



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:56 am GMT

PDB ID : 1JLF  
Title : CRYSTAL STRUCTURE OF Y188C MUTANT HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH NEVIRAPINE  
Authors : Ren, J.; Nichols, C.; Bird, L.; Chamberlain, P.; Weaver, K.; Short, S.; Stuart, D.I.; Stammers, D.K.  
Deposited on : 2001-07-16  
Resolution : 2.60 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

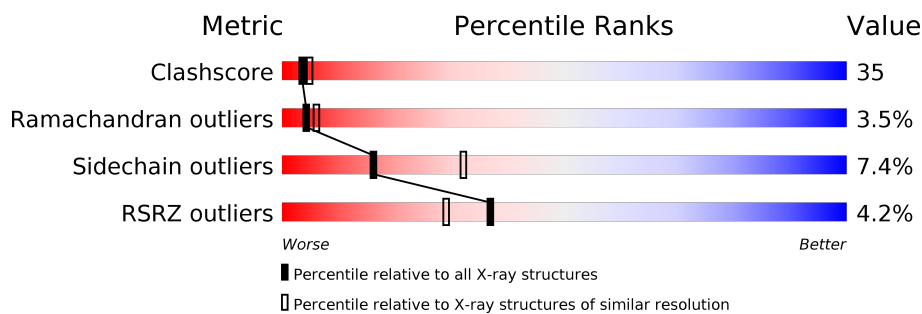
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 4% 38% 51% 7% . .
2	B	440	 4% 40% 47% . 8%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7829 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called HIV-1 RT A-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			4404	2847	734	814	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	CYS	TYR	ENGINEERED	UNP P04585
A	280	CSD	CYS	OXIDIZED CYS	UNP P04585

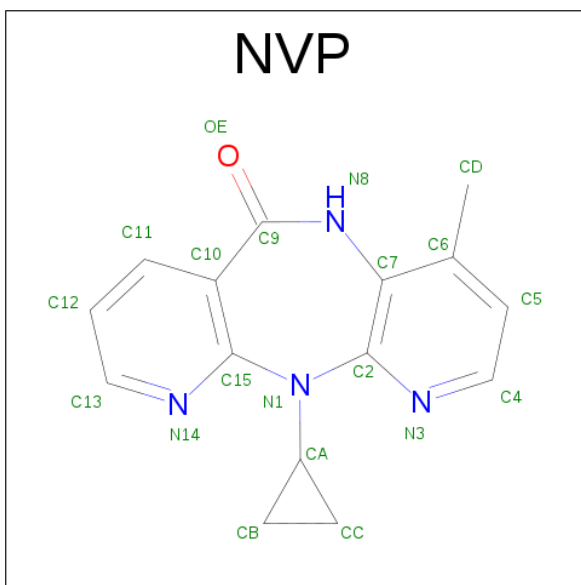
- Molecule 2 is a protein called HIV-1 RT B-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3345	2173	557	607	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	188	CYS	TYR	ENGINEERED	UNP P04585

- Molecule 3 is 11-CYCLOPROPYL-5,11-DIHYDRO-4-METHYL-6H-DIPYRIDO[3,2-B:2',3'-E][1,4]DIAZEPIN-6-ONE (three-letter code: NVP) (formula: C<sub>15</sub>H<sub>14</sub>N<sub>4</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	15	4	1		

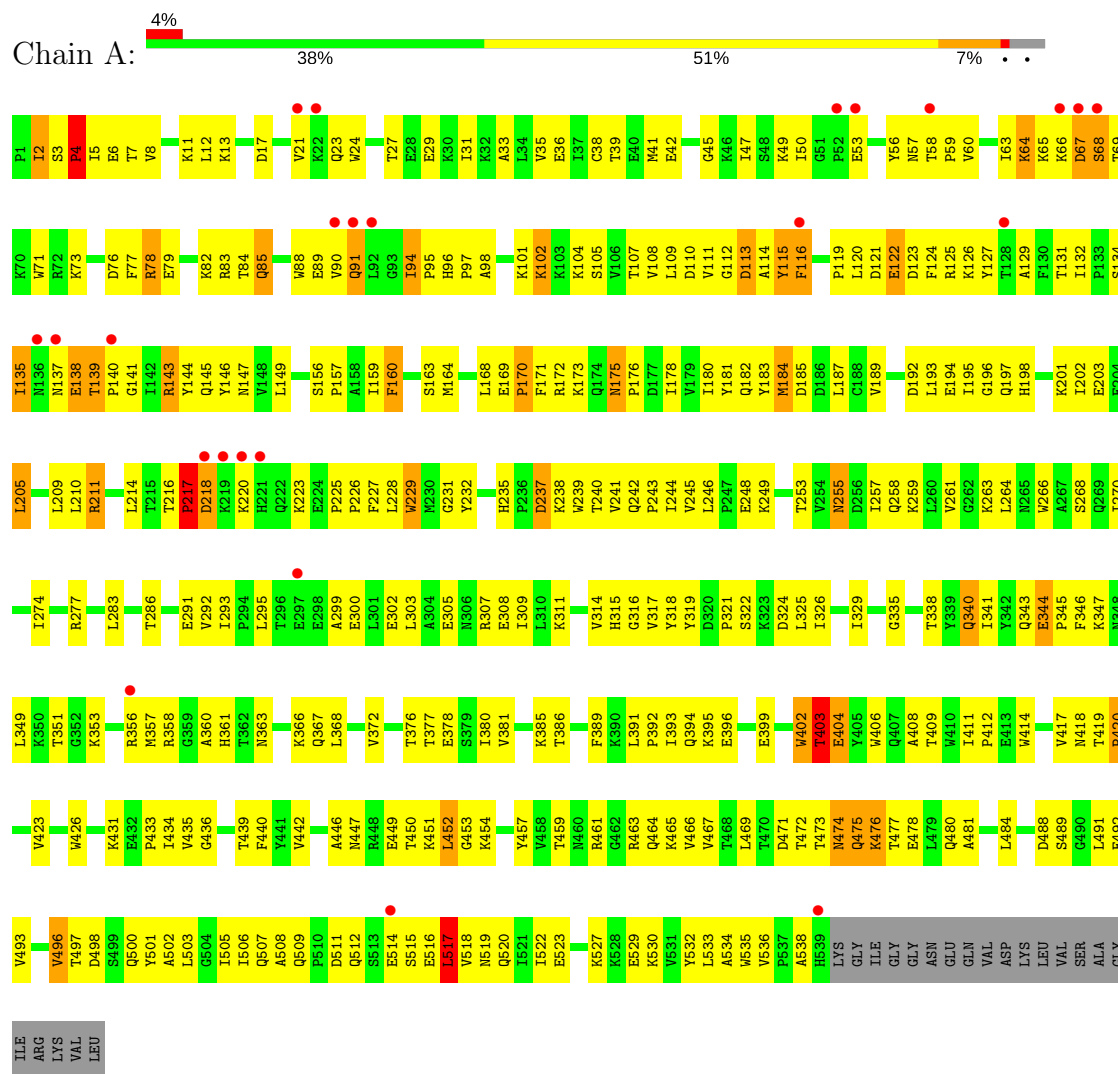
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	34	Total O 34 34	0	0
4	B	26	Total O 26 26	0	0

