Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:05 PM GMT

PDB ID	:	1NHV
Title	:	Hepatitis C virus RNA polymerase in complex with non-nucleoside analogue inhibitor
Authors	:	Wang, M.; Ng, K.K.S.; Cherney, M.M.; Chan, L.; Yannopoulos, C.G.; Bedard, J.; Morin, N.; Nguyen-Ba, N.; Alaoui-Ismaili, M.H.; Bethell, R.C.; James, M.N.G.
Deposited on	:	2002-12-19
Resolution	:	2.90 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:

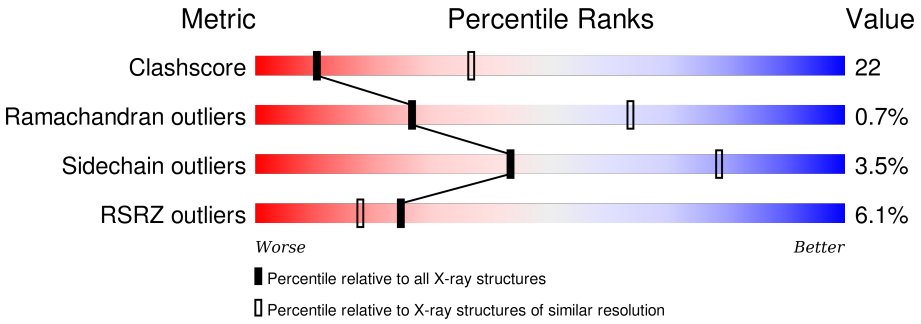
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	578	6% 56% 39%
1	B	578	6% 59% 36%

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
2	154	A	5001	-	-	-	X
2	154	B	6001	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8779 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.

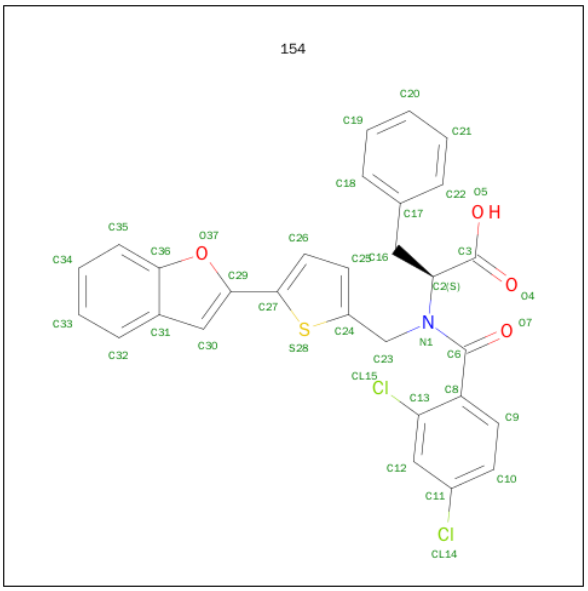
- Molecule 1 is a protein called HEPATITIS C VIRUS NS5B RNA-DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4340	2738	765	806	31			
1	B	561	Total	C	N	O	S	0	0	0
			4365	2753	771	810	31			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ALA	-	EXPRESSION TAG	UNP P26663
A	-6	SER	-	EXPRESSION TAG	UNP P26663
A	-5	HIS	-	EXPRESSION TAG	UNP P26663
A	-4	HIS	-	EXPRESSION TAG	UNP P26663
A	-3	HIS	-	EXPRESSION TAG	UNP P26663
A	-2	HIS	-	EXPRESSION TAG	UNP P26663
A	-1	HIS	-	EXPRESSION TAG	UNP P26663
A	0	HIS	-	EXPRESSION TAG	UNP P26663
B	-7	ALA	-	EXPRESSION TAG	UNP P26663
B	-6	SER	-	EXPRESSION TAG	UNP P26663
B	-5	HIS	-	EXPRESSION TAG	UNP P26663
B	-4	HIS	-	EXPRESSION TAG	UNP P26663
B	-3	HIS	-	EXPRESSION TAG	UNP P26663
B	-2	HIS	-	EXPRESSION TAG	UNP P26663
B	-1	HIS	-	EXPRESSION TAG	UNP P26663
B	0	HIS	-	EXPRESSION TAG	UNP P26663

- Molecule 2 is (2S)-2-[(5-BENZOFURAN-2-YL-THIOPHEN-2-YLMETHYL)-(2,4-DICHLORO-BENZOYL)-AMINO]-3-PHENYL-PROPIONIC ACID (three-letter code: 154) (formula: $C_{29}H_{21}Cl_2NO_4S$).



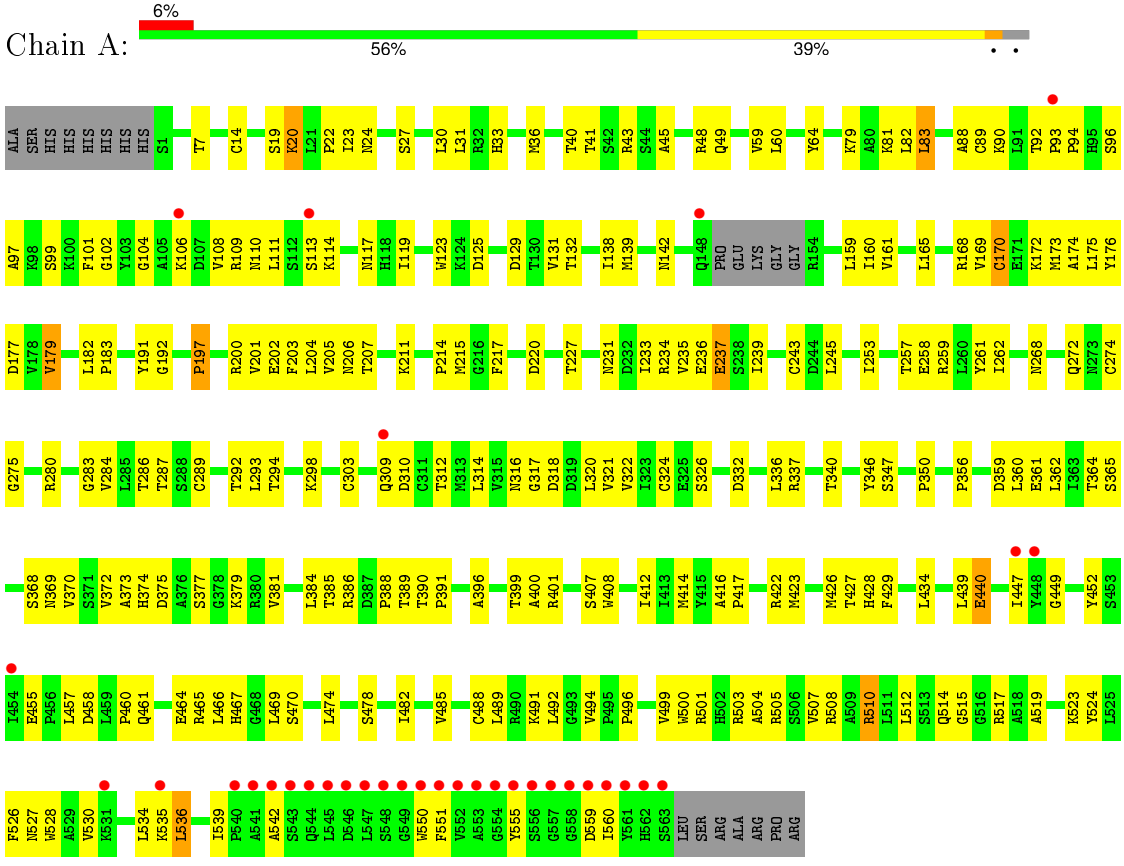
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			37	29	2	1	4	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			37	29	2	1	4	1		

