



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:08 AM GMT

PDB ID : 3DRR
Title : HIV reverse transcriptase Y181C mutant in complex with inhibitor R8e
Authors : Yan, Y.
Deposited on : 2008-07-11
Resolution : 2.89 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

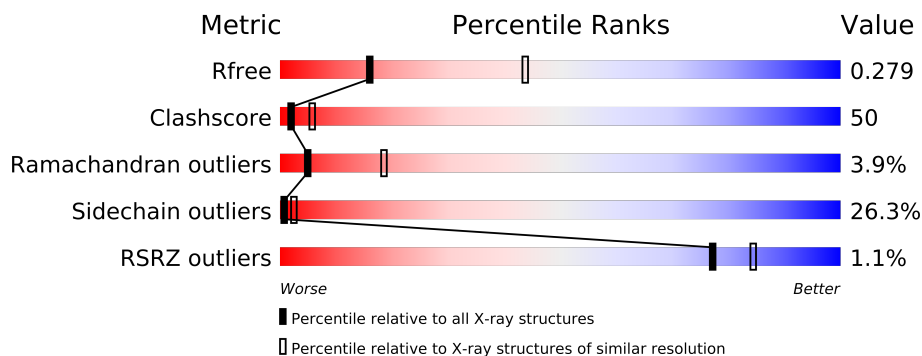
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.89 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	563	
2	B	443	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8249 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4536	2928	760	839	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP P04585
A	-1	ASN	-	EXPRESSION TAG	UNP P04585
A	0	SER	-	EXPRESSION TAG	UNP P04585
A	181	CYS	TYR	ENGINEERED	UNP P04585

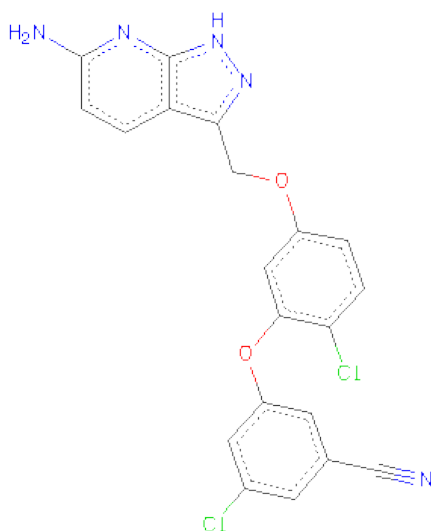
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3338	2170	554	607	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	EXPRESSION TAG	UNP P04585
B	-1	ASN	-	EXPRESSION TAG	UNP P04585
B	0	SER	-	EXPRESSION TAG	UNP P04585
B	181	CYS	TYR	ENGINEERED	UNP P04585

- Molecule 3 is 3-{5-[(6-AMINO-1H-PYRAZOLO[3,4-B]PYRIDIN-3-YL)METHOXY]-2-CHLOROPHENOXY}-5-CHLOROBENZONITRILE (three-letter code: R8E) (formula: C₂₀H₁₃Cl₂N₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
3	A	1	29	20	2	5	2	0	0

- Molecule 4 is water.

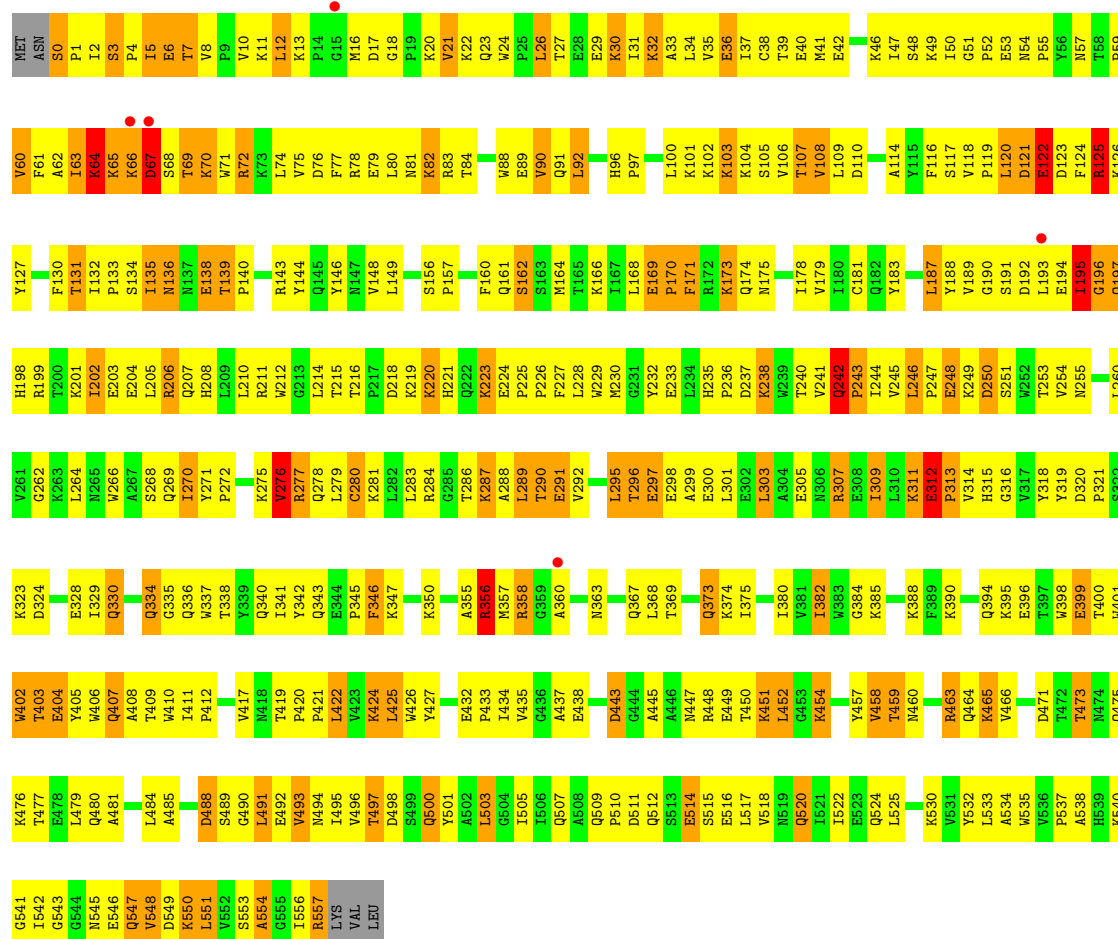
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	195	195	195	0	0
4	B	151	151	151	0	0

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

• Molecule 1: Reverse transcriptase/ribonucleaseH

Chain A: 



A62	I135	T215	R277	Q343	E413
I63	Y144	THR	Q278	E344	
K64	Y146	PRO	L279	P345	F416
K65	Y149	ASP	C280	F346	V417
Q145	L149	LYS	K281	K347	N418
D67	P150	LYS	L282	K348	T419
S68	W153	HIS	L283	L349	P420
T69	W154	GLN	K284	Y354	P421
K70	W155	LYS	G285	L422	L422
W71	W156	GLU	T286	A355	V423
K73	Q154	PRO	K287	R356	K424
L74	G155	PRO	A288	MET	L425
V75	G156	PHE	L289	ARG	W426
D76	P157	LEU	T290	GLY	Y427
F77	A158	TRP	E291	ALA	Q428
R78	I159	MET	V292	H361	LEU
E79	F160	G231	I293	T362	GLU
L80	S163	Y232	P294	N363	LYS
N81	K166	E233	L295	D364	GLY
K82	I167	L234	T296	V365	PRO
R83	E168	D237	E297	K366	ILE
Q85	L169	K238	E298	Q367	VAL
D86	R172	V241	A299	L368	GLY
F87	K173	Q242	E300	T369	ALA
W88	Q174	Q243	L301	E370	GLU
E89	M175	I244	E302	A371	THR
Q91	P176	V245	L303	V372	PHE
V90	D177	K246	E304	Q373	
L92	I178	L247	N305	K374	
P95	V179	E248	R307	I375	
H96	I180	K249	E308	T376	
P97	S251	D250	I309	T377	
A98	C181	W252	K310	T382	
G99	Q182	T253	K311	W383	
L100	L187	V254	P312	G384	
K101	Y188	N255	V314	K385	
K102	V189	D256	Y319	T386	
K103	I195	I257	D320	P387	
V108	R199	Q258	P321	F388	
V111	T200	K259	S322	F389	
Y115	K201	L260	K323	L391	
F116	I202	V261	D324	P392	
S117	E203	G262	L325	I393	
V118	E204	N265	Q326	Q394	
P119	L205	V266	Q330	K395	
L120	R206	A267	K331	E396	
D121	Q207	S268	Q332	T397	
E122	H208	Q269	K333	W398	
	L209	I270	Q335	E399	
	L210	Y271	W401	T400	
R125	K211	P272	Q336	W402	
K126	W212	G273	W337	T403	
Y127	G213	I274	V338	E404	
T128	L214	K275	Y339	Y405	
A129		V276	Q340	W406	
			I341	Q407	
			Y342		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.93Å 154.68Å 154.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.89 47.14 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.89) 99.6 (47.14-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.91 (at 2.91Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.183 , 0.269 0.192 , 0.279	Depositor DCC
R_{free} test set	1617 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 31972 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8249	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: R8E

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	0.64	0/4652	0.88	4/6320 (0.1%)
2	B	0.63	0/3431	0.84	4/4661 (0.1%)
All	All	0.64	0/8083	0.86	8/10981 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	GLU	C-N-CD	-13.44	91.04	120.60
2	B	420	PRO	C-N-CD	-11.79	94.67	120.60
2	B	51	GLY	C-N-CD	-6.55	106.19	120.60
1	A	216	THR	C-N-CD	6.06	141.12	128.40
1	A	242	GLN	C-N-CD	-6.05	107.30	120.60
2	B	419	THR	C-N-CD	-5.82	107.80	120.60
2	B	233	GLU	N-CA-C	5.54	125.95	111.00
1	A	149	LEU	C-N-CD	5.25	139.43	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts i

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4536	0	4591	499	0
2	B	3338	0	3365	325	0
3	A	29	0	13	5	0
4	A	195	0	0	15	0
4	B	151	0	0	8	0
All	All	8249	0	7969	796	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 50.

