



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:40 PM GMT

PDB ID : 1Y8E  
Title : VCP:Suramin Complex  
Authors : Ganesh, V.K.; Muthuvel, S.K.; Smith, S.A.; Kotwal, G.J.; Murthy, K.H.  
Deposited on : 2004-12-12  
Resolution : 2.20 Å(reported)

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

---

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

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

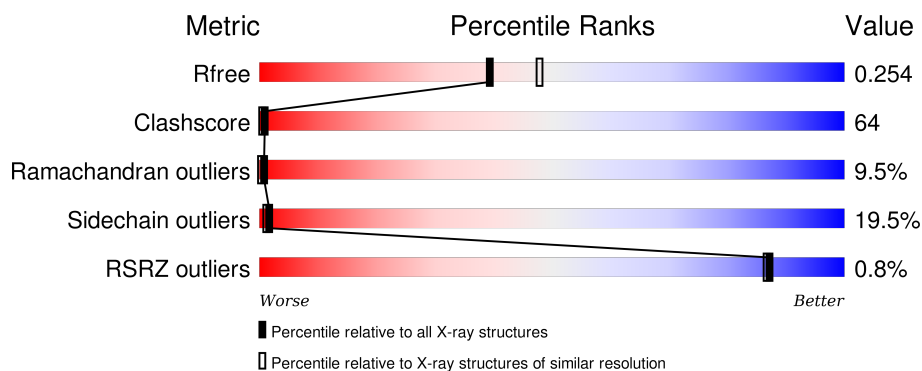
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	244	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 19%, yellow 33%, green 49%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>49%</span> <span>33%</span> <span>14%</span> <span>5%</span> </div> </div>
1	B	244	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 37%, yellow 41%, orange 57%, red 62%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>37%</span> <span>41%</span> <span>16%</span> <span>5%</span> </div> </div>

## 2 Entry composition [i](#)

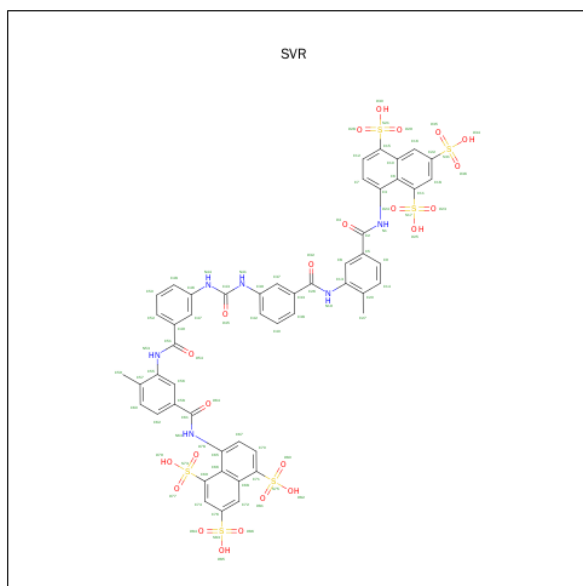
There are 3 unique types of molecules in this entry. The entry contains 4375 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Complement control protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1860	1156	315	369	20			
1	B	243	Total	C	N	O	S	0	0	0
			1849	1150	314	366	19			

- Molecule 2 is 8,8'-[CARBONYLBIS[IMINO-3,1-PHENYLENECARBONYLIMINO(4-METHYL-3,1-PHENYLENE)CARBONYLIMINO]]BIS-1,3,5-NAPHTHALENETRISULFONIC ACID (three-letter code: SVR) (formula: C<sub>51</sub>H<sub>40</sub>N<sub>6</sub>O<sub>23</sub>S<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			86	51	6	23	6		
2	B	1	Total	C	N	O	S	0	0
			86	51	6	23	6		