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.

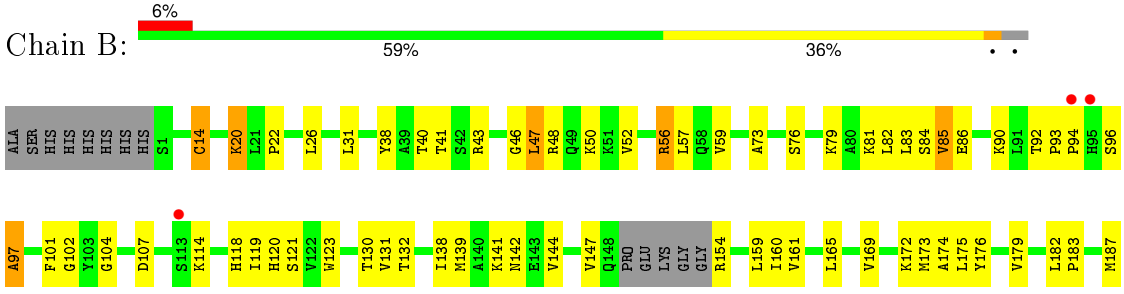
- Molecule 1: HEPATITIS C VIRUS NS5B RNA-DEPENDENT RNA POLYMERASE

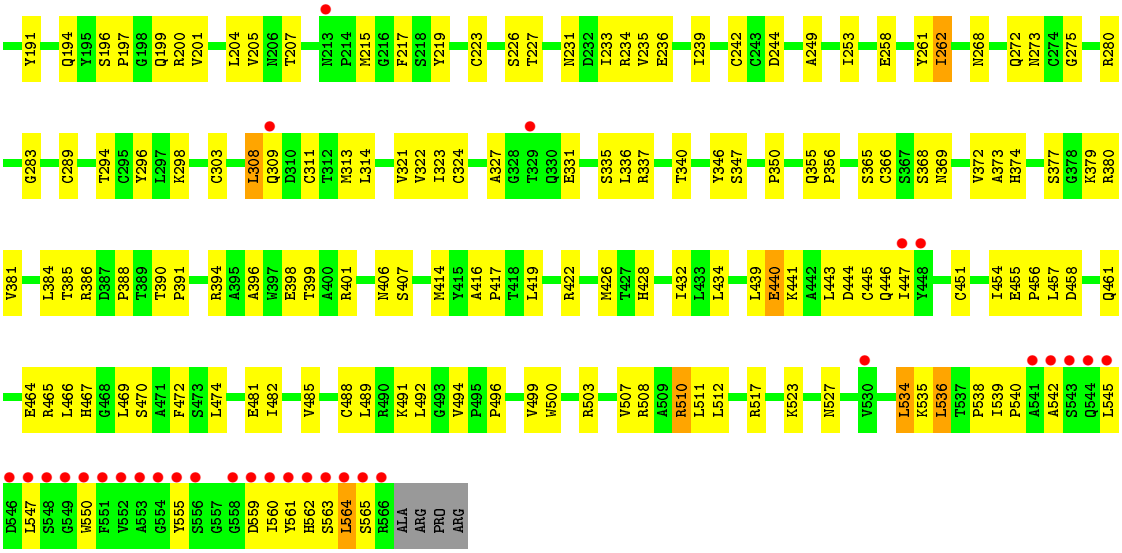
Chain A:



- Molecule 1: HEPATITIS C VIRUS NS5B RNA-DEPENDENT RNA POLYMERASE

Chain B:




Y191 Q194 Y195 S196 P197 G198 Q199 R200 V201 L204 V205 N206 T207 N213 P214 M215 C216 F217 S218 Y219 C223 S226 T227 N231 D232 I233 R234 V235 E236 I239 C242 C243 D244 A249 I253 E258 Y261 I262 N268 Q272 N273 C274 G275 R280
G283 C289 T294 C295 Y296 L297 K298 C303 L308 Q309 D310 C311 T312 M313 L314 V321 V322 I323 C324 A327 G328 T329 Q330 E331 S335 L336 R337 T340 Y346 S347 P350 Q355 P356 S365 C366 S367 S368 N369 V372 A373 H374 S377 G378 K379 R380
V381 L384 T385 R386 D387 P388 T389 T390 P391 R394 A395 A396 W397 E398 T399 A400 R401 N406 S407 M414 Y415 A416 P417 T418 L419 R422 M426 T427 H428 I432 L433 L434 L439 E440 K441 A442 L443 D444 C445 Q446 I447 Y448 C451 I454 E455 P456 L457 D458 Q461
E464 R465 L466 H467 G468 L469 S470 A471 F472 S473 L474 E481 I482 V485 C488 L489 R490 K491 L492 G493 V494 P495 P496 V499 W500 R503 V507 R508 A509 R510 L511 L512 R517 K523 N527 V530 L534 K535 L536 T537 P538 I539 P540 A541 A542 S543 Q544 L545
D546 L547 S548 G549 W550 F551 V552 A553 G554 Y555 S556 G557 G558 D559 I560 Y561 H562 S563 L564 S565 R566 ALA ARG PRO ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.50Å 107.83Å 126.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.74 – 2.90 39.74 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.1 (39.74-2.90) 94.2 (39.74-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.280 0.247 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.951	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	2 of 25058 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8779	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.98 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.5035e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 154

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.40	0/4434	0.65	0/6017
1	B	0.40	0/4459	0.64	0/6050
All	All	0.40	0/8893	0.64	0/12067

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4340	0	4357	203	0
1	B	4365	0	4386	177	0
2	A	37	0	20	4	0
2	B	37	0	20	0	0
All	All	8779	0	8783	378	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 22.