All (796) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:65:LYS:HE3	1:A:70:LYS:HG2	1.19	1.16
1:A:255:ASN:HB2	1:A:289:LEU:HD22	1.16	1.14
1:A:63:ILE:HD11	1:A:74:LEU:HD21	1.19	1.13
2:B:260:LEU:HD22	2:B:264:LEU:HD12	1.30	1.13
1:A:473:THR:HG23	1:A:476:LYS:HD2	1.20	1.11
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.24	1.10
1:A:63:ILE:HD12	1:A:72:ARG:HG3	1.22	1.10
1:A:175:ASN:HB3	1:A:178:ILE:HD13	1.34	1.07
1:A:195:ILE:HG23	1:A:199:ARG:HD2	1.36	1.07
1:A:296:THR:HG22	1:A:299:ALA:H	1.11	1.06
1:A:21:VAL:HG22	1:A:59:PRO:HD3	1.40	1.04
1:A:175:ASN:HD21	1:A:201:LYS:NZ	1.56	1.03
2:B:362:THR:HG22	2:B:366:LYS:HG2	1.42	1.00
1:A:64:LYS:HZ1	1:A:69:THR:HG22	1.20	1.00
1:A:175:ASN:ND2	1:A:201:LYS:HZ2	1.59	0.99
1:A:500:GLN:HG3	2:B:422:LEU:HD11	1.46	0.97
2:B:422:LEU:HA	2:B:425:LEU:HD21	1.46	0.96
2:B:175:ASN:HB3	2:B:178:ILE:HG13	1.45	0.96
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.04	0.95
2:B:111:VAL:HG21	2:B:187:LEU:HD22	1.50	0.94
2:B:258:GLN:HG3	2:B:283:LEU:HD21	1.52	0.90
2:B:298:GLU:HA	2:B:301:LEU:CD1	2.02	0.90
1:A:63:ILE:HG12	1:A:74:LEU:HD11	1.52	0.90
2:B:125:ARG:HB3	2:B:145:GLN:HE21	1.35	0.90
1:A:65:LYS:HE3	1:A:70:LYS:CG	2.02	0.89
1:A:104:LYS:CB	1:A:192:ASP:HA	2.03	0.89
2:B:279:LEU:HA	2:B:282:LEU:HD11	1.53	0.89
2:B:24:TRP:CE3	2:B:25:PRO:HD2	2.08	0.88
1:A:287:LYS:HE2	1:A:287:LYS:HA	1.54	0.88
1:A:255:ASN:HB2	1:A:289:LEU:CD2	2.03	0.87
2:B:362:THR:CG2	2:B:366:LYS:HG2	2.04	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:298:GLU:HA	2:B:301:LEU:HG	1.56	0.87
1:A:296:THR:CG2	1:A:299:ALA:H	1.86	0.87
1:A:500:GLN:HG3	2:B:422:LEU:CD1	2.04	0.87
1:A:473:THR:CG2	1:A:476:LYS:HD2	2.03	0.87
2:B:65:LYS:HE3	2:B:68:SER:CB	2.05	0.87
1:A:143:ARG:HH11	1:A:143:ARG:HG3	1.39	0.85
1:A:233:GLU:HG2	1:A:235:HIS:CE1	2.11	0.85
1:A:131:THR:HG23	1:A:143:ARG:HD2	1.56	0.85
1:A:466:VAL:CG2	1:A:551:LEU:HD23	2.07	0.84
1:A:63:ILE:HD12	1:A:72:ARG:CG	2.07	0.84
1:A:296:THR:HG22	1:A:299:ALA:N	1.92	0.84
1:A:206:ARG:CZ	1:A:218:ASP:HA	2.07	0.83
2:B:65:LYS:HE3	2:B:68:SER:HB3	1.58	0.83
2:B:344:GLU:CB	2:B:347:LYS:HD3	2.07	0.83
1:A:63:ILE:CD1	1:A:74:LEU:HD21	2.07	0.82
1:A:125:ARG:HG2	1:A:146:TYR:O	1.78	0.82
1:A:241:VAL:HG23	1:A:244:ILE:HD11	1.62	0.82
2:B:254:VAL:HG21	2:B:288:ALA:O	1.79	0.81
2:B:268:SER:O	2:B:269:GLN:HG3	1.80	0.81
1:A:5:ILE:HG22	1:A:212:TRP:CE3	2.16	0.81
2:B:298:GLU:HA	2:B:301:LEU:CG	2.12	0.80
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.64	0.80
1:A:65:LYS:HD3	1:A:70:LYS:O	1.82	0.80
1:A:7:THR:HG22	4:A:629:HOH:O	1.81	0.80
1:A:175:ASN:HD21	1:A:201:LYS:HZ2	0.82	0.79
1:A:3:SER:OG	1:A:5:ILE:HG23	1.82	0.79
1:A:223:LYS:H	1:A:223:LYS:HD2	1.46	0.79
1:A:223:LYS:CD	1:A:223:LYS:H	1.95	0.79
2:B:425:LEU:HD23	2:B:425:LEU:H	1.47	0.79
2:B:18:GLY:HA3	2:B:56:TYR:CE1	2.18	0.79
1:A:206:ARG:NH1	1:A:218:ASP:HA	1.98	0.78
2:B:253:THR:HG23	2:B:289:LEU:O	1.83	0.78
1:A:5:ILE:HG22	1:A:212:TRP:HE3	1.48	0.78
1:A:35:VAL:O	1:A:39:THR:HG23	1.82	0.78
2:B:172:ARG:HH21	2:B:180:ILE:HB	1.47	0.78
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.18	0.77
1:A:298:GLU:HA	1:A:301:LEU:HD12	1.66	0.77
2:B:274:ILE:HG23	2:B:306:ASN:ND2	1.99	0.77
2:B:284:ARG:H	2:B:287:LYS:HZ2	1.32	0.77
2:B:366:LYS:O	2:B:370:GLU:HG3	1.84	0.77
2:B:241:VAL:CG2	2:B:243:PRO:HG3	2.15	0.76
1:A:195:ILE:CG2	1:A:199:ARG:HD2	2.12	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:271:TYR:CE1	1:A:314:VAL:HG23	2.20	0.76
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.67	0.76
1:A:516:GLU:O	1:A:520:GLN:HG2	1.86	0.76
1:A:204:GLU:HB2	4:A:660:HOH:O	1.84	0.76
1:A:181:CYS:HB2	1:A:188:TYR:HB2	1.66	0.76
1:A:65:LYS:HG2	1:A:68:SER:HB3	1.67	0.76
1:A:278:GLN:HG2	1:A:298:GLU:HB2	1.66	0.76
1:A:91:GLN:HE21	1:A:92:LEU:N	1.84	0.76
1:A:79:GLU:CG	1:A:83:ARG:HH21	1.98	0.76
1:A:515:SER:HB3	1:A:518:VAL:HG23	1.68	0.75
2:B:279:LEU:HA	2:B:282:LEU:CD1	2.15	0.75
1:A:287:LYS:HE2	1:A:287:LYS:CA	2.09	0.75
1:A:473:THR:HG23	1:A:476:LYS:CD	2.11	0.75
1:A:330:GLN:NE2	1:A:340:GLN:HE22	1.82	0.75
2:B:298:GLU:CD	2:B:298:GLU:H	1.89	0.74
1:A:5:ILE:HG12	1:A:6:GLU:N	2.00	0.74
2:B:260:LEU:HD22	2:B:264:LEU:CD1	2.15	0.74
1:A:511:ASP:OD2	1:A:512:GLN:HG3	1.87	0.74
1:A:278:GLN:HG2	1:A:298:GLU:CB	2.17	0.74
2:B:8:VAL:HG11	2:B:159:ILE:HG12	1.68	0.74
1:A:2:ILE:HD11	1:A:46:LYS:NZ	2.02	0.74
2:B:373:GLN:HE22	2:B:407:GLN:H	1.33	0.74
2:B:418:ASN:O	2:B:420:PRO:HD3	1.87	0.74
2:B:344:GLU:HB3	2:B:347:LYS:HD3	1.67	0.74
1:A:76:ASP:OD2	1:A:78:ARG:HG3	1.88	0.74
1:A:219:LYS:HG3	1:A:220:LYS:H	1.53	0.73
1:A:424:LYS:HE2	1:A:426:TRP:CH2	2.23	0.73
1:A:64:LYS:NZ	1:A:69:THR:HG22	2.01	0.73
1:A:466:VAL:HG23	1:A:551:LEU:HD23	1.69	0.73
1:A:134:SER:OG	1:A:139:THR:HB	1.89	0.73
2:B:298:GLU:CA	2:B:301:LEU:HG	2.19	0.73
1:A:435:VAL:HG23	2:B:290:THR:HG21	1.71	0.73
1:A:211:ARG:HD3	1:A:211:ARG:O	1.88	0.73
2:B:303:LEU:O	2:B:307:ARG:HB2	1.89	0.72
2:B:344:GLU:HB2	2:B:347:LYS:HD3	1.70	0.72
1:A:458:VAL:HG13	1:A:548:VAL:HG13	1.71	0.72
2:B:335:GLY:HA3	2:B:356:ARG:HG2	1.70	0.72
1:A:201:LYS:HE2	1:A:204:GLU:OE2	1.89	0.72
1:A:96:HIS:HB3	1:A:382:ILE:HD13	1.70	0.72
2:B:282:LEU:HB3	2:B:293:ILE:CD1	2.19	0.71
1:A:277:ARG:NH1	1:A:278:GLN:NE2	2.37	0.71
1:A:90:VAL:HG12	1:A:91:GLN:N	2.05	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:34:LEU:CD2	2:B:73:LYS:HB2	2.21	0.71
1:A:277:ARG:CD	1:A:334:GLN:HE21	2.03	0.71
2:B:270:ILE:HB	2:B:346:PHE:HB3	1.71	0.71
2:B:125:ARG:CB	2:B:145:GLN:HE21	2.03	0.71
1:A:450:THR:OG1	1:A:452:LEU:HB2	1.91	0.70
1:A:454:LYS:HB2	1:A:556:ILE:HG13	1.72	0.70
1:A:175:ASN:ND2	1:A:201:LYS:NZ	2.27	0.70
1:A:52:PRO:HD2	1:A:53:GLU:OE2	1.91	0.70
2:B:271:TYR:CD1	2:B:310:LEU:HD12	2.25	0.70
1:A:503:LEU:HD22	1:A:507:GLN:HG3	1.74	0.70
1:A:65:LYS:CE	1:A:70:LYS:HG2	2.10	0.70
2:B:270:ILE:HG13	2:B:346:PHE:O	1.92	0.70
1:A:424:LYS:HE2	1:A:426:TRP:CZ2	2.27	0.70
1:A:324:ASP:OD2	1:A:388:LYS:HE2	1.90	0.70
1:A:373:GLN:OE1	2:B:400:THR:HG21	1.91	0.70
2:B:284:ARG:H	2:B:287:LYS:NZ	1.88	0.69
2:B:8:VAL:HG11	2:B:159:ILE:CG1	2.22	0.69
2:B:306:ASN:O	2:B:310:LEU:HD22	1.92	0.69
2:B:282:LEU:HB3	2:B:293:ILE:HD11	1.75	0.69
1:A:535:TRP:CZ3	1:A:537:PRO:HD3	2.27	0.69
1:A:57:ASN:ND2	1:A:131:THR:OG1	2.25	0.69
2:B:50:ILE:HG21	2:B:145:GLN:HB2	1.75	0.69
1:A:13:LYS:O	1:A:16:MET:HB2	1.93	0.69
1:A:12:LEU:HD23	1:A:124:PHE:HE1	1.57	0.69
1:A:330:GLN:HE22	1:A:340:GLN:NE2	1.85	0.69
2:B:267:ALA:O	2:B:270:ILE:HG23	1.93	0.68
1:A:63:ILE:HG12	1:A:74:LEU:CD1	2.22	0.68
2:B:293:ILE:O	2:B:293:ILE:HG13	1.92	0.68
1:A:23:GLN:NE2	1:A:26:LEU:HD21	2.08	0.68
2:B:116:PHE:HB2	4:B:465:HOH:O	1.92	0.68
1:A:454:LYS:NZ	1:A:554:ALA:O	2.27	0.68
2:B:373:GLN:NE2	2:B:407:GLN:H	1.91	0.68
2:B:256:ASP:O	2:B:260:LEU:HB2	1.92	0.68
1:A:79:GLU:HG3	1:A:83:ARG:HE	1.58	0.68
2:B:87:PHE:CZ	2:B:159:ILE:HD11	2.29	0.68
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.29	0.68
2:B:28:GLU:O	2:B:32:LYS:HG2	1.94	0.68
2:B:337:TRP:HE1	2:B:367:GLN:NE2	1.92	0.67
1:A:104:LYS:HB2	1:A:191:SER:O	1.95	0.67
2:B:8:VAL:CG1	2:B:159:ILE:HG12	2.24	0.67
1:A:320:ASP:OD2	1:A:323:LYS:NZ	2.28	0.67
1:A:203:GLU:OE2	1:A:206:ARG:NH1	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:422:LEU:HA	2:B:425:LEU:CD2	2.24	0.67