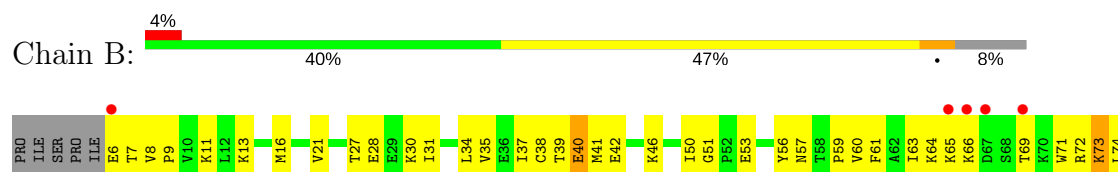
### 3 Residue-property plots

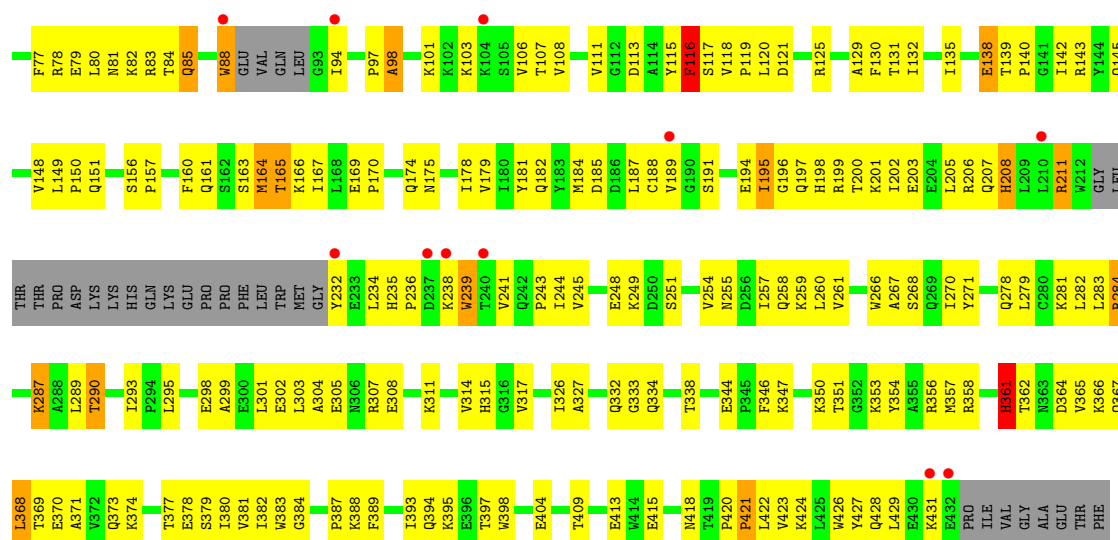
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: HIV-1 RT A-chain



#### • Molecule 2: HIV-1 RT B-chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.30Å 109.20Å 72.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.60 19.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.99-2.60) 99.3 (19.99-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.59Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.237 , 0.303 0.224 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	70.0	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 93.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7829	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, NVP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.47	0/4512	0.69	0/6133
2	B	0.45	0/3438	0.70	0/4667
All	All	0.46	0/7950	0.69	0/10800

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	4404	0	4450	314	0
2	B	3345	0	3373	242	0
3	A	20	0	14	0	0
4	A	34	0	0	5	0
4	B	26	0	0	4	0
All	All	7829	0	7837	545	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 35.

All (545) 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:502:ALA:HA	1:A:505:ILE:HD12	1.42	1.01
2:B:195:ILE:HG23	2:B:196:GLY:H	1.30	0.94
1:A:2:ILE:HG22	1:A:3:SER:H	1.33	0.91
1:A:380:ILE:HD11	1:A:386:THR:HG22	1.52	0.89
1:A:238:LYS:HB2	1:A:316:GLY:O	1.72	0.88
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.54	0.88
1:A:335:GLY:HA2	1:A:367:GLN:OE1	1.72	0.88
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.56	0.85
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.58	0.85
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.59	0.84
1:A:475:GLN:N	1:A:475:GLN:HE21	1.76	0.84
2:B:164:MET:O	2:B:167:ILE:HG12	1.77	0.83
1:A:226:PRO:HB3	1:A:235:HIS:ND1	1.93	0.83
2:B:178:ILE:HG12	2:B:191:SER:HB3	1.58	0.82
2:B:31:ILE:O	2:B:35:VAL:HG23	1.80	0.82
1:A:503:LEU:HA	1:A:506:ILE:HD12	1.60	0.81
2:B:195:ILE:HG23	2:B:196:GLY:N	1.96	0.81
1:A:195:ILE:HG13	1:A:196:GLY:N	1.96	0.81
2:B:79:GLU:O	2:B:83:ARG:HG3	1.81	0.81
1:A:17:ASP:O	1:A:83:ARG:HD3	1.79	0.80
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.64	0.80
1:A:516:GLU:O	1:A:520:GLN:HG3	1.83	0.78
2:B:241:VAL:CG1	2:B:350:LYS:HA	2.14	0.77
2:B:366:LYS:O	2:B:370:GLU:HB2	1.83	0.77
1:A:141:GLY:HA2	4:A:1035:HOH:O	1.84	0.77
1:A:65:LYS:HG2	1:A:66:LYS:H	1.50	0.77
1:A:2:ILE:HG22	1:A:3:SER:N	1.99	0.76
1:A:66:LYS:HD2	1:A:66:LYS:H	1.50	0.76
1:A:515:SER:OG	1:A:518:VAL:HG23	1.86	0.76
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.69	0.75
1:A:516:GLU:O	1:A:519:ASN:HB2	1.85	0.75
1:A:110:ASP:O	1:A:217:PRO:HD2	1.87	0.75
1:A:94:ILE:H	1:A:94:ILE:HD13	1.50	0.75
2:B:241:VAL:HG12	2:B:350:LYS:HA	1.67	0.74
2:B:206:ARG:HB3	2:B:206:ARG:NH1	2.01	0.74
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.21	0.74
1:A:211:ARG:HB3	1:A:211:ARG:NH1	2.01	0.74
2:B:245:VAL:HG11	2:B:431:LYS:HB2	1.71	0.73
1:A:64:LYS:H	1:A:64:LYS:HD2	1.51	0.73
1:A:116:PHE:HE1	1:A:146:TYR:HE1	1.36	0.73
1:A:446:ALA:HB2	1:A:453:GLY:HA3	1.71	0.73
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.18	0.72