All (378) 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:336:LEU:HD12	1:A:356:PRO:HD3	1.50	0.92
1:B:510:ARG:HG2	1:B:510:ARG:HH11	1.41	0.85
1:A:215:MET:HB2	1:A:326:SER:HB2	1.60	0.83
1:A:192:GLY:HA3	1:A:316:ASN:OD1	1.78	0.82
1:B:268:ASN:HD21	1:B:272:GLN:HB2	1.44	0.81
1:B:175:LEU:HD21	1:B:253:ILE:HG12	1.62	0.81
1:B:327:ALA:O	1:B:331:GLU:HB3	1.81	0.80
1:B:470:SER:O	1:B:474:LEU:HG	1.82	0.79
1:B:314:LEU:HB3	1:B:321:VAL:HG13	1.63	0.79
1:A:496:PRO:HG2	1:A:499:VAL:HG23	1.63	0.79
1:B:381:VAL:HG11	1:B:474:LEU:HD22	1.66	0.77
1:B:48:ARG:HG2	1:B:159:LEU:HD13	1.67	0.77
1:B:336:LEU:HD12	1:B:356:PRO:HD3	1.66	0.76
1:B:550:TRP:HZ2	1:B:564:LEU:HD13	1.49	0.75
1:B:83:LEU:HB2	1:B:173:MET:HA	1.69	0.74
1:A:455:GLU:HB2	1:A:458:ASP:OD2	1.86	0.74
1:B:14:CYS:HB2	1:B:139:MET:SD	2.28	0.73
1:B:555:TYR:CG	1:B:560:ILE:HG13	2.22	0.73
1:A:321:VAL:HG21	1:A:365:SER:HB3	1.70	0.73
1:A:321:VAL:CG2	1:A:365:SER:HB3	2.19	0.72
1:A:466:LEU:HD21	1:A:551:PHE:HE2	1.53	0.72
1:B:527:ASN:HD21	1:B:534:LEU:HB2	1.53	0.72
1:B:461:GLN:HG3	1:B:539:ILE:HG21	1.71	0.70
1:B:231:ASN:O	1:B:235:VAL:HG23	1.90	0.70
1:A:94:PRO:HG3	1:A:109:ARG:CZ	2.22	0.70
1:A:170:CYS:HA	1:A:173:MET:HE3	1.72	0.70
1:A:501:ARG:NH1	2:A:5001:154:H26	2.07	0.69
1:B:422:ARG:HA	1:B:426:MET:CE	2.23	0.69
1:A:20:LYS:H	1:A:20:LYS:HD2	1.58	0.69
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.22	0.69
1:B:555:TYR:CD1	1:B:560:ILE:HG13	2.27	0.69
1:B:141:LYS:HE3	1:B:160:ILE:HD13	1.75	0.69
1:B:41:THR:HG23	1:B:43:ARG:HB2	1.74	0.68
1:B:416:ALA:HB3	1:B:417:PRO:HD3	1.76	0.68
1:A:48:ARG:HG2	1:A:159:LEU:HD13	1.75	0.68
1:B:510:ARG:NH1	1:B:510:ARG:HG2	2.07	0.68
1:A:175:LEU:O	1:A:179:VAL:HG22	1.94	0.67
1:A:555:TYR:CG	1:A:560:ILE:HG13	2.30	0.67
1:A:422:ARG:HA	1:A:426:MET:HE2	1.76	0.67
1:A:510:ARG:HH11	1:A:510:ARG:HG2	1.59	0.67
1:B:52:VAL:HG12	1:B:223:CYS:SG	2.35	0.67
1:B:227:THR:HB	1:B:347:SER:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:HD12	1:A:173:MET:O	1.96	0.66
1:B:41:THR:HG23	1:B:43:ARG:H	1.60	0.66
1:B:385:THR:HG21	1:B:481:GLU:OE1	1.96	0.66
1:B:197:PRO:O	1:B:201:VAL:HG23	1.96	0.66
1:B:439:LEU:O	1:B:456:PRO:HB2	1.95	0.65
1:B:390:THR:HB	1:B:391:PRO:HD3	1.77	0.65
1:A:390:THR:HB	1:A:391:PRO:HD3	1.79	0.65
1:A:336:LEU:CD1	1:A:356:PRO:HD3	2.26	0.65
1:A:204:LEU:HD21	1:A:314:LEU:CD2	2.27	0.65
1:B:527:ASN:ND2	1:B:534:LEU:HB2	2.12	0.65
1:A:268:ASN:HD21	1:A:272:GLN:HB2	1.62	0.65
1:B:268:ASN:ND2	1:B:272:GLN:HB2	2.12	0.64
1:A:268:ASN:ND2	1:A:272:GLN:HB2	2.12	0.64
1:A:523:LYS:O	1:A:527:ASN:HB2	1.96	0.64
1:A:422:ARG:HA	1:A:426:MET:CE	2.27	0.64
1:B:550:TRP:CZ2	1:B:564:LEU:HD13	2.32	0.63
1:A:434:LEU:HD13	1:A:510:ARG:HB3	1.78	0.63
1:A:227:THR:HB	1:A:347:SER:O	1.98	0.63
1:A:22:PRO:HG2	1:A:401:ARG:HG3	1.80	0.63
1:B:374:HIS:CE1	1:B:380:ARG:HG3	2.33	0.63
1:B:201:VAL:O	1:B:205:VAL:HG23	1.98	0.63
1:A:204:LEU:HD21	1:A:314:LEU:HD22	1.80	0.63
1:A:527:ASN:HD21	1:A:534:LEU:H	1.46	0.62
1:B:503:ARG:O	1:B:507:VAL:HG23	1.99	0.62
1:A:14:CYS:HB2	1:A:139:MET:SD	2.39	0.62
1:A:527:ASN:ND2	1:A:534:LEU:HB2	2.15	0.62
1:B:465:ARG:HH11	1:B:465:ARG:HG3	1.65	0.62
1:B:41:THR:CG2	1:B:43:ARG:HB2	2.30	0.61
1:A:466:LEU:CD2	1:A:551:PHE:HE2	2.13	0.60
1:B:422:ARG:HA	1:B:426:MET:HE2	1.84	0.60
1:B:445:CYS:SG	1:B:454:ILE:HD12	2.42	0.60
1:B:496:PRO:HG2	1:B:499:VAL:HG23	1.82	0.60
1:B:372:VAL:HG23	1:B:381:VAL:O	2.00	0.60
1:A:452:TYR:OH	1:A:550:TRP:HA	2.01	0.60
1:B:56:ARG:N	1:B:56:ARG:HD3	2.17	0.60
1:B:488:CYS:O	1:B:492:LEU:HD13	2.02	0.60
1:B:485:VAL:O	1:B:489:LEU:HG	2.02	0.60
1:B:414:MET:HE2	1:B:447:ILE:HG23	1.82	0.60
1:A:217:PHE:CE1	1:A:322:VAL:HB	2.36	0.60
1:B:455:GLU:HB2	1:B:458:ASP:OD2	2.02	0.59
1:B:217:PHE:CE1	1:B:322:VAL:HB	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.84	0.59
1:A:470:SER:O	1:A:474:LEU:HG	2.03	0.59
1:A:510:ARG:NH1	1:A:510:ARG:HG2	2.15	0.59
1:A:478:SER:O	1:A:482:ILE:HG13	2.02	0.59
1:B:139:MET:O	1:B:160:ILE:HG22	2.02	0.59
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.85	0.59
1:A:31:LEU:HD12	1:A:492:LEU:HD23	1.85	0.59
1:A:129:ASP:O	1:A:259:ARG:NH1	2.35	0.59
1:A:233:ILE:HD13	1:A:262:ILE:HA	1.86	0.58
1:A:104:GLY:O	1:A:108:VAL:HG23	2.04	0.57
1:A:515:GLY:HA2	1:A:519:ALA:HB2	1.86	0.57