1:A:244:ILE:HD12	1:A:244:ILE:N	2.09	0.67
1:A:410:TRP:CZ3	2:B:363:ASN:HB3	2.30	0.67
1:A:32:LYS:NZ	1:A:36:GLU:OE2	2.26	0.67
1:A:241:VAL:CG2	1:A:244:ILE:HD11	2.25	0.66
1:A:402:TRP:CE3	1:A:403:THR:HB	2.29	0.66
1:A:369:THR:HG22	1:A:411:ILE:HD11	1.77	0.66
2:B:308:GLU:O	2:B:311:LYS:HG2	1.95	0.66
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.31	0.66
1:A:89:GLU:CB	1:A:92:LEU:HD11	2.26	0.66
1:A:312:GLU:HB2	4:A:737:HOH:O	1.96	0.66
1:A:169:GLU:O	1:A:173:LYS:HE2	1.96	0.66
1:A:358:ARG:NH1	2:B:396:GLU:OE2	2.28	0.66
1:A:65:LYS:HE2	1:A:72:ARG:CZ	2.25	0.66
1:A:266:TRP:O	1:A:269:GLN:HG3	1.95	0.66
2:B:18:GLY:HA3	2:B:56:TYR:CD1	2.31	0.65
2:B:28:GLU:HG3	2:B:135:ILE:CD1	2.26	0.65
1:A:134:SER:HB3	1:A:139:THR:O	1.96	0.65
1:A:277:ARG:HD2	1:A:334:GLN:HE21	1.62	0.65
2:B:274:ILE:HG22	2:B:275:LYS:N	2.11	0.65
2:B:260:LEU:O	2:B:264:LEU:HB2	1.97	0.65
2:B:195:ILE:O	2:B:199:ARG:HG3	1.96	0.65
2:B:98:ALA:O	2:B:101:LYS:NZ	2.29	0.65
1:A:233:GLU:HG2	1:A:235:HIS:HE1	1.60	0.64
1:A:503:LEU:HD22	1:A:507:GLN:CG	2.27	0.64
2:B:253:THR:O	2:B:257:ILE:HG12	1.98	0.64
1:A:278:GLN:CG	1:A:298:GLU:HB2	2.27	0.64
1:A:249:LYS:HG2	1:A:251:SER:O	1.97	0.64
2:B:108:VAL:HB	2:B:232:TYR:HD2	1.62	0.64
2:B:95:PRO:HG3	4:B:562:HOH:O	1.96	0.64
2:B:306:ASN:O	2:B:309:ILE:HB	1.98	0.64
2:B:279:LEU:HD23	2:B:302:GLU:OE1	1.97	0.64
2:B:373:GLN:O	2:B:377:THR:HG23	1.98	0.64
2:B:30:LYS:HG2	2:B:62:ALA:HB3	1.80	0.64
1:A:106:VAL:HG22	1:A:227:PHE:CE2	2.33	0.63
1:A:5:ILE:HG12	1:A:6:GLU:O	1.98	0.63
2:B:159:ILE:HG22	2:B:160:PHE:N	2.12	0.63
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.79	0.63
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.27	0.63
1:A:175:ASN:CB	1:A:178:ILE:HD13	2.20	0.63
2:B:274:ILE:HG22	2:B:275:LYS:H	1.61	0.63
1:A:206:ARG:HH22	1:A:218:ASP:HB3	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:553:SER:HA	1:A:557:ARG:HD3	1.80	0.63
1:A:489:SER:HB2	1:A:493:VAL:CG1	2.28	0.63
1:A:465:LYS:HG3	1:A:466:VAL:N	2.13	0.63
1:A:2:ILE:HG12	4:A:698:HOH:O	1.98	0.63
1:A:102:LYS:HZ3	1:A:237:ASP:CB	2.12	0.63
2:B:396:GLU:O	2:B:400:THR:HG22	1.99	0.62
1:A:17:ASP:O	1:A:83:ARG:HD3	1.98	0.62
2:B:92:LEU:HD23	4:B:492:HOH:O	1.98	0.62
1:A:171:PHE:O	1:A:175:ASN:HB2	1.98	0.62
1:A:277:ARG:HD2	1:A:334:GLN:NE2	2.13	0.62
1:A:131:THR:HG23	1:A:143:ARG:CD	2.29	0.62
1:A:102:LYS:NZ	1:A:237:ASP:HB3	2.14	0.62
2:B:214:LEU:HD23	2:B:214:LEU:N	2.15	0.62
1:A:249:LYS:HG3	1:A:250:ASP:H	1.65	0.61
2:B:72:ARG:HH11	2:B:72:ARG:HG3	1.65	0.61
1:A:235:HIS:HB3	1:A:236:PRO:CD	2.30	0.61
1:A:498:ASP:OD2	1:A:538:ALA:HB2	2.00	0.61
1:A:303:LEU:O	1:A:307:ARG:HG3	2.00	0.61
2:B:258:GLN:HG3	2:B:283:LEU:CD2	2.28	0.61
1:A:434:ILE:HG21	1:A:492:GLU:OE1	1.99	0.61
1:A:406:TRP:HZ3	2:B:392:PRO:CB	2.13	0.61
2:B:274:ILE:O	2:B:275:LYS:HD3	2.00	0.61
2:B:87:PHE:CZ	2:B:92:LEU:HD12	2.36	0.61
1:A:135:ILE:O	1:A:136:ASN:HB2	2.01	0.60
2:B:273:GLY:O	2:B:275:LYS:NZ	2.30	0.60
2:B:266:TRP:CE3	2:B:426:TRP:HB3	2.37	0.60
1:A:89:GLU:HB2	1:A:92:LEU:HD11	1.81	0.60
2:B:97:PRO:HG3	4:B:522:HOH:O	2.00	0.60
2:B:324:ASP:O	2:B:343:GLN:HG2	2.00	0.60
1:A:131:THR:CG2	1:A:143:ARG:HD2	2.32	0.60
1:A:79:GLU:HG2	1:A:83:ARG:HH21	1.66	0.60
2:B:64:LYS:NZ	2:B:69:THR:O	2.34	0.60
1:A:107:THR:HG23	1:A:198:HIS:CE1	2.37	0.60
2:B:261:VAL:O	2:B:265:ASN:HB3	2.01	0.60
1:A:223:LYS:NZ	4:A:627:HOH:O	2.24	0.60
1:A:363:ASN:HA	1:A:511:ASP:OD2	2.02	0.60
1:A:360:ALA:HA	1:A:514:GLU:OE1	2.02	0.60
1:A:65:LYS:HE2	1:A:72:ARG:NH1	2.17	0.60
1:A:277:ARG:NH1	1:A:278:GLN:HE21	1.97	0.60
2:B:241:VAL:HG23	2:B:243:PRO:HG3	1.83	0.60
2:B:295:LEU:HD12	2:B:299:ALA:HB3	1.82	0.59
2:B:87:PHE:CE1	2:B:92:LEU:HD12	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:170:PRO:O	1:A:173:LYS:N	2.27	0.59
1:A:253:THR:HA	1:A:291:GLU:O	2.02	0.59
1:A:219:LYS:HG3	1:A:220:LYS:N	2.17	0.59
1:A:244:ILE:HD12	1:A:244:ILE:H	1.66	0.59
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.38	0.59
2:B:175:ASN:N	2:B:176:PRO:HD3	2.18	0.59
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.37	0.59
1:A:437:ALA:HB3	1:A:494:ASN:HD21	1.68	0.59
1:A:66:LYS:O	1:A:67:ASP:HB2	2.02	0.59
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.31	0.58
2:B:90:VAL:O	2:B:90:VAL:HG23	2.03	0.58
2:B:320:ASP:OD2	2:B:323:LYS:HD2	2.02	0.58
1:A:400:THR:O	1:A:404:GLU:HG3	2.03	0.58
2:B:422:LEU:HB3	2:B:426:TRP:CZ2	2.38	0.58
1:A:70:LYS:NZ	1:A:72:ARG:NH2	2.51	0.58
1:A:70:LYS:NZ	1:A:72:ARG:HH21	2.01	0.58
2:B:323:LYS:NZ	2:B:344:GLU:OE2	2.30	0.58
1:A:238:LYS:HB2	1:A:315:HIS:HD2	1.68	0.58
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.83	0.58
1:A:108:VAL:HG13	1:A:223:LYS:HD3	1.86	0.58
1:A:384:GLY:O	2:B:27:THR:HB	2.03	0.58
2:B:76:ASP:OD2	2:B:78:ARG:HG3	2.03	0.58
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.38	0.58
1:A:27:THR:OG1	1:A:30:LYS:HG3	2.03	0.58
1:A:287:LYS:HG2	1:A:291:GLU:OE1	2.02	0.58
1:A:60:VAL:HG21	1:A:130:PHE:HD2	1.68	0.58
2:B:241:VAL:HG21	2:B:243:PRO:HG3	1.86	0.58
1:A:195:ILE:HG23	1:A:199:ARG:CD	2.24	0.58
2:B:271:TYR:O	2:B:274:ILE:HG12	2.04	0.58
1:A:106:VAL:HA	1:A:189:VAL:O	2.04	0.57
1:A:90:VAL:HG12	1:A:91:GLN:H	1.68	0.57
1:A:420:PRO:HA	1:A:421:PRO:C	2.24	0.57
2:B:65:LYS:HE2	2:B:70:LYS:O	2.04	0.57
1:A:465:LYS:HG3	1:A:466:VAL:H	1.69	0.57
1:A:23:GLN:HG3	1:A:24:TRP:O	2.05	0.57
1:A:230:MET:HA	1:A:230:MET:HE2	1.86	0.57
1:A:29:GLU:HG2	4:A:669:HOH:O	2.04	0.57
1:A:21:VAL:HG22	1:A:59:PRO:CD	2.26	0.57
2:B:11:LYS:HG2	2:B:11:LYS:O	2.05	0.57
2:B:13:LYS:HB2	2:B:16:MET:HE3	1.86	0.57
1:A:405:TYR:CE2	1:A:407:GLN:HG2	2.39	0.57
1:A:330:GLN:NE2	1:A:338:THR:HG23	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.87	0.57
1:A:105:SER:O	1:A:190:GLY:HA2	2.05	0.57
1:A:373:GLN:HE22	2:B:401:TRP:HE1	1.51	0.57
2:B:34:LEU:HD23	2:B:73:LYS:HB2	1.87	0.57
2:B:13:LYS:HB2	2:B:16:MET:CE	2.35	0.57
1:A:122:GLU:HB2	4:A:624:HOH:O	2.05	0.57
2:B:65:LYS:HD3	2:B:65:LYS:N	2.19	0.56
2:B:399:GLU:HG2	4:B:512:HOH:O	2.03	0.56
1:A:195:ILE:HD13	1:A:199:ARG:CD	2.35	0.56
1:A:434:ILE:HD12	1:A:434:ILE:H	1.70	0.56
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.87	0.56
1:A:445:ALA:O	1:A:477:THR:HG21	2.05	0.56
1:A:346:PHE:N	1:A:346:PHE:CD1	2.70	0.56
1:A:171:PHE:HA	1:A:174:GLN:HE21	1.71	0.56
1:A:175:ASN:HB3	1:A:178:ILE:CD1	2.22	0.56
1:A:296:THR:HG22	1:A:299:ALA:CB	2.36	0.56
2:B:362:THR:HG23	2:B:366:LYS:NZ	2.20	0.56
1:A:369:THR:HG21	1:A:398:TRP:CH2	2.41	0.56
1:A:143:ARG:NH1	1:A:143:ARG:HG3	2.14	0.56
2:B:122:GLU:HA	2:B:125:ARG:NE	2.21	0.56
1:A:203:GLU:HA	1:A:206:ARG:HG3	1.88	0.56
1:A:277:ARG:HD3	1:A:334:GLN:HE21	1.69	0.56
1:A:406:TRP:CZ2	2:B:418:ASN:HA	2.40	0.56
2:B:275:LYS:H	2:B:306:ASN:HD21	1.54	0.56
2:B:167:ILE:HG12	2:B:212:TRP:CG	2.41	0.56
1:A:70:LYS:HZ3	1:A:72:ARG:NH2	2.04	0.56
2:B:65:LYS:HD2	2:B:72:ARG:HB2	1.87	0.56
1:A:193:LEU:HD13	1:A:197:GLN:HB2	1.86	0.56
1:A:41:MET:HB2	1:A:47:ILE:HG12	1.88	0.56
1:A:104:LYS:CG	1:A:192:ASP:HA	2.35	0.56
1:A:2:ILE:HD11	1:A:46:LYS:HZ2	1.67	0.56
1:A:399:GLU:O	1:A:402:TRP:HE3	1.89	0.56
1:A:107:THR:OG1	1:A:202:ILE:HD11	2.05	0.56
1:A:102:LYS:O	1:A:103:LYS:NZ	2.29	0.56
1:A:88:TRP:HE3	1:A:88:TRP:HA	1.70	0.56
1:A:547:GLN:HA	1:A:550:LYS:HE2	1.88	0.56
