



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:26 PM GMT

PDB ID : 1FM6  
Title : THE 2.1 ANGSTROM RESOLUTION CRYSTAL STRUCTURE OF THE HETERODIMER OF THE HUMAN RXRALPHA AND PPARGAMMA LIGAND BINDING DOMAINS RESPECTIVELY BOUND WITH 9-CIS RETINOIC ACID AND ROSIGLITAZONE AND CO-ACTIVATOR PEPTIDES.  
Authors : Gampe Jr., R.T.; Montana, V.G.; Lambert, M.H.; Miller, A.B.; Bledsoe, R.K.; Milburn, M.V.; Kliewer, S.A.; Willson, T.M.; Xu, H.E.  
Deposited on : 2000-08-16  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

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

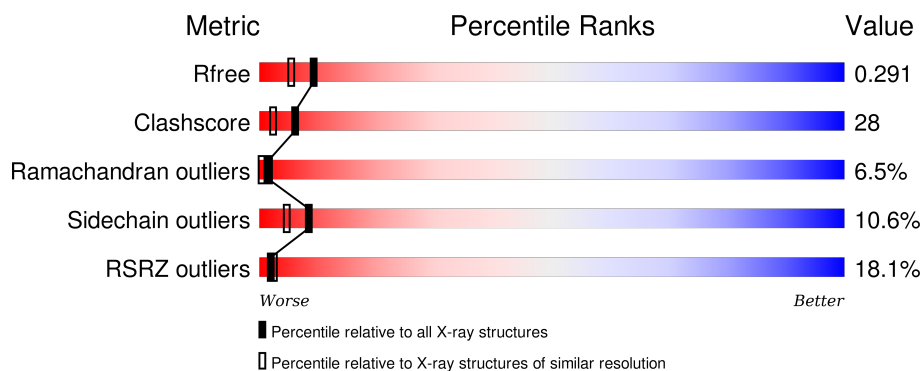
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	238	<div> <div>21%</div> <div>58%</div> <div>31%</div> <div>7%</div> <div>• •</div> </div>
1	U	238	<div> <div>22%</div> <div>51%</div> <div>36%</div> <div>9%</div> <div>• •</div> </div>
2	D	272	<div> <div>13%</div> <div>61%</div> <div>30%</div> <div>8%</div> <div>•</div> </div>
2	X	272	<div> <div>15%</div> <div>60%</div> <div>29%</div> <div>10%</div> <div>•</div> </div>
3	B	25	<div> <div>20%</div> <div>16%</div> <div>•</div> <div>60%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	E	25	
3	V	25	
3	Y	25	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	9CR	A	501	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8838 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 RETINOIC ACID RECEPTOR RXR-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1754	1117	306	321	10			
1	U	232	Total	C	N	O	S	0	0	0
			1754	1117	306	321	10			

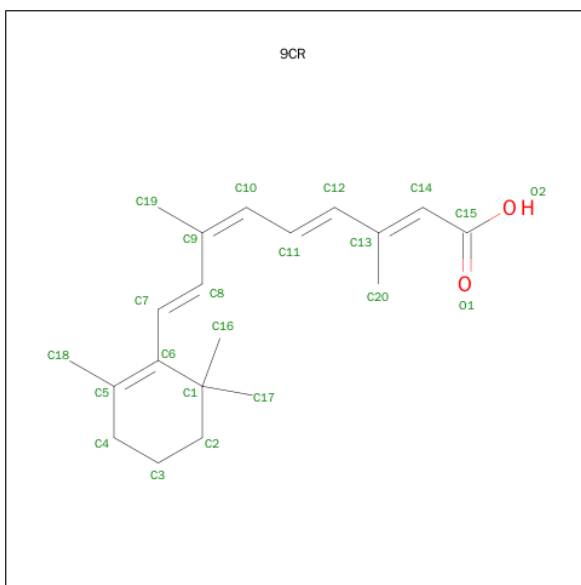
- Molecule 2 is a protein called PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	272	Total	C	N	O	S	0	0	0
			2183	1409	356	408	10			
2	X	272	Total	C	N	O	S	0	0	0
			2142	1377	347	408	10			

- Molecule 3 is a protein called STEROID RECEPTOR COACTIVATOR.

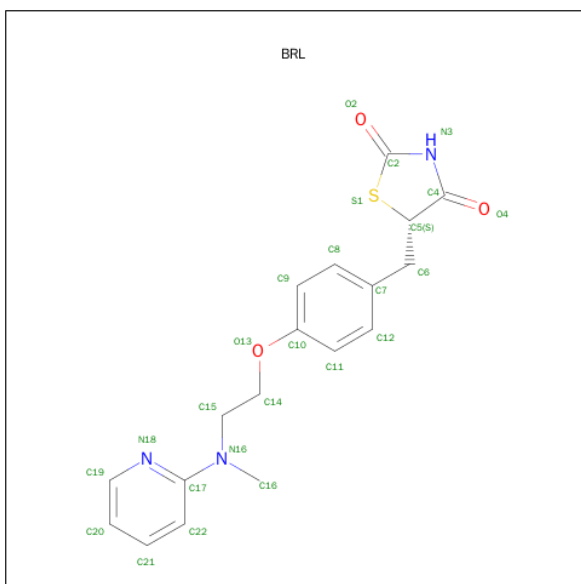
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	10	Total	C	N	O	0	0	0
			86	55	18	13			
3	V	15	Total	C	N	O	0	0	0
			127	79	27	21			
3	E	16	Total	C	N	O	0	0	0
			129	79	27	23			
3	Y	13	Total	C	N	O	0	0	0
			117	73	25	19			

- Molecule 4 is (9CIS)-RETINOIC ACID (three-letter code: 9CR) (formula: C<sub>20</sub>H<sub>28</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			22	20	2		
4	U	1	Total	C	O	0	0
			22	20	2		

- Molecule 5 is 2,4-THIAZOLIDINEDIONE, 5-[[4-[2-(METHYL-2-PYRIDINYLAMINO)ETHOXY]PHENYL]METHYL]-(9CL) (three-letter code: BRL) (formula: C<sub>18</sub>H<sub>19</sub>N<sub>3</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	S	0	0
			25	18	3	3	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	X	1	Total	C	N	O	S	0	0
			25	18	3	3	1		

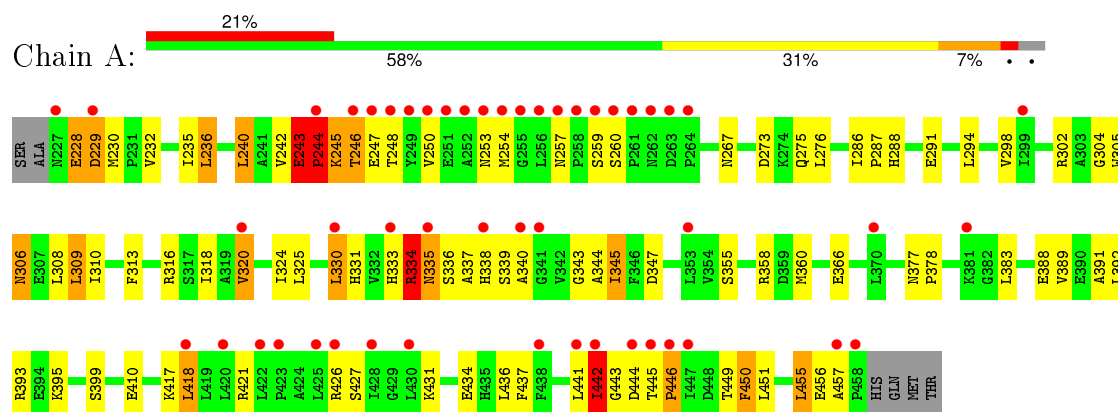
- Molecule 6 is water.

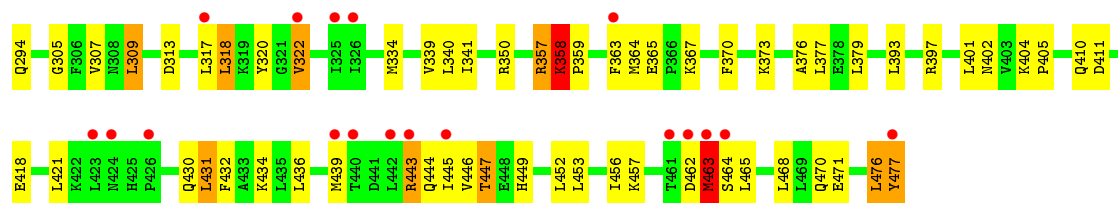
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	64	Total	O	0	0
			64	64		
6	D	151	Total	O	0	0
			151	151		
6	U	79	Total	O	0	0
			79	79		
6	X	132	Total	O	0	0
			132	132		
6	B	3	Total	O	0	0
			3	3		
6	V	8	Total	O	0	0
			8	8		
6	E	9	Total	O	0	0
			9	9		
6	Y	6	Total	O	0	0
			6	6		