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.69	0.72
1:A:2:ILE:HD11	1:A:45:GLY:HA3	1.71	0.72
1:A:27:THR:O	1:A:31:ILE:HG13	1.90	0.72
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.71	0.72
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.05	0.71
1:A:23:GLN:HG2	1:A:131:THR:O	1.89	0.71
2:B:420:PRO:HG3	4:B:1024:HOH:O	1.90	0.71
1:A:480:GLN:HE21	1:A:484:LEU:HG	1.54	0.71
2:B:107:THR:HA	2:B:232:TYR:O	1.91	0.71
2:B:365:VAL:O	2:B:369:THR:HG23	1.91	0.71
2:B:61:PHE:CE1	2:B:74:LEU:HD23	2.25	0.71
1:A:175:ASN:HB2	1:A:178:ILE:HD13	1.71	0.70
1:A:523:GLU:O	1:A:527:LYS:HG3	1.91	0.70
1:A:96:HIS:HD2	1:A:98:ALA:H	1.40	0.70
2:B:426:TRP:O	2:B:429:LEU:HB2	1.90	0.70
2:B:78:ARG:O	2:B:82:LYS:HG3	1.92	0.70
2:B:98:ALA:O	2:B:101:LYS:HG2	1.92	0.69
2:B:191:SER:HG	2:B:198:HIS:HD1	1.37	0.69
1:A:109:LEU:HG	1:A:216:THR:HG21	1.74	0.69
2:B:379:SER:CB	2:B:387:PRO:HD3	2.23	0.69
1:A:135:ILE:O	1:A:138:GLU:HG3	1.93	0.68
1:A:3:SER:HB3	1:A:5:ILE:HG13	1.74	0.68
2:B:139:THR:HG22	2:B:140:PRO:O	1.93	0.68
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.29	0.67
2:B:160:PHE:CD1	2:B:160:PHE:O	2.47	0.67
2:B:108:VAL:HA	2:B:187:LEU:O	1.93	0.67
1:A:65:LYS:HD3	1:A:67:ASP:OD2	1.92	0.67
2:B:205:LEU:O	2:B:208:HIS:HB2	1.95	0.67
1:A:211:ARG:HB3	1:A:211:ARG:HH11	1.57	0.67
2:B:281:LYS:NZ	2:B:284:ARG:HH22	1.93	0.67
1:A:180:ILE:HG23	1:A:189:VAL:HG22	1.76	0.66
2:B:195:ILE:HG13	2:B:199:ARG:NE	2.10	0.66
2:B:239:TRP:CZ2	2:B:378:GLU:HG2	2.30	0.66
2:B:254:VAL:O	2:B:258:GLN:HG3	1.95	0.66
2:B:195:ILE:CG2	2:B:196:GLY:H	2.06	0.66
1:A:171:PHE:O	1:A:175:ASN:ND2	2.29	0.65
2:B:161:GLN:O	2:B:165:THR:HG22	1.97	0.65
1:A:94:ILE:HB	1:A:229:TRP:HH2	1.60	0.65
1:A:110:ASP:OD1	1:A:217:PRO:HG2	1.97	0.65
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.79	0.65
1:A:357:MET:HB3	1:A:367:GLN:NE2	2.12	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:GLU:HA	1:A:530:LYS:O	1.97	0.65
1:A:3:SER:HB3	1:A:4:PRO:HD2	1.78	0.65
1:A:64:LYS:HE3	1:A:71:TRP:CZ3	2.31	0.65
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.32	0.64
2:B:118:VAL:HG13	2:B:119:PRO:HD2	1.79	0.64
2:B:161:GLN:HB3	4:B:1052:HOH:O	1.97	0.64
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.63	0.64
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.80	0.64
2:B:131:THR:OG1	2:B:143:ARG:HD2	1.98	0.64
1:A:164:MET:O	1:A:168:LEU:HG	1.97	0.64
2:B:125:ARG:HB3	2:B:145:GLN:HE21	1.61	0.64
1:A:255:ASN:O	1:A:259:LYS:HG2	1.97	0.64
1:A:31:ILE:HD12	1:A:135:ILE:HD12	1.79	0.64
1:A:135:ILE:O	1:A:135:ILE:HG22	1.98	0.64
2:B:88:TRP:C	2:B:88:TRP:HE3	2.02	0.64
1:A:377:THR:O	1:A:381:VAL:HG23	1.99	0.63
2:B:163:SER:O	2:B:167:ILE:HG23	1.98	0.63
2:B:356:ARG:HB2	2:B:367:GLN:HG2	1.80	0.62
1:A:143:ARG:HG2	1:A:143:ARG:HH11	1.62	0.62
1:A:293:ILE:HD12	1:A:293:ILE:N	2.14	0.62
1:A:95:PRO:O	1:A:229:TRP:HZ3	1.80	0.62
1:A:418:ASN:C	1:A:420:PRO:HD3	2.20	0.62
1:A:248:GLU:O	1:A:249:LYS:HD3	1.99	0.61
2:B:427:TYR:C	2:B:429:LEU:H	2.03	0.61
1:A:2:ILE:CG2	1:A:3:SER:H	2.11	0.61
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.81	0.61
1:A:175:ASN:HB2	1:A:178:ILE:CD1	2.30	0.61
1:A:2:ILE:HD11	1:A:45:GLY:CA	2.30	0.61
1:A:261:VAL:HA	1:A:264:LEU:HD12	1.80	0.61
1:A:408:ALA:HB2	2:B:368:LEU:HD12	1.81	0.61
2:B:380:ILE:O	2:B:384:GLY:HA2	2.00	0.61
1:A:268:SER:HB3	1:A:353:LYS:HE2	1.82	0.61
1:A:246:LEU:HD12	1:A:307:ARG:HA	1.83	0.61
2:B:41:MET:HB3	2:B:46:LYS:HB2	1.83	0.61
1:A:418:ASN:O	1:A:420:PRO:HD3	2.01	0.61
1:A:108:VAL:HG11	1:A:223:LYS:HB2	1.83	0.60
1:A:2:ILE:HD11	1:A:45:GLY:C	2.21	0.60
1:A:3:SER:CB	1:A:5:ILE:HG13	2.31	0.60
2:B:332:GLN:NE2	2:B:428:GLN:HB2	2.16	0.60
2:B:94:ILE:HD11	2:B:182:GLN:H	1.67	0.60
2:B:194:GLU:OE2	2:B:195:ILE:HG22	2.01	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ILE:O	1:A:261:VAL:HG23	2.02	0.60
1:A:108:VAL:O	1:A:108:VAL:HG13	2.01	0.60
1:A:451:LYS:O	1:A:472:THR:N	2.35	0.60
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.36	0.59
2:B:35:VAL:O	2:B:39:THR:HG23	2.02	0.59
1:A:195:ILE:HG13	1:A:196:GLY:H	1.65	0.59
1:A:66:LYS:HD2	1:A:66:LYS:N	2.16	0.59
1:A:17:ASP:OD1	1:A:56:TYR:HE1	1.85	0.59
2:B:108:VAL:H	2:B:232:TYR:N	2.00	0.59
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.83	0.59
2:B:278:GLN:HG3	2:B:298:GLU:HB3	1.84	0.59
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.84	0.59
2:B:248:GLU:HG2	2:B:307:ARG:NH2	2.17	0.59
1:A:57:ASN:HA	1:A:129:ALA:O	2.03	0.59
1:A:475:GLN:HA	1:A:478:GLU:OE2	2.03	0.58
2:B:175:ASN:ND2	2:B:201:LYS:HD2	2.18	0.58
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.21	0.58
1:A:474:ASN:O	1:A:478:GLU:HG3	2.02	0.58
1:A:465:LYS:HG2	1:A:466:VAL:N	2.17	0.58
1:A:112:GLY:O	1:A:114:ALA:N	2.32	0.58
1:A:111:VAL:HG22	1:A:185:ASP:HB3	1.86	0.58
1:A:64:LYS:H	1:A:64:LYS:CD	2.16	0.58
2:B:63:ILE:HG22	2:B:65:LYS:H	1.68	0.58
2:B:64:LYS:HE2	2:B:71:TRP:CZ2	2.38	0.58
2:B:50:ILE:HG21	2:B:145:GLN:HB3	1.85	0.58
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.39	0.58
2:B:379:SER:OG	2:B:387:PRO:HD3	2.03	0.58
1:A:307:ARG:O	1:A:311:LYS:HG3	2.03	0.58
1:A:475:GLN:H	1:A:475:GLN:HE21	1.49	0.57
2:B:77:PHE:CD2	2:B:80:LEU:HD23	2.39	0.57
1:A:42:GLU:HA	1:A:47:ILE:HG13	1.87	0.57
1:A:94:ILE:H	1:A:94:ILE:CD1	2.16	0.57
1:A:376:THR:O	1:A:380:ILE:HG12	2.04	0.57
2:B:350:LYS:HE2	2:B:378:GLU:OE1	2.05	0.57
1:A:380:ILE:CD1	1:A:386:THR:HG22	2.30	0.57
1:A:360:ALA:HA	1:A:514:GLU:OE2	2.03	0.57
2:B:64:LYS:HG2	2:B:71:TRP:CE3	2.40	0.57
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.86	0.57
1:A:63:ILE:C	1:A:63:ILE:HD12	2.25	0.57
2:B:281:LYS:HZ3	2:B:284:ARG:HH22	1.53	0.57
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.33	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:TRP:HH2	2:B:378:GLU:HA	1.69	0.57
1:A:102:LYS:NZ	1:A:102:LYS:HB2	2.18	0.57