1:A:369:ASN:O	1:A:384:LEU:HD12	2.03	0.57
1:B:346:TYR:O	1:B:347:SER:HB3	2.04	0.57
1:A:201:VAL:O	1:A:205:VAL:HG23	2.04	0.57
1:B:398:GLU:HA	1:B:401:ARG:O	2.05	0.57
1:A:515:GLY:CA	1:A:519:ALA:HB2	2.34	0.57
1:A:176:TYR:HE1	1:A:560:ILE:HD12	1.69	0.57
1:B:434:LEU:HD13	1:B:510:ARG:HB3	1.87	0.57
1:A:175:LEU:HD21	1:A:253:ILE:HG12	1.86	0.57
1:B:147:VAL:HG12	1:B:154:ARG:HG2	1.87	0.57
1:A:524:TYR:CD2	1:A:536:LEU:HG	2.40	0.57
1:A:179:VAL:HG12	1:A:289:CYS:CB	2.35	0.56
1:B:369:ASN:O	1:B:384:LEU:HD12	2.05	0.56
1:A:292:THR:OG1	1:A:317:GLY:HA2	2.04	0.56
1:B:123:TRP:HH2	1:B:174:ALA:HB2	1.69	0.56
1:B:48:ARG:CG	1:B:159:LEU:HD13	2.34	0.56
1:A:422:ARG:HG2	1:A:426:MET:HE2	1.87	0.56
1:B:197:PRO:HB2	1:B:467:HIS:HE1	1.71	0.56
1:A:461:GLN:CG	1:A:539:ILE:HG21	2.35	0.56
1:A:499:VAL:O	1:A:503:ARG:HG3	2.05	0.56
1:B:422:ARG:HG2	1:B:426:MET:HE2	1.88	0.56
1:A:340:THR:CG2	1:A:350:PRO:HG3	2.36	0.56
1:B:374:HIS:HA	1:B:379:LYS:O	2.06	0.56
1:A:284:VAL:HG22	1:A:287:THR:OG1	2.06	0.56
1:B:131:VAL:HG12	1:B:132:THR:N	2.21	0.56
1:A:501:ARG:NH1	1:A:505:ARG:NH2	2.53	0.55
1:B:309:GLN:O	1:B:324:CYS:HB2	2.06	0.55
1:A:45:ALA:O	1:A:49:GLN:HG3	2.07	0.55
1:B:97:ALA:O	1:B:165:LEU:HD22	2.06	0.55
1:B:440:GLU:HB3	1:B:457:LEU:HD12	1.89	0.55
1:A:236:GLU:OE2	1:A:280:ARG:NH2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ALA:HB3	1:A:417:PRO:HD3	1.89	0.55
1:A:217:PHE:CZ	1:A:322:VAL:HB	2.42	0.54
1:A:440:GLU:OE1	1:A:440:GLU:N	2.40	0.54
1:A:457:LEU:HB3	1:A:517:ARG:HB3	1.88	0.54
1:A:165:LEU:HD13	1:A:168:ARG:HH21	1.72	0.54
1:A:215:MET:C	1:A:215:MET:SD	2.86	0.53
1:B:196:SER:OG	1:B:199:GLN:HG3	2.08	0.53
1:B:451:CYS:O	1:B:561:TYR:CD2	2.61	0.53
1:B:233:ILE:HD13	1:B:262:ILE:HA	1.90	0.53
1:A:123:TRP:CH2	1:A:174:ALA:HB2	2.43	0.53
1:B:249:ALA:O	1:B:253:ILE:HG13	2.08	0.53
1:B:368:SER:HA	1:B:386:ARG:HB3	1.90	0.53
1:A:202:GLU:HG2	1:A:206:ASN:ND2	2.24	0.53
1:A:359:ASP:HB3	1:A:362:LEU:HD12	1.89	0.53
1:A:123:TRP:HH2	1:A:174:ALA:HB2	1.74	0.53
1:A:83:LEU:CB	1:A:173:MET:HA	2.39	0.53
1:A:527:ASN:HD21	1:A:534:LEU:N	2.07	0.53
1:A:423:MET:HE1	2:A:5001:154:H21	1.90	0.53
1:A:60:LEU:HD13	1:A:64:TYR:CE2	2.44	0.53
1:A:175:LEU:HD13	1:A:286:THR:CG2	2.39	0.52
1:A:182:LEU:HD22	1:A:293:LEU:HD11	1.91	0.52
1:B:94:PRO:HD3	1:B:561:TYR:CD2	2.43	0.52
1:B:396:ALA:O	1:B:399:THR:HB	2.09	0.52
1:A:110:ASN:O	1:A:111:LEU:HB2	2.10	0.52
1:B:294:THR:HG22	1:B:298:LYS:HE3	1.91	0.52
1:B:93:PRO:HB2	1:B:96:SER:HB2	1.90	0.52
1:A:364:THR:HA	1:A:368:SER:O	2.11	0.51
1:A:464:GLU:OE2	1:A:469:LEU:HD21	2.10	0.51
1:B:235:VAL:O	1:B:239:ILE:HG13	2.10	0.51
1:A:48:ARG:CG	1:A:159:LEU:HD13	2.40	0.51
1:A:519:ALA:O	1:A:523:LYS:HB2	2.09	0.51
1:B:31:LEU:HG	1:B:492:LEU:HB3	1.90	0.51
1:A:197:PRO:HB2	1:A:467:HIS:HE1	1.75	0.51
1:B:38:TYR:CD2	1:B:154:ARG:HD2	2.46	0.51
1:A:504:ALA:HB1	1:A:526:PHE:CD1	2.46	0.51
1:B:73:ALA:O	1:B:76:SER:HB2	2.11	0.51
1:B:535:LYS:HG3	1:B:536:LEU:H	1.76	0.51
1:A:33:HIS:HB2	1:A:492:LEU:O	2.11	0.51
1:B:187:MET:HG2	1:B:296:TYR:CG	2.46	0.51
1:B:337:ARG:HB3	1:B:337:ARG:NH1	2.26	0.51
1:A:31:LEU:HD23	1:A:31:LEU:C	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLN:HG2	1:A:539:ILE:HG21	1.93	0.51
1:B:207:THR:HG22	1:B:323:ILE:HG21	1.93	0.51
1:A:408:TRP:O	1:A:412:ILE:HG13	2.11	0.51
1:B:446:GLN:HE21	1:B:451:CYS:HB2	1.76	0.51
1:A:30:LEU:O	1:A:494:VAL:HA	2.10	0.51
1:A:197:PRO:O	1:A:201:VAL:HG23	2.11	0.50
1:B:47:LEU:O	1:B:50:LYS:HB2	2.11	0.50
1:A:527:ASN:HD21	1:A:534:LEU:HB2	1.75	0.50
1:A:231:ASN:O	1:A:235:VAL:HG23	2.11	0.50
1:A:508:ARG:CZ	1:A:512:LEU:HD11	2.41	0.50
1:B:545:LEU:HB3	1:B:547:LEU:HD13	1.93	0.50
1:A:202:GLU:HG2	1:A:206:ASN:HD21	1.75	0.50
1:B:182:LEU:HB3	1:B:183:PRO:HD3	1.93	0.50
1:B:523:LYS:O	1:B:527:ASN:HB2	2.12	0.50
1:B:422:ARG:HA	1:B:426:MET:HE3	1.91	0.50
1:A:138:ILE:HG23	1:A:138:ILE:O	2.10	0.50
1:B:236:GLU:OE2	1:B:280:ARG:NH2	2.39	0.50
1:B:491:LYS:HG2	1:B:492:LEU:HD12	1.93	0.50
1:A:7:THR:HG23	1:A:275:GLY:HA2	1.94	0.50
1:A:388:PRO:HG2	1:A:488:CYS:SG	2.52	0.50
1:B:508:ARG:CZ	1:B:512:LEU:HD11	2.42	0.50
1:B:439:LEU:HD23	1:B:457:LEU:HD21	1.93	0.49
1:A:381:VAL:HG11	1:A:474:LEU:HD22	1.93	0.49
1:B:46:GLY:O	1:B:50:LYS:HD3	2.11	0.49
1:A:447:ILE:HB	1:A:452:TYR:HE2	1.77	0.49