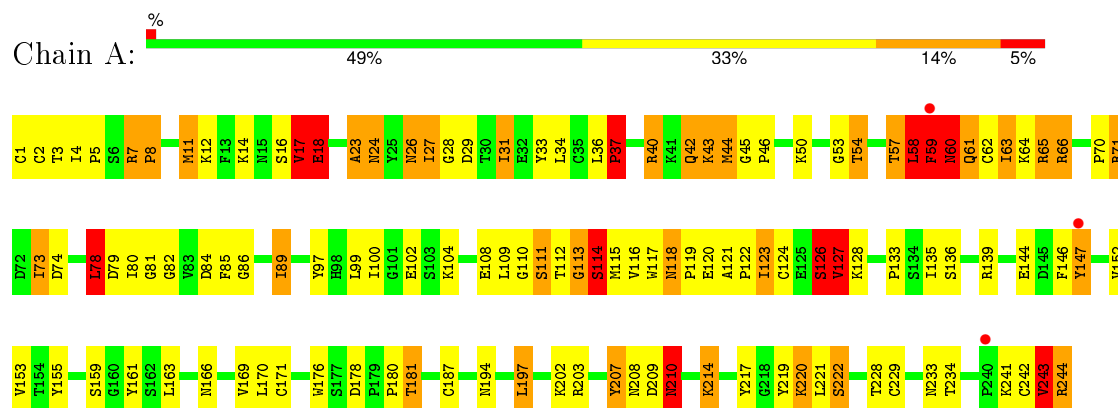
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	276	Total 276	O 276	0	0
3	B	218	Total 218	O 218	0	0

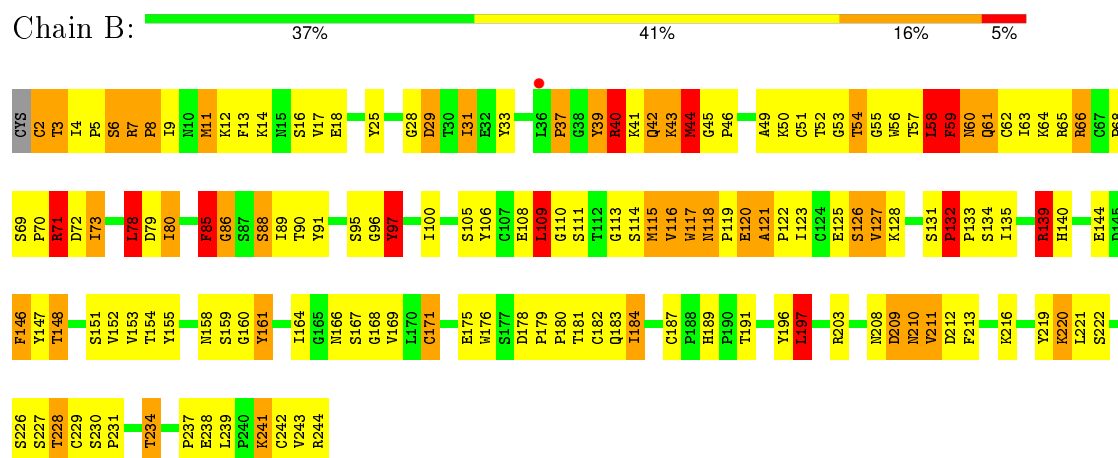
### 3 Residue-property plots

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: Complement control protein



#### • Molecule 1: Complement control protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.10Å 125.10Å 149.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	150.00 – 2.20 29.88 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.5 (150.00-2.20) 100.0 (29.88-2.20)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.13 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.195 , 0.215 0.213 , 0.254	Depositor DCC
$R_{free}$ test set	6280 reflections (10.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.6	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 229.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 62783 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4375	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: SVR

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	0.48	0/1909	1.47	32/2589 (1.2%)
1	B	0.51	1/1898 (0.1%)	1.33	22/2574 (0.9%)
All	All	0.49	1/3807 (0.0%)	1.40	54/5163 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	LYS	N-CA	5.08	1.56	1.46