1:A:49:LYS:HB2	1:A:144:TYR:CE2	2.40	0.57
1:A:295:LEU:HB2	1:A:300:GLU:OE1	2.04	0.57
2:B:178:ILE:HG12	2:B:191:SER:CB	2.31	0.57
1:A:302:GLU:HA	4:A:1006:HOH:O	2.05	0.56
2:B:236:PRO:O	2:B:239:TRP:HB2	2.05	0.56
2:B:332:GLN:HE22	2:B:428:GLN:HB2	1.69	0.56
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.87	0.56
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.03	0.56
2:B:245:VAL:HG23	2:B:245:VAL:O	2.04	0.56
2:B:27:THR:O	2:B:31:ILE:HG13	2.06	0.56
1:A:108:VAL:HG11	1:A:227:PHE:CE1	2.40	0.56
1:A:21:VAL:HG11	1:A:59:PRO:HD3	1.87	0.56
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.40	0.56
2:B:393:ILE:HG12	2:B:394:GLN:N	2.20	0.56
1:A:228:LEU:HD22	1:A:242:GLN:OE1	2.05	0.56
1:A:41:MET:SD	1:A:73:LYS:HE3	2.46	0.56
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.05	0.56
2:B:206:ARG:CZ	2:B:206:ARG:HB3	2.35	0.56
2:B:332:GLN:HE22	2:B:424:LYS:HD3	1.69	0.56
2:B:9:PRO:HA	2:B:121:ASP:OD2	2.06	0.56
2:B:241:VAL:HG12	2:B:351:THR:H	1.71	0.56
1:A:169:GLU:CB	1:A:170:PRO:HD3	2.34	0.56
1:A:241:VAL:O	1:A:243:PRO:HD3	2.05	0.56
1:A:402:TRP:CH2	2:B:362:THR:HA	2.41	0.56
2:B:373:GLN:O	2:B:377:THR:HG23	2.06	0.55
1:A:110:ASP:O	1:A:216:THR:HG23	2.07	0.55
2:B:125:ARG:CB	2:B:145:GLN:HE21	2.19	0.55
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.46	0.55
1:A:122:GLU:CD	1:A:122:GLU:H	2.09	0.55
1:A:33:ALA:O	1:A:36:GLU:HB3	2.07	0.55
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.41	0.55
2:B:197:GLN:O	2:B:201:LYS:HB2	2.05	0.55
2:B:301:LEU:O	2:B:304:ALA:N	2.39	0.55
1:A:134:SER:OG	1:A:138:GLU:HB2	2.06	0.55
1:A:396:GLU:CD	1:A:396:GLU:H	2.10	0.55
1:A:65:LYS:HG2	1:A:66:LYS:N	2.21	0.55
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.41	0.55
1:A:497:THR:O	1:A:535:TRP:HA	2.07	0.55
2:B:235:HIS:N	2:B:236:PRO:HD3	2.21	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.89	0.55
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.42	0.55
2:B:88:TRP:C	2:B:88:TRP:CE3	2.80	0.55
1:A:475:GLN:NE2	1:A:475:GLN:N	2.52	0.55
1:A:317:VAL:HG12	1:A:318:TYR:N	2.22	0.55
1:A:474:ASN:O	1:A:477:THR:OG1	2.24	0.55
1:A:122:GLU:C	1:A:124:PHE:H	2.10	0.54
1:A:102:LYS:HB3	1:A:318:TYR:HB2	1.88	0.54
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.89	0.54
1:A:111:VAL:HG22	1:A:185:ASP:CA	2.38	0.54
2:B:245:VAL:CG1	2:B:431:LYS:HB2	2.37	0.54
1:A:139:THR:HB	1:A:140:PRO:CD	2.38	0.54
1:A:125:ARG:NE	1:A:147:ASN:HA	2.23	0.54
2:B:255:ASN:OD1	2:B:259:LYS:HE2	2.07	0.54
1:A:111:VAL:HG23	1:A:114:ALA:HB2	1.90	0.54
2:B:308:GLU:OE1	2:B:311:LYS:HD2	2.07	0.54
1:A:418:ASN:OD1	1:A:420:PRO:HD3	2.07	0.53
1:A:436:GLY:O	1:A:461:ARG:NH2	2.40	0.53
1:A:168:LEU:O	1:A:172:ARG:HB2	2.09	0.53
1:A:389:PHE:HB2	1:A:414:TRP:HB3	1.91	0.53
2:B:125:ARG:CB	2:B:145:GLN:NE2	2.71	0.53
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.89	0.53
1:A:125:ARG:HG2	1:A:146:TYR:O	2.08	0.53
1:A:65:LYS:CG	1:A:66:LYS:H	2.19	0.53
2:B:57:ASN:HA	2:B:129:ALA:O	2.09	0.53
2:B:244:ILE:HG23	2:B:429:LEU:HB3	1.90	0.53
2:B:39:THR:O	2:B:42:GLU:HB3	2.08	0.53
2:B:57:ASN:HB2	2:B:143:ARG:HH12	1.72	0.53
1:A:419:THR:HG22	1:A:419:THR:O	2.07	0.53
1:A:143:ARG:HG2	1:A:143:ARG:NH1	2.23	0.53
1:A:473:THR:CG2	1:A:476:LYS:HG3	2.39	0.53
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.44	0.53
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.91	0.53
2:B:161:GLN:HA	2:B:161:GLN:HE21	1.72	0.53
2:B:27:THR:HG22	2:B:28:GLU:N	2.24	0.53
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.43	0.53
2:B:63:ILE:HG22	2:B:65:LYS:N	2.23	0.53
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.44	0.53
1:A:228:LEU:HA	1:A:232:TYR:O	2.09	0.53
2:B:115:TYR:O	2:B:117:SER:N	2.42	0.53
1:A:454:LYS:HA	1:A:467:VAL:O	2.08	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:LYS:HD3	1:A:471:ASP:OD2	2.08	0.52
2:B:106:VAL:HA	2:B:189:VAL:O	2.09	0.52
2:B:374:LYS:O	2:B:378:GLU:HG3	2.09	0.52
1:A:11:LYS:O	1:A:85:GLN:HB3	2.10	0.52
1:A:248:GLU:HB2	1:A:307:ARG:NH2	2.25	0.52
2:B:156:SER:HB2	2:B:157:PRO:CD	2.40	0.52
2:B:427:TYR:C	2:B:429:LEU:N	2.63	0.52
1:A:408:ALA:HB3	2:B:393:ILE:HB	1.92	0.52
2:B:315:HIS:O	2:B:317:VAL:HG23	2.10	0.52
1:A:451:LYS:HB3	1:A:471:ASP:HA	1.91	0.52
2:B:169:GLU:HB2	2:B:170:PRO:CD	2.37	0.52
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.10	0.51
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.92	0.51
2:B:344:GLU:HB3	2:B:347:LYS:NZ	2.25	0.51
2:B:53:GLU:N	2:B:53:GLU:OE1	2.42	0.51
2:B:303:LEU:O	2:B:307:ARG:HG3	2.11	0.51
2:B:428:GLN:O	2:B:428:GLN:HG2	2.10	0.51
2:B:97:PRO:O	2:B:98:ALA:C	2.48	0.51
1:A:240:THR:HG22	1:A:241:VAL:N	2.26	0.51
1:A:446:ALA:CB	1:A:453:GLY:HA3	2.39	0.51
1:A:465:LYS:HG2	1:A:466:VAL:H	1.76	0.51
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.93	0.51
2:B:232:TYR:HB3	2:B:234:LEU:HD11	1.92	0.51
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.93	0.51
2:B:281:LYS:HG2	2:B:284:ARG:NH2	2.25	0.50
2:B:11:LYS:N	2:B:85:GLN:OE1	2.32	0.50
1:A:183:TYR:CD1	1:A:184:MET:HB2	2.45	0.50
1:A:283:LEU:O	1:A:286:THR:HG23	2.10	0.50
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.41	0.50
1:A:98:ALA:HB2	1:A:349:LEU:O	2.10	0.50
1:A:181:TYR:HB2	2:B:138:GLU:OE1	2.11	0.50
2:B:37:ILE:O	2:B:40:GLU:HB2	2.12	0.50
1:A:346:PHE:N	1:A:346:PHE:CD2	2.77	0.50
1:A:319:TYR:OH	1:A:385:LYS:HD3	2.10	0.50
2:B:6:GLU:HG2	2:B:7:THR:H	1.77	0.50
2:B:98:ALA:HA	2:B:101:LYS:NZ	2.27	0.50
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.93	0.50
1:A:517:LEU:O	1:A:518:VAL:C	2.49	0.50
1:A:96:HIS:CD2	1:A:97:PRO:HD2	2.47	0.50
1:A:2:ILE:CD1	1:A:45:GLY:HA3	2.39	0.50
1:A:357:MET:HE2	4:A:1041:HOH:O	2.12	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:VAL:HA	1:A:534:ALA:O	2.12	0.50
2:B:195:ILE:O	2:B:198:HIS:HB3	2.12	0.50
1:A:268:SER:CB	1:A:353:LYS:HE2	2.42	0.50