1:A:237:GLU:HG3	1:A:257:THR:OG1	2.12	0.49
1:B:239:ILE:O	1:B:242:CYS:HB2	2.12	0.49
1:A:375:ASP:OD1	1:A:377:SER:N	2.44	0.49
1:A:309:GLN:O	1:A:324:CYS:HB2	2.12	0.49
1:A:179:VAL:HG12	1:A:289:CYS:HB3	1.95	0.49
1:A:59:VAL:HG13	1:B:59:VAL:HG13	1.94	0.49
1:A:457:LEU:O	1:A:460:PRO:HD2	2.12	0.49
1:A:83:LEU:HB2	1:A:173:MET:HA	1.95	0.49
1:A:175:LEU:HD12	1:A:261:TYR:OH	2.12	0.49
1:A:294:THR:CG2	1:A:298:LYS:HE3	2.43	0.49
1:A:99:SER:C	1:A:101:PHE:H	2.15	0.49
1:A:346:TYR:O	1:A:347:SER:HB3	2.12	0.49
1:B:337:ARG:CB	1:B:337:ARG:HH11	2.25	0.49
1:A:485:VAL:O	1:A:489:LEU:HG	2.12	0.49
1:A:447:ILE:HG21	1:A:551:PHE:CE1	2.48	0.48
1:A:182:LEU:CD2	1:A:293:LEU:HD11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ARG:O	1:A:507:VAL:HG23	2.13	0.48
1:A:360:LEU:C	1:A:362:LEU:H	2.17	0.48
1:B:419:LEU:HD22	1:B:482:ILE:HG12	1.95	0.48
1:B:141:LYS:CE	1:B:160:ILE:HD13	2.43	0.48
1:A:414:MET:HE1	1:A:551:PHE:CE1	2.48	0.48
1:B:294:THR:O	1:B:298:LYS:HG3	2.14	0.48
1:B:561:TYR:CG	1:B:562:HIS:N	2.82	0.48
1:B:234:ARG:NH1	1:B:258:GLU:OE2	2.39	0.48
1:A:139:MET:O	1:A:160:ILE:HG22	2.13	0.48
1:B:381:VAL:HG11	1:B:474:LEU:CD2	2.42	0.47
1:B:233:ILE:CD1	1:B:262:ILE:HA	2.43	0.47
1:A:359:ASP:O	1:A:362:LEU:HB2	2.13	0.47
1:B:340:THR:CG2	1:B:350:PRO:HG3	2.44	0.47
1:A:24:ASN:ND2	1:A:400:ALA:HA	2.29	0.47
1:A:292:THR:OG1	1:A:317:GLY:N	2.46	0.47
1:A:523:LYS:HE2	1:A:534:LEU:HD23	1.96	0.47
1:A:88:ALA:HB1	1:A:169:VAL:HG13	1.96	0.47
1:A:183:PRO:HB2	1:A:191:TYR:CE2	2.49	0.47
1:A:19:SER:H	1:A:20:LYS:NZ	2.12	0.47
1:B:38:TYR:CG	1:B:154:ARG:HD2	2.50	0.47
1:A:236:GLU:O	1:A:239:ILE:HB	2.15	0.47
1:A:234:ARG:NH1	1:A:258:GLU:OE2	2.41	0.47
1:A:414:MET:HE1	1:A:551:PHE:HE1	1.80	0.47
1:A:182:LEU:HB3	1:A:183:PRO:HD3	1.95	0.47
1:B:104:GLY:O	1:B:107:ASP:HB2	2.14	0.47
1:A:292:THR:OG1	1:A:317:GLY:CA	2.64	0.46
1:A:182:LEU:HD11	1:A:239:ILE:HG22	1.96	0.46
1:A:59:VAL:CG1	1:B:59:VAL:HG13	2.44	0.46
1:A:461:GLN:HG3	1:A:539:ILE:HG21	1.95	0.46
1:A:22:PRO:HG2	1:A:401:ARG:CG	2.43	0.46
1:A:396:ALA:O	1:A:399:THR:HB	2.15	0.46
1:B:84:SER:O	1:B:85:VAL:C	2.54	0.46
1:A:161:VAL:O	1:A:283:GLY:N	2.44	0.46
1:B:123:TRP:CH2	1:B:174:ALA:HB2	2.50	0.46
1:A:508:ARG:HE	1:A:530:VAL:HG11	1.81	0.46
1:A:81:LYS:N	1:A:177:ASP:OD2	2.37	0.46
1:B:388:PRO:HG2	1:B:488:CYS:SG	2.55	0.46
1:B:43:ARG:HH11	1:B:43:ARG:HG3	1.81	0.46
1:B:102:GLY:O	1:B:114:LYS:HE2	2.15	0.46
1:A:204:LEU:HD21	1:A:314:LEU:HD23	1.98	0.46
1:A:399:THR:O	1:A:399:THR:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:HIS:HB2	1:B:500:TRP:CZ3	2.51	0.45
1:A:20:LYS:H	1:A:20:LYS:CD	2.24	0.45
1:A:89:CYS:HB3	1:A:108:VAL:O	2.16	0.45
1:A:439:LEU:O	1:A:457:LEU:HG	2.17	0.45
1:A:412:ILE:HD13	1:A:426:MET:HG2	1.98	0.45
1:B:26:LEU:HD13	1:B:432:ILE:HD13	1.97	0.45
1:A:215:MET:HB2	1:A:326:SER:CB	2.39	0.45
1:A:458:ASP:CG	1:A:517:ARG:HH22	2.20	0.45
1:A:59:VAL:HG13	1:B:59:VAL:CG1	2.46	0.45
1:B:161:VAL:O	1:B:283:GLY:N	2.42	0.45
1:B:419:LEU:CD2	1:B:482:ILE:HG12	2.47	0.45
1:B:273:ASN:ND2	1:B:275:GLY:H	2.14	0.45
1:B:464:GLU:OE2	1:B:538:PRO:HA	2.17	0.45
1:A:374:HIS:HA	1:A:379:LYS:O	2.16	0.45
1:B:563:SER:O	1:B:565:SER:N	2.50	0.45
1:B:219:TYR:CZ	1:B:350:PRO:HB3	2.52	0.45
1:A:211:LYS:HB2	1:A:214:PRO:HB3	1.98	0.45
1:B:499:VAL:O	1:B:503:ARG:HG3	2.16	0.45
1:B:489:LEU:HD22	1:B:494:VAL:HG11	1.98	0.44
1:B:26:LEU:HD13	1:B:432:ILE:CD1	2.47	0.44
1:B:79:LYS:HA	1:B:244:ASP:HB3	1.99	0.44
1:A:466:LEU:CD2	1:A:551:PHE:CE2	2.98	0.44
1:B:464:GLU:OE2	1:B:469:LEU:HD21	2.17	0.44
1:B:138:ILE:HG23	1:B:138:ILE:O	2.16	0.44
1:A:408:TRP:HB2	1:A:429:PHE:CE2	2.53	0.44
1:A:539:ILE:HB	1:A:542:ALA:HB2	1.98	0.44
1:B:492:LEU:HD12	1:B:492:LEU:N	2.32	0.44
1:A:461:GLN:HB3	1:A:542:ALA:HA	1.99	0.44
1:B:179:VAL:HG12	1:B:289:CYS:CB	2.47	0.44
1:B:204:LEU:HD21	1:B:314:LEU:CD2	2.48	0.44
1:B:313:MET:HG2	1:B:322:VAL:HG22	1.99	0.44
1:A:465:ARG:HD3	1:A:542:ALA:O	2.16	0.44
1:B:81:LYS:HE2	1:B:81:LYS:HA	1.98	0.44
1:B:144:VAL:HB	1:B:394:ARG:HG2	2.00	0.44
1:B:422:ARG:NH2	1:B:472:PHE:O	2.51	0.44
1:A:508:ARG:NE	1:A:530:VAL:HG11	2.33	0.44
1:A:526:PHE:C	1:A:528:TRP:H	2.21	0.44
1:B:441:LYS:O	1:B:443:LEU:HG	2.18	0.44
1:B:492:LEU:N	1:B:492:LEU:CD1	2.81	0.44
1:A:535:LYS:HG3	1:A:536:LEU:H	1.83	0.44