### 3 Residue-property plots

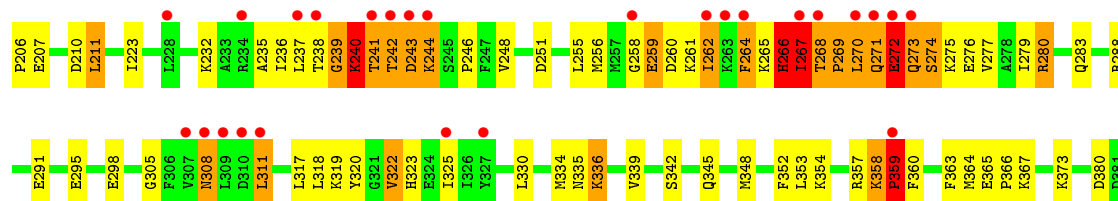
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: RETINOIC ACID RECEPTOR RXR-ALPHA





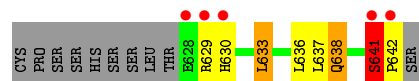
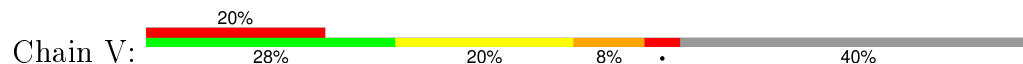
• Molecule 2: PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA



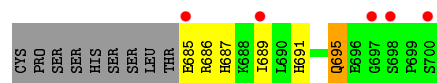
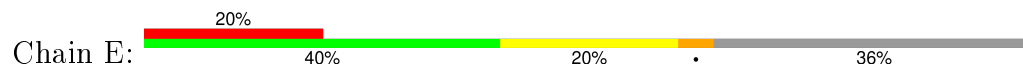
• Molecule 3: STEROID RECEPTOR COACTIVATOR



• Molecule 3: STEROID RECEPTOR COACTIVATOR



• Molecule 3: STEROID RECEPTOR COACTIVATOR



• Molecule 3: STEROID RECEPTOR COACTIVATOR





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.26 Å   222.36 Å   55.29 Å 90.00°   98.59°   90.00°	Depositor
Resolution (Å)	20.00 – 2.10 44.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.8 (20.00-2.10) 87.7 (44.00-2.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.10 Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.250   ,   0.292 0.249   ,   0.291	Depositor DCC
$R_{free}$ test set	6054 reflections (10.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.2	Xtriage
Anisotropy	0.749	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 59964 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8838	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9CR, BRL

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	0.34	0/1789	0.69	2/2414 (0.1%)
1	U	0.35	0/1789	0.64	0/2414
2	D	0.36	0/2221	0.65	1/2992 (0.0%)
2	X	0.34	0/2178	0.68	2/2938 (0.1%)
3	B	0.33	0/87	0.69	0/116
3	E	0.33	0/131	0.64	0/175
3	V	0.32	0/129	0.68	0/171
3	Y	0.31	0/118	0.65	0/156
All	All	0.35	0/8442	0.67	5/11376 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	GLU	C-N-CD	-10.26	98.02	120.60
2	X	266	HIS	N-CA-C	6.78	129.30	111.00
1	A	243	GLU	C-N-CA	5.98	147.12	122.00
2	X	206	PRO	N-CA-CB	5.44	109.83	103.30
2	D	206	PRO	N-CA-CB	5.37	109.74	103.30

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	1754	0	1733	78	0
1	U	1754	0	1733	137	0
2	D	2183	0	2243	135	0
2	X	2142	0	2162	101	0
3	B	86	0	86	9	0
3	E	129	0	125	16	0
3	V	127	0	131	14	0
3	Y	117	0	123	17	0
4	A	22	0	27	1	0
4	U	22	0	27	2	0
5	D	25	0	19	4	0
5	X	25	0	19	1	0
6	A	64	0	0	3	0
6	B	3	0	0	0	0
6	D	151	0	0	5	0
6	E	9	0	0	1	0
6	U	79	0	0	10	0
6	V	8	0	0	1	0
6	X	132	0	0	6	0
6	Y	6	0	0	0	0
All	All	8838	0	8428	476	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 28.

