



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:25 PM GMT

PDB ID : 1TL3  
Title : Crystal structure of hiv-1 reverse transcriptase in complex with gw450557  
Authors : Hopkins, A.L.; Ren, J.; Stuart, D.I.; Stammers, D.K.  
Deposited on : 2004-06-09  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

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

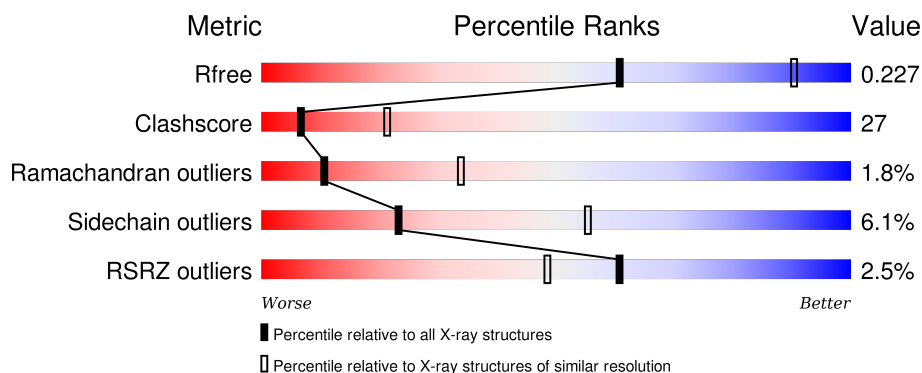
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	B	440	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7612 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 Pol polyprotein, Reverse transcriptase, Chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			4247	2754	701	784	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	OXIDIZED CYS	UNP P04585

- Molecule 2 is a protein called Pol polyprotein, Reverse transcriptase, Chain B.

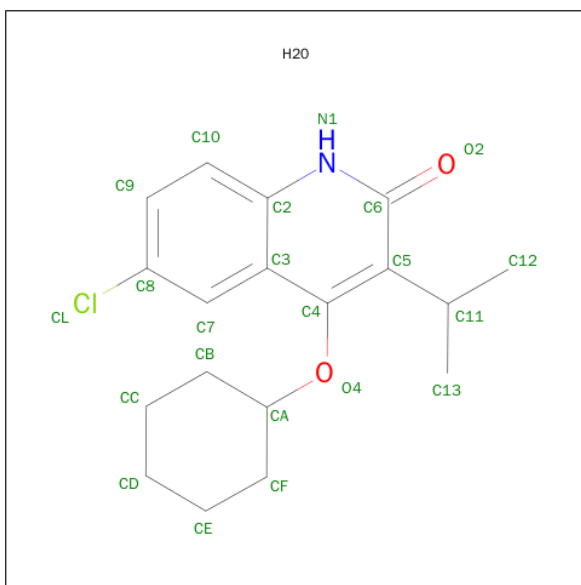
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3328	2173	548	600	7			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 4 is 6-CHLORO-4-(CYCLOHEXYLOXY)-3-ISOPROPYLQUINOLIN-2(1H)-ONE (three-letter code: H20) (formula:  $C_{18}H_{22}ClNO_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			22	18	1	1	2		

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 ( $\text{RSRZ} > 2$ ). 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.

- Chain A:

LEU	VAL	SER	ALA	GLY	ILE	ARG	LYS	VAL	LEU
K476	W402	L479	Q480	Q481	W406	Q407	A408	E492	D498
									S499
									Q500
									Y501
									A502
									L503
									G504
									I505
									I506
									Q507
									A508
									Q509
									P510
									E514
									L517
									V518
									N519
									Q520
									I521
									I522
									E523
									Q524
									L525
									I526
									K527
									K528
									E529
									K530
									W535
									P537
									ALA
									HIS
									GLY
									GLY
									ILE
									GLY
									GLY
									ASN
									GLU
									GLN
									VAL
									ASP
									P570

PRO  
ILE  
SER  
P4  
I5  
E6  
T7  
V8  
P9  
K11  
L12  
K13  
P14  
D17  
G18  
P19  
K20  
W24  
T27  
E28  
E29  
K30  
I37  
C38  
T39  
E40  
M41  
E42  
K43  
I47  
I50  
E53  
M54  
P55  
P56  
F61  
A62  
I63  
L63  
LYS  
LYS  
LYS  
ASP  
SER  
THR  
K70  
W71  
K72  
K73  
L74  
E70