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	TYR	CA-CB-CG	10.06	132.51	113.40
1	A	97	TYR	CA-CB-CG	7.54	127.72	113.40
1	A	7	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	219	TYR	CA-CB-CG	6.96	126.62	113.40
1	B	7	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	B	197	LEU	CA-CB-CG	6.93	131.23	115.30
1	A	197	LEU	CA-CB-CG	6.91	131.19	115.30
1	A	66	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	B	40	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	40	ARG	NE-CZ-NH1	6.67	123.63	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	LEU	CA-C-N	-6.65	102.57	117.20
1	A	65	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	65	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	A	78	LEU	CA-CB-CG	6.48	130.21	115.30
1	A	57	THR	C-N-CA	6.40	137.69	121.70
1	A	114	SER	N-CA-CB	6.38	120.07	110.50
1	B	78	LEU	CA-CB-CG	6.28	129.74	115.30
1	B	66	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	17	VAL	C-N-CA	6.13	137.04	121.70
1	B	116	VAL	CA-C-N	-6.12	103.75	117.20
1	B	203	ARG	CD-NE-CZ	6.12	132.16	123.60
1	A	57	THR	CA-C-N	-6.00	104.00	117.20
1	A	139	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	B	139	ARG	CD-NE-CZ	5.88	131.84	123.60
1	A	203	ARG	CD-NE-CZ	5.87	131.82	123.60
1	A	147	TYR	CA-CB-CG	5.78	124.38	113.40
1	A	139	ARG	CD-NE-CZ	5.77	131.68	123.60
1	A	71	ARG	CD-NE-CZ	5.75	131.65	123.60
1	B	71	ARG	CD-NE-CZ	5.72	131.61	123.60
1	B	58	LEU	CA-C-N	-5.72	104.62	117.20
1	B	139	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	71	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	59	PHE	CA-C-N	-5.64	104.78	117.20
1	A	23	ALA	CB-CA-C	5.62	118.53	110.10
1	A	210	ASN	O-C-N	-5.50	113.90	122.70
1	B	85	PHE	CB-CG-CD1	-5.49	116.95	120.80
1	A	163	LEU	CA-CB-CG	5.48	127.90	115.30
1	B	66	ARG	CD-NE-CZ	5.45	131.23	123.60
1	B	116	VAL	C-N-CA	5.38	135.14	121.70
1	B	65	ARG	CD-NE-CZ	5.37	131.12	123.60
1	B	71	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	243	VAL	CA-C-N	-5.26	105.63	117.20
1	B	46	PRO	CA-N-CD	-5.25	104.14	111.50
1	A	65	ARG	CD-NE-CZ	5.21	130.90	123.60
1	A	18	GLU	C-N-CA	5.21	134.72	121.70
1	A	161	TYR	CA-CB-CG	5.21	123.29	113.40
1	A	221	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	40	ARG	CD-NE-CZ	5.18	130.85	123.60
1	A	203	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	211	VAL	CB-CA-C	-5.13	101.64	111.40
1	A	66	ARG	CD-NE-CZ	5.10	130.74	123.60
1	A	18	GLU	CA-C-N	-5.07	106.05	117.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	ARG	CD-NE-CZ	5.03	130.64	123.60
1	A	217	TYR	CA-CB-CG	-5.02	103.86	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	ASN	Mainchain

## 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	1860	0	1752	160	0
1	B	1849	0	1738	317	0
2	A	86	0	40	8	0
2	B	86	0	40	8	0
3	A	276	0	0	32	1
3	B	218	0	0	22	0
All	All	4375	0	3570	475	1

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 64.