All (476) 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:335:ASN:HD22	1:A:336:SER:N	1.45	1.12
1:A:267:ASN:HD22	1:A:330:LEU:HD11	1.16	1.10
2:D:262:ILE:HA	2:D:265:LYS:HB2	1.41	1.02
3:E:685:GLU:HG2	3:E:686:ARG:H	1.27	0.99
1:U:306:ASN:O	1:U:310:ILE:HG22	1.64	0.95
1:U:289:PHE:O	1:U:292:LEU:HD22	1.66	0.95
2:X:280:ARG:HH11	2:X:280:ARG:HG2	1.29	0.95
1:A:335:ASN:HD22	1:A:336:SER:H	1.14	0.93
1:A:267:ASN:HD22	1:A:330:LEU:CD1	1.85	0.90
2:D:273:GLN:HA	2:D:280:ARG:HD3	1.54	0.90
2:D:261:LYS:HG2	2:D:265:LYS:HE3	1.52	0.89
1:U:345:ILE:HD13	1:U:431:LYS:HD3	1.55	0.87
1:U:452:MET:HE3	1:U:452:MET:HA	1.56	0.87
2:D:268:THR:H	2:D:269:PRO:HD2	1.38	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:270:LEU:HD22	2:D:287:PHE:CG	2.10	0.86
1:A:294:LEU:HD11	3:B:638:GLN:HE21	1.43	0.84
1:A:267:ASN:ND2	1:A:330:LEU:HD11	1.92	0.83
2:D:476:LEU:HG	2:D:477:TYR:H	1.44	0.82
2:D:264:PHE:C	2:D:264:PHE:HD1	1.84	0.81
2:D:262:ILE:HD13	2:D:265:LYS:HD2	1.63	0.81
2:D:471:GLU:OE2	3:E:689:ILE:HG22	1.81	0.81
1:U:244:PRO:HD2	6:U:527:HOH:O	1.83	0.79
2:D:271:GLN:HE22	2:D:280:ARG:CG	1.95	0.79
2:D:268:THR:N	2:D:269:PRO:HD2	1.94	0.79
2:D:271:GLN:HG3	2:D:283:GLN:OE1	1.83	0.78
2:X:244:LYS:HE3	2:X:246:PRO:HG3	1.66	0.78
2:D:271:GLN:HE22	2:D:280:ARG:CD	1.96	0.78
1:A:243:GLU:HB2	1:A:244:PRO:O	1.84	0.77
1:U:302:ARG:HH12	1:U:457:ALA:HA	1.49	0.77
3:Y:689:ILE:O	3:Y:692:ARG:HG2	1.84	0.77
2:D:240:LYS:O	2:D:241:THR:HG22	1.85	0.76
2:D:264:PHE:CD1	2:D:264:PHE:C	2.57	0.76
1:U:243:GLU:HA	1:U:244:PRO:O	1.85	0.76
1:U:276:LEU:HD11	1:U:305:TRP:CD1	2.22	0.75
1:A:383:LEU:HD21	1:A:389:VAL:HG21	1.67	0.75
2:X:238:THR:HG23	2:X:239:GLY:N	2.02	0.75
2:X:238:THR:HG23	2:X:239:GLY:H	1.52	0.75
1:A:230:MET:CE	1:A:235:ILE:HD11	2.17	0.75
1:U:238:ALA:O	1:U:242:VAL:HG22	1.86	0.75
2:D:269:PRO:HB3	2:D:272:GLU:OE2	1.86	0.74
1:U:335:ASN:ND2	1:U:336:SER:H	1.85	0.74
1:U:243:GLU:HB3	1:U:244:PRO:HA	1.70	0.74
2:D:457:LYS:HA	2:D:463:MET:HG3	1.70	0.74
1:U:335:ASN:HD22	1:U:336:SER:H	1.33	0.73
2:D:271:GLN:HE22	2:D:280:ARG:HG2	1.53	0.73
2:D:443:ARG:HD2	2:D:477:TYR:CE2	2.22	0.73
3:Y:684:THR:HB	3:Y:685:GLU:OE2	1.89	0.73
1:U:318:ILE:HD12	1:U:319:ALA:N	2.04	0.73
1:U:442:ILE:HD12	1:U:443:GLY:N	2.04	0.72
2:X:269:PRO:HG2	2:X:270:LEU:H	1.53	0.72
2:X:261:LYS:O	2:X:262:ILE:O	2.08	0.72
1:A:417:LYS:HE2	6:A:555:HOH:O	1.90	0.72
2:D:471:GLU:CD	3:E:689:ILE:HG22	2.10	0.72
3:Y:696:GLU:HG2	3:Y:696:GLU:O	1.90	0.72
2:D:268:THR:O	2:D:269:PRO:O	2.07	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:206:PRO:HA	6:D:624:HOH:O	1.89	0.71
2:D:273:GLN:HA	2:D:280:ARG:CD	2.21	0.70
2:D:237:LEU:H	2:D:237:LEU:HD12	1.57	0.70
1:A:445:THR:O	1:A:446:PRO:O	2.10	0.69
2:D:357:ARG:HG3	2:D:358:LYS:H	1.56	0.69
2:X:262:ILE:C	2:X:264:PHE:H	1.94	0.69
1:A:294:LEU:HD11	3:B:638:GLN:NE2	2.08	0.69
2:D:377:LEU:HB2	2:D:379:LEU:CD1	2.22	0.69
2:X:320:TYR:CE1	2:X:476:LEU:HD23	2.28	0.68
1:A:333:HIS:HD2	1:A:335:ASN:ND2	1.91	0.68
3:E:686:ARG:HH12	3:E:691:HIS:CD2	2.12	0.68
1:U:310:ILE:C	1:U:310:ILE:HD13	2.13	0.68
2:X:411:ASP:HB2	6:X:515:HOH:O	1.92	0.68
2:D:404:LYS:HB3	2:D:405:PRO:HD3	1.75	0.68
2:D:411:ASP:HB2	6:D:556:HOH:O	1.93	0.67
2:X:279:ILE:O	2:X:283:GLN:HG3	1.95	0.67
2:D:273:GLN:C	2:D:275:LYS:H	1.97	0.67
2:X:273:GLN:O	2:X:275:LYS:N	2.28	0.67
2:D:377:LEU:HB2	2:D:379:LEU:HD11	1.76	0.67
3:E:691:HIS:HB3	6:E:408:HOH:O	1.95	0.67
1:U:417:LYS:HE3	6:X:542:HOH:O	1.94	0.67
2:D:262:ILE:CA	2:D:265:LYS:HB2	2.23	0.66
1:A:320:VAL:HG21	1:A:331:HIS:CE1	2.29	0.66
2:D:443:ARG:HD2	2:D:477:TYR:HE2	1.61	0.65
1:A:298:VAL:HG13	3:B:633:LEU:HD12	1.78	0.65
2:D:262:ILE:HA	2:D:265:LYS:HD2	1.78	0.65
1:A:335:ASN:ND2	1:A:336:SER:H	1.90	0.65
2:X:258:GLY:O	2:X:259:GLU:HG3	1.96	0.65
2:X:280:ARG:NH1	2:X:280:ARG:HG2	2.04	0.65
1:A:437:PHE:HE1	1:A:455:LEU:O	1.79	0.65
1:U:310:ILE:HD12	1:U:425:LEU:HD12	1.79	0.64
1:U:293:PRO:O	1:U:297:GLN:HG3	1.97	0.64
2:D:260:ASP:O	2:D:263:LYS:HB2	1.97	0.64
3:E:685:GLU:CG	3:E:686:ARG:H	2.06	0.64
2:D:271:GLN:NE2	2:D:280:ARG:HG2	2.12	0.64
1:U:334:ARG:NH1	1:U:347:ASP:OD1	2.31	0.64
1:U:456:GLU:O	1:U:458:PRO:HD3	1.98	0.64
1:A:335:ASN:ND2	1:A:336:SER:N	2.31	0.64
2:D:357:ARG:HG3	2:D:358:LYS:N	2.13	0.64
2:X:474:LYS:HD3	3:Y:686:ARG:HH21	1.63	0.63
2:X:264:PHE:O	2:X:265:LYS:C	2.36	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:GLU:O	1:A:456:GLU:HG3	1.97	0.63
2:D:358:LYS:HB2	2:D:359:PRO:CD	2.29	0.63
1:U:298:VAL:HG13	3:V:633:LEU:CD1	2.28	0.63
1:U:229:ASP:O	1:U:230:MET:HB2	1.98	0.63
2:D:262:ILE:HA	2:D:265:LYS:CB	2.25	0.63
2:X:336:LYS:HD2	2:X:336:LYS:H	1.63	0.63
1:A:228:GLU:O	1:A:229:ASP:HB2	1.99	0.63
2:X:311:LEU:HD22	3:Y:691:HIS:CE1	2.35	0.62
3:Y:685:GLU:OE1	3:Y:686:ARG:HG2	1.99	0.62
2:D:237:LEU:N	2:D:237:LEU:HD12	2.14	0.62
2:D:468:LEU:HD13	3:E:689:ILE:CG2	2.30	0.62
1:A:273:ASP:OD1	1:A:449:THR:O	2.16	0.62
2:D:358:LYS:CB	2:D:359:PRO:CD	2.77	0.62
2:D:233:ALA:O	2:D:237:LEU:CD1	2.46	0.62
2:D:370:PHE:HB2	2:D:445:ILE:HD11	1.81	0.62
2:D:270:LEU:HD22	2:D:287:PHE:CD1	2.35	0.62
1:A:236:LEU:HD22	1:A:240:LEU:HD22	1.82	0.62
1:U:334:ARG:NH1	1:U:338:HIS:NE2	2.48	0.61
1:U:334:ARG:HH11	1:U:334:ARG:HG3	1.64	0.61
2:X:311:LEU:HD22	3:Y:691:HIS:HE1	1.65	0.61
1:U:447:ILE:HD13	1:U:447:ILE:H	1.66	0.61
6:U:564:HOH:O	2:X:373:LYS:HD3	2.00	0.61
2:D:357:ARG:CG	2:D:358:LYS:H	2.09	0.61
2:X:363:PHE:CB	2:X:452:LEU:HD21	2.31	0.61
3:B:634:HIS:CE1	3:B:638:GLN:HE22	2.19	0.61
1:U:242:VAL:HG23	1:U:242:VAL:O	2.01	0.60
2:X:237:LEU:HD13	2:X:335:ASN:HD22	1.66	0.60
1:U:297:GLN:HE21	3:V:637:LEU:HD22	1.65	0.60
2:X:363:PHE:HB3	2:X:452:LEU:HD21	1.83	0.60
2:X:443:ARG:O	2:X:447:THR:HG23	2.02	0.60
2:D:443:ARG:O	2:D:447:THR:HG23	2.02	0.60
1:U:422:LEU:HB3	2:X:440:THR:HG21	1.83	0.60
3:E:685:GLU:HG2	3:E:686:ARG:N	2.06	0.60
2:D:379:LEU:HD12	2:D:379:LEU:N	2.17	0.60
2:X:463:MET:O	2:X:464:SER:HB2	2.00	0.59
1:U:423:PRO:HG3	2:X:440:THR:HG22	1.84	0.59
1:U:310:ILE:HA	1:U:313:PHE:CE2	2.38	0.59
2:D:269:PRO:C	2:D:270:LEU:HG	2.21	0.59
1:U:310:ILE:HD12	1:U:425:LEU:CD1	2.32	0.59
1:U:264:PRO:C	1:U:266:THR:H	2.06	0.59
1:U:353:LEU:HD22	1:U:428:ILE:HD12	1.85	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:297:GLN:NE2	3:V:637:LEU:HD22	2.17	0.59
2:D:468:LEU:HD13	3:E:689:ILE:HG23	1.85	0.59
1:U:231:PRO:HG2	1:U:234:ARG:HB2	1.84	0.59
1:U:335:ASN:N	1:U:335:ASN:HD22	2.01	0.59
1:U:445:THR:N	1:U:446:PRO:HD3	2.18	0.58
1:U:394:GLU:OE2	2:X:434:LYS:HE2	2.02	0.58
3:V:641:SER:H	3:V:642:PRO:CD	2.16	0.58
3:V:642:PRO:HB2	6:V:269:HOH:O	2.04	0.58
1:U:322:ASP:HB3	1:U:331:HIS:NE2	2.18	0.58
2:X:262:ILE:C	2:X:264:PHE:N	2.57	0.58
2:X:477:TYR:HD1	2:X:477:TYR:OXT	1.87	0.58
2:X:238:THR:CG2	2:X:239:GLY:H	2.16	0.57
1:U:335:ASN:HD22	1:U:336:SER:N	2.02	0.57
1:U:229:ASP:O	1:U:230:MET:CB	2.52	0.57
2:D:271:GLN:HE22	2:D:280:ARG:HD2	1.69	0.57
1:U:456:GLU:O	1:U:456:GLU:HG3	2.04	0.57
2:X:334:MET:HG2	2:X:339:VAL:HB	1.84	0.57
1:U:310:ILE:HD11	1:U:353:LEU:CD2	2.34	0.57
1:U:302:ARG:NH1	1:U:457:ALA:HA	2.19	0.57
2:X:405:PRO:O	2:X:409:ILE:HG13	2.05	0.57
2:D:244:LYS:HE3	2:D:245:SER:O	2.04	0.57
2:D:262:ILE:HD13	2:D:265:LYS:CD	2.34	0.57
1:U:454:MET:CE	3:V:633:LEU:HG	2.35	0.57
1:U:335:ASN:ND2	1:U:336:SER:N	2.53	0.56
1:U:440:LYS:HD2	1:U:452:MET:HE1	1.86	0.56
1:U:427:SER:HB2	2:X:443:ARG:HG3	1.87	0.56
1:U:457:ALA:HB3	6:U:545:HOH:O	2.05	0.56
1:U:447:ILE:HD13	1:U:447:ILE:N	2.20	0.56
1:U:364:LYS:NZ	6:U:508:HOH:O	2.38	0.56
2:D:379:LEU:HD13	6:D:506:HOH:O	2.05	0.56
2:D:271:GLN:CD	2:D:271:GLN:O	2.44	0.56
2:X:422:LYS:O	2:X:422:LYS:HE3	2.06	0.56
1:A:232:VAL:HG23	1:A:399:SER:HB3	1.88	0.56
1:A:441:LEU:O	1:A:442:ILE:HB	2.04	0.56
2:D:241:THR:HG23	2:D:241:THR:O	2.06	0.56
2:X:365:GLU:HB3	2:X:366:PRO:HD3	1.87	0.56
2:D:318:LEU:O	2:D:322:VAL:HB	2.05	0.56
2:D:259:GLU:O	2:D:262:ILE:HG12	2.05	0.56
1:A:288:HIS:HA	1:A:291:GLU:HG3	1.87	0.56
2:X:441:ASP:O	2:X:445:ILE:HG12	2.06	0.56
2:X:276:GLU:HA	6:X:525:HOH:O	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:358:ARG:NH1	6:U:523:HOH:O	2.39	0.55
2:X:317:LEU:HD11	2:X:406:ILE:HD13	1.88	0.55
1:U:242:VAL:HG11	1:U:282:TRP:HB2	1.89	0.55
1:U:298:VAL:HG13	3:V:633:LEU:HD13	1.88	0.55
1:U:264:PRO:O	1:U:266:THR:N	2.35	0.55
2:X:358:LYS:O	2:X:360:PHE:N	2.40	0.55
1:A:338:HIS:C	1:A:340:ALA:H	2.09	0.55
1:U:242:VAL:HB	1:U:278:THR:HG22	1.88	0.55
2:X:272:GLU:O	2:X:273:GLN:HB3	2.07	0.55
2:D:430:GLN:O	2:D:434:LYS:HG3	2.06	0.55
1:A:243:GLU:HB3	1:A:244:PRO:HB2	1.88	0.55
2:X:476:LEU:HD22	2:X:477:TYR:CD1	2.42	0.55
2:D:465:LEU:HB3	2:D:470:GLN:HG2	1.89	0.55
2:X:238:THR:CG2	2:X:239:GLY:N	2.69	0.55
2:X:269:PRO:O	2:X:272:GLU:HG3	2.07	0.55
1:A:267:ASN:ND2	1:A:330:LEU:CD1	2.61	0.55
1:U:310:ILE:HA	1:U:313:PHE:CD2	2.41	0.55
1:A:310:ILE:HA	1:A:313:PHE:CE2	2.42	0.55
1:A:246:THR:O	1:A:248:THR:N	2.38	0.55
2:X:236:ILE:CG2	2:X:246:PRO:HG2	2.37	0.54
2:D:364:MET:SD	5:D:503:BRL:H11	2.48	0.54
1:U:243:GLU:HB3	1:U:244:PRO:CA	2.37	0.54
2:X:267:ILE:O	2:X:268:THR:OG1	2.23	0.54
2:D:471:GLU:CG	3:E:687:HIS:HA	2.38	0.54
1:U:231:PRO:HB2	1:U:233:GLU:OE1	2.07	0.54
1:U:241:ALA:O	1:U:243:GLU:N	2.40	0.54
1:A:391:ALA:O	1:A:395:LYS:HG3	2.08	0.54
1:A:426:ARG:NH2	6:A:513:HOH:O	2.41	0.54
2:D:261:LYS:CG	2:D:265:LYS:HE3	2.34	0.53
2:X:325:ILE:HG12	2:X:388:ILE:HG23	1.91	0.53
1:A:242:VAL:O	1:A:243:GLU:O	2.25	0.53
2:X:357:ARG:O	2:X:360:PHE:HB2	2.07	0.53
2:D:260:ASP:HB3	2:D:263:LYS:HD2	1.90	0.53
1:U:294:LEU:O	1:U:294:LEU:HD12	2.08	0.53
2:D:268:THR:N	2:D:269:PRO:CD	2.71	0.53
1:A:343:GLY:O	1:A:345:ILE:N	2.42	0.53
2:D:273:GLN:HB3	2:D:280:ARG:NE	2.24	0.53
1:A:320:VAL:HG22	6:A:537:HOH:O	2.09	0.53
2:D:282:PHE:CZ	2:D:286:GLN:NE2	2.77	0.53
1:A:306:ASN:H	1:A:306:ASN:HD22	1.55	0.53
2:X:364:MET:SD	5:X:504:BRL:H11	2.49	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:357:ARG:NH1	2:D:358:LYS:HB2	2.24	0.52
1:U:437:PHE:CE1	1:U:455:LEU:O	2.62	0.52
2:D:256:MET:O	2:D:260:ASP:OD2	2.27	0.52
1:A:243:GLU:HB2	1:A:244:PRO:C	2.29	0.52
1:U:334:ARG:NH1	1:U:347:ASP:CG	2.63	0.52
3:V:638:GLN:HG3	3:V:638:GLN:O	2.08	0.52
1:U:305:TRP:CD1	1:U:305:TRP:C	2.81	0.52
1:A:345:ILE:HG12	1:A:431:LYS:HD2	1.91	0.52
2:D:357:ARG:HH11	2:D:358:LYS:HB2	1.74	0.52
1:U:324:ILE:HG12	1:U:332:VAL:HG22	1.92	0.52
2:D:313:ASP:O	2:D:317:LEU:HG	2.10	0.52
2:X:262:ILE:O	2:X:264:PHE:N	2.38	0.52
2:D:262:ILE:HD13	2:D:265:LYS:NZ	2.25	0.52
2:D:273:GLN:CA	2:D:280:ARG:HD3	2.33	0.52
2:D:252:MET:HG3	2:D:277:VAL:HG21	1.92	0.51
2:X:270:LEU:O	2:X:272:GLU:HG2	2.10	0.51
1:U:390:GLU:O	1:U:394:GLU:HG3	2.10	0.51
2:X:270:LEU:O	2:X:272:GLU:N	2.40	0.51
2:X:354:LYS:HD2	2:X:365:GLU:OE1	2.11	0.51
3:E:686:ARG:HA	3:E:686:ARG:NE	2.26	0.51
1:A:437:PHE:CE1	1:A:455:LEU:HG	2.46	0.51
2:X:259:GLU:CD	2:X:266:HIS:CB	2.79	0.51
1:U:334:ARG:O	1:U:338:HIS:HD2	1.93	0.51