Q151  
R83  
T84  
E89  
V90  
Q91  
G93  
I94  
P95  
L100  
K101  
K104  
S105  
I106  
T107  
Q182  
I108  
I109  
D110  
V111  
G112  
D113  
A114  
V115  
F116  
S117  
V118  
P119  
L120  
D121  
E122  
R125  
K126  
I127  
T128  
A129  
I132  
P133  
S134  
I135  
N136  
H137  
E138  
T139  
P140  
G141  
I142  
R143  
Q145  
Y146  
L149  
E150  
P156  
F160  
M164  
L168  
E169  
P170  
F171  
R172  
L100  
K101  
T178  
V179  
I180  
Y181  
Q182  
I183  
M184  
D185  
I186  
L187  
Y188  
V189  
G190  
S191  
D192  
L193  
E194  
I195  
G196  
Q197  
H198  
K201  
I202  
E203  
E204  
L205  
R206  
Q207  
H208  
L209  
K287  
L210  
E288  
L289  
T290  
E291  
V292  
I293  
E298  
L303  
Q222  
K223  
E224  
P226  
F227  
L228  
W229  
K230  
G231  
Y232  
E233  
L234  
H235  
K238  
W239  
T240  
V241  
Q242  
K243  
I244  
V245  
L246  
Q247  
E248  
K249  
T253  
V254  
M255  
D256  
I257  
L260  
V261  
L193  
N265  
I270  
Y271  
K277  
Q278  
L279  
L282  
L283  
T286  
K287  
E288  
L289  
T290  
E291  
V292  
I293  
E298  
L303  
Q222  
K223  
E224  
P226  
F227  
L228  
W229  
K230  
G231  
Y232  
E233  
L234  
H235  
K238  
W239  
T240  
V241  
Q242  
K243  
I244  
V245  
L246  
Q247  
E248  
K249  
T253  
V254  
M255  
D256  
I257  
L260  
V261  
L193  
N265  
I270  
Y271  
K277  
Q278  
L279  
L282  
L283  
T286  
K287  
E288  
L289  
T290  
E291  
V292  
I293  
E298  
L303  
Q222  
K223  
E224  
P226  
F227  
L228  
W229  
K230  
G231  
Y232  
E233  
L234  
H235  
K238  
W239  
T240  
V241  
Q242  
K243  
I244  
V245  
L246  
Q247  
E248  
K249  
T253  
V254  
M255  
D256  
I257  
L260  
V261  
L193  
N265  
I270  
Y271  
K277  
Q278  
L279  
L282  
L283  
T286  
K287  
E288  
L289  
T290  
E291  
V292  
I293  
E2

- Chain B:
- 
- 2% 43% 45% 9%

[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.00 Å   115.20 Å   65.30 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.85 – 2.80 29.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.5 (29.85-2.80) 92.5 (29.84-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.80 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.206   ,   0.286 0.197   ,   0.227	Depositor DCC
$R_{free}$ test set	1171 reflections (4.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.8	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 78.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 24373 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7612	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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, H2O

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	0.50	0/4352	0.71	0/5918
2	B	0.49	0/3425	0.70	0/4652
All	All	0.50	0/7777	0.70	0/10570

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	4247	0	4275	234	0
2	B	3328	0	3353	202	0
3	A	15	0	0	1	0
4	A	22	0	22	2	0
All	All	7612	0	7650	414	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 27.

All (414) 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:500:GLN:HE21	2:B:422:LEU:HD12	1.31	0.94
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.49	0.92
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.51	0.92
2:B:234:LEU:HD21	2:B:377:THR:HG21	1.52	0.91
1:A:253:THR:HG22	1:A:255:ASN:H	1.37	0.88
1:A:500:GLN:NE2	2:B:422:LEU:HD12	1.89	0.88
2:B:227:PHE:HB3	2:B:231:GLY:HA2	1.55	0.88
2:B:66:LYS:HE3	2:B:230:MET:HG3	1.58	0.86
2:B:266:TRP:O	2:B:269:GLN:HG2	1.77	0.85
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.76	0.84
1:A:354:TYR:HD2	1:A:374:LYS:HD2	1.43	0.83
2:B:362:THR:HG22	2:B:366:LYS:HD3	1.60	0.82
1:A:101:LYS:N	1:A:101:LYS:HD2	1.96	0.80
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.17	0.80
2:B:193:LEU:H	2:B:193:LEU:HD12	1.49	0.77
1:A:500:GLN:HE21	2:B:422:LEU:CD1	1.97	0.77
2:B:348:ASN:HD22	2:B:351:THR:CG2	1.99	0.76
2:B:227:PHE:HB3	2:B:231:GLY:CA	2.15	0.76
1:A:469:LEU:HD21	1:A:480:GLN:HG3	1.68	0.75
2:B:203:GLU:HG3	2:B:207:GLN:NE2	2.02	0.74
1:A:91:GLN:HE21	2:B:137:ASN:HB3	1.52	0.74
1:A:206:ARG:HG2	1:A:216:THR:OG1	1.87	0.73
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.70	0.73
2:B:295:LEU:HD12	2:B:295:LEU:N	2.02	0.73
2:B:193:LEU:N	2:B:193:LEU:HD12	2.03	0.73
2:B:40:GLU:HG3	2:B:44:GLU:OE2	1.89	0.73
1:A:113:ASP:HB2	1:A:116:PHE:CD2	2.24	0.73
1:A:28:GLU:OE1	1:A:135:ILE:HG22	1.89	0.71
1:A:111:VAL:HG12	1:A:114:ALA:HB2	1.71	0.71
2:B:239:TRP:HB3	2:B:350:LYS:NZ	2.07	0.70
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.27	0.69
1:A:480:GLN:HG2	1:A:517:LEU:HD11	1.75	0.69
1:A:178:ILE:HG12	1:A:191:SER:HB3	1.75	0.69
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.75	0.69
1:A:507:GLN:HE22	2:B:421:PRO:HB3	1.58	0.68
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.74	0.68
2:B:242:GLN:HG2	2:B:353:LYS:HG2	1.75	0.68
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.28	0.68
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.29	0.68
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.76	0.67
1:A:239:TRP:NE1	1:A:316:GLY:HA3	2.10	0.67
1:A:354:TYR:CD2	1:A:374:LYS:HD2	2.29	0.66