1:A:164:MET:O	1:A:168:LEU:HD12	2.06	0.56
2:B:275:LYS:HE3	2:B:305:GLU:OE1	2.06	0.56
2:B:103:LYS:CE	2:B:179:VAL:HG23	2.36	0.56
1:A:226:PRO:O	1:A:228:LEU:HD12	2.05	0.56
1:A:305:GLU:O	1:A:309:ILE:HG13	2.05	0.56
1:A:465:LYS:O	1:A:466:VAL:HG23	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:490:GLY:O	1:A:492:GLU:N	2.40	0.55
2:B:12:LEU:HD23	2:B:17:ASP:HA	1.87	0.55
2:B:129:ALA:HA	2:B:144:TYR:O	2.06	0.55
2:B:332:GLN:HA	2:B:424:LYS:HE3	1.88	0.55
2:B:14:PRO:HA	4:B:541:HOH:O	2.05	0.55
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.07	0.55
1:A:245:VAL:O	1:A:247:PRO:HD3	2.07	0.55
2:B:246:LEU:HD11	2:B:310:LEU:CD2	2.36	0.55
2:B:274:ILE:C	2:B:275:LYS:HD3	2.26	0.55
1:A:238:LYS:HB2	1:A:315:HIS:CD2	2.41	0.55
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.35	0.55
1:A:540:LYS:O	1:A:542:ILE:N	2.40	0.55
1:A:311:LYS:O	1:A:312:GLU:HB3	2.04	0.55
2:B:72:ARG:HH11	2:B:72:ARG:CG	2.18	0.55
2:B:252:TRP:HB3	2:B:257:ILE:HD13	1.89	0.55
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.27	0.55
1:A:262:GLY:HA2	4:A:675:HOH:O	2.07	0.55
1:A:369:THR:HG21	1:A:398:TRP:CZ3	2.41	0.55
2:B:80:LEU:O	2:B:84:THR:HG23	2.07	0.55
1:A:106:VAL:HG22	1:A:227:PHE:HE2	1.68	0.55
1:A:194:GLU:H	1:A:194:GLU:CD	2.10	0.55
2:B:398:TRP:O	2:B:402:TRP:HD1	1.90	0.55
2:B:267:ALA:O	2:B:271:TYR:HB2	2.06	0.55
2:B:344:GLU:HB3	2:B:347:LYS:HZ2	1.72	0.55
1:A:26:LEU:CD2	1:A:133:PRO:HG3	2.37	0.55
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.42	0.55
1:A:173:LYS:HZ2	1:A:173:LYS:HA	1.72	0.54
2:B:8:VAL:HG23	4:B:498:HOH:O	2.07	0.54
1:A:406:TRP:CZ3	1:A:407:GLN:HB2	2.42	0.54
1:A:426:TRP:O	1:A:427:TYR:HB3	2.08	0.54
1:A:319:TYR:OH	1:A:385:LYS:HE2	2.06	0.54
1:A:229:TRP:CD2	1:A:230:MET:HB2	2.42	0.54
1:A:460:ASN:HD22	2:B:288:ALA:N	2.05	0.54
1:A:8:VAL:O	1:A:10:VAL:HG23	2.08	0.54
2:B:298:GLU:HA	2:B:301:LEU:HD12	1.87	0.54
1:A:171:PHE:HA	1:A:174:GLN:NE2	2.22	0.54
2:B:369:THR:HG22	2:B:370:GLU:N	2.22	0.54
2:B:422:LEU:O	2:B:425:LEU:HD23	2.06	0.54
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.43	0.54
2:B:425:LEU:H	2:B:425:LEU:CD2	2.17	0.54
2:B:204:GLU:O	2:B:208:HIS:HD2	1.90	0.54
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:70:LYS:HZ1	1:A:72:ARG:HH21	1.55	0.53
1:A:183:TYR:HB3	1:A:188:TYR:HE1	1.72	0.53
1:A:290:THR:HB	4:A:633:HOH:O	2.08	0.53
1:A:433:PRO:CG	2:B:255:ASN:HD22	2.21	0.53
2:B:253:THR:HG22	2:B:255:ASN:N	2.24	0.53
1:A:91:GLN:HE21	1:A:92:LEU:H	1.54	0.53
2:B:428:GLN:HA	2:B:428:GLN:NE2	2.23	0.53
2:B:261:VAL:O	2:B:265:ASN:N	2.27	0.53
2:B:246:LEU:HD11	2:B:310:LEU:HD21	1.89	0.53
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.43	0.53
1:A:515:SER:CB	1:A:518:VAL:HG23	2.36	0.53
1:A:2:ILE:CD1	1:A:46:LYS:HZ2	2.22	0.53
1:A:193:LEU:HB3	1:A:197:GLN:HG2	1.89	0.53
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.91	0.53
1:A:454:LYS:HD3	1:A:556:ILE:HD11	1.91	0.53
1:A:411:ILE:HG23	1:A:412:PRO:HD2	1.91	0.53
1:A:194:GLU:O	1:A:196:GLY:N	2.42	0.53
1:A:120:LEU:HD12	1:A:121:ASP:N	2.24	0.53
1:A:447:ASN:OD1	1:A:449:GLU:HG2	2.09	0.53
2:B:297:GLU:O	2:B:301:LEU:HG	2.09	0.52
2:B:64:LYS:O	2:B:65:LYS:O	2.27	0.52
2:B:12:LEU:HD12	2:B:84:THR:HG22	1.91	0.52
1:A:51:GLY:O	1:A:143:ARG:NH1	2.42	0.52
2:B:11:LYS:HE2	2:B:11:LYS:N	2.23	0.52
2:B:371:ALA:O	2:B:375:ILE:HG13	2.09	0.52
1:A:104:LYS:HG3	1:A:192:ASP:O	2.09	0.52
1:A:171:PHE:N	1:A:174:GLN:NE2	2.57	0.52
1:A:410:TRP:CE3	2:B:363:ASN:CB	2.93	0.52
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.44	0.52
1:A:454:LYS:CD	1:A:556:ILE:HD11	2.39	0.52
1:A:178:ILE:HD12	1:A:178:ILE:H	1.75	0.52
1:A:277:ARG:HH11	1:A:278:GLN:NE2	2.07	0.52
1:A:202:ILE:HG22	1:A:203:GLU:N	2.25	0.52
2:B:373:GLN:HE22	2:B:407:GLN:N	2.06	0.52
1:A:48:SER:O	1:A:144:TYR:HA	2.10	0.52
2:B:296:THR:O	2:B:300:GLU:OE1	2.27	0.52
2:B:362:THR:HG23	2:B:366:LYS:CE	2.39	0.52
1:A:406:TRP:HZ2	2:B:418:ASN:OD1	1.93	0.52
2:B:267:ALA:O	2:B:271:TYR:N	2.43	0.52
2:B:257:ILE:HA	2:B:260:LEU:HB2	1.90	0.52
1:A:464:GLN:HG2	1:A:465:LYS:N	2.24	0.52
1:A:270:ILE:O	1:A:272:PRO:HD3	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:417:VAL:O	1:A:417:VAL:HG13	2.10	0.52
2:B:34:LEU:HD21	2:B:73:LYS:HB2	1.90	0.52
2:B:326:ILE:O	2:B:341:ILE:HA	2.10	0.52
2:B:80:LEU:O	2:B:80:LEU:HD22	2.09	0.52
2:B:87:PHE:HE1	2:B:159:ILE:HD12	1.75	0.52
1:A:433:PRO:CG	2:B:255:ASN:ND2	2.73	0.51
1:A:12:LEU:CD2	1:A:124:PHE:HE1	2.22	0.51
1:A:230:MET:CA	1:A:230:MET:CE	2.88	0.51
2:B:189:VAL:HB	2:B:202:ILE:HD11	1.91	0.51
2:B:256:ASP:O	2:B:260:LEU:N	2.43	0.51
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.40	0.51
2:B:271:TYR:HD1	2:B:310:LEU:HD12	1.72	0.51
1:A:102:LYS:HZ3	1:A:237:ASP:HB3	1.75	0.51
1:A:355:ALA:O	1:A:356:ARG:O	2.28	0.51
1:A:219:LYS:O	1:A:220:LYS:HG2	2.10	0.51
2:B:331:LYS:O	2:B:424:LYS:NZ	2.35	0.51
1:A:100:LEU:O	1:A:318:TYR:HB3	2.10	0.51
2:B:99:GLY:O	2:B:102:LYS:HB2	2.10	0.51
1:A:79:GLU:OE1	1:A:82:LYS:HE2	2.10	0.51
2:B:257:ILE:O	2:B:261:VAL:HG13	2.10	0.51
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.09	0.51
1:A:435:VAL:HG23	2:B:290:THR:CG2	2.40	0.51
1:A:542:ILE:O	1:A:545:ASN:HB3	2.11	0.51
1:A:497:THR:O	1:A:535:TRP:HA	2.11	0.51
1:A:497:THR:OG1	1:A:498:ASP:N	2.43	0.51
2:B:282:LEU:HB3	2:B:293:ILE:HD13	1.91	0.51
1:A:92:LEU:HD22	1:A:92:LEU:N	2.26	0.51
1:A:298:GLU:CA	1:A:301:LEU:HD12	2.38	0.51
2:B:268:SER:HB3	2:B:274:ILE:HB	1.93	0.51
2:B:273:GLY:O	2:B:275:LYS:HD3	2.10	0.51
2:B:60:VAL:CG2	2:B:73:LYS:HD2	2.41	0.51
1:A:400:THR:O	1:A:404:GLU:OE2	2.29	0.51
1:A:434:ILE:HD13	1:A:493:VAL:O	2.11	0.51
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.58	0.51
1:A:50:ILE:HG13	1:A:143:ARG:CB	2.40	0.51
1:A:363:ASN:O	1:A:367:GLN:HG3	2.10	0.51
1:A:432:GLU:HB3	1:A:433:PRO:HD2	1.93	0.50
1:A:296:THR:HG23	1:A:298:GLU:OE2	2.11	0.50
1:A:12:LEU:CD2	1:A:124:PHE:CE1	2.94	0.50
1:A:295:LEU:N	1:A:295:LEU:HD23	2.26	0.50
1:A:62:ALA:HA	1:A:72:ARG:O	2.11	0.50
1:A:70:LYS:HG3	1:A:71:TRP:N	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:166:LYS:CE	2:B:166:LYS:HA	2.40	0.50
1:A:406:TRP:CH2	1:A:407:GLN:HB2	2.46	0.50
1:A:91:GLN:NE2	1:A:92:LEU:H	2.08	0.50
1:A:2:ILE:HG22	1:A:2:ILE:O	2.11	0.50
1:A:135:ILE:O	1:A:138:GLU:OE2	2.29	0.50
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.92	0.50
1:A:63:ILE:CD1	1:A:72:ARG:HG3	2.17	0.50
1:A:104:LYS:HB2	1:A:192:ASP:CA	2.18	0.50
1:A:249:LYS:HG3	1:A:250:ASP:N	2.27	0.50
2:B:362:THR:HG23	2:B:366:LYS:HE3	1.94	0.50
1:A:406:TRP:HZ3	2:B:392:PRO:CA	2.23	0.50
1:A:233:GLU:HB3	1:A:240:THR:HG22	1.93	0.50
2:B:8:VAL:O	2:B:121:ASP:HB2	2.12	0.50
1:A:26:LEU:HD23	1:A:133:PRO:HG3	1.93	0.50
1:A:402:TRP:CE3	1:A:403:THR:CB	2.95	0.50
1:A:489:SER:CB	1:A:493:VAL:CG1	2.90	0.50
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.92	0.50
1:A:156:SER:N	1:A:157:PRO:CD	2.75	0.50
2:B:199:ARG:NH1	2:B:233:GLU:OE2	2.45	0.50
2:B:210:LEU:O	2:B:210:LEU:HG	2.12	0.50
1:A:65:LYS:HE2	1:A:72:ARG:HD2	1.94	0.49
1:A:475:GLN:NE2	1:A:501:TYR:CG	2.80	0.49
2:B:61:PHE:HE2	2:B:76:ASP:HB2	1.77	0.49
1:A:104:LYS:N	1:A:192:ASP:OD2	2.44	0.49
2:B:244:ILE:CG2	2:B:263:LYS:HE2	2.42	0.49
2:B:244:ILE:HD13	2:B:266:TRP:CH2	2.47	0.49
1:A:400:THR:O	1:A:403:THR:HG22	2.12	0.49