1:B:160:ILE:HG23	1:B:160:ILE:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:VAL:HG12	1:B:289:CYS:SG	2.59	0.43
1:A:113:SER:O	1:A:117:ASN:ND2	2.52	0.43
1:A:23:ILE:HG23	1:A:27:SER:CB	2.47	0.43
1:B:187:MET:HG2	1:B:296:TYR:CD2	2.53	0.43
1:B:52:VAL:HB	1:B:226:SER:OG	2.18	0.43
1:B:215:MET:SD	1:B:215:MET:C	2.97	0.43
1:B:308:LEU:CD1	1:B:335:SER:HB3	2.48	0.43
1:B:372:VAL:CG2	1:B:373:ALA:N	2.81	0.43
1:B:337:ARG:HB3	1:B:337:ARG:HH11	1.83	0.43
1:B:175:LEU:HD12	1:B:261:TYR:OH	2.19	0.43
1:A:555:TYR:CD1	1:A:560:ILE:HG13	2.53	0.43
1:B:313:MET:HE3	1:B:313:MET:HB2	1.79	0.43
1:A:496:PRO:HG2	1:A:499:VAL:CG2	2.42	0.43
1:A:125:ASP:O	1:A:129:ASP:HB3	2.19	0.43
1:A:172:LYS:CE	1:A:559:ASP:O	2.67	0.43
1:A:422:ARG:HD3	2:A:5001:154:CL14	2.55	0.43
1:A:510:ARG:O	1:A:514:GLN:HG2	2.18	0.43
1:A:33:HIS:HB3	1:A:36:MET:CG	2.49	0.43
1:B:517:ARG:HH11	1:B:517:ARG:HG2	1.84	0.43
1:A:160:ILE:HG23	1:A:160:ILE:O	2.19	0.43
1:B:94:PRO:HD3	1:B:561:TYR:CG	2.54	0.43
1:A:30:LEU:O	1:A:494:VAL:HG13	2.18	0.43
1:B:56:ARG:N	1:B:56:ARG:CD	2.82	0.43
1:A:368:SER:CB	1:A:384:LEU:HD11	2.49	0.43
1:A:526:PHE:HA	1:A:528:TRP:NE1	2.33	0.43
1:B:440:GLU:N	1:B:440:GLU:OE1	2.50	0.43
1:A:504:ALA:HB1	1:A:526:PHE:HD1	1.83	0.42
1:A:372:VAL:HG22	1:A:373:ALA:N	2.34	0.42
1:B:406:ASN:ND2	1:B:443:LEU:HB3	2.33	0.42
1:A:102:GLY:C	1:A:114:LYS:HE3	2.40	0.42
1:A:235:VAL:O	1:A:239:ILE:HG13	2.19	0.42
1:A:97:ALA:O	1:A:165:LEU:HD22	2.19	0.42
1:A:428:HIS:HB2	1:A:500:TRP:CZ3	2.55	0.42
1:B:176:TYR:HE1	1:B:560:ILE:HD12	1.84	0.42
1:B:561:TYR:CD1	1:B:562:HIS:N	2.88	0.42
1:B:82:LEU:HD12	1:B:173:MET:O	2.20	0.42
1:B:217:PHE:CZ	1:B:322:VAL:HB	2.54	0.42
1:A:79:LYS:HG2	1:A:79:LYS:O	2.20	0.42
1:A:320:LEU:HD12	1:A:321:VAL:H	1.85	0.42
1:A:447:ILE:C	1:A:449:GLY:N	2.73	0.42
1:B:523:LYS:HG3	1:B:534:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:ILE:O	1:B:542:ALA:HB3	2.19	0.42
2:A:5001:154:H231	2:A:5001:154:H162	1.72	0.41
1:A:92:THR:HA	1:A:93:PRO:HD3	1.93	0.41
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.59	0.41
1:B:22:PRO:HG2	1:B:401:ARG:HG3	2.02	0.41
1:B:535:LYS:O	1:B:536:LEU:HB2	2.20	0.41
1:B:308:LEU:HB3	1:B:311:CYS:SG	2.60	0.41
1:A:385:THR:OG1	1:A:386:ARG:N	2.53	0.41
1:A:203:PHE:CE2	1:A:314:LEU:HD13	2.54	0.41
1:A:31:LEU:HG	1:A:492:LEU:HB3	2.00	0.41
1:B:130:THR:O	1:B:130:THR:OG1	2.36	0.41
1:A:427:THR:HA	1:A:526:PHE:CZ	2.55	0.41
1:A:40:THR:O	1:A:142:ASN:HA	2.20	0.41
1:A:33:HIS:ND1	1:A:491:LYS:O	2.53	0.41
1:A:92:THR:HG21	1:A:165:LEU:HD11	2.03	0.41
1:A:207:THR:CG2	1:A:312:THR:HG21	2.50	0.41
1:A:361:GLU:HG2	1:A:370:VAL:O	2.21	0.41
1:A:215:MET:CB	1:A:326:SER:HB2	2.41	0.41
1:B:545:LEU:HB3	1:B:547:LEU:CD1	2.50	0.41
1:A:368:SER:HB2	1:A:384:LEU:HD11	2.03	0.41
1:A:340:THR:HG21	1:A:350:PRO:HG3	2.02	0.41
1:B:118:HIS:O	1:B:121:SER:N	2.54	0.41
1:B:434:LEU:HD21	1:B:511:LEU:HD23	2.03	0.41
1:A:200:ARG:O	1:A:204:LEU:HG	2.20	0.41
1:A:132:THR:O	1:A:259:ARG:HB3	2.21	0.41
1:B:92:THR:HA	1:B:93:PRO:HD3	1.94	0.41
1:A:41:THR:OG1	1:A:43:ARG:HB2	2.21	0.41
1:A:243:CYS:HB2	1:A:245:LEU:HG	2.03	0.41
1:A:326:SER:OG	1:A:332:ASP:OD2	2.37	0.41
1:B:465:ARG:HH11	1:B:465:ARG:CG	2.33	0.41
1:A:389:THR:HA	1:A:488:CYS:SG	2.61	0.41
1:B:191:TYR:O	1:B:194:GLN:HG2	2.21	0.41
1:B:20:LYS:HZ3	1:B:20:LYS:H	1.68	0.41
1:B:336:LEU:CD1	1:B:356:PRO:HD3	2.45	0.40
1:A:96:SER:O	1:A:97:ALA:C	2.59	0.40
1:B:444:ASP:HB3	1:B:451:CYS:SG	2.61	0.40
1:B:200:ARG:HH21	1:B:365:SER:HB2	1.86	0.40
1:B:172:LYS:NZ	1:B:559:ASP:HB3	2.36	0.40
1:A:439:LEU:HG	1:A:457:LEU:CD2	2.52	0.40
1:A:123:TRP:HE3	1:A:170:CYS:SG	2.45	0.40
1:B:96:SER:O	1:B:97:ALA:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:HH11	1:A:43:ARG:HG3	1.85	0.40
1:B:386:ARG:NH2	1:B:391:PRO:HD3	2.37	0.40
1:B:510:ARG:CG	1:B:510:ARG:NH1	2.80	0.40
1:A:359:ASP:OD1	1:A:359:ASP:C	2.60	0.40
1:A:310:ASP:O	1:A:324:CYS:HA	2.21	0.40
1:B:101:PHE:CD2	1:B:118:HIS:CE1	3.09	0.40
1:B:40:THR:O	1:B:142:ASN:HA	2.22	0.40
1:B:346:TYR:O	1:B:347:SER:CB	2.70	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	554/578 (96%)	508 (92%)	44 (8%)	2 (0%)	39	74
1	B	557/578 (96%)	504 (90%)	47 (8%)	6 (1%)	17	51
All	All	1111/1156 (96%)	1012 (91%)	91 (8%)	8 (1%)	26	63