1:U:273:ASP:OD1	1:U:450:PHE:HB3	2.11	0.50
3:Y:684:THR:O	3:Y:691:HIS:CD2	2.64	0.50
2:X:380:ASP:OD1	2:X:382:SER:OG	2.26	0.50
1:U:276:LEU:CD1	1:U:305:TRP:CD1	2.92	0.50
1:A:298:VAL:HG22	3:B:637:LEU:HD12	1.93	0.50
4:U:502:9CR:H8	4:U:502:9CR:H19	1.93	0.50
1:U:411:GLN:NE2	1:U:414:ARG:HH11	2.09	0.50
2:D:233:ALA:O	2:D:237:LEU:HD12	2.11	0.50
1:U:378:PRO:HG3	1:U:390:GLU:OE1	2.12	0.50
1:U:310:ILE:CD1	1:U:425:LEU:CD1	2.89	0.50
2:X:336:LYS:H	2:X:336:LYS:CD	2.20	0.50
1:U:305:TRP:HZ3	6:U:545:HOH:O	1.95	0.50
2:D:237:LEU:CD1	2:D:237:LEU:H	2.22	0.50
2:D:367:LYS:HD2	2:D:367:LYS:N	2.27	0.50
2:X:342:SER:CB	2:X:345:GLN:HB2	2.42	0.50
1:U:310:ILE:HD11	1:U:353:LEU:HD23	1.93	0.49
2:D:273:GLN:O	2:D:274:SER:HB2	2.13	0.49
2:X:244:LYS:HD2	2:X:244:LYS:C	2.32	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:251:ASP:HA	2:X:352:PHE:CD1	2.47	0.49
1:U:426:ARG:NH1	6:U:512:HOH:O	2.34	0.49
2:D:273:GLN:HB3	2:D:280:ARG:CZ	2.42	0.49
1:U:333:HIS:HB2	1:U:335:ASN:HD21	1.77	0.49
2:D:261:LYS:O	2:D:265:LYS:HG3	2.12	0.49
3:E:685:GLU:O	3:E:686:ARG:HB3	2.11	0.49
1:U:345:ILE:HD13	1:U:431:LYS:CD	2.34	0.49
2:D:363:PHE:CZ	2:D:364:MET:HG2	2.48	0.49
1:A:360:MET:CE	1:A:418:LEU:HD13	2.42	0.49
1:A:316:ARG:NH1	1:A:325:LEU:O	2.42	0.49
1:U:334:ARG:HH12	1:U:347:ASP:CG	2.17	0.48
1:U:427:SER:HB2	2:X:443:ARG:CG	2.43	0.48
2:X:268:THR:O	2:X:272:GLU:OE2	2.30	0.48
1:U:326:LEU:HD12	1:U:330:LEU:HB3	1.95	0.48
1:A:445:THR:N	1:A:446:PRO:CD	2.76	0.48
2:D:270:LEU:O	2:D:271:GLN:HB2	2.12	0.48
2:D:421:LEU:HD22	2:D:431:LEU:HD13	1.94	0.48
1:A:304:GLY:O	1:A:308:LEU:HG	2.13	0.48
2:D:471:GLU:HG2	3:E:687:HIS:HA	1.94	0.48
2:X:240:LYS:O	2:X:241:THR:O	2.32	0.48
2:X:444:GLN:O	2:X:448:GLU:HB2	2.13	0.48
1:U:353:LEU:HD22	1:U:428:ILE:CD1	2.44	0.48
2:X:242:THR:O	2:X:242:THR:OG1	2.32	0.48
1:U:334:ARG:NH1	1:U:347:ASP:OD2	2.44	0.48
1:A:392:LEU:HD23	1:A:395:LYS:HD2	1.96	0.48
1:A:427:SER:HB3	2:D:443:ARG:HG3	1.96	0.48
1:U:335:ASN:N	1:U:335:ASN:ND2	2.62	0.48
2:X:273:GLN:O	2:X:273:GLN:HG3	2.13	0.48
1:U:454:MET:HE2	3:V:633:LEU:HG	1.96	0.47
2:D:401:LEU:C	2:D:402:ASN:HD22	2.17	0.47
1:U:302:ARG:HH22	1:U:457:ALA:N	2.12	0.47
2:X:411:ASP:OD1	2:X:415:GLN:NE2	2.47	0.47
1:U:444:ASP:O	1:U:445:THR:C	2.52	0.47
2:D:449:HIS:HE2	5:D:503:BRL:C2	2.27	0.47
1:U:306:ASN:O	1:U:310:ILE:CG2	2.50	0.47
2:D:357:ARG:HD2	2:D:358:LYS:HG2	1.96	0.47
2:D:307:VAL:HG22	6:D:540:HOH:O	2.14	0.47
2:D:462:ASP:O	2:D:463:MET:C	2.51	0.47
2:X:260:ASP:OD2	2:X:261:LYS:N	2.46	0.47
1:U:445:THR:O	1:U:446:PRO:O	2.33	0.47
2:D:259:GLU:C	2:D:261:LYS:H	2.17	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:358:LYS:CB	2:D:359:PRO:HD3	2.43	0.47
1:A:441:LEU:O	1:A:442:ILE:CB	2.62	0.47
2:D:363:PHE:CE1	2:D:364:MET:HG2	2.49	0.47
2:D:267:ILE:O	2:D:267:ILE:HG22	2.14	0.47
1:U:318:ILE:C	1:U:318:ILE:HD12	2.33	0.47
2:X:264:PHE:C	2:X:266:HIS:N	2.66	0.47
1:U:252:ALA:O	1:U:329:GLY:O	2.33	0.47
2:X:305:GLY:O	2:X:308:ASN:ND2	2.41	0.47
2:D:257:MET:O	2:D:261:LYS:HB2	2.15	0.47
4:A:501:9CR:H8	4:A:501:9CR:H19	1.97	0.47
2:D:207:GLU:O	2:D:210:ASP:HB2	2.15	0.47
3:Y:692:ARG:HG3	3:Y:693:LEU:N	2.30	0.47
1:U:298:VAL:HG22	3:V:633:LEU:HD13	1.96	0.47
2:X:232:LYS:O	2:X:235:ALA:HB3	2.15	0.46
2:D:273:GLN:C	2:D:275:LYS:N	2.65	0.46
2:X:460:GLU:O	2:X:461:THR:C	2.52	0.46
2:D:286:GLN:NE2	2:D:465:LEU:HD12	2.30	0.46
1:U:264:PRO:C	1:U:266:THR:N	2.69	0.46
1:A:313:PHE:CD1	1:A:313:PHE:C	2.88	0.46
2:D:462:ASP:OD1	2:D:462:ASP:N	2.42	0.46
2:D:377:LEU:CB	2:D:379:LEU:HD11	2.44	0.46
2:D:373:LYS:O	2:D:376:ALA:HB3	2.16	0.46
1:U:292:LEU:HB2	1:U:293:PRO:HD2	1.98	0.46
2:D:237:LEU:HD11	2:D:340:LEU:HD11	1.98	0.46
2:D:358:LYS:HB2	2:D:359:PRO:HD2	1.96	0.46
1:A:437:PHE:CE1	1:A:455:LEU:O	2.65	0.46
1:U:437:PHE:HE1	1:U:455:LEU:O	1.98	0.46
1:A:434:GLU:HG3	6:D:626:HOH:O	2.15	0.46
2:D:264:PHE:O	2:D:264:PHE:HD1	1.96	0.46
1:A:451:LEU:O	1:A:455:LEU:HB2	2.15	0.46
1:A:338:HIS:HD2	1:A:343:GLY:HA3	1.80	0.46
2:X:325:ILE:HD11	2:X:392:ILE:HG13	1.97	0.46
1:U:440:LYS:HD2	1:U:452:MET:CE	2.46	0.46
2:D:379:LEU:CD1	2:D:379:LEU:N	2.79	0.46
2:X:477:TYR:OXT	2:X:477:TYR:CD1	2.67	0.46
1:U:242:VAL:HB	1:U:278:THR:CG2	2.46	0.46
1:U:287:PRO:O	1:U:288:HIS:HB2	2.16	0.46
1:U:348:ARG:O	1:U:352:GLU:HG3	2.16	0.45
2:X:274:SER:O	2:X:275:LYS:C	2.54	0.45
1:U:334:ARG:HH11	1:U:334:ARG:CG	2.29	0.45
1:U:280:VAL:HG11	3:V:636:LEU:HB3	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:290:VAL:O	2:D:294:GLN:HG3	2.16	0.45
1:U:293:PRO:HB2	1:U:296:ASP:OD2	2.16	0.45
2:D:271:GLN:O	2:D:272:GLU:C	2.55	0.45
1:A:449:THR:HG22	1:A:450:PHE:H	1.82	0.45
2:X:272:GLU:HB2	2:X:273:GLN:H	1.37	0.45
3:V:641:SER:H	3:V:642:PRO:HD2	1.82	0.45
1:U:231:PRO:HG3	1:U:234:ARG:HD3	1.97	0.45
1:A:287:PRO:O	1:A:288:HIS:HB2	2.17	0.45
2:D:334:MET:HG2	2:D:339:VAL:HB	1.98	0.45
1:A:273:ASP:OD2	1:U:237:GLU:OE2	2.35	0.45
1:U:455:LEU:HA	1:U:455:LEU:HD23	1.80	0.45
1:A:377:ASN:HA	1:A:393:ARG:NH2	2.32	0.45
1:U:228:GLU:O	1:U:228:GLU:CG	2.64	0.45
1:A:449:THR:O	1:A:451:LEU:N	2.43	0.45
2:X:271:GLN:HG3	6:X:563:HOH:O	2.16	0.45
1:U:335:ASN:ND2	1:U:335:ASN:H	2.15	0.45
2:D:237:LEU:CD1	2:D:340:LEU:HD11	2.47	0.45
2:D:379:LEU:H	2:D:379:LEU:CD1	2.30	0.45
1:U:363:ASP:OD1	1:U:366:GLU:HG3	2.16	0.45
1:U:292:LEU:CD2	1:U:297:GLN:HG2	2.47	0.44
1:A:228:GLU:O	1:A:229:ASP:CB	2.62	0.44
1:U:370:LEU:O	1:U:374:VAL:HG23	2.18	0.44
2:D:242:THR:HG23	2:D:242:THR:O	2.17	0.44
1:U:452:MET:CE	1:U:452:MET:HA	2.39	0.44
1:U:333:HIS:HB2	1:U:335:ASN:ND2	2.32	0.44
2:X:319:LYS:NZ	3:Y:687:HIS:HE1	2.16	0.44
2:X:259:GLU:OE1	2:X:266:HIS:CB	2.64	0.44
1:U:355:SER:HB2	6:U:523:HOH:O	2.18	0.44
1:U:454:MET:HE3	3:V:633:LEU:HG	1.99	0.44
3:E:695:GLN:HB3	3:E:695:GLN:HE21	1.48	0.44
1:U:292:LEU:HD23	1:U:292:LEU:C	2.38	0.44
2:X:242:THR:O	2:X:243:ASP:HB3	2.18	0.44
2:X:348:MET:SD	2:X:353:LEU:HD21	2.57	0.44
1:U:384:SER:O	1:U:385:ASN:HB2	2.18	0.44
2:D:232:LYS:O	2:D:235:ALA:HB3	2.17	0.44
2:X:288:ARG:NH1	2:X:288:ARG:O	2.49	0.44
2:D:358:LYS:HB3	2:D:359:PRO:HD3	1.98	0.44
2:D:379:LEU:H	2:D:379:LEU:HD12	1.83	0.44
1:U:305:TRP:CG	1:U:306:ASN:N	2.85	0.43
2:X:255:LEU:O	2:X:258:GLY:O	2.36	0.43
1:U:445:THR:N	1:U:446:PRO:CD	2.81	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:685:GLU:CG	3:E:686:ARG:N	2.74	0.43
1:A:331:HIS:C	1:A:331:HIS:CD2	2.92	0.43
2:X:336:LYS:N	2:X:336:LYS:HD2	2.32	0.43
1:A:377:ASN:HA	1:A:378:PRO:HD3	1.77	0.43
2:X:453:LEU:HD12	2:X:453:LEU:HA	1.85	0.43
1:A:333:HIS:HD2	1:A:335:ASN:CG	2.22	0.43
2:X:477:TYR:HA	6:X:551:HOH:O	2.17	0.43
2:X:363:PHE:O	2:X:367:LYS:HD3	2.18	0.43
1:U:407:LYS:C	1:U:409:PRO:HD3	2.38	0.43
1:A:343:GLY:O	1:A:344:ALA:HB3	2.19	0.43
1:A:294:LEU:HD21	3:B:634:HIS:NE2	2.34	0.43
2:D:233:ALA:O	2:D:237:LEU:HD13	2.18	0.43
1:A:318:ILE:HG23	1:A:358:ARG:HB2	2.00	0.43
1:U:242:VAL:HG11	1:U:282:TRP:CA	2.48	0.43
1:U:411:GLN:HA	1:U:412:PRO:HD2	1.78	0.43
1:A:245:LYS:O	1:A:246:THR:O	2.36	0.43
2:D:436:LEU:O	2:D:439:MET:HB2	2.19	0.43
1:U:292:LEU:HD21	1:U:297:GLN:HG2	2.00	0.43
1:A:275:GLN:NE2	1:A:275:GLN:HA	2.34	0.43
2:D:305:GLY:O	2:D:309:LEU:HD13	2.18	0.43
1:U:310:ILE:HD11	1:U:353:LEU:HD21	2.01	0.43
2:D:271:GLN:O	2:D:271:GLN:CG	2.67	0.43
2:D:241:THR:O	2:D:241:THR:CG2	2.67	0.43
2:X:266:HIS:C	2:X:267:ILE:HG13	2.39	0.43
1:A:305:TRP:O	1:A:309:LEU:HB2	2.19	0.43
2:D:275:LYS:O	2:D:276:GLU:O	2.37	0.43
3:B:638:GLN:HB3	3:B:638:GLN:HE21	1.55	0.43
2:X:211:LEU:HB3	2:X:419:LEU:HD23	2.01	0.43
2:D:443:ARG:HD3	2:D:443:ARG:HA	1.87	0.42
1:U:334:ARG:O	1:U:338:HIS:CD2	2.73	0.42
2:X:358:LYS:HA	2:X:359:PRO:HD2	1.85	0.42
1:U:332:VAL:CG2	1:U:332:VAL:O	2.67	0.42
2:X:342:SER:HB3	2:X:345:GLN:HB2	2.02	0.42
1:U:437:PHE:HB3	6:U:577:HOH:O	2.19	0.42
1:U:312:SER:OG	1:U:371:ARG:CZ	2.67	0.42
1:U:243:GLU:CB	1:U:244:PRO:HA	2.46	0.42
1:U:308:LEU:HD11	1:U:371:ARG:O	2.19	0.42
1:A:306:ASN:ND2	1:A:306:ASN:H	2.17	0.42
1:A:360:MET:HE1	1:A:418:LEU:HD13	2.00	0.42
2:X:322:VAL:HG12	2:X:323:HIS:N	2.34	0.42
1:A:334:ARG:O	1:A:337:ALA:HB3	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:348:ARG:O	1:U:352:GLU:CG	2.68	0.42
2:X:363:PHE:CB	2:X:452:LEU:CD2	2.98	0.42
1:A:338:HIS:HD2	1:A:343:GLY:CA	2.32	0.42
1:U:352:GLU:HG3	1:U:428:ILE:HD11	2.00	0.42
1:U:266:THR:O	1:U:270:GLN:HB2	2.20	0.42
2:D:320:TYR:CB	2:D:397:ARG:HD2	2.50	0.42
2:D:275:LYS:O	2:D:280:ARG:CG	2.68	0.42
1:A:298:VAL:O	1:A:302:ARG:HG3	2.20	0.42
1:U:423:PRO:CG	2:X:440:THR:HG22	2.47	0.42
6:U:533:HOH:O	3:V:630:HIS:HB3	2.20	0.42
3:B:633:LEU:HD13	3:B:633:LEU:C	2.40	0.42
3:Y:688:LYS:HB3	3:Y:688:LYS:NZ	2.35	0.42
1:A:335:ASN:C	1:A:335:ASN:HD22	2.05	0.41
2:X:280:ARG:NH1	2:X:280:ARG:CG	2.75	0.41
2:D:281:ILE:HG23	5:D:503:BRL:H22	2.02	0.41
2:X:342:SER:HB2	2:X:345:GLN:HB2	2.00	0.41
1:A:443:GLY:O	1:A:444:ASP:HB2	2.20	0.41
2:D:219:TYR:O	2:D:222:TYR:HB3	2.20	0.41
3:E:686:ARG:NH1	3:E:686:ARG:O	2.52	0.41
1:U:276:LEU:HD13	1:U:309:LEU:HD11	2.02	0.41
3:Y:686:ARG:CZ	3:Y:686:ARG:HB3	2.49	0.41
1:A:324:ILE:HG22	1:A:325:LEU:N	2.35	0.41
2:X:319:LYS:HZ2	3:Y:687:HIS:HE1	1.68	0.41
3:B:634:HIS:HE1	3:B:638:GLN:HE22	1.66	0.41
2:D:477:TYR:C	2:D:477:TYR:CD1	2.93	0.41
3:Y:684:THR:CA	3:Y:691:HIS:NE2	2.84	0.41
2:D:341:ILE:HG22	5:D:503:BRL:H152	2.02	0.41
2:D:350:ARG:NH2	2:D:365:GLU:OE2	2.51	0.41
1:U:345:ILE:CD1	1:U:431:LYS:HD3	2.38	0.41
1:A:243:GLU:CB	1:A:244:PRO:C	2.89	0.41
1:U:229:ASP:HB3	1:U:395:LYS:HD3	2.03	0.41
1:A:334:ARG:HD2	1:A:347:ASP:OD1	2.21	0.41
2:D:393:LEU:O	2:D:410:GLN:HB2	2.21	0.41
3:Y:684:THR:N	3:Y:691:HIS:CE1	2.89	0.41
2:X:367:LYS:HD2	2:X:367:LYS:N	2.36	0.41
1:U:394:GLU:O	2:X:430:GLN:NE2	2.49	0.41
1:U:228:GLU:O	1:U:228:GLU:CD	2.59	0.41
2:D:446:VAL:HG11	2:D:477:TYR:HE1	1.85	0.41
3:Y:685:GLU:H	3:Y:685:GLU:CD	2.24	0.41
2:D:418:GLU:HG3	2:D:432:PHE:CG	2.56	0.41
2:D:250:TYR:CD1	2:D:250:TYR:N	2.88	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:291:GLU:O	2:X:295:GLU:HG3	2.21	0.41
2:X:264:PHE:O	2:X:266:HIS:CB	2.70	0.40
2:X:207:GLU:HB3	2:X:210:ASP:OD2	2.20	0.40
2:X:223:ILE:HD11	6:X:587:HOH:O	2.20	0.40
4:U:502:9CR:H8	4:U:502:9CR:H10	1.87	0.40
2:D:367:LYS:HD2	2:D:367:LYS:H	1.84	0.40
2:D:418:GLU:HG3	2:D:432:PHE:CD2	2.56	0.40
2:D:476:LEU:HG	2:D:477:TYR:N	2.23	0.40
3:Y:684:THR:HB	3:Y:685:GLU:H	1.74	0.40
1:A:366:GLU:HG2	1:A:418:LEU:HD21	2.03	0.40
2:D:452:LEU:O	2:D:456:ILE:HG13	2.22	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	230/238 (97%)	191 (83%)	21 (9%)	18 (8%)	1	0
1	U	230/238 (97%)	191 (83%)	24 (10%)	15 (6%)	1	0
2	D	270/272 (99%)	240 (89%)	15 (6%)	15 (6%)	2	0
2	X	270/272 (99%)	235 (87%)	16 (6%)	19 (7%)	1	0
3	B	8/25 (32%)	7 (88%)	1 (12%)	0	100	100
3	E	14/25 (56%)	13 (93%)	1 (7%)	0	100	100
3	V	13/25 (52%)	10 (77%)	2 (15%)	1 (8%)	1	0
3	Y	11/25 (44%)	10 (91%)	1 (9%)	0	100	100
All	All	1046/1120 (93%)	897 (86%)	81 (8%)	68 (6%)	1	0