1:A:104:LYS:HG3	1:A:192:ASP:C	2.32	0.49
1:A:298:GLU:OE2	1:A:298:GLU:N	2.29	0.49
2:B:87:PHE:CE1	2:B:159:ILE:HD12	2.48	0.49
1:A:13:LYS:HE3	1:A:84:THR:O	2.11	0.49
2:B:12:LEU:HD22	2:B:127:TYR:CZ	2.46	0.49
1:A:79:GLU:HG3	1:A:83:ARG:NE	2.26	0.49
2:B:303:LEU:O	2:B:307:ARG:N	2.30	0.49
1:A:106:VAL:CG2	1:A:227:PHE:CE2	2.95	0.49
1:A:79:GLU:HG3	1:A:83:ARG:HH21	1.76	0.49
1:A:369:THR:CG2	1:A:398:TRP:CZ3	2.95	0.49
1:A:297:GLU:O	1:A:301:LEU:HG	2.13	0.49
1:A:91:GLN:NE2	1:A:92:LEU:N	2.58	0.49
1:A:230:MET:HE2	1:A:230:MET:CA	2.43	0.49
2:B:10:VAL:HG11	2:B:153:TRP:CH2	2.48	0.49
2:B:80:LEU:HD22	2:B:84:THR:HG23	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:20:LYS:HG2	1:A:55:PRO:O	2.13	0.49
2:B:274:ILE:CG2	2:B:275:LYS:H	2.25	0.49
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.38	0.49
2:B:87:PHE:O	2:B:91:GLN:HB3	2.13	0.49
1:A:403:THR:HG22	1:A:404:GLU:HG3	1.95	0.49
1:A:475:GLN:NE2	1:A:501:TYR:CD1	2.81	0.49
2:B:428:GLN:O	2:B:428:GLN:NE2	2.34	0.49
1:A:406:TRP:CZ3	1:A:407:GLN:CB	2.95	0.49
2:B:241:VAL:C	2:B:243:PRO:HD3	2.34	0.49
1:A:402:TRP:CZ3	1:A:403:THR:HB	2.47	0.49
1:A:296:THR:HG21	4:A:750:HOH:O	2.14	0.48
1:A:12:LEU:HD23	1:A:124:PHE:CE1	2.43	0.48
2:B:87:PHE:HZ	2:B:159:ILE:HD11	1.77	0.48
1:A:495:ILE:HB	1:A:533:LEU:HD13	1.95	0.48
1:A:64:LYS:HE2	1:A:69:THR:C	2.32	0.48
2:B:257:ILE:H	2:B:257:ILE:HG12	1.39	0.48
2:B:275:LYS:N	2:B:306:ASN:HD21	2.10	0.48
2:B:87:PHE:CE1	2:B:159:ILE:CD1	2.96	0.48
1:A:540:LYS:O	1:A:542:ILE:HG13	2.13	0.48
1:A:532:TYR:HE2	1:A:534:ALA:HB2	1.76	0.48
1:A:402:TRP:CZ3	1:A:403:THR:CB	2.96	0.48
1:A:116:PHE:HA	1:A:148:VAL:HG21	1.96	0.48
1:A:500:GLN:HG3	2:B:422:LEU:CG	2.43	0.48
1:A:443:ASP:HB2	1:A:548:VAL:HB	1.96	0.48
2:B:419:THR:HA	2:B:420:PRO:HD2	1.78	0.48
2:B:279:LEU:CD2	2:B:279:LEU:H	2.27	0.48
1:A:64:LYS:O	1:A:65:LYS:HD2	2.13	0.48
2:B:301:LEU:O	2:B:305:GLU:HB2	2.13	0.48
1:A:106:VAL:CG1	3:A:601:R8E:C18	2.91	0.48
2:B:88:TRP:CZ2	2:B:154:LYS:HE3	2.47	0.48
1:A:5:ILE:CG1	1:A:6:GLU:N	2.74	0.48
1:A:556:ILE:HD13	1:A:556:ILE:N	2.28	0.48
1:A:312:GLU:HA	1:A:313:PRO:HD3	1.56	0.48
1:A:396:GLU:HB2	4:A:611:HOH:O	2.14	0.48
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.95	0.48
2:B:312:GLU:O	2:B:313:PRO:O	2.32	0.48
1:A:105:SER:HB3	1:A:198:HIS:CE1	2.49	0.47
1:A:92:LEU:CD2	1:A:92:LEU:N	2.77	0.47
1:A:454:LYS:HD3	1:A:556:ILE:CG1	2.44	0.47
1:A:547:GLN:OE1	2:B:285:GLY:HA2	2.14	0.47
2:B:65:LYS:CE	2:B:68:SER:HB3	2.38	0.47
2:B:66:LYS:HG2	2:B:407:GLN:HE22	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:547:GLN:N	1:A:547:GLN:HE21	2.12	0.47
2:B:120:LEU:O	2:B:125:ARG:NH2	2.47	0.47
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.96	0.47
1:A:27:THR:OG1	1:A:30:LYS:HD2	2.14	0.47
1:A:29:GLU:HG3	1:A:30:LYS:N	2.30	0.47
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.97	0.47
1:A:406:TRP:CE2	1:A:407:GLN:HB3	2.50	0.47
2:B:274:ILE:CG2	2:B:275:LYS:N	2.77	0.47
1:A:404:GLU:H	1:A:404:GLU:HG3	1.55	0.47
1:A:403:THR:CG2	1:A:404:GLU:N	2.77	0.47
1:A:492:GLU:HA	1:A:530:LYS:O	2.15	0.47
2:B:283:LEU:HA	2:B:287:LYS:NZ	2.30	0.47
1:A:410:TRP:CE3	2:B:363:ASN:HB3	2.50	0.47
2:B:250:ASP:O	2:B:251:SER:HB3	2.15	0.47
1:A:65:LYS:NZ	1:A:72:ARG:NH1	2.62	0.47
1:A:433:PRO:HG3	2:B:255:ASN:ND2	2.30	0.47
1:A:518:VAL:O	1:A:522:ILE:HD12	2.15	0.47
2:B:87:PHE:CZ	2:B:159:ILE:CD1	2.96	0.47
1:A:219:LYS:C	1:A:221:HIS:H	2.18	0.47
1:A:219:LYS:CG	1:A:220:LYS:N	2.78	0.47
1:A:194:GLU:C	1:A:196:GLY:N	2.67	0.47
2:B:271:TYR:CD1	2:B:310:LEU:CD1	2.97	0.47
1:A:101:LYS:O	3:A:601:R8E:H11	2.15	0.47
1:A:12:LEU:HD13	1:A:83:ARG:HB3	1.97	0.47
2:B:420:PRO:O	2:B:422:LEU:N	2.48	0.47
2:B:253:THR:HB	2:B:256:ASP:OD1	2.15	0.47
2:B:428:GLN:NE2	2:B:428:GLN:CA	2.79	0.46
1:A:277:ARG:HH11	1:A:278:GLN:HE22	1.63	0.46
2:B:325:LEU:HD12	2:B:385:LYS:HG3	1.97	0.46
2:B:125:ARG:HG2	2:B:146:TYR:O	2.16	0.46
1:A:270:ILE:HD11	1:A:316:GLY:CA	2.45	0.46
1:A:228:LEU:HD12	1:A:228:LEU:N	2.31	0.46
2:B:253:THR:HG22	2:B:255:ASN:H	1.80	0.46
2:B:391:LEU:HA	2:B:392:PRO:HD2	1.79	0.46
2:B:268:SER:C	2:B:270:ILE:H	2.18	0.46
1:A:3:SER:HB2	1:A:117:SER:O	2.15	0.46
1:A:402:TRP:CE3	1:A:403:THR:N	2.83	0.46
1:A:337:TRP:CD1	1:A:337:TRP:N	2.83	0.46
1:A:489:SER:CB	1:A:493:VAL:HG11	2.46	0.46
2:B:268:SER:O	2:B:270:ILE:HG22	2.15	0.46
2:B:306:ASN:HA	2:B:309:ILE:HD12	1.97	0.46
1:A:291:GLU:HG3	1:A:292:VAL:N	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:241:VAL:HG23	2:B:243:PRO:CG	2.46	0.46
1:A:524:GLN:NE2	1:A:524:GLN:HA	2.30	0.46
2:B:13:LYS:CB	2:B:16:MET:HE3	2.46	0.46
2:B:281:LYS:O	2:B:284:ARG:HD3	2.16	0.46
1:A:406:TRP:C	1:A:406:TRP:CE3	2.89	0.46
1:A:266:TRP:CD2	1:A:269:GLN:NE2	2.84	0.46
1:A:489:SER:HB2	1:A:493:VAL:HG13	1.97	0.46
1:A:275:LYS:HB3	1:A:336:GLN:HE22	1.79	0.46
2:B:279:LEU:CD2	2:B:279:LEU:N	2.79	0.46
1:A:108:VAL:HG22	1:A:223:LYS:HE3	1.98	0.46
1:A:173:LYS:CA	1:A:173:LYS:NZ	2.79	0.45
1:A:50:ILE:HG13	1:A:143:ARG:HB3	1.98	0.45
1:A:47:ILE:HD12	1:A:144:TYR:CD1	2.52	0.45
1:A:65:LYS:CE	1:A:72:ARG:NH1	2.79	0.45
2:B:246:LEU:CD1	2:B:310:LEU:HD23	2.45	0.45
2:B:258:GLN:HE22	2:B:289:LEU:CD2	2.30	0.45
2:B:271:TYR:CE1	2:B:310:LEU:HD12	2.50	0.45
1:A:202:ILE:CG2	1:A:203:GLU:N	2.79	0.45
1:A:335:GLY:O	1:A:355:ALA:HA	2.16	0.45
1:A:443:ASP:O	1:A:481:ALA:HB2	2.16	0.45
1:A:134:SER:OG	1:A:135:ILE:N	2.50	0.45
2:B:363:ASN:O	2:B:367:GLN:HG3	2.17	0.45
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.75	0.45
2:B:279:LEU:O	2:B:282:LEU:HD12	2.16	0.45
2:B:87:PHE:CZ	2:B:92:LEU:CD1	3.00	0.45
1:A:42:GLU:OE1	1:A:49:LYS:HE3	2.17	0.45
2:B:79:GLU:O	2:B:83:ARG:HG2	2.16	0.45
2:B:270:ILE:HD12	2:B:346:PHE:HA	1.98	0.45
1:A:270:ILE:CD1	1:A:316:GLY:HA3	2.46	0.45
1:A:60:VAL:HG13	1:A:75:VAL:HG22	1.98	0.45
1:A:61:PHE:CE2	1:A:63:ILE:HG23	2.52	0.45
1:A:65:LYS:HB3	1:A:68:SER:O	2.16	0.45
1:A:406:TRP:CD2	1:A:407:GLN:HB3	2.51	0.45
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.99	0.45
1:A:503:LEU:HA	1:A:503:LEU:HD23	1.79	0.45
1:A:33:ALA:O	1:A:37:ILE:HG13	2.17	0.45
1:A:173:LYS:NZ	1:A:173:LYS:HA	2.32	0.45
1:A:50:ILE:HG13	1:A:143:ARG:HB2	1.99	0.45
1:A:3:SER:HA	1:A:4:PRO:HD2	1.47	0.45
2:B:244:ILE:HG23	2:B:263:LYS:HE2	1.99	0.45
1:A:206:ARG:NH2	1:A:218:ASP:HB3	2.30	0.45
1:A:169:GLU:OE2	1:A:173:LYS:HE3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:107:THR:CG2	1:A:198:HIS:CE1	3.00	0.44
1:A:537:PRO:HB2	1:A:540:LYS:HG3	1.98	0.44
1:A:248:GLU:HG2	1:A:248:GLU:H	1.49	0.44
1:A:29:GLU:HG3	1:A:30:LYS:HG3	1.98	0.44
2:B:66:LYS:HG2	2:B:407:GLN:NE2	2.32	0.44
2:B:153:TRP:CH2	2:B:155:GLY:HA3	2.52	0.44
2:B:330:GLN:CD	2:B:340:GLN:HE22	2.19	0.44
1:A:422:LEU:HD12	1:A:422:LEU:HA	1.64	0.44
2:B:8:VAL:HG11	2:B:159:ILE:HG13	1.97	0.44
1:A:400:THR:HG22	1:A:404:GLU:OE2	2.17	0.44
1:A:64:LYS:HZ1	1:A:69:THR:CG2	2.10	0.44
1:A:460:ASN:HD21	2:B:288:ALA:HB2	1.83	0.44
1:A:433:PRO:HG2	2:B:255:ASN:HD22	1.81	0.44
2:B:72:ARG:NH1	2:B:72:ARG:CG	2.79	0.44
1:A:498:ASP:N	1:A:498:ASP:OD1	2.49	0.44
1:A:411:ILE:HG22	1:A:412:PRO:O	2.18	0.44
2:B:81:ASN:ND2	2:B:154:LYS:HG3	2.32	0.44
2:B:319:TYR:O	2:B:321:PRO:HD3	2.18	0.44
1:A:1:PRO:O	1:A:2:ILE:HD13	2.17	0.44
1:A:30:LYS:HE2	1:A:61:PHE:HE1	1.82	0.44
2:B:270:ILE:HD12	2:B:346:PHE:CB	2.48	0.44