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	VAL
1	A	90	LYS
1	B	564	LEU
1	A	536	LEU
1	B	97	ALA
1	B	536	LEU
1	B	90	LYS
1	B	540	PRO

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	476/492 (97%)	461 (97%)	15 (3%)	46 81
1	B	479/492 (97%)	461 (96%)	18 (4%)	40 76
All	All	955/984 (97%)	922 (96%)	33 (4%)	43 78

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	83	LEU
1	A	106	LYS
1	A	131	VAL
1	A	170	CYS
1	A	179	VAL
1	A	197	PRO
1	A	220	ASP
1	A	237	GLU
1	A	303	CYS
1	A	318	ASP
1	A	337	ARG
1	A	407	SER
1	A	440	GLU
1	A	510	ARG
1	B	14	CYS
1	B	20	LYS
1	B	47	LEU
1	B	56	ARG
1	B	57	LEU
1	B	86	GLU
1	B	120	HIS
1	B	262	ILE
1	B	303	CYS
1	B	308	LEU
1	B	355	GLN
1	B	366	CYS

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Mol	Chain	Res	Type
1	B	377	SER
1	B	407	SER
1	B	440	GLU
1	B	466	LEU
1	B	510	ARG
1	B	534	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	273	ASN
1	A	467	HIS
1	A	527	ASN
1	A	544	GLN
1	B	49	GLN
1	B	184	GLN
1	B	206	ASN
1	B	231	ASN
1	B	273	ASN
1	B	406	ASN
1	B	446	GLN
1	B	467	HIS
1	B	527	ASN
1	B	544	GLN
1	B	562	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (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	$\#\|Z\| > 2$
2	154	A	5001	-	32,41,41	2.31	17 (53%)	35,58,58	1.23	5 (14%)
2	154	B	6001	-	32,41,41	2.15	14 (43%)	35,58,58	1.38	6 (17%)