1:A:39:THR:O	1:A:42:GLU:HB3	2.12	0.50
2:B:118:VAL:CG1	2:B:119:PRO:HD2	2.41	0.50
2:B:64:LYS:HE2	2:B:71:TRP:CE2	2.47	0.50
1:A:357:MET:HB3	1:A:367:GLN:HE22	1.76	0.49
1:A:94:ILE:HB	1:A:229:TRP:CH2	2.45	0.49
2:B:125:ARG:HB2	2:B:145:GLN:NE2	2.27	0.49
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.94	0.49
2:B:46:LYS:HE2	2:B:116:PHE:HD1	1.77	0.49
2:B:266:TRP:CZ3	2:B:426:TRP:CG	3.00	0.49
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.41	0.49
2:B:107:THR:O	2:B:188:CYS:HA	2.12	0.49
1:A:465:LYS:NZ	1:A:488:ASP:OD1	2.43	0.49
1:A:50:ILE:HG23	1:A:145:GLN:HG2	1.93	0.49
1:A:129:ALA:HA	1:A:144:TYR:O	2.13	0.48
1:A:402:TRP:CG	1:A:403:THR:N	2.80	0.48
1:A:498:ASP:HA	1:A:536:VAL:O	2.13	0.48
2:B:244:ILE:CG2	2:B:429:LEU:HD23	2.42	0.48
1:A:107:THR:HG22	1:A:108:VAL:N	2.29	0.48
2:B:77:PHE:HD2	2:B:80:LEU:HD23	1.78	0.48
1:A:340:GLN:CB	1:A:351:THR:HG22	2.43	0.48
1:A:77:PHE:O	1:A:79:GLU:N	2.47	0.48
1:A:218:ASP:HB3	1:A:220:LYS:H	1.78	0.48
2:B:206:ARG:CB	2:B:206:ARG:HH11	2.27	0.48
1:A:164:MET:HE1	1:A:214:LEU:HD13	1.94	0.48
2:B:170:PRO:O	2:B:174:GLN:HG3	2.14	0.48
2:B:354:TYR:OH	2:B:370:GLU:HB3	2.14	0.48
1:A:244:ILE:HD11	1:A:263:LYS:HB3	1.96	0.48
2:B:165:THR:HG23	2:B:166:LYS:H	1.77	0.48
1:A:108:VAL:CG1	1:A:223:LYS:HB2	2.42	0.48
1:A:164:MET:CE	1:A:214:LEU:HD13	2.44	0.48
1:A:95:PRO:O	1:A:229:TRP:CZ3	2.65	0.48
2:B:344:GLU:CB	2:B:347:LYS:HE3	2.44	0.48
2:B:356:ARG:HH11	2:B:356:ARG:HG3	1.78	0.48
2:B:423:VAL:O	2:B:427:TYR:CD2	2.67	0.48
2:B:64:LYS:HG2	2:B:71:TRP:CZ3	2.49	0.48
1:A:394:GLN:HB3	1:A:396:GLU:OE1	2.13	0.47
2:B:98:ALA:C	2:B:101:LYS:HZ3	2.18	0.47
2:B:175:ASN:HD21	2:B:201:LYS:HD2	1.77	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:PHE:HD1	2:B:160:PHE:O	1.95	0.47
2:B:191:SER:OG	2:B:198:HIS:ND1	2.38	0.47
2:B:195:ILE:HG13	2:B:199:ARG:HE	1.79	0.47
1:A:508:ALA:O	1:A:509:GLN:C	2.52	0.47
2:B:301:LEU:HD11	2:B:305:GLU:HG3	1.97	0.47
2:B:56:TYR:O	2:B:57:ASN:HB2	2.14	0.47
1:A:102:LYS:NZ	1:A:237:ASP:HA	2.29	0.47
1:A:198:HIS:O	1:A:201:LYS:N	2.47	0.47
1:A:135:ILE:CG2	1:A:135:ILE:O	2.63	0.47
1:A:102:LYS:HZ3	1:A:237:ASP:HA	1.79	0.47
2:B:202:ILE:O	2:B:205:LEU:HB3	2.15	0.47
2:B:259:LYS:O	2:B:260:LEU:C	2.51	0.47
1:A:160:PHE:CD2	1:A:160:PHE:C	2.88	0.47
1:A:88:TRP:HE3	1:A:88:TRP:HA	1.80	0.47
2:B:232:TYR:HB3	2:B:234:LEU:CD1	2.45	0.47
1:A:345:PRO:O	1:A:346:PHE:HB2	2.14	0.47
1:A:439:THR:O	1:A:459:THR:HA	2.15	0.47
1:A:475:GLN:NE2	1:A:475:GLN:CA	2.78	0.47
1:A:17:ASP:OD1	1:A:56:TYR:CE1	2.67	0.47
1:A:501:TYR:CD2	1:A:501:TYR:C	2.89	0.47
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.14	0.47
1:A:463:ARG:HG2	1:A:464:GLN:N	2.30	0.46
1:A:108:VAL:O	1:A:108:VAL:CG1	2.64	0.46
1:A:308:GLU:O	1:A:311:LYS:N	2.46	0.46
2:B:282:LEU:HD13	2:B:295:LEU:CD2	2.45	0.46
1:A:518:VAL:O	1:A:522:ILE:HG13	2.15	0.46
1:A:66:LYS:O	1:A:68:SER:N	2.48	0.46
2:B:94:ILE:HG13	2:B:181:TYR:HE2	1.80	0.46
1:A:473:THR:HG23	1:A:476:LYS:H	1.79	0.46
1:A:194:GLU:O	1:A:195:ILE:C	2.54	0.46
1:A:2:ILE:CG2	1:A:3:SER:N	2.71	0.46
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.31	0.46
2:B:308:GLU:OE1	2:B:308:GLU:HA	2.15	0.46
1:A:111:VAL:HG22	1:A:185:ASP:CB	2.46	0.46
1:A:363:ASN:O	1:A:366:LYS:HB3	2.16	0.46
2:B:198:HIS:O	2:B:201:LYS:HB3	2.16	0.46
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.51	0.46
2:B:115:TYR:C	2:B:117:SER:N	2.69	0.46
1:A:253:THR:HA	1:A:291:GLU:O	2.16	0.46
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.46	0.46
2:B:121:ASP:N	4:B:1049:HOH:O	2.35	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:GLY:O	2:B:334:GLN:HB2	2.16	0.46
1:A:238:LYS:HG3	1:A:239:TRP:N	2.30	0.45
2:B:165:THR:HG23	2:B:166:LYS:N	2.30	0.45
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.51	0.45
1:A:184:MET:HB3	1:A:185:ASP:H	1.43	0.45
1:A:53:GLU:HG3	1:A:53:GLU:O	2.17	0.45
1:A:241:VAL:CG2	1:A:314:VAL:HG23	2.47	0.45
1:A:411:ILE:HG22	1:A:412:PRO:O	2.16	0.45
2:B:268:SER:HA	2:B:271:TYR:O	2.17	0.45
1:A:507:GLN:OE1	2:B:421:PRO:HG3	2.14	0.45
2:B:63:ILE:HG22	2:B:64:LYS:N	2.31	0.45
1:A:475:GLN:CA	1:A:475:GLN:HE21	2.25	0.45
1:A:59:PRO:HG2	1:A:76:ASP:CB	2.45	0.45
1:A:408:ALA:CB	2:B:368:LEU:HD12	2.44	0.45
1:A:399:GLU:O	1:A:403:THR:HG22	2.17	0.45
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.99	0.45
2:B:94:ILE:HG13	2:B:94:ILE:O	2.16	0.45
1:A:299:ALA:O	1:A:303:LEU:HB3	2.16	0.45
1:A:409:THR:O	2:B:364:ASP:HB2	2.16	0.45
1:A:452:LEU:HD23	1:A:469:LEU:O	2.16	0.45
2:B:195:ILE:CG1	2:B:199:ARG:NE	2.79	0.45
1:A:90:VAL:O	1:A:91:GLN:C	2.55	0.45
1:A:115:TYR:OH	1:A:157:PRO:HG3	2.16	0.45
1:A:501:TYR:CD2	1:A:501:TYR:O	2.70	0.45
1:A:402:TRP:CD1	1:A:402:TRP:C	2.89	0.45
2:B:356:ARG:NH2	2:B:361:HIS:HB3	2.32	0.45
1:A:511:ASP:O	1:A:512:GLN:HB3	2.17	0.45
2:B:125:ARG:HB3	2:B:145:GLN:NE2	2.29	0.45
2:B:249:LYS:HD2	2:B:251:SER:O	2.17	0.45
2:B:338:THR:CG2	2:B:353:LYS:HE2	2.47	0.45
1:A:277:ARG:HD2	4:A:1038:HOH:O	2.18	0.44
1:A:69:THR:HG22	1:A:69:THR:O	2.17	0.44
2:B:377:THR:O	2:B:381:VAL:HG23	2.16	0.44
1:A:109:LEU:HG	1:A:216:THR:CG2	2.44	0.44
1:A:149:LEU:HD11	1:A:159:ILE:HG21	1.99	0.44
2:B:196:GLY:O	2:B:200:THR:HG23	2.18	0.44
2:B:254:VAL:HG21	2:B:287:LYS:HG2	1.99	0.44
1:A:193:LEU:HD13	1:A:197:GLN:HB3	2.00	0.44
2:B:211:ARG:O	2:B:211:ARG:HG3	2.18	0.44
2:B:234:LEU:C	2:B:236:PRO:HD3	2.38	0.44
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.52	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:HA	1:A:319:TYR:O	2.17	0.44
2:B:164:MET:HG2	2:B:182:GLN:NE2	2.33	0.44
2:B:303:LEU:HD22	2:B:307:ARG:NE	2.32	0.44
1:A:232:TYR:HE2	1:A:239:TRP:CZ3	2.36	0.44
2:B:195:ILE:HD11	2:B:199:ARG:HD3	1.99	0.44
2:B:279:LEU:O	2:B:282:LEU:HB2	2.17	0.44
2:B:255:ASN:HB2	2:B:289:LEU:HG	1.99	0.44
1:A:122:GLU:OE1	1:A:122:GLU:N	2.46	0.44
2:B:257:ILE:O	2:B:261:VAL:HG23	2.17	0.44