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	GLU
1	A	244	PRO
1	A	246	THR
1	A	247	GLU
1	A	253	ASN
1	A	254	MET
1	A	257	ASN
1	A	260	SER
1	A	442	ILE
1	A	446	PRO
2	D	265	LYS
2	D	269	PRO
2	D	271	GLN
2	D	273	GLN
2	D	276	GLU
2	D	357	ARG
2	D	358	LYS
2	D	463	MET
1	U	230	MET
1	U	253	ASN
1	U	259	SER
1	U	263	ASP
1	U	264	PRO
1	U	443	GLY
1	U	446	PRO
2	X	240	LYS
2	X	241	THR
2	X	259	GLU
2	X	262	ILE
2	X	270	LEU
2	X	271	GLN
2	X	273	GLN
2	X	274	SER
2	X	359	PRO
1	A	339	SER
2	D	243	ASP
1	U	242	VAL
1	U	322	ASP
2	X	243	ASP
2	X	269	PRO
2	X	272	GLU
1	A	245	LYS
2	D	260	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	D	464	SER
2	D	476	LEU
1	U	254	MET
2	X	264	PHE
1	A	229	ASP
1	A	259	SER
1	A	334	ARG
1	A	455	LEU
2	D	272	GLU
1	U	243	GLU
1	U	244	PRO
1	U	257	ASN
2	X	266	HIS
2	X	267	ILE
2	X	463	MET
1	A	250	VAL
2	D	241	THR
3	V	641	SER
1	U	265	VAL
2	X	268	THR
2	X	358	LYS
1	A	457	ALA
2	X	239	GLY
2	D	268	THR
1	U	260	SER

