91
4	A	999	GWE	C2-C7-C8	2.51	123.99	119.65
4	A	999	GWE	C15-O2-C1	2.44	123.15	117.55
4	A	999	GWE	C8-C9-C10	2.43	120.35	118.52
4	A	999	GWE	C1-C2-C7	-2.35	119.34	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	999	GWE	C11-C10-C9	-2.29	120.23	123.48
4	A	999	GWE	C22-C17-C18	-2.25	117.92	120.62
4	A	999	GWE	O4-S1-O5	-2.18	110.59	117.62
4	A	999	GWE	O2-C15-C16	-2.12	104.57	110.78
4	A	999	GWE	F2-C14-C12	-2.00	108.35	112.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	532/560 (95%)	-0.25	0 100 100	18, 59, 103, 141	0
2	B	400/440 (90%)	-0.22	2 (0%) 88 39	25, 58, 105, 133	0
All	All	932/1000 (93%)	-0.24	2 (0%) 93 61	18, 59, 103, 141	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	434	ILE	3.3
2	B	437	ALA	2.0

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

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	CSD	A	280	8/9	0.14	-0.68	38,60,64,65	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GWE	A	999	36/36	0.17	-0.42	27,51,72,77	0
3	PO4	B	1300	5/5	0.26	-0.58	124,130,137,145	0
3	PO4	A	1301	5/5	0.12	-1.10	101,110,114,124	0

6.5 Other polymers

There are no such residues in this entry.