2:B:279:LEU:HD23	2:B:299:ALA:HB1	2.00	0.44
2:B:308:GLU:O	2:B:311:LYS:HB2	2.18	0.44
2:B:314:VAL:HG13	2:B:317:VAL:CG2	2.47	0.44
2:B:30:LYS:NZ	2:B:404:GLU:OE2	2.46	0.44
2:B:34:LEU:CD2	2:B:73:LYS:HG2	2.48	0.44
1:A:402:TRP:O	1:A:404:GLU:N	2.51	0.44
1:A:457:TYR:C	1:A:457:TYR:CD1	2.91	0.44
2:B:115:TYR:CD1	2:B:156:SER:HB3	2.52	0.44
2:B:195:ILE:CG2	2:B:196:GLY:N	2.67	0.44
2:B:266:TRP:CZ3	2:B:426:TRP:CD1	3.04	0.44
1:A:517:LEU:O	1:A:520:GLN:N	2.51	0.43
1:A:489:SER:HB2	1:A:493:VAL:HG22	2.00	0.43
2:B:357:MET:O	2:B:358:ARG:C	2.56	0.43
1:A:344:GLU:O	1:A:345:PRO:C	2.57	0.43
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.00	0.43
2:B:72:ARG:CZ	2:B:409:THR:HG22	2.48	0.43
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.50	0.43
1:A:60:VAL:O	1:A:60:VAL:HG13	2.17	0.43
2:B:367:GLN:O	2:B:371:ALA:N	2.46	0.43
1:A:38:CYS:O	1:A:42:GLU:HB2	2.18	0.43
1:A:426:TRP:N	1:A:426:TRP:CD1	2.87	0.43
1:A:64:LYS:CD	1:A:64:LYS:N	2.82	0.43
2:B:132:ILE:HB	2:B:142:ILE:HD12	2.00	0.43
2:B:60:VAL:O	2:B:61:PHE:HB3	2.18	0.43
1:A:314:VAL:O	1:A:314:VAL:HG23	2.18	0.43
1:A:338:THR:HG22	1:A:353:LYS:HB3	2.01	0.43
1:A:66:LYS:C	1:A:68:SER:H	2.22	0.43
2:B:203:GLU:OE2	2:B:206:ARG:NH1	2.52	0.43
1:A:77:PHE:C	1:A:79:GLU:N	2.72	0.43
1:A:149:LEU:HG	1:A:156:SER:HA	2.01	0.43
1:A:402:TRP:CZ2	2:B:362:THR:HA	2.54	0.43
2:B:382:ILE:HB	2:B:383:TRP:CE3	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:VAL:HG23	2:B:9:PRO:HD2	2.01	0.43
1:A:319:TYR:O	1:A:321:PRO:HD3	2.18	0.43
2:B:301:LEU:HG	2:B:302:GLU:N	2.32	0.43
1:A:170:PRO:O	1:A:171:PHE:C	2.57	0.43
1:A:3:SER:HB3	1:A:4:PRO:CD	2.48	0.42
2:B:282:LEU:HD22	2:B:293:ILE:CG2	2.49	0.42
1:A:211:ARG:CB	1:A:211:ARG:HH11	2.31	0.42
1:A:132:ILE:O	1:A:141:GLY:HA3	2.18	0.42
1:A:84:THR:O	1:A:85:GLN:O	2.36	0.42
2:B:182:GLN:HB2	2:B:187:LEU:HD12	1.99	0.42
1:A:111:VAL:HG22	1:A:185:ASP:HA	2.02	0.42
1:A:132:ILE:O	1:A:132:ILE:HG22	2.19	0.42
1:A:65:LYS:CG	1:A:66:LYS:N	2.82	0.42
2:B:239:TRP:CH2	2:B:378:GLU:HA	2.51	0.42
1:A:169:GLU:O	1:A:173:LYS:HD3	2.20	0.42
2:B:279:LEU:HG	2:B:302:GLU:OE2	2.19	0.42
2:B:422:LEU:C	2:B:424:LYS:N	2.71	0.42
1:A:308:GLU:O	1:A:309:ILE:C	2.57	0.42
2:B:211:ARG:CG	2:B:211:ARG:O	2.67	0.42
1:A:293:ILE:CD1	1:A:293:ILE:N	2.81	0.42
1:A:35:VAL:O	1:A:39:THR:OG1	2.38	0.42
1:A:433:PRO:HG3	1:A:532:TYR:CE2	2.53	0.42
1:A:137:ASN:OD1	1:A:137:ASN:O	2.38	0.42
1:A:202:ILE:HG22	1:A:203:GLU:N	2.35	0.42
1:A:225:PRO:HG3	1:A:227:PHE:CZ	2.55	0.42
1:A:33:ALA:HB2	1:A:71:TRP:CD1	2.55	0.42
1:A:402:TRP:C	1:A:404:GLU:H	2.22	0.42
2:B:41:MET:HG2	2:B:46:LYS:HD2	2.02	0.42
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.50	0.42
2:B:206:ARG:CB	2:B:206:ARG:NH1	2.74	0.42
2:B:356:ARG:HG3	2:B:356:ARG:NH1	2.34	0.42
1:A:163:SER:O	1:A:164:MET:C	2.57	0.42
1:A:205:LEU:O	1:A:209:LEU:HG	2.19	0.42
1:A:258:GLN:O	1:A:259:LYS:C	2.57	0.42
1:A:419:THR:O	1:A:420:PRO:C	2.56	0.42
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.84	0.42
1:A:338:THR:HG22	1:A:353:LYS:CB	2.49	0.41
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.20	0.41
2:B:157:PRO:HG3	2:B:184:MET:HA	2.02	0.41
2:B:388:LYS:HE2	2:B:415:GLU:HB3	2.02	0.41
1:A:235:HIS:O	1:A:238:LYS:O	2.38	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:HD13	1:A:309:ILE:HD12	2.02	0.41
1:A:149:LEU:HD21	1:A:160:PHE:N	2.35	0.41
1:A:245:VAL:O	1:A:245:VAL:HG23	2.19	0.41
1:A:255:ASN:HD22	1:A:255:ASN:HA	1.58	0.41
1:A:29:GLU:HG2	1:A:71:TRP:HE1	1.85	0.41
2:B:197:GLN:HG3	2:B:197:GLN:H	1.72	0.41
1:A:13:LYS:HG2	1:A:85:GLN:HA	2.03	0.41
2:B:278:GLN:NE2	2:B:278:GLN:HA	2.35	0.41
2:B:395:LYS:NZ	4:B:1060:HOH:O	2.47	0.41
2:B:82:LYS:HD3	2:B:413:GLU:OE1	2.20	0.41
2:B:61:PHE:HE1	2:B:63:ILE:HD11	1.85	0.41
1:A:134:SER:CB	1:A:138:GLU:HB2	2.49	0.41
1:A:231:GLY:C	1:A:242:GLN:HB3	2.41	0.41
1:A:368:LEU:O	1:A:372:VAL:HG23	2.20	0.41
1:A:8:VAL:O	1:A:121:ASP:HB2	2.19	0.41
2:B:206:ARG:O	2:B:207:GLN:C	2.59	0.41
2:B:332:GLN:NE2	2:B:424:LYS:HE2	2.36	0.41
1:A:225:PRO:HA	1:A:226:PRO:C	2.40	0.41
1:A:324:ASP:O	1:A:343:GLN:HG2	2.19	0.41
1:A:41:MET:HB2	1:A:47:ILE:CD1	2.51	0.41
1:A:58:THR:CG2	1:A:76:ASP:O	2.69	0.41
2:B:393:ILE:HD11	2:B:397:THR:HG22	2.03	0.41
2:B:80:LEU:O	2:B:81:ASN:C	2.58	0.41
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.56	0.41
1:A:378:GLU:HG3	4:A:1010:HOH:O	2.20	0.41
1:A:64:LYS:HE3	1:A:71:TRP:HZ3	1.81	0.41
1:A:498:ASP:CG	1:A:538:ALA:HB2	2.41	0.41
2:B:51:GLY:HA3	2:B:53:GLU:OE1	2.21	0.41
1:A:326:ILE:O	1:A:341:ILE:HA	2.21	0.41
1:A:96:HIS:CD2	1:A:98:ALA:H	2.29	0.41
2:B:28:GLU:CG	2:B:135:ILE:HD11	2.50	0.41
1:A:270:ILE:CG2	1:A:314:VAL:HG21	2.51	0.41
1:A:78:ARG:O	1:A:82:LYS:HG2	2.20	0.41
2:B:281:LYS:HZ2	2:B:284:ARG:HH22	1.68	0.41
2:B:314:VAL:HG13	2:B:317:VAL:HG21	2.03	0.41
2:B:393:ILE:HG12	2:B:394:GLN:H	1.86	0.41
2:B:422:LEU:O	2:B:423:VAL:C	2.59	0.41
2:B:130:PHE:CD1	2:B:130:PHE:C	2.94	0.40
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.80	0.40
2:B:111:VAL:HG22	2:B:185:ASP:O	2.20	0.40
2:B:361:HIS:CD2	2:B:361:HIS:N	2.88	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:GLU:HB3	2:B:347:LYS:HE3	2.03	0.40
1:A:124:PHE:O	1:A:127:TYR:CD2	2.74	0.40
1:A:329:ILE:O	1:A:392:PRO:HD3	2.21	0.40
1:A:491:LEU:HB3	1:A:529:GLU:HB2	2.02	0.40
1:A:175:ASN:CB	1:A:178:ILE:HD13	2.46	0.40
1:A:84:THR:HG22	1:A:85:GLN:O	2.21	0.40
2:B:116:PHE:HA	2:B:148:VAL:HG21	2.03	0.40
2:B:326:ILE:HG22	2:B:327:ALA:N	2.35	0.40
2:B:13:LYS:HE3	2:B:84:THR:O	2.20	0.40
1:A:408:ALA:HB3	2:B:393:ILE:CB	2.51	0.40
2:B:195:ILE:O	2:B:196:GLY:C	2.60	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	536/560 (96%)	439 (82%)	72 (13%)	25 (5%)	<b>3</b>	<b>3</b>
2	B	398/440 (90%)	343 (86%)	47 (12%)	8 (2%)	<b>9</b>	<b>17</b>
All	All	934/1000 (93%)	782 (84%)	119 (13%)	33 (4%)	<b>4</b>	<b>6</b>