### 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	182/205 (89%)	161 (88%)	21 (12%)	7	3
1	U	182/205 (89%)	160 (88%)	22 (12%)	6	3
2	D	244/245 (100%)	226 (93%)	18 (7%)	17	13
2	X	236/245 (96%)	212 (90%)	24 (10%)	9	5
3	B	9/24 (38%)	7 (78%)	2 (22%)	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	14/24 (58%)	13 (93%)	1 (7%)	18	14
3	V	14/24 (58%)	10 (71%)	4 (29%)	0	0
3	Y	13/24 (54%)	10 (77%)	3 (23%)	1	0
All	All	894/996 (90%)	799 (89%)	95 (11%)	8	5

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	GLU
1	A	236	LEU
1	A	240	LEU
1	A	244	PRO
1	A	276	LEU
1	A	286	ILE
1	A	306	ASN
1	A	309	LEU
1	A	320	VAL
1	A	330	LEU
1	A	334	ARG
1	A	335	ASN
1	A	345	ILE
1	A	355	SER
1	A	388	GLU
1	A	410	GLU
1	A	418	LEU
1	A	421	ARG
1	A	436	LEU
1	A	442	ILE
1	A	450	PHE
2	D	234	ARG
2	D	251	ASP
2	D	256	MET
2	D	264	PHE
2	D	267	ILE
2	D	269	PRO
2	D	270	LEU
2	D	309	LEU
2	D	318	LEU
2	D	322	VAL
2	D	358	LYS
2	D	431	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	443	ARG
2	D	444	GLN
2	D	447	THR
2	D	453	LEU
2	D	463	MET
2	D	477	TYR
1	U	243	GLU
1	U	264	PRO
1	U	266	THR
1	U	270	GLN
1	U	276	LEU
1	U	285	ARG
1	U	292	LEU
1	U	302	ARG
1	U	305	TRP
1	U	308	LEU
1	U	310	ILE
1	U	320	VAL
1	U	332	VAL
1	U	335	ASN
1	U	353	LEU
1	U	381	LYS
1	U	420	LEU
1	U	422	LEU
1	U	426	ARG
1	U	447	ILE
1	U	450	PHE
1	U	452	MET
2	X	211	LEU
2	X	240	LYS
2	X	242	THR
2	X	244	LYS
2	X	248	VAL
2	X	256	MET
2	X	267	ILE
2	X	272	GLU
2	X	277	VAL
2	X	280	ARG
2	X	298	GLU
2	X	308	ASN
2	X	311	LEU
2	X	318	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	X	322	VAL
2	X	330	LEU
2	X	336	LYS
2	X	359	PRO
2	X	422	LYS
2	X	453	LEU
2	X	459	THR
2	X	465	LEU
2	X	476	LEU
2	X	477	TYR
3	B	630	HIS
3	B	638	GLN
3	V	629	ARG
3	V	633	LEU
3	V	638	GLN
3	V	641	SER
3	E	695	GLN
3	Y	684	THR
3	Y	685	GLU
3	Y	691	HIS