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:LEU:H	2:B:193:LEU:CD1	2.08	0.66
1:A:249:LYS:NZ	1:A:256:ASP:HB3	2.10	0.66
2:B:203:GLU:HG3	2:B:207:GLN:HE22	1.61	0.66
1:A:206:ARG:HH21	1:A:217:PRO:C	2.00	0.66
2:B:295:LEU:HD12	2:B:295:LEU:H	1.58	0.66
2:B:110:ASP:HB3	2:B:226:PRO:HG2	1.78	0.65
1:A:111:VAL:CG1	1:A:114:ALA:HB2	2.27	0.65
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.78	0.65
2:B:254:VAL:HG23	2:B:291:GLU:O	1.97	0.65
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.32	0.64
1:A:24:TRP:HZ3	1:A:61:PHE:HB3	1.62	0.64
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.32	0.64
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.61	0.64
1:A:91:GLN:NE2	2:B:137:ASN:HB3	2.12	0.64
1:A:62:ALA:C	1:A:63:ILE:HD12	2.18	0.64
1:A:360:ALA:HB1	1:A:514:GLU:OE1	1.97	0.64
2:B:66:LYS:HG2	2:B:230:MET:HA	1.80	0.64
1:A:228:LEU:H	1:A:228:LEU:HD12	1.61	0.64
1:A:206:ARG:HH21	1:A:218:ASP:HA	1.63	0.63
2:B:234:LEU:HD21	2:B:377:THR:CG2	2.26	0.63
1:A:476:LYS:HD2	1:A:476:LYS:O	1.98	0.63
1:A:507:GLN:NE2	2:B:421:PRO:HB3	2.13	0.63
1:A:476:LYS:HD3	1:A:517:LEU:HD12	1.79	0.63
2:B:183:TYR:CE1	2:B:184:MET:HG2	2.32	0.63
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.33	0.63
1:A:319:TYR:OH	1:A:385:LYS:HE2	1.98	0.63
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.80	0.62
2:B:254:VAL:O	2:B:258:GLN:HG3	1.99	0.62
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.81	0.62
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.35	0.62
1:A:330:GLN:HG2	1:A:338:THR:OG1	1.99	0.62
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.81	0.62
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.82	0.62
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.34	0.61
1:A:206:ARG:NH2	1:A:218:ASP:HA	2.15	0.61
2:B:249:LYS:HG3	2:B:252:TRP:CE2	2.36	0.61
1:A:105:SER:HB2	1:A:198:HIS:CD2	2.35	0.61
2:B:63:ILE:HD11	2:B:72:ARG:HD3	1.83	0.61
2:B:169:GLU:O	2:B:173:LYS:HG3	2.01	0.61
2:B:98:ALA:O	2:B:101:LYS:HG2	2.00	0.61
2:B:66:LYS:NZ	2:B:67:ASP:HB2	2.16	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLU:OE2	2:B:40:GLU:HA	2.01	0.60
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.35	0.60
1:A:136:ASN:OD1	1:A:139:THR:HG23	1.99	0.60
1:A:95:PRO:HB3	2:B:136:ASN:O	2.01	0.60
1:A:115:TYR:CD1	1:A:156:SER:HB3	2.37	0.60
2:B:66:LYS:HE3	2:B:230:MET:CG	2.31	0.60
1:A:249:LYS:HZ1	1:A:256:ASP:HB3	1.65	0.60
1:A:90:VAL:HG12	1:A:91:GLN:N	2.16	0.60
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.36	0.60
1:A:40:GLU:HA	1:A:40:GLU:OE2	2.02	0.60
2:B:168:LEU:C	2:B:170:PRO:HD2	2.22	0.59
1:A:396:GLU:HG3	1:A:397:THR:N	2.18	0.59
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.84	0.59
2:B:66:LYS:CG	2:B:230:MET:HA	2.31	0.59
1:A:125:ARG:HG2	1:A:146:TYR:O	2.03	0.59
1:A:253:THR:HG22	1:A:255:ASN:N	2.14	0.59
1:A:240:THR:OG1	1:A:241:VAL:N	2.35	0.59
1:A:24:TRP:CZ3	1:A:61:PHE:HB3	2.37	0.59
1:A:358:ARG:HD3	1:A:370:GLU:CD	2.22	0.59
1:A:206:ARG:HB3	1:A:206:ARG:HH11	1.68	0.58
1:A:522:ILE:O	1:A:526:ILE:HG13	2.04	0.58
2:B:297:GLU:O	2:B:301:LEU:HG	2.03	0.58
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.85	0.58
1:A:56:TYR:O	1:A:143:ARG:NH2	2.30	0.58
2:B:193:LEU:HD22	2:B:201:LYS:HD3	1.86	0.57
1:A:277:ARG:HH11	1:A:277:ARG:HG3	1.68	0.57
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.85	0.57
1:A:61:PHE:N	1:A:61:PHE:HD2	2.01	0.57
1:A:411:ILE:O	1:A:412:PRO:O	2.22	0.57
1:A:228:LEU:HA	1:A:232:TYR:O	2.05	0.57
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.40	0.57
1:A:132:ILE:HB	1:A:142:ILE:HG13	1.87	0.57
2:B:174:GLN:C	2:B:176:PRO:HD3	2.25	0.56
1:A:13:LYS:HE3	1:A:84:THR:O	2.06	0.56
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.51	0.56
1:A:376:THR:HG23	1:A:386:THR:HG22	1.86	0.56
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.41	0.56
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.41	0.56
1:A:61:PHE:N	1:A:61:PHE:CD2	2.72	0.56
1:A:18:GLY:HA3	1:A:56:TYR:CE1	2.40	0.56
2:B:167:ILE:O	2:B:208:HIS:HE1	1.89	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:HD23	1:A:282:LEU:HD11	1.87	0.55
2:B:166:LYS:O	2:B:169:GLU:HG3	2.06	0.55
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.07	0.55
2:B:332:GLN:HA	2:B:424:LYS:HE3	1.89	0.55
1:A:246:LEU:HD22	1:A:260:LEU:HD11	1.88	0.55
1:A:412:PRO:HG3	2:B:401:TRP:HZ2	1.72	0.55
1:A:24:TRP:HZ3	1:A:61:PHE:CG	2.25	0.55