All (475) 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:B:29:ASP:HB2	1:B:51:CYS:CB	1.21	1.57
1:B:89:ILE:HB	1:B:105:SER:CB	1.36	1.53
1:B:29:ASP:CB	1:B:51:CYS:HB2	1.35	1.37
1:B:208:ASN:HB3	1:B:229:CYS:CB	1.61	1.30
1:B:153:VAL:CB	1:B:169:VAL:HB	1.63	1.27
1:A:100:ILE:O	1:A:122:PRO:CB	1.83	1.26
1:B:97:TYR:HA	1:B:126:SER:O	1.08	1.26
1:B:153:VAL:HB	1:B:169:VAL:CB	1.67	1.22

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:CB	1:A:169:VAL:HB	1.67	1.22
1:B:29:ASP:CB	1:B:51:CYS:CB	1.94	1.21
1:B:45:GLY:O	1:B:111:SER:HA	1.39	1.19
1:B:211:VAL:O	1:B:227:SER:HB2	1.36	1.19
1:B:3:THR:HB	1:B:55:GLY:CA	1.73	1.19
1:B:89:ILE:CB	1:B:105:SER:HB3	1.75	1.17
1:B:220:LYS:HA	1:B:220:LYS:HE3	1.24	1.16
1:B:161:TYR:HE1	1:B:184:ILE:HG13	1.08	1.16
1:A:153:VAL:HB	1:A:169:VAL:CB	1.76	1.15
1:B:89:ILE:CB	1:B:105:SER:CB	2.26	1.13
1:B:208:ASN:CB	1:B:229:CYS:HB3	1.78	1.13
1:B:43:LYS:HA	1:B:110:GLY:CA	1.76	1.13
1:A:89:ILE:HD11	1:A:117:TRP:HZ3	1.01	1.13
1:A:89:ILE:HD11	1:A:117:TRP:CZ3	1.84	1.12
1:B:230:SER:HB2	1:B:234:THR:HB	1.31	1.12
1:B:31:ILE:HB	1:B:49:ALA:HB3	1.30	1.12
1:A:46:PRO:HD2	1:A:58:LEU:HD13	1.26	1.12
1:B:97:TYR:CA	1:B:126:SER:O	2.00	1.09
1:B:60:ASN:C	1:B:60:ASN:HD22	1.50	1.09
1:A:100:ILE:O	1:A:122:PRO:HB3	1.45	1.09
1:B:208:ASN:HB2	1:B:229:CYS:H	1.11	1.08
1:B:78:LEU:HD12	1:B:91:TYR:CE1	1.89	1.08
1:B:43:LYS:HA	1:B:110:GLY:HA2	1.30	1.08
1:B:96:GLY:HA2	1:B:127:VAL:HG12	1.33	1.07
1:A:100:ILE:O	1:A:122:PRO:HB2	1.51	1.06
1:B:220:LYS:HA	1:B:220:LYS:CE	1.78	1.05
1:A:46:PRO:CD	1:A:58:LEU:HD13	1.85	1.05
1:B:31:ILE:HB	1:B:49:ALA:CB	1.88	1.04
1:B:12:LYS:HD2	1:B:33:TYR:CG	1.91	1.04
1:A:43:LYS:HD3	1:A:115:MET:CG	1.89	1.03
1:B:89:ILE:HB	1:B:105:SER:HB2	1.38	1.02
1:B:220:LYS:CA	1:B:220:LYS:HE3	1.89	1.01
1:A:208:ASN:HB3	1:A:229:CYS:HB3	1.38	1.01
1:B:89:ILE:O	1:B:105:SER:HB2	1.59	1.00
1:B:85:PHE:H	1:B:85:PHE:HD1	1.05	1.00
1:B:89:ILE:C	1:B:105:SER:HB2	1.82	1.00
1:B:3:THR:HB	1:B:55:GLY:HA2	1.03	1.00
1:B:121:ALA:N	1:B:122:PRO:HD2	1.77	0.99
1:B:12:LYS:CE	1:B:60:ASN:HA	1.92	0.99
1:B:96:GLY:CA	1:B:127:VAL:HG12	1.93	0.99
1:B:43:LYS:HB2	1:B:115:MET:HG2	1.43	0.98