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

Mol	Chain	Res	Type
1	A	267	ASN
1	A	270	GLN
1	A	275	GLN
1	A	306	ASN
1	A	331	HIS
1	A	333	HIS
1	A	335	ASN
1	A	338	HIS
2	D	266	HIS
2	D	271	GLN
2	D	402	ASN
2	D	451	GLN
1	U	270	GLN
1	U	275	GLN
1	U	297	GLN
1	U	333	HIS
1	U	335	ASN
1	U	406	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	U	411	GLN
1	U	435	HIS
2	X	402	ASN
2	X	415	GLN
2	X	451	GLN
3	B	638	GLN
3	E	695	GLN
3	Y	687	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	9CR	A	501	-	19,22,22	4.01	9 (47%)	26,30,30	2.59	13 (50%)
5	BRL	D	503	-	26,27,27	2.29	11 (42%)	31,36,36	2.83	11 (35%)
4	9CR	U	502	-	19,22,22	3.89	9 (47%)	26,30,30	2.79	12 (46%)
5	BRL	X	504	-	26,27,27	2.15	10 (38%)	31,36,36	2.98	10 (32%)

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
4	9CR	A	501	-	-	0/13/32/32	0/1/1/1
5	BRL	D	503	-	-	0/14/26/26	0/3/3/3
4	9CR	U	502	-	-	0/13/32/32	0/1/1/1
5	BRL	X	504	-	-	0/14/26/26	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	503	BRL	C2-N3	-4.28	1.32	1.37
5	X	504	BRL	C2-N3	-4.22	1.32	1.37
5	D	503	BRL	C4-N3	-2.48	1.34	1.37
5	D	503	BRL	C11-C10	2.08	1.42	1.38
5	X	504	BRL	C8-C7	2.16	1.43	1.38
5	X	504	BRL	C15-N16	2.22	1.53	1.46
5	D	503	BRL	C8-C7	2.29	1.43	1.38
5	X	504	BRL	C11-C10	2.32	1.43	1.38
5	X	504	BRL	O13-C10	2.33	1.43	1.37
4	U	502	9CR	C14-C13	2.35	1.38	1.35
5	D	503	BRL	O13-C10	2.44	1.43	1.37
5	D	503	BRL	C12-C7	2.51	1.44	1.38
5	X	504	BRL	C12-C7	2.59	1.44	1.38
4	A	501	9CR	C2-C3	2.63	1.59	1.52
4	U	502	9CR	C2-C3	2.65	1.59	1.52
4	A	501	9CR	C14-C13	2.88	1.39	1.35
4	A	501	9CR	C4-C5	2.95	1.57	1.51
4	U	502	9CR	C20-C13	2.98	1.57	1.50
5	X	504	BRL	C22-C17	2.99	1.46	1.39
5	D	503	BRL	C22-C17	3.00	1.46	1.39
4	U	502	9CR	C2-C1	3.13	1.61	1.54
5	D	503	BRL	C17-N18	3.14	1.40	1.34
4	U	502	9CR	C4-C5	3.19	1.57	1.51
5	X	504	BRL	C17-N18	3.21	1.41	1.34
5	D	503	BRL	C16-N16	3.34	1.51	1.46
5	X	504	BRL	C16-N16	3.46	1.51	1.46
4	A	501	9CR	C2-C1	3.66	1.62	1.54
4	A	501	9CR	C20-C13	3.70	1.58	1.50
5	D	503	BRL	C5-C4	3.84	1.55	1.52
4	A	501	9CR	C16-C1	3.88	1.62	1.53
5	D	503	BRL	C9-C10	4.27	1.47	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	502	9CR	C10-C9	4.30	1.41	1.35
5	X	504	BRL	C9-C10	4.34	1.47	1.38
4	A	501	9CR	C10-C9	4.54	1.41	1.35
4	U	502	9CR	C16-C1	5.10	1.64	1.53
4	A	501	9CR	C5-C6	9.33	1.49	1.34
4	U	502	9CR	C5-C6	9.43	1.49	1.34
4	U	502	9CR	C1-C6	9.82	1.67	1.53
4	A	501	9CR	C1-C6	10.72	1.69	1.53