1:A:115:TYR:O	1:A:149:LEU:HB2	2.06	0.55
1:A:40:GLU:OE2	1:A:43:LYS:HD3	2.07	0.55
2:B:183:TYR:OH	2:B:386:THR:HG23	2.07	0.55
2:B:195:ILE:HG23	2:B:196:GLY:N	2.22	0.54
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.88	0.54
1:A:257:ILE:O	1:A:261:VAL:HG23	2.06	0.54
1:A:498:ASP:HA	1:A:536:VAL:O	2.08	0.54
2:B:276:VAL:O	2:B:277:ARG:C	2.45	0.54
2:B:298:GLU:CD	2:B:298:GLU:H	2.11	0.54
1:A:332:GLN:HG2	1:A:332:GLN:O	2.08	0.54
2:B:197:GLN:O	2:B:201:LYS:HG3	2.07	0.54
1:A:228:LEU:N	1:A:228:LEU:HD12	2.22	0.54
1:A:216:THR:HB	1:A:217:PRO:HD2	1.90	0.53
2:B:125:ARG:HB3	2:B:145:GLN:NE2	2.23	0.53
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.90	0.53
1:A:265:ASN:N	1:A:265:ASN:HD22	2.05	0.53
2:B:305:GLU:O	2:B:309:ILE:HG13	2.09	0.53
1:A:406:TRP:O	2:B:331:LYS:HB3	2.08	0.53
2:B:295:LEU:CD1	2:B:295:LEU:N	2.72	0.53
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.90	0.53
2:B:182:GLN:HA	2:B:187:LEU:HD12	1.91	0.53
2:B:66:LYS:HZ2	2:B:67:ASP:HB2	1.72	0.53
1:A:469:LEU:HD21	1:A:480:GLN:CG	2.38	0.53
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.44	0.53
2:B:199:ARG:CZ	2:B:233:GLU:OE1	2.56	0.53
1:A:441:TYR:HB2	1:A:458:VAL:HG23	1.90	0.53
1:A:498:ASP:O	1:A:535:TRP:NE1	2.41	0.53
1:A:116:PHE:CD2	1:A:116:PHE:N	2.77	0.53
2:B:63:ILE:HG21	2:B:74:LEU:HD22	1.91	0.52
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.91	0.52
2:B:66:LYS:HD2	2:B:67:ASP:N	2.25	0.52
2:B:195:ILE:CG2	2:B:196:GLY:N	2.73	0.52
1:A:399:GLU:HG3	1:A:402:TRP:CE3	2.45	0.52
2:B:208:HIS:HA	2:B:211:ARG:HD3	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HG13	1:A:6:GLU:N	2.23	0.52
1:A:521:ILE:O	1:A:524:GLN:HB2	2.09	0.52
1:A:362:THR:HG22	1:A:366:LYS:HD3	1.93	0.51
1:A:505:ILE:O	1:A:510:PRO:HD3	2.10	0.51
2:B:229:TRP:CE3	2:B:229:TRP:HA	2.46	0.51
2:B:64:LYS:HE2	2:B:68:SER:O	2.10	0.51
2:B:202:ILE:HG21	2:B:227:PHE:HE1	1.74	0.51
2:B:175:ASN:N	2:B:176:PRO:HD3	2.25	0.51
1:A:37:ILE:O	1:A:41:MET:HG3	2.11	0.51
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.45	0.51
1:A:91:GLN:C	1:A:93:GLY:H	2.14	0.51
2:B:239:TRP:HB3	2:B:350:LYS:HZ1	1.74	0.51
2:B:239:TRP:CZ3	2:B:378:GLU:HG2	2.46	0.51
1:A:292:VAL:C	1:A:293:ILE:HD12	2.31	0.51
2:B:380:ILE:O	2:B:384:GLY:N	2.43	0.51
1:A:142:ILE:HD12	1:A:144:TYR:OH	2.11	0.51
1:A:101:LYS:HD2	1:A:101:LYS:H	1.73	0.51
1:A:175:ASN:OD1	1:A:201:LYS:HE3	2.11	0.51
1:A:129:ALA:HA	1:A:144:TYR:O	2.11	0.51
1:A:210:LEU:C	1:A:212:TRP:N	2.63	0.50
1:A:30:LYS:CD	1:A:62:ALA:HB3	2.40	0.50
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.10	0.50
2:B:195:ILE:HD11	2:B:233:GLU:HG3	1.93	0.50
2:B:57:ASN:HD22	2:B:143:ARG:HH11	1.58	0.50
1:A:476:LYS:CD	1:A:517:LEU:HD12	2.41	0.50
2:B:278:GLN:NE2	2:B:298:GLU:HB2	2.26	0.50
2:B:295:LEU:H	2:B:295:LEU:CD1	2.22	0.50
2:B:203:GLU:CG	2:B:207:GLN:HE22	2.24	0.50
1:A:472:THR:CB	1:A:476:LYS:HE3	2.42	0.50
1:A:63:ILE:N	1:A:63:ILE:HD12	2.27	0.50
2:B:348:ASN:HD22	2:B:351:THR:HG21	1.76	0.49
1:A:116:PHE:HE1	3:A:1302:PO4:O1	1.94	0.49
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.47	0.49
1:A:107:THR:HG21	1:A:222:GLN:NE2	2.27	0.49
1:A:226:PRO:HA	1:A:234:LEU:O	2.12	0.49
2:B:142:ILE:HG22	2:B:144:TYR:CE2	2.48	0.49
2:B:339:TYR:CD1	2:B:375:ILE:HD11	2.47	0.49
1:A:61:PHE:CE2	1:A:74:LEU:HG	2.47	0.49
1:A:279:LEU:HA	1:A:282:LEU:CD1	2.43	0.49
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.42	0.49
1:A:380:ILE:HD13	2:B:27:THR:HG22	1.95	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LYS:HG2	1:A:351:THR:N	2.27	0.49
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.94	0.49
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.47	0.49
2:B:125:ARG:HB3	2:B:145:GLN:HE21	1.76	0.49
2:B:12:LEU:HD22	2:B:83:ARG:O	2.13	0.49
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.94	0.49
1:A:472:THR:OG1	1:A:476:LYS:HE3	2.13	0.49
2:B:393:ILE:HG12	2:B:394:GLN:N	2.28	0.49
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.11	0.49
1:A:391:LEU:C	1:A:417:VAL:HG12	2.33	0.49
1:A:210:LEU:C	1:A:212:TRP:H	2.16	0.49
1:A:47:ILE:HD12	1:A:144:TYR:CD2	2.48	0.48
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.48	0.48
1:A:106:VAL:HA	1:A:189:VAL:O	2.13	0.48
1:A:426:TRP:N	1:A:426:TRP:CD1	2.81	0.48
2:B:335:GLY:O	2:B:355:ALA:HA	2.14	0.48
1:A:376:THR:HG23	1:A:386:THR:CG2	2.43	0.48
1:A:169:GLU:O	1:A:172:ARG:HB2	2.14	0.48
2:B:66:LYS:HG2	2:B:230:MET:CA	2.42	0.48