2:B:298:GLU:N	2:B:298:GLU:CD	2.65	0.44
2:B:254:VAL:O	2:B:258:GLN:HB2	2.17	0.44
1:A:106:VAL:CG2	1:A:227:PHE:HE2	2.31	0.44
1:A:420:PRO:HA	1:A:422:LEU:HD13	1.99	0.44
1:A:97:PRO:HG2	1:A:232:TYR:CD1	2.52	0.44
1:A:96:HIS:ND1	1:A:97:PRO:HD2	2.32	0.44
1:A:194:GLU:HA	4:A:775:HOH:O	2.18	0.44
2:B:249:LYS:HB3	2:B:249:LYS:HE2	1.31	0.43
2:B:80:LEU:HD13	2:B:153:TRP:CD1	2.53	0.43
2:B:422:LEU:HB3	2:B:426:TRP:CE2	2.53	0.43
2:B:271:TYR:HB3	2:B:274:ILE:HD11	2.00	0.43
2:B:243:PRO:O	2:B:245:VAL:HG23	2.18	0.43
1:A:522:ILE:HA	1:A:525:LEU:HD12	2.00	0.43
2:B:244:ILE:HG23	2:B:263:LYS:CE	2.48	0.43
1:A:218:ASP:HB2	4:A:725:HOH:O	2.16	0.43
1:A:20:LYS:HE2	1:A:55:PRO:HB2	2.00	0.43
2:B:43:LYS:C	2:B:45:GLY:H	2.22	0.43
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.70	0.43
2:B:270:ILE:HD12	2:B:346:PHE:CD2	2.53	0.43
1:A:466:VAL:HG23	1:A:551:LEU:CD2	2.42	0.43
1:A:12:LEU:HA	1:A:12:LEU:HD22	1.69	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:424:LYS:HE2	1:A:426:TRP:CE2	2.53	0.43
1:A:47:ILE:HD12	1:A:144:TYR:CG	2.54	0.43
1:A:319:TYR:CZ	1:A:321:PRO:HA	2.52	0.43
1:A:295:LEU:HB3	1:A:300:GLU:HG2	2.00	0.43
2:B:252:TRP:HB3	2:B:257:ILE:CD1	2.48	0.43
1:A:110:ASP:OD1	1:A:223:LYS:HE2	2.18	0.43
1:A:235:HIS:O	3:A:601:R8E:C22	2.66	0.43
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.72	0.43
1:A:457:TYR:OH	1:A:488:ASP:OD2	2.25	0.43
2:B:287:LYS:H	2:B:287:LYS:HG2	1.68	0.43
1:A:208:HIS:O	1:A:212:TRP:HD1	2.02	0.43
2:B:108:VAL:HB	2:B:232:TYR:CD2	2.48	0.43
2:B:86:ASP:HA	2:B:90:VAL:HG22	2.00	0.43
1:A:54:ASN:HA	1:A:55:PRO:HD3	1.85	0.43
2:B:63:ILE:HD13	2:B:74:LEU:HB2	2.01	0.43
1:A:402:TRP:CZ3	1:A:403:THR:OG1	2.69	0.43
2:B:416:PHE:N	2:B:416:PHE:CD2	2.86	0.43
1:A:8:VAL:O	1:A:121:ASP:HB2	2.19	0.43
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.00	0.43
2:B:336:GLN:HE21	2:B:336:GLN:HB2	1.48	0.43
1:A:63:ILE:HD11	4:A:644:HOH:O	2.17	0.43
2:B:253:THR:CG2	2:B:255:ASN:H	2.32	0.43
1:A:178:ILE:HD12	1:A:178:ILE:N	2.33	0.43
1:A:195:ILE:HD13	1:A:199:ARG:CG	2.49	0.43
1:A:139:THR:HA	1:A:140:PRO:HD3	1.52	0.43
2:B:23:GLN:OE1	2:B:60:VAL:HG12	2.19	0.43
1:A:65:LYS:HE2	1:A:72:ARG:CD	2.49	0.43
2:B:305:GLU:O	2:B:309:ILE:HD12	2.18	0.43
1:A:270:ILE:HG13	1:A:270:ILE:O	2.18	0.43
2:B:118:VAL:HG21	2:B:160:PHE:HD1	1.84	0.43
1:A:77:PHE:O	1:A:81:ASN:HB2	2.19	0.43
2:B:234:LEU:HA	2:B:234:LEU:HD23	1.75	0.43
1:A:162:SER:CB	2:B:52:PRO:HG3	2.49	0.43
1:A:236:PRO:HA	3:A:601:R8E:N24	2.34	0.42
1:A:238:LYS:HD2	1:A:315:HIS:CG	2.54	0.42
1:A:447:ASN:O	1:A:451:LYS:N	2.46	0.42
1:A:277:ARG:HE	1:A:336:GLN:CD	2.23	0.42
2:B:244:ILE:CD1	2:B:266:TRP:CH2	3.02	0.42
1:A:230:MET:HA	1:A:230:MET:CE	2.49	0.42
1:A:38:CYS:HB3	1:A:144:TYR:CZ	2.53	0.42
1:A:194:GLU:C	1:A:196:GLY:H	2.21	0.42
2:B:428:GLN:HE21	2:B:428:GLN:C	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:271:TYR:HA	1:A:272:PRO:HD2	1.63	0.42
2:B:199:ARG:NH1	2:B:233:GLU:OE1	2.53	0.42
2:B:330:GLN:NE2	2:B:340:GLN:HE22	2.18	0.42
2:B:339:TYR:O	2:B:340:GLN:HG3	2.19	0.42
1:A:438:GLU:OE1	1:A:459:THR:OG1	2.26	0.42
1:A:225:PRO:HB3	3:A:601:R8E:N25	2.34	0.42
1:A:244:ILE:H	1:A:244:ILE:CD1	2.32	0.42
1:A:419:THR:HA	1:A:420:PRO:HD2	1.85	0.42
1:A:80:LEU:HD11	1:A:124:PHE:CZ	2.55	0.42
1:A:138:GLU:H	1:A:138:GLU:HG3	1.46	0.42
1:A:23:GLN:NE2	1:A:26:LEU:CD2	2.81	0.42
1:A:75:VAL:HG11	1:A:77:PHE:CZ	2.55	0.42
1:A:170:PRO:HB2	1:A:171:PHE:H	1.51	0.42
1:A:485:ALA:O	1:A:489:SER:HB3	2.19	0.42
1:A:438:GLU:OE2	1:A:463:ARG:NH2	2.39	0.42
1:A:401:TRP:HB2	1:A:425:LEU:HD21	2.01	0.42
1:A:102:LYS:NZ	1:A:237:ASP:CB	2.75	0.42
1:A:105:SER:HB2	1:A:198:HIS:ND1	2.34	0.42
1:A:80:LEU:HD13	1:A:127:TYR:HB3	2.02	0.42
2:B:54:ASN:HD21	2:B:126:LYS:CA	2.33	0.42
1:A:501:TYR:CZ	1:A:505:ILE:CD1	3.02	0.42
2:B:58:THR:HG23	2:B:76:ASP:O	2.20	0.42
2:B:13:LYS:CB	2:B:16:MET:CE	2.98	0.42
2:B:150:PRO:HG2	2:B:153:TRP:CB	2.50	0.42
1:A:65:LYS:HE2	1:A:72:ARG:NE	2.35	0.41
2:B:260:LEU:CD2	2:B:264:LEU:HD12	2.23	0.41
2:B:13:LYS:HE2	2:B:16:MET:HE3	2.01	0.41
1:A:246:LEU:HA	1:A:247:PRO:HD2	1.65	0.41
1:A:173:LYS:N	1:A:173:LYS:HZ3	2.17	0.41
1:A:240:THR:HG23	1:A:241:VAL:O	2.19	0.41
1:A:424:LYS:HE2	1:A:426:TRP:CZ3	2.55	0.41
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.55	0.41
1:A:65:LYS:CG	1:A:68:SER:HB3	2.45	0.41
2:B:249:LYS:HD2	2:B:252:TRP:CZ3	2.55	0.41
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.55	0.41
2:B:33:ALA:O	2:B:37:ILE:HD12	2.20	0.41
2:B:294:PRO:HB3	4:B:451:HOH:O	2.19	0.41
2:B:203:GLU:HA	2:B:203:GLU:OE1	2.19	0.41
2:B:253:THR:HG22	2:B:255:ASN:CB	2.50	0.41
2:B:253:THR:O	2:B:257:ILE:CG1	2.66	0.41
1:A:21:VAL:O	1:A:57:ASN:HB3	2.20	0.41
2:B:195:ILE:HA	2:B:195:ILE:HD12	1.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:271:TYR:HA	2:B:271:TYR:HD2	1.63	0.41
1:A:105:SER:HB2	4:A:603:HOH:O	2.20	0.41
2:B:335:GLY:O	2:B:355:ALA:HA	2.20	0.41
1:A:452:LEU:HA	1:A:452:LEU:HD22	1.84	0.41
2:B:363:ASN:ND2	2:B:363:ASN:H	2.18	0.41
2:B:81:ASN:CG	2:B:154:LYS:HG3	2.41	0.41
1:A:509:GLN:N	1:A:510:PRO:CD	2.83	0.41
1:A:104:LYS:HG3	1:A:192:ASP:CA	2.50	0.41
2:B:362:THR:HG23	2:B:366:LYS:HG2	1.97	0.41
1:A:210:LEU:C	1:A:212:TRP:N	2.73	0.41
1:A:356:ARG:CZ	1:A:358:ARG:HG3	2.50	0.41
1:A:34:LEU:HB3	1:A:132:ILE:HD13	2.02	0.41
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.02	0.41
1:A:342:TYR:CD1	1:A:342:TYR:C	2.93	0.41
1:A:242:GLN:HA	1:A:243:PRO:HD3	1.84	0.41
2:B:156:SER:HB2	2:B:157:PRO:HD3	2.02	0.41
1:A:169:GLU:CB	1:A:170:PRO:CD	2.94	0.41
1:A:520:GLN:HG2	1:A:520:GLN:H	1.57	0.41
2:B:91:GLN:HB3	2:B:92:LEU:H	1.76	0.41
1:A:96:HIS:CB	1:A:382:ILE:HD13	2.45	0.41
1:A:194:GLU:N	1:A:194:GLU:CD	2.74	0.41
1:A:276:VAL:O	1:A:280:CYS:HB2	2.21	0.41
1:A:109:LEU:HB2	1:A:187:LEU:HB2	2.03	0.41
1:A:406:TRP:HE3	1:A:406:TRP:O	2.04	0.41
1:A:464:GLN:HG2	1:A:465:LYS:H	1.84	0.41
1:A:466:VAL:CG2	1:A:551:LEU:CD2	2.91	0.41
2:B:396:GLU:O	2:B:400:THR:CG2	2.66	0.41
1:A:0:SER:HA	1:A:1:PRO:HD3	1.74	0.41
2:B:13:LYS:HD2	2:B:85:GLN:HB3	2.03	0.41
1:A:214:LEU:HA	1:A:214:LEU:HD23	1.76	0.41
1:A:480:GLN:HA	1:A:480:GLN:NE2	2.35	0.41
1:A:254:VAL:HG21	1:A:288:ALA:O	2.21	0.41
1:A:296:THR:HG23	1:A:297:GLU:N	2.36	0.41
1:A:105:SER:CB	1:A:198:HIS:ND1	2.84	0.41
1:A:406:TRP:CE3	1:A:407:GLN:CA	3.04	0.40
2:B:30:LYS:CG	2:B:62:ALA:HB3	2.50	0.40
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.91	0.40
1:A:206:ARG:HH22	1:A:218:ASP:CB	2.33	0.40
2:B:54:ASN:HD21	2:B:126:LYS:CB	2.35	0.40
2:B:22:LYS:O	2:B:59:PRO:HG3	2.21	0.40
1:A:109:LEU:O	1:A:187:LEU:HB2	2.20	0.40
2:B:421:PRO:O	2:B:425:LEU:HD22	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:287:LYS:CE	1:A:287:LYS:HA	2.39	0.40
1:A:26:LEU:HD22	1:A:133:PRO:HG3	2.03	0.40
2:B:167:ILE:HG12	2:B:212:TRP:CD1	2.57	0.40
1:A:27:THR:O	1:A:31:ILE:HG13	2.21	0.40
1:A:108:VAL:HG12	1:A:227:PHE:CE1	2.56	0.40
1:A:63:ILE:HG13	1:A:74:LEU:HG	2.02	0.40
2:B:354:TYR:OH	2:B:370:GLU:OE2	2.40	0.40
1:A:324:ASP:O	1:A:343:GLN:HG2	2.22	0.40
2:B:382:ILE:HG22	2:B:383:TRP:CG	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	556/563 (99%)	466 (84%)	62 (11%)	28 (5%)	3	11
2	B	398/443 (90%)	350 (88%)	39 (10%)	9 (2%)	10	36
All	All	954/1006 (95%)	816 (86%)	101 (11%)	37 (4%)	5	18