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
2	154	A	5001	-	-	0/20/28/28	0/4/5/5
2	154	B	6001	-	-	0/20/28/28	0/4/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6001	154	C19-C18	2.01	1.43	1.38
2	B	6001	154	C12-C11	2.21	1.42	1.38
2	A	5001	154	C12-C13	2.24	1.42	1.38
2	A	5001	154	C12-C11	2.26	1.42	1.38
2	B	6001	154	C12-C13	2.28	1.42	1.38
2	A	5001	154	C19-C18	2.33	1.43	1.38
2	B	6001	154	C22-C17	2.43	1.44	1.38
2	A	5001	154	C21-C22	2.44	1.43	1.38
2	B	6001	154	C18-C17	2.44	1.44	1.38
2	A	5001	154	C18-C17	2.48	1.44	1.38
2	A	5001	154	C16-C2	2.51	1.58	1.54
2	A	5001	154	C10-C11	2.51	1.42	1.38
2	A	5001	154	C8-C13	2.61	1.43	1.39
2	B	6001	154	C34-C35	2.70	1.42	1.36
2	A	5001	154	C22-C17	2.72	1.44	1.38
2	B	6001	154	C33-C32	2.73	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6001	154	C34-C33	2.82	1.45	1.38
2	A	5001	154	C23-C24	2.84	1.55	1.51
2	A	5001	154	C33-C32	2.85	1.43	1.36
2	B	6001	154	C2-N1	2.86	1.51	1.47
2	B	6001	154	C16-C2	2.89	1.59	1.54
2	B	6001	154	C23-N1	2.92	1.51	1.46
2	A	5001	154	C34-C35	2.94	1.43	1.36
2	A	5001	154	C34-C33	2.98	1.45	1.38
2	B	6001	154	C35-C36	3.02	1.44	1.38
2	A	5001	154	C35-C36	3.29	1.45	1.38
2	A	5001	154	C2-N1	3.35	1.52	1.47
2	B	6001	154	C8-C13	3.36	1.44	1.39
2	A	5001	154	C23-N1	3.85	1.53	1.46
2	A	5001	154	C6-N1	4.79	1.43	1.35
2	B	6001	154	C6-N1	4.89	1.43	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	6001	154	C12-C13-C8	-3.55	119.22	121.59
2	B	6001	154	O7-C6-C8	-2.56	114.92	120.14
2	A	5001	154	O7-C6-C8	-2.28	115.50	120.14
2	A	5001	154	C12-C13-C8	-2.23	120.10	121.59
2	B	6001	154	C23-N1-C6	2.13	123.22	117.55
2	A	5001	154	C17-C16-C2	2.48	118.78	113.95
2	B	6001	154	C17-C16-C2	2.66	119.13	113.95
2	A	5001	154	C24-C23-N1	2.77	117.82	113.45
2	B	6001	154	C8-C6-N1	2.97	122.00	117.78
2	A	5001	154	C8-C6-N1	3.13	122.23	117.78
2	B	6001	154	C24-C23-N1	3.14	118.39	113.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5001	154	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	558/578 (96%)	0.08	34 (6%)	25	18	8, 28, 63, 102	0
1	B	561/578 (97%)	0.20	34 (6%)	25	18	9, 29, 70, 99	0
All	All	1119/1156 (96%)	0.14	68 (6%)	25	18	8, 29, 68, 102	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	549	GLY	11.1
1	B	563	SER	9.2
1	B	550	TRP	8.8
1	A	550	TRP	8.8
1	A	561	TYR	8.2
1	B	561	TYR	7.9
1	B	548	SER	7.5
1	B	566	ARG	6.8
1	B	565	SER	6.8
1	A	548	SER	6.7
1	A	549	GLY	6.6
1	A	563	SER	6.6
1	A	560	ILE	6.6
1	B	544	GLN	6.5
1	B	546	ASP	6.4
1	A	562	HIS	6.0
1	B	542	ALA	5.9
1	B	556	SER	5.9
1	B	543	SER	5.7
1	B	560	ILE	5.6
1	A	556	SER	5.3
1	B	564	LEU	5.3
1	A	546	ASP	5.2
1	A	448	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	541	ALA	4.8
1	A	544	GLN	4.7
1	B	545	LEU	4.6
1	A	559	ASP	4.6
1	A	542	ALA	4.6
1	B	547	LEU	4.5
1	A	545	LEU	4.1
1	B	559	ASP	4.0
1	B	551	PHE	3.9
1	A	547	LEU	3.9
1	A	543	SER	3.9
1	B	555	TYR	3.8
1	B	562	HIS	3.7
1	B	558	GLY	3.6
1	A	541	ALA	3.3
1	B	329	THR	3.1
1	A	555	TYR	2.9
1	B	552	VAL	2.9
1	A	540	PRO	2.8
1	A	535	LYS	2.6
1	B	447	ILE	2.6
1	A	447	ILE	2.5
1	A	552	VAL	2.5
1	B	113	SER	2.5
1	B	94	PRO	2.5
1	B	554	GLY	2.5
1	A	106	LYS	2.4
1	B	448	TYR	2.4
1	B	95	HIS	2.4
1	A	557	GLY	2.3
1	A	553	ALA	2.2
1	A	93	PRO	2.2
1	B	553	ALA	2.2
1	A	531	LYS	2.2
1	A	148	GLN	2.2
1	A	554	GLY	2.2
1	B	309	GLN	2.1
1	B	213	ASN	2.1
1	A	558	GLY	2.1
1	A	309	GLN	2.1
1	A	113	SER	2.1
1	B	530	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	454	ILE	2.1
1	A	551	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	154	A	5001	37/37	0.81	0.30	2.28	37,44,58,59	0
2	154	B	6001	37/37	0.79	0.35	2.27	40,46,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.