2:B:191:SER:HB2	2:B:193:LEU:CD1	2.43	0.48
1:A:329:ILE:HG22	1:A:330:GLN:N	2.29	0.48
2:B:169:GLU:N	2:B:170:PRO:HD2	2.28	0.48
1:A:486:LEU:O	1:A:528:LYS:NZ	2.45	0.48
1:A:470:THR:O	1:A:471:ASP:HB2	2.13	0.48
1:A:523:GLU:O	1:A:527:LYS:HG2	2.14	0.48
1:A:253:THR:CG2	1:A:289:LEU:O	2.62	0.48
2:B:173:LYS:O	2:B:176:PRO:HD3	2.14	0.48
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.43	0.48
1:A:278:GLN:HA	1:A:278:GLN:NE2	2.29	0.48
2:B:154:LYS:O	2:B:157:PRO:HD2	2.14	0.48
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.79	0.47
1:A:89:GLU:O	1:A:90:VAL:C	2.52	0.47
2:B:31:ILE:HD12	2:B:135:ILE:HD11	1.96	0.47
1:A:358:ARG:NH2	2:B:394:GLN:HG2	2.29	0.47
2:B:205:LEU:O	2:B:209:LEU:HG	2.14	0.47
1:A:235:HIS:HB2	1:A:238:LYS:O	2.14	0.47
1:A:492:GLU:OE1	1:A:530:LYS:HD2	2.14	0.47
2:B:257:ILE:O	2:B:260:LEU:HB3	2.14	0.47
1:A:340:GLN:HA	1:A:351:THR:HA	1.96	0.47
2:B:270:ILE:O	2:B:272:PRO:HD3	2.14	0.47
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.49	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:HD23	1:A:343:GLN:HG2	1.95	0.47
2:B:117:SER:O	2:B:118:VAL:CG2	2.63	0.47
2:B:12:LEU:O	2:B:13:LYS:C	2.51	0.47
2:B:105:SER:O	2:B:190:GLY:HA2	2.15	0.47
2:B:376:THR:O	2:B:377:THR:C	2.54	0.47
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.97	0.47
1:A:206:ARG:NH2	1:A:217:PRO:O	2.47	0.46
1:A:469:LEU:CD2	1:A:480:GLN:HG3	2.39	0.46
2:B:163:SER:O	2:B:167:ILE:HG13	2.16	0.46
2:B:397:THR:O	2:B:400:THR:HB	2.15	0.46
2:B:57:ASN:ND2	2:B:143:ARG:NH1	2.55	0.46
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.49	0.46
2:B:229:TRP:HZ3	2:B:407:GLN:HB2	1.81	0.46
1:A:517:LEU:HA	1:A:520:GLN:NE2	2.30	0.46
1:A:254:VAL:HG22	1:A:293:ILE:CD1	2.46	0.46
1:A:402:TRP:CG	1:A:403:THR:N	2.83	0.46
1:A:194:GLU:O	1:A:195:ILE:C	2.53	0.46
2:B:244:ILE:HD13	2:B:266:TRP:HZ3	1.79	0.46
2:B:27:THR:OG1	2:B:30:LYS:HG2	2.16	0.46
2:B:328:GLU:HG2	2:B:390:LYS:HD2	1.97	0.46
1:A:218:ASP:O	1:A:222:GLN:HG3	2.16	0.46
1:A:202:ILE:HG22	1:A:203:GLU:N	2.31	0.46
4:A:999:H20:HB1	4:A:999:H20:H122	1.98	0.46
2:B:79:GLU:O	2:B:83:ARG:HG3	2.16	0.46
1:A:253:THR:HB	1:A:256:ASP:OD2	2.16	0.46
1:A:180:ILE:HA	1:A:188:TYR:O	2.16	0.46
2:B:167:ILE:HG23	2:B:212:TRP:CE3	2.51	0.45
1:A:24:TRP:HZ3	1:A:61:PHE:CB	2.26	0.45
2:B:332:GLN:HB2	2:B:336:GLN:O	2.17	0.45
1:A:254:VAL:HG23	1:A:291:GLU:O	2.15	0.45
2:B:129:ALA:HA	2:B:144:TYR:O	2.16	0.45
2:B:24:TRP:CD1	2:B:25:PRO:HD2	2.51	0.45
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.50	0.45
2:B:189:VAL:HG11	2:B:202:ILE:HD13	1.98	0.45
2:B:193:LEU:CD2	2:B:201:LYS:HD2	2.46	0.45
2:B:193:LEU:CD2	2:B:201:LYS:CD	2.95	0.45
1:A:116:PHE:H	1:A:116:PHE:HD2	1.63	0.45
1:A:417:VAL:O	1:A:417:VAL:HG13	2.17	0.45
1:A:270:ILE:HG23	1:A:271:TYR:N	2.30	0.45
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.48	0.45
1:A:424:LYS:NZ	1:A:426:TRP:CD2	2.76	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PRO:HB3	2:B:289:LEU:HD23	1.98	0.45
1:A:283:LEU:O	1:A:286:THR:HG23	2.17	0.45
1:A:193:LEU:HD13	1:A:197:GLN:HG3	1.98	0.45
1:A:72:ARG:HG2	1:A:73:LYS:N	2.32	0.45
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.97	0.45
2:B:17:ASP:OD1	2:B:56:TYR:OH	2.27	0.45
2:B:193:LEU:HD22	2:B:201:LYS:CD	2.46	0.44
1:A:90:VAL:HG12	1:A:91:GLN:H	1.79	0.44
2:B:183:TYR:CD1	2:B:184:MET:HG2	2.51	0.44
1:A:328:GLU:O	1:A:339:TYR:HA	2.17	0.44
1:A:317:VAL:HG13	1:A:318:TYR:N	2.32	0.44
1:A:479:LEU:HD11	1:A:501:TYR:CE2	2.52	0.44
2:B:208:HIS:NE2	2:B:212:TRP:HZ3	2.15	0.44
1:A:420:PRO:HA	1:A:421:PRO:C	2.37	0.44
2:B:229:TRP:CZ3	2:B:407:GLN:HB2	2.53	0.44
2:B:66:LYS:CE	2:B:230:MET:HG3	2.37	0.44
1:A:520:GLN:HE21	1:A:520:GLN:HB2	1.61	0.44
1:A:398:TRP:NE1	1:A:411:ILE:HD12	2.32	0.44
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.53	0.44
1:A:13:LYS:HB3	1:A:14:PRO:HD2	1.99	0.44
2:B:303:LEU:O	2:B:306:ASN:HB2	2.18	0.44
2:B:81:ASN:OD1	2:B:153:TRP:HD1	2.00	0.44
1:A:164:MET:O	1:A:168:LEU:HG	2.18	0.44
1:A:110:ASP:O	1:A:112:GLY:N	2.51	0.43
1:A:287:LYS:HG3	1:A:287:LYS:H	1.72	0.43
2:B:297:GLU:HA	2:B:300:GLU:HB2	2.00	0.43
1:A:361:HIS:O	1:A:362:THR:HG23	2.18	0.43
2:B:38:CYS:O	2:B:47:ILE:HD11	2.18	0.43
2:B:103:LYS:HE3	2:B:192:ASP:OD1	2.18	0.43
2:B:332:GLN:HG3	2:B:338:THR:HG23	2.00	0.43
2:B:135:ILE:HG22	2:B:136:ASN:N	2.33	0.43
1:A:406:TRP:HH2	2:B:418:ASN:OD1	2.01	0.43
2:B:257:ILE:HG21	2:B:283:LEU:HD13	2.00	0.43