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	504	BRL	C4-N3-C2	-9.22	112.02	118.32
5	D	503	BRL	C4-N3-C2	-8.42	112.57	118.32
4	U	502	9CR	C16-C1-C6	-6.21	100.57	110.30
4	A	501	9CR	C16-C1-C6	-4.37	103.44	110.30
5	X	504	BRL	C6-C5-S1	-4.27	108.53	113.00
5	X	504	BRL	O2-C2-N3	-4.14	121.03	125.72
5	X	504	BRL	C5-S1-C2	-4.10	90.59	92.90
4	A	501	9CR	C19-C9-C10	-4.02	116.96	122.90
5	D	503	BRL	O2-C2-N3	-4.01	121.18	125.72
4	U	502	9CR	C19-C9-C10	-3.80	117.29	122.90
5	D	503	BRL	C5-S1-C2	-3.44	90.96	92.90
5	D	503	BRL	C6-C5-S1	-3.04	109.82	113.00
5	D	503	BRL	O4-C4-N3	-2.89	121.33	124.83
5	D	503	BRL	C22-C17-N18	-2.82	117.97	123.17
5	X	504	BRL	C22-C17-N18	-2.78	118.04	123.17
4	A	501	9CR	C1-C6-C5	-2.62	118.81	122.66
4	A	501	9CR	C16-C1-C2	-2.62	99.39	108.79
5	D	503	BRL	O2-C2-S1	-2.59	122.19	124.68
5	X	504	BRL	O2-C2-S1	-2.49	122.29	124.68
5	X	504	BRL	O4-C4-N3	-2.30	122.05	124.83
4	U	502	9CR	C1-C6-C5	-2.26	119.35	122.66
4	A	501	9CR	C4-C5-C6	-2.22	119.95	122.78
4	U	502	9CR	C11-C10-C9	-2.14	124.11	127.20
4	U	502	9CR	C16-C1-C2	-2.08	101.34	108.79
4	A	501	9CR	C11-C10-C9	-2.06	124.22	127.20
5	D	503	BRL	C4-C5-S1	-2.03	103.97	105.89
4	A	501	9CR	C2-C1-C6	2.15	113.77	110.36
4	A	501	9CR	C7-C6-C5	2.18	126.35	121.37
4	U	502	9CR	C7-C6-C5	2.28	126.59	121.37
4	U	502	9CR	C8-C7-C6	2.40	134.53	127.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	9CR	C8-C7-C6	2.68	135.37	127.32
4	U	502	9CR	C20-C13-C12	2.81	122.77	118.10
4	A	501	9CR	C20-C13-C12	2.87	122.88	118.10
4	U	502	9CR	C2-C1-C6	2.92	114.99	110.36
5	D	503	BRL	C19-N18-C17	3.10	120.93	116.92
5	X	504	BRL	C19-N18-C17	3.31	121.21	116.92
4	A	501	9CR	C19-C9-C8	3.57	124.04	118.10
4	U	502	9CR	C19-C9-C8	3.99	124.73	118.10
5	D	503	BRL	C5-C4-N3	4.17	115.88	111.96
5	X	504	BRL	C5-C4-N3	4.32	116.01	111.96
4	A	501	9CR	C7-C8-C9	4.91	133.71	126.22
4	U	502	9CR	C7-C8-C9	5.52	134.63	126.22
4	A	501	9CR	C17-C1-C6	6.64	120.71	110.30
4	U	502	9CR	C17-C1-C6	6.80	120.96	110.30
5	D	503	BRL	S1-C2-N3	8.48	116.62	110.38
5	X	504	BRL	S1-C2-N3	8.56	116.68	110.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	9CR	1	0
5	D	503	BRL	4	0
4	U	502	9CR	2	0
5	X	504	BRL	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	232/238 (97%)	1.65	50 (21%) 1 1	32, 54, 120, 134	0
1	U	232/238 (97%)	1.62	53 (22%) 1 1	31, 51, 119, 126	0
2	D	272/272 (100%)	1.01	36 (13%) 4 6	31, 46, 93, 119	0
2	X	272/272 (100%)	0.82	40 (14%) 3 5	31, 51, 88, 100	0
3	B	10/25 (40%)	0.44	0 100 100	55, 64, 75, 81	0
3	E	16/25 (64%)	1.52	5 (31%) 1 1	53, 63, 81, 86	0
3	V	15/25 (60%)	2.98	5 (33%) 0 1	59, 72, 101, 104	0
3	Y	13/25 (52%)	1.43	3 (23%) 1 1	61, 75, 85, 93	0
All	All	1062/1120 (94%)	1.27	192 (18%) 2 2	31, 51, 99, 134	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	259	SER	22.2
2	D	271	GLN	22.1
1	A	259	SER	20.9
1	A	261	PRO	19.3
1	U	260	SER	19.3
1	A	258	PRO	19.2
1	A	252	ALA	17.3
1	U	254	MET	16.9
1	U	257	ASN	14.8
1	A	256	LEU	14.0
1	A	248	THR	13.8
1	U	258	PRO	13.4
3	V	642	PRO	13.4
2	D	272	GLU	12.4
1	U	252	ALA	12.1
2	D	264	PHE	11.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	U	256	LEU	11.0
1	A	254	MET	10.5
1	U	457	ALA	10.4
2	D	242	THR	10.2
2	D	270	LEU	10.1
3	V	641	SER	10.0
2	D	267	ILE	9.9
1	A	255	GLY	9.6
1	U	250	VAL	9.5
1	A	262	ASN	9.4
2	D	266	HIS	9.4
1	A	247	GLU	9.3
1	U	247	GLU	9.2
1	A	458	PRO	9.1
2	D	243	ASP	8.5
1	U	227	ASN	8.5
1	A	250	VAL	8.5
1	U	248	THR	8.1
1	A	249	TYR	8.0
1	A	457	ALA	7.8
1	A	445	THR	7.8
1	U	246	THR	7.6
1	U	255	GLY	7.5
1	A	260	SER	7.4
1	A	251	GLU	7.2
1	A	246	THR	7.0
1	A	442	ILE	7.0
1	U	444	ASP	6.8
1	A	227	ASN	6.5
2	D	262	ILE	6.4
2	D	263	LYS	6.3
1	U	262	ASN	6.2
2	X	241	THR	6.2
2	X	262	ILE	6.0
1	U	445	THR	5.9
2	D	268	THR	5.8
1	A	444	ASP	5.6
2	X	243	ASP	5.6
1	U	244	PRO	5.3
3	V	628	GLU	5.3
2	X	308	ASN	5.3
2	D	265	LYS	5.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	U	253	ASN	5.3
2	D	477	TYR	5.1
1	U	261	PRO	5.0
1	A	257	ASN	5.0
2	D	269	PRO	5.0
1	A	446	PRO	4.9
2	D	241	THR	4.7
2	X	238	THR	4.7
3	E	685	GLU	4.6
3	V	629	ARG	4.5
2	X	311	LEU	4.5
2	X	267	ILE	4.5
3	Y	691	HIS	4.4
1	U	446	PRO	4.4
2	X	263	LYS	4.4
2	X	461	THR	4.3
1	A	438	PHE	4.3
2	X	477	TYR	4.3
2	D	260	ASP	4.2
2	D	463	MET	4.0
1	A	253	ASN	4.0
1	A	263	ASP	3.9
2	X	264	PHE	3.9
2	X	237	LEU	3.8
1	A	244	PRO	3.8
2	X	271	GLN	3.8
2	X	307	VAL	3.7
2	X	463	MET	3.7
3	E	700	SER	3.7
2	D	461	THR	3.7
1	A	299	ILE	3.7
1	U	422	LEU	3.6
1	U	251	GLU	3.6
2	D	273	GLN	3.5
2	X	446	VAL	3.5
1	U	425	LEU	3.5
1	U	249	TYR	3.5
2	D	442	LEU	3.4
2	X	268	THR	3.4
2	X	244	LYS	3.3
1	U	458	PRO	3.3
1	U	339	SER	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	440	THR	3.2
1	A	320	VAL	3.2
1	A	330	LEU	3.1
2	X	440	THR	3.1
1	A	447	ILE	3.1
2	D	322	VAL	3.1
1	A	425	LEU	3.1
1	U	340	ALA	3.0
2	X	428	SER	3.0
1	U	424	ALA	3.0
1	U	427	SER	2.9
3	Y	684	THR	2.9
1	U	370	LEU	2.8
2	X	228	LEU	2.8
2	X	439	MET	2.8
1	A	422	LEU	2.8
2	X	242	THR	2.8
1	U	428	ILE	2.8
2	X	442	LEU	2.8
2	D	326	ILE	2.8
1	A	264	PRO	2.7
1	U	264	PRO	2.7
1	U	243	GLU	2.7
1	A	353	LEU	2.7
1	U	447	ILE	2.7
1	U	245	LYS	2.7
2	D	240	LYS	2.7
1	A	338	HIS	2.7
2	D	439	MET	2.7
2	X	309	LEU	2.7
2	X	476	LEU	2.7
3	E	697	GLY	2.7
3	E	698	SER	2.6
1	A	335	ASN	2.6
1	U	419	LEU	2.6
1	U	321	LYS	2.6
2	D	325	ILE	2.6
2	D	464	SER	2.5
2	D	423	LEU	2.5
1	A	341	GLY	2.5
2	X	325	ILE	2.5
1	A	441	LEU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	229	ASP	2.5
2	X	425	HIS	2.5
2	X	423	LEU	2.5
1	U	426	ARG	2.5
1	A	370	LEU	2.4
2	X	445	ILE	2.4
2	D	445	ILE	2.4
3	Y	695	GLN	2.4
2	X	359	PRO	2.4
1	A	418	LEU	2.4
1	A	333	HIS	2.4
1	U	263	ASP	2.4
2	X	272	GLU	2.4
2	X	234	ARG	2.4
2	X	270	LEU	2.3
1	U	322	ASP	2.3
1	A	428	ILE	2.3
2	D	363	PHE	2.3
1	U	456	GLU	2.3
1	A	381	LYS	2.3
1	U	423	PRO	2.3
1	A	340	ALA	2.3
1	A	420	LEU	2.3
1	U	309	LEU	2.3
1	A	423	PRO	2.2
1	U	443	GLY	2.2
2	X	273	GLN	2.2
1	U	374	VAL	2.2
3	V	630	HIS	2.2
1	A	430	LEU	2.2
2	X	426	PRO	2.2
2	X	258	GLY	2.2
1	U	420	LEU	2.2
1	A	426	ARG	2.2
2	D	443	ARG	2.2
2	D	424	ASN	2.2
1	U	418	LEU	2.1
2	D	462	ASP	2.1
1	U	308	LEU	2.1
1	U	373	ILE	2.1
2	X	327	TYR	2.1
3	E	689	ILE	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	U	305	TRP	2.1
2	X	310	ASP	2.1
1	U	441	LEU	2.1
2	D	317	LEU	2.1
1	U	431	LYS	2.0
2	D	426	PRO	2.0
2	X	447	THR	2.0
2	D	244	LYS	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, 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
4	9CR	A	501	22/22	0.86	0.26	3.80	44,61,71,72	0
4	9CR	U	502	22/22	0.90	0.23	1.90	41,49,63,64	0
5	BRL	D	503	25/25	0.93	0.17	0.44	41,45,47,49	0
5	BRL	X	504	25/25	0.94	0.17	0.02	37,40,48,48	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.