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	217	PRO
1	A	218	ASP
2	B	98	ALA
2	B	195	ILE
2	B	361	HIS
1	A	67	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	85	GLN
1	A	91	GLN
1	A	113	ASP
1	A	138	GLU
2	B	66	LYS
2	B	116	PHE
2	B	208	HIS
1	A	68	SER
1	A	78	ARG
1	A	126	LYS
1	A	170	PRO
1	A	315	HIS
1	A	361	HIS
1	A	517	LEU
1	A	115	TYR
1	A	116	PHE
1	A	403	THR
1	A	4	PRO
1	A	135	ILE
1	A	476	LYS
2	B	85	GLN
1	A	123	ASP
2	B	421	PRO
1	A	139	THR
1	A	176	PRO
1	A	420	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	483/499 (97%)	439 (91%)	44 (9%)	11	21
2	B	368/400 (92%)	349 (95%)	19 (5%)	27	52
All	All	851/899 (95%)	788 (93%)	63 (7%)	16	32

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	6	GLU
1	A	24	TRP
1	A	64	LYS
1	A	89	GLU
1	A	94	ILE
1	A	102	LYS
1	A	105	SER
1	A	113	ASP
1	A	120	LEU
1	A	122	GLU
1	A	143	ARG
1	A	160	PHE
1	A	175	ASN
1	A	182	GLN
1	A	184	MET
1	A	187	LEU
1	A	205	LEU
1	A	210	LEU
1	A	211	ARG
1	A	217	PRO
1	A	229	TRP
1	A	237	ASP
1	A	255	ASN
1	A	266	TRP
1	A	305	GLU
1	A	322	SER
1	A	325	LEU
1	A	340	GLN
1	A	344	GLU
1	A	358	ARG
1	A	402	TRP
1	A	403	THR
1	A	404	GLU
1	A	417	VAL
1	A	431	LYS
1	A	449	GLU
1	A	452	LEU
1	A	474	ASN
1	A	475	GLN
1	A	496	VAL
1	A	500	GLN
1	A	517	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	533	LEU
2	B	40	GLU
2	B	69	THR
2	B	73	LYS
2	B	88	TRP
2	B	113	ASP
2	B	116	PHE
2	B	138	GLU
2	B	164	MET
2	B	165	THR
2	B	211	ARG
2	B	238	LYS
2	B	239	TRP
2	B	243	PRO
2	B	283	LEU
2	B	284	ARG
2	B	287	LYS
2	B	290	THR
2	B	361	HIS
2	B	368	LEU