1:A:279:LEU:HA	1:A:282:LEU:HD12	1.99	0.43
2:B:27:THR:O	2:B:28:GLU:C	2.57	0.43
1:A:134:SER:HB3	1:A:140:PRO:O	2.18	0.43
1:A:61:PHE:HD2	1:A:61:PHE:H	1.66	0.43
2:B:169:GLU:OE2	2:B:170:PRO:HD3	2.18	0.43
1:A:197:GLN:HE21	1:A:201:LYS:HG2	1.84	0.43
1:A:245:VAL:HG23	1:A:245:VAL:O	2.18	0.43
1:A:356:ARG:CZ	1:A:358:ARG:HG2	2.47	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:LEU:HA	2:B:187:LEU:HD12	1.91	0.43
1:A:108:VAL:HA	1:A:187:LEU:O	2.19	0.43
2:B:76:ASP:C	2:B:78:ARG:H	2.21	0.43
1:A:10:VAL:HG12	1:A:11:LYS:N	2.34	0.43
1:A:403:THR:CG2	2:B:334:GLN:H	2.32	0.43
2:B:170:PRO:HG2	2:B:171:PHE:H	1.82	0.43
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.87	0.43
1:A:210:LEU:O	1:A:212:TRP:N	2.51	0.43
1:A:91:GLN:OE1	2:B:140:PRO:HA	2.19	0.42
1:A:277:ARG:NH1	1:A:277:ARG:HG3	2.32	0.42
1:A:390:LYS:HD2	1:A:415:GLU:OE2	2.18	0.42
2:B:320:ASP:O	2:B:343:GLN:NE2	2.43	0.42
1:A:206:ARG:CB	1:A:206:ARG:HH11	2.32	0.42
1:A:61:PHE:CD2	1:A:74:LEU:O	2.72	0.42
2:B:142:ILE:CG2	2:B:144:TYR:CE2	3.02	0.42
1:A:340:GLN:HB3	1:A:340:GLN:HE21	1.61	0.42
1:A:17:ASP:O	1:A:83:ARG:HD3	2.19	0.42
2:B:282:LEU:HB3	2:B:293:ILE:HG21	2.02	0.42
2:B:306:ASN:HA	2:B:309:ILE:HD12	2.02	0.42
1:A:254:VAL:HG22	1:A:293:ILE:HD11	2.02	0.42
2:B:232:TYR:HA	2:B:232:TYR:HD2	1.72	0.42
1:A:207:GLN:NE2	1:A:207:GLN:HA	2.34	0.42
2:B:327:ALA:O	2:B:389:PHE:HA	2.20	0.42
2:B:425:LEU:HD23	2:B:425:LEU:O	2.19	0.42
2:B:207:GLN:HA	2:B:210:LEU:HD12	2.02	0.42
1:A:226:PRO:HG3	1:A:235:HIS:CE1	2.54	0.42
1:A:53:GLU:O	1:A:55:PRO:HD3	2.20	0.42
1:A:465:LYS:HD2	1:A:484:LEU:HD22	2.02	0.42
1:A:50:ILE:CG2	1:A:145:GLN:HG2	2.49	0.42
1:A:320:ASP:OD2	1:A:322:SER:OG	2.35	0.42
1:A:500:GLN:O	1:A:503:LEU:HB3	2.19	0.42
1:A:332:GLN:HB3	1:A:336:GLN:HB3	2.02	0.42
2:B:117:SER:C	2:B:118:VAL:HG23	2.40	0.42
1:A:188:TYR:CD2	4:A:999:H2O:HF1	2.55	0.42
1:A:108:VAL:HG13	1:A:223:LYS:HB2	2.01	0.42
2:B:241:VAL:O	2:B:243:PRO:HD3	2.20	0.42
2:B:379:SER:CB	2:B:387:PRO:HD3	2.50	0.41
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.55	0.41
1:A:19:PRO:HD3	1:A:80:LEU:HD13	2.02	0.41
1:A:114:ALA:CB	1:A:160:PHE:CE2	3.02	0.41
1:A:319:TYR:O	1:A:321:PRO:HD3	2.19	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:VAL:O	1:A:522:ILE:HG13	2.20	0.41
2:B:66:LYS:HG3	2:B:230:MET:HA	2.02	0.41
2:B:117:SER:O	2:B:118:VAL:HG23	2.20	0.41
2:B:284:ARG:O	2:B:287:LYS:NZ	2.47	0.41
2:B:146:TYR:CE2	2:B:150:PRO:HA	2.56	0.41
1:A:50:ILE:HD12	1:A:54:ASN:CB	2.51	0.41
1:A:8:VAL:O	1:A:121:ASP:HB2	2.20	0.41
1:A:427:TYR:CE2	1:A:509:GLN:HG2	2.55	0.41
2:B:203:GLU:CD	2:B:207:GLN:HE22	2.24	0.41
2:B:380:ILE:O	2:B:381:VAL:C	2.59	0.41
1:A:100:LEU:O	1:A:318:TYR:HB3	2.21	0.41
2:B:229:TRP:HE3	2:B:229:TRP:HA	1.82	0.41
2:B:372:VAL:HG13	2:B:389:PHE:CZ	2.55	0.41
2:B:325:LEU:O	2:B:387:PRO:HA	2.20	0.41
1:A:434:ILE:HB	1:A:437:ALA:HB3	2.02	0.41
1:A:183:TYR:HE1	1:A:184:MET:CE	2.34	0.41
1:A:104:LYS:HB2	1:A:104:LYS:HE3	1.91	0.41
1:A:255:ASN:HB2	1:A:289:LEU:O	2.21	0.41
1:A:405:TYR:O	2:B:331:LYS:HD3	2.21	0.41
1:A:239:TRP:CD1	1:A:316:GLY:C	2.94	0.41
2:B:368:LEU:O	2:B:372:VAL:HG23	2.21	0.41
2:B:285:GLY:O	2:B:287:LYS:N	2.54	0.41
2:B:367:GLN:HA	2:B:370:GLU:OE1	2.21	0.41
2:B:317:VAL:O	2:B:317:VAL:HG12	2.21	0.41
1:A:27:THR:O	1:A:30:LYS:N	2.53	0.41
2:B:282:LEU:CD2	2:B:296:THR:HG23	2.51	0.41
2:B:228:LEU:HD23	2:B:228:LEU:HA	1.79	0.41
1:A:219:LYS:HD2	1:A:222:GLN:NE2	2.34	0.40
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.56	0.40
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.86	0.40
1:A:486:LEU:HD13	1:A:524:GLN:HB2	2.03	0.40
2:B:328:GLU:CG	2:B:390:LYS:HD2	2.51	0.40
2:B:85:GLN:O	2:B:85:GLN:HG3	2.22	0.40
2:B:46:LYS:HA	2:B:148:VAL:HG13	2.03	0.40
1:A:91:GLN:C	1:A:93:GLY:N	2.75	0.40
2:B:303:LEU:HD22	2:B:307:ARG:HG3	2.04	0.40
2:B:203:GLU:OE2	2:B:207:GLN:NE2	2.48	0.40
1:A:205:LEU:HD22	1:A:209:LEU:HG	2.03	0.40
1:A:246:LEU:HA	1:A:247:PRO:HD3	1.98	0.40
1:A:118:VAL:HG13	1:A:119:PRO:HD2	2.02	0.40
1:A:206:ARG:HH21	1:A:218:ASP:CA	2.31	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:HG13	2:B:199:ARG:HE	1.87	0.40
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.51	0.40
1:A:298:GLU:OE2	1:A:298:GLU:N	2.50	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	510/560 (91%)	454 (89%)	45 (9%)	11 (2%)	8	28
2	B	393/440 (89%)	340 (86%)	48 (12%)	5 (1%)	15	44
All	All	903/1000 (90%)	794 (88%)	93 (10%)	16 (2%)	11	34