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	90	VAL
1	A	136	ASN
1	A	170	PRO
1	A	286	THR
1	A	356	ARG
1	A	491	LEU
2	B	65	LYS
2	B	313	PRO
2	B	421	PRO
1	A	64	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	171	PHE
1	A	195	ILE
1	A	196	GLY
1	A	243	PRO
1	A	541	GLY
1	A	543	GLY
2	B	18	GLY
1	A	18	GLY
1	A	67	ASP
1	A	121	ASP
1	A	122	GLU
1	A	313	PRO
2	B	91	GLN
2	B	237	ASP
2	B	272	PRO
2	B	277	ARG
1	A	125	ARG
1	A	139	THR
1	A	554	ALA
2	B	251	SER
1	A	312	GLU
1	A	346	PHE
1	A	345	PRO
1	A	276	VAL
1	A	119	PRO
1	A	135	ILE

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	498/503 (99%)	368 (74%)	130 (26%)	1	2
2	B	368/403 (91%)	270 (73%)	98 (27%)	1	2
All	All	866/906 (96%)	638 (74%)	228 (26%)	1	2

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	5	ILE
1	A	6	GLU
1	A	7	THR
1	A	11	LYS
1	A	12	LEU
1	A	21	VAL
1	A	22	LYS
1	A	26	LEU
1	A	30	LYS
1	A	32	LYS
1	A	36	GLU
1	A	40	GLU
1	A	60	VAL
1	A	63	ILE
1	A	64	LYS
1	A	65	LYS
1	A	66	LYS
1	A	67	ASP
1	A	69	THR
1	A	70	LYS
1	A	72	ARG
1	A	82	LYS
1	A	92	LEU
1	A	103	LYS
1	A	107	THR
1	A	108	VAL
1	A	118	VAL
1	A	120	LEU
1	A	122	GLU
1	A	123	ASP
1	A	125	ARG
1	A	126	LYS
1	A	131	THR
1	A	138	GLU
1	A	161	GLN
1	A	162	SER
1	A	166	LYS
1	A	169	GLU
1	A	173	LYS
1	A	179	VAL
1	A	187	LEU
1	A	195	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	197	GLN
1	A	202	ILE
1	A	205	LEU
1	A	206	ARG
1	A	207	GLN
1	A	215	THR
1	A	220	LYS
1	A	223	LYS
1	A	224	GLU
1	A	238	LYS
1	A	242	GLN
1	A	246	LEU
1	A	248	GLU
1	A	250	ASP
1	A	260	LEU
1	A	268	SER
1	A	270	ILE
1	A	276	VAL
1	A	277	ARG
1	A	279	LEU
1	A	280	CYS
1	A	281	LYS
1	A	284	ARG
1	A	287	LYS
1	A	289	LEU
1	A	290	THR
1	A	291	GLU
1	A	295	LEU
1	A	296	THR
1	A	297	GLU
1	A	303	LEU
1	A	307	ARG
1	A	309	ILE
1	A	311	LYS
1	A	330	GLN
1	A	334	GLN
1	A	341	ILE
1	A	347	LYS
1	A	350	LYS
1	A	356	ARG
1	A	357	MET
1	A	358	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	368	LEU
1	A	373	GLN
1	A	374	LYS
1	A	380	ILE
1	A	382	ILE
1	A	394	GLN
1	A	395	LYS
1	A	399	GLU
1	A	402	TRP
1	A	403	THR
1	A	404	GLU
1	A	407	GLN
1	A	409	THR
1	A	422	LEU
1	A	424	LYS
1	A	425	LEU
1	A	443	ASP
1	A	448	ARG
1	A	451	LYS
1	A	452	LEU
1	A	454	LYS
1	A	458	VAL
1	A	459	THR
1	A	463	ARG
1	A	465	LYS
1	A	471	ASP
1	A	473	THR
1	A	479	LEU
1	A	488	ASP
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL
1	A	497	THR
1	A	500	GLN
1	A	503	LEU
1	A	514	GLU
1	A	517	LEU
1	A	520	GLN
1	A	546	GLU
1	A	547	GLN
1	A	548	VAL
1	A	549	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	550	LYS
1	A	551	LEU
1	A	557	ARG
2	B	6	GLU
2	B	10	VAL
2	B	11	LYS
2	B	12	LEU
2	B	17	ASP
2	B	22	LYS
2	B	24	TRP
2	B	27	THR
2	B	29	GLU
2	B	30	LYS
2	B	32	LYS
2	B	40	GLU
2	B	46	LYS
2	B	48	SER
2	B	49	LYS
2	B	63	ILE
2	B	64	LYS
2	B	65	LYS
2	B	66	LYS
2	B	68	SER
2	B	69	THR
2	B	70	LYS
2	B	72	ARG
2	B	73	LYS
2	B	79	GLU
2	B	80	LEU
2	B	83	ARG
2	B	89	GLU
2	B	91	GLN
2	B	101	LYS
2	B	102	LYS
2	B	111	VAL
2	B	117	SER
2	B	120	LEU
2	B	126	LYS
2	B	159	ILE
2	B	163	SER
2	B	166	LYS
2	B	169	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	173	LYS
2	B	174	GLN
2	B	178	ILE
2	B	182	GLN
2	B	187	LEU
2	B	195	ILE
2	B	205	LEU
2	B	206	ARG
2	B	214	LEU
2	B	232	TYR
2	B	233	GLU
2	B	238	LYS
2	B	242	GLN
2	B	248	GLU
2	B	249	LYS
2	B	253	THR
2	B	254	VAL
2	B	256	ASP
2	B	257	ILE
2	B	259	LYS
2	B	260	LEU
2	B	265	ASN
2	B	268	SER
2	B	269	GLN
2	B	271	TYR
2	B	275	LYS
2	B	276	VAL
2	B	277	ARG
2	B	278	GLN
2	B	282	LEU
2	B	283	LEU
2	B	286	THR
2	B	287	LYS
2	B	290	THR
2	B	291	GLU
2	B	293	ILE
2	B	295	LEU
2	B	297	GLU
2	B	298	GLU
2	B	300	GLU
2	B	303	LEU
2	B	305	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	307	ARG
2	B	310	LEU
2	B	311	LYS
2	B	314	VAL
2	B	323	LYS
2	B	336	GLN
2	B	347	LYS
2	B	349	LEU
2	B	362	THR
2	B	369	THR
2	B	377	THR
2	B	388	LYS
2	B	394	GLN
2	B	400	THR
2	B	403	THR
2	B	413	GLU
2	B	428	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	91	GLN
1	A	147	ASN
1	A	161	GLN
1	A	174	GLN
1	A	175	ASN
1	A	222	GLN
1	A	235	HIS
1	A	258	GLN
1	A	278	GLN
1	A	315	HIS
1	A	330	GLN
1	A	334	GLN
1	A	460	ASN
1	A	480	GLN
1	A	494	ASN
1	A	519	ASN
1	A	524	GLN
1	A	547	GLN
2	B	54	ASN
2	B	137	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	145	GLN
2	B	161	GLN
2	B	175	ASN
2	B	208	HIS
2	B	255	ASN
2	B	258	GLN
2	B	306	ASN
2	B	330	GLN
2	B	336	GLN
2	B	340	GLN
2	B	361	HIS
2	B	367	GLN
2	B	373	GLN
2	B	407	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	R8E	A	601	-	32,32,32	2.23	7 (21%)	42,45,45	4.27	16 (38%)