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	57	ASN
1	A	96	HIS
1	A	137	ASN
1	A	174	GLN
1	A	175	ASN
1	A	255	ASN
1	A	278	GLN
1	A	332	GLN
1	A	336	GLN
1	A	474	ASN
1	A	475	GLN
1	A	480	GLN
1	A	500	GLN
1	A	512	GLN
2	B	57	ASN
2	B	145	GLN
2	B	147	ASN
2	B	161	GLN

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
2	B	182	GLN
2	B	197	GLN
2	B	278	GLN
2	B	332	GLN
2	B	361	HIS
2	B	394	GLN
2	B	428	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	CSD	A	280	1	4,7,8	1.32	0	2,8,10	3.42	1 (50%)

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	4.66	114.34	105.61

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](#)

1 ligand 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	$\# Z  > 2$
3	NVP	A	999	-	15,23,23	1.45	5 (33%)	14,34,34	1.21	1 (7%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	NVP	C13-N14	2.09	1.36	1.32
3	A	999	NVP	C5-C4	2.15	1.43	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	NVP	C12-C11	2.15	1.41	1.36
3	A	999	NVP	C4-N3	2.36	1.37	1.32
3	A	999	NVP	C10-C15	2.59	1.43	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	NVP	C4-C5-C6	-2.27	118.42	120.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	538/560 (96%)	-0.01	24 (4%) 34 26	18, 79, 126, 150	0
2	B	404/440 (91%)	-0.14	16 (3%) 39 31	29, 73, 119, 150	0
All	All	942/1000 (94%)	-0.06	40 (4%) 37 29	18, 77, 123, 150	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	SER	7.5
1	A	66	LYS	5.9
2	B	232	TYR	5.3
1	A	91	GLN	5.3
2	B	67	ASP	4.9
1	A	53	GLU	4.9
1	A	67	ASP	4.2
2	B	88	TRP	4.1
2	B	69	THR	4.1
1	A	219	LYS	3.7
2	B	65	LYS	3.7
1	A	514	GLU	3.6
2	B	94	ILE	3.5
1	A	221	HIS	3.5
2	B	66	LYS	3.3
1	A	21	VAL	3.2
1	A	52	PRO	3.2
1	A	356	ARG	3.1
1	A	22	LYS	3.0
2	B	432	GLU	3.0
1	A	220	LYS	2.9
2	B	210	LEU	2.8
1	A	137	ASN	2.8
2	B	431	LYS	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	92	LEU	2.6
2	B	237	ASP	2.4
2	B	104	LYS	2.4
2	B	240	THR	2.3
2	B	189	VAL	2.3
1	A	128	THR	2.3
2	B	238	LYS	2.3
1	A	539	HIS	2.3
1	A	218	ASP	2.3
1	A	136	ASN	2.2
1	A	116	PHE	2.2
1	A	297	GLU	2.1
1	A	90	VAL	2.1
1	A	140	PRO	2.0
2	B	6	GLU	2.0
1	A	58	THR	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	0.97	0.14	-	76,87,108,126	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( $\text{\AA}^2$ )	Q<0.9
3	NVP	A	999	20/20	0.90	0.29	1.69	80,99,112,116	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.