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	111	VAL
1	A	195	ILE
1	A	402	TRP
1	A	412	PRO
1	A	472	THR
2	B	136	ASN
1	A	230	MET
1	A	345	PRO
2	B	77	PHE
2	B	277	ARG
1	A	356	ARG
2	B	286	THR
1	A	501	TYR
2	B	250	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	170	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	466/499 (93%)	433 (93%)	33 (7%)	18	46
2	B	366/400 (92%)	348 (95%)	18 (5%)	31	65
All	All	832/899 (92%)	781 (94%)	51 (6%)	23	55

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	20	LYS
1	A	24	TRP
1	A	39	THR
1	A	61	PHE
1	A	105	SER
1	A	107	THR
1	A	110	ASP
1	A	135	ILE
1	A	138	GLU
1	A	151	GLN
1	A	182	GLN
1	A	185	ASP
1	A	202	ILE
1	A	205	LEU
1	A	206	ARG
1	A	265	ASN
1	A	287	LYS
1	A	303	LEU
1	A	317	VAL
1	A	330	GLN
1	A	336	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	340	GLN
1	A	345	PRO
1	A	356	ARG
1	A	362	THR
1	A	396	GLU
1	A	443	ASP
1	A	458	VAL
1	A	476	LYS
1	A	487	GLN
1	A	514	GLU
1	A	517	LEU
2	B	60	VAL
2	B	73	LYS
2	B	122	GLU
2	B	205	LEU
2	B	206	ARG
2	B	212	TRP
2	B	232	TYR
2	B	233	GLU
2	B	240	THR
2	B	249	LYS
2	B	250	ASP
2	B	295	LEU
2	B	298	GLU
2	B	303	LEU
2	B	405	TYR
2	B	410	TRP
2	B	413	GLU
2	B	414	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	197	GLN
1	A	207	GLN
1	A	208	HIS
1	A	222	GLN
1	A	265	ASN
1	A	278	GLN
1	A	330	GLN
1	A	336	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	373	GLN
1	A	407	GLN
1	A	475	GLN
1	A	480	GLN
1	A	500	GLN
1	A	507	GLN
1	A	512	GLN
1	A	520	GLN
2	B	57	ASN
2	B	137	ASN
2	B	147	ASN
2	B	278	GLN
2	B	336	GLN
2	B	348	ASN
2	B	394	GLN
2	B	407	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	0.76	0	3,8,10	4.35	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(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	7.37	117.69	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](#)