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	R8E	A	601	-	-	0/9/11/11	0/2/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	R8E	C2-C26	-8.29	1.22	1.44
3	A	601	R8E	C16-C17	4.55	1.48	1.39
3	A	601	R8E	C23-N25	3.40	1.45	1.35
3	A	601	R8E	C18-N24	-2.84	1.31	1.34
3	A	601	R8E	C5-C4	-2.70	1.33	1.38
3	A	601	R8E	C17-C18	-2.32	1.37	1.43
3	A	601	R8E	C26-N27	-2.23	1.09	1.14

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	R8E	C17-C16-N20	-16.47	105.31	110.46
3	A	601	R8E	C2-C1-C6	-14.62	110.92	119.51
3	A	601	R8E	C5-C6-CL28	-6.71	110.86	119.14
3	A	601	R8E	N25-C23-N24	-6.60	114.71	118.15
3	A	601	R8E	C8-C13-CL29	-4.96	112.98	119.45
3	A	601	R8E	C1-C6-CL28	4.78	125.05	119.14
3	A	601	R8E	C3-C2-C26	-4.42	113.69	119.50
3	A	601	R8E	C4-C5-C6	4.35	122.77	117.70
3	A	601	R8E	C21-C22-C23	-3.53	116.35	119.78
3	A	601	R8E	C8-O7-C4	3.31	128.15	117.67
3	A	601	R8E	C15-O14-C10	2.92	125.47	117.66
3	A	601	R8E	C1-C2-C3	2.71	124.81	119.73
3	A	601	R8E	O14-C15-C16	-2.66	104.91	110.59
3	A	601	R8E	C22-C21-C17	-2.61	117.27	121.15
3	A	601	R8E	C17-C18-N24	-2.57	119.12	125.25
3	A	601	R8E	C12-C13-CL29	2.21	123.29	118.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	558/563 (99%)	-0.11	5 (0%) 81 88	21, 50, 83, 112	0
2	B	404/443 (91%)	-0.13	6 (1%) 70 79	24, 49, 100, 118	0
All	All	962/1006 (95%)	-0.12	11 (1%) 77 84	21, 50, 94, 118	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	LEU	3.4
2	B	90	VAL	3.1
2	B	270	ILE	2.9
2	B	67	ASP	2.7
1	A	66	LYS	2.7
2	B	252	TRP	2.6
1	A	360	ALA	2.6
2	B	311	LYS	2.3
1	A	15	GLY	2.2
1	A	67	ASP	2.2
2	B	362	THR	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	R8E	A	601	29/29	0.21	0.39	42,52,75,78	0

6.5 Other polymers ⓘ

There are no such residues in this entry.