4 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	1.07	0	6,6,6	0.27	0
3	PO4	A	1301	-	4,4,4	1.08	0	6,6,6	0.27	0
3	PO4	A	1302	-	4,4,4	1.13	0	6,6,6	0.27	0
4	H2O	A	999	-	23,24,24	2.19	8 (34%)	26,34,34	2.09	6 (23%)

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
3	PO4	A	1302	-	-	0/0/0/0	0/0/0/0
4	H2O	A	999	-	-	0/8/16/16	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	H2O	C8-CL	-2.69	1.68	1.74
4	A	999	H2O	CE-CF	2.19	1.59	1.53
4	A	999	H2O	C10-C9	2.47	1.41	1.36
4	A	999	H2O	O4-C4	3.30	1.45	1.38
4	A	999	H2O	C6-N1	3.35	1.39	1.33
4	A	999	H2O	C4-C5	3.80	1.41	1.36
4	A	999	H2O	CB-CA	4.07	1.61	1.51
4	A	999	H2O	CF-CA	5.49	1.65	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	H2O	C5-C6-N1	-3.91	118.94	125.18
4	A	999	H2O	C3-C2-N1	-3.12	120.60	123.45
4	A	999	H2O	C6-C5-C11	-2.08	116.27	122.83
4	A	999	H2O	C13-C11-C12	2.04	115.30	110.33
4	A	999	H2O	CE-CF-CA	2.41	116.90	110.54
4	A	999	H2O	C6-N1-C2	7.63	121.38	116.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1302	PO4	1	0
4	A	999	H2O	2	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	516/560 (92%)	-0.32	13 (2%)	61 48	20, 58, 100, 131	0
2	B	401/440 (91%)	-0.18	10 (2%)	61 48	18, 57, 104, 126	0
All	All	917/1000 (91%)	-0.26	23 (2%)	61 48	18, 58, 101, 131	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	469	LEU	4.3
2	B	88	TRP	4.1
1	A	468	THR	3.3
2	B	294	PRO	3.2
2	B	362	THR	3.0
1	A	137	ASN	3.0
1	A	72	ARG	3.0
1	A	243	PRO	2.8
2	B	237	ASP	2.7
2	B	214	LEU	2.7
1	A	63	ILE	2.5
1	A	467	VAL	2.5
1	A	140	PRO	2.5
2	B	87	PHE	2.4
2	B	67	ASP	2.3
2	B	334	GLN	2.2
2	B	212	TRP	2.2
1	A	474	ASN	2.2
1	A	471	ASP	2.1
2	B	356	ARG	2.1
1	A	472	THR	2.1
1	A	455	ALA	2.1
1	A	61	PHE	2.0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CSD	A	280	8/9	0.95	0.14	-	50,52,65,75	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PO4	A	1301	5/5	0.91	0.15	0.85	117,124,127,128	0
3	PO4	A	1302	5/5	0.95	0.22	0.70	134,137,138,141	0
3	PO4	A	1300	5/5	0.88	0.18	0.64	113,116,121,122	0
4	H2O	A	999	22/22	0.97	0.17	0.48	24,41,52,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.