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:SER:CB	1:B:234:THR:HB	1.94	0.97
1:B:78:LEU:HD12	1:B:91:TYR:HE1	1.23	0.97
1:B:133:PRO:HD3	1:B:176:TRP:CZ2	2.01	0.96
1:B:3:THR:CB	1:B:55:GLY:HA2	1.95	0.96
1:B:208:ASN:CB	1:B:229:CYS:H	1.77	0.96
1:B:29:ASP:HB3	1:B:51:CYS:HB2	1.43	0.96
1:B:164:ILE:HD11	1:B:183:GLN:HB2	1.45	0.95
1:B:161:TYR:CE1	1:B:184:ILE:HG13	2.01	0.95
1:B:78:LEU:HD13	1:B:80:ILE:CD1	1.97	0.95
1:B:2:CYS:SG	1:B:56:TRP:HE3	1.90	0.95
1:B:31:ILE:CB	1:B:49:ALA:HB3	1.97	0.94
1:B:42:GLN:O	1:B:110:GLY:HA3	1.66	0.94
1:B:196:TYR:CE2	1:B:216:LYS:HB2	2.03	0.94
1:B:70:PRO:HG2	1:B:80:ILE:HD11	1.49	0.93
1:A:153:VAL:HG23	1:A:169:VAL:O	1.68	0.93
1:A:42:GLN:HG3	1:A:63:ILE:HD11	1.49	0.92
1:B:171:CYS:HB2	1:B:175:GLU:O	1.69	0.92
1:B:12:LYS:HE3	1:B:60:ASN:CB	2.00	0.91
1:B:230:SER:HB2	1:B:234:THR:CB	2.01	0.91
1:A:43:LYS:HD3	1:A:115:MET:HG3	1.52	0.91
1:A:50:LYS:NZ	1:B:88:SER:HB2	1.86	0.91
1:B:78:LEU:HD13	1:B:80:ILE:HD11	1.51	0.91
1:B:53:GLY:O	1:B:54:THR:OG1	1.89	0.90
1:B:6:SER:HB2	1:B:11:MET:SD	2.11	0.90
1:B:96:GLY:HA2	1:B:127:VAL:CG1	2.01	0.90
1:B:64:LYS:HE2	1:B:66:ARG:HH12	1.37	0.90
1:B:89:ILE:CB	1:B:105:SER:HB2	1.97	0.90
1:B:208:ASN:HB3	1:B:229:CYS:HB3	0.90	0.89
1:B:60:ASN:C	1:B:60:ASN:ND2	2.19	0.89
1:B:226:SER:O	1:B:237:PRO:HD2	1.72	0.89
1:A:153:VAL:HB	1:A:169:VAL:HB	0.91	0.88
1:B:12:LYS:HE3	1:B:60:ASN:HB2	1.54	0.88
1:B:29:ASP:HB2	1:B:51:CYS:HB3	0.89	0.87
1:B:12:LYS:HE3	1:B:60:ASN:CA	2.04	0.87
1:B:12:LYS:HE2	1:B:61:GLN:H	1.40	0.87
1:B:16:SER:O	1:B:18:GLU:N	2.09	0.86
1:A:153:VAL:CG2	1:A:169:VAL:HB	2.06	0.86
1:A:42:GLN:NE2	1:A:43:LYS:HG3	1.91	0.86
1:B:211:VAL:O	1:B:227:SER:CB	2.24	0.85
1:B:120:GLU:C	1:B:122:PRO:HD2	1.95	0.85
1:A:85:PHE:HB2	1:A:114:SER:OG	1.76	0.85

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:LYS:CE	1:B:243:VAL:HG12	2.07	0.85
1:B:70:PRO:CG	1:B:80:ILE:HD11	2.07	0.84
1:B:121:ALA:N	1:B:122:PRO:CD	2.38	0.84
1:B:42:GLN:C	1:B:110:GLY:HA3	1.97	0.84
1:B:208:ASN:CB	1:B:229:CYS:CB	2.47	0.84
1:A:144:GLU:HG3	3:A:595:HOH:O	1.77	0.84
1:B:220:LYS:HE3	1:B:221:LEU:H	1.43	0.84
1:A:85:PHE:CD2	1:A:114:SER:HA	2.14	0.83
1:B:78:LEU:HD11	1:B:89:ILE:CG2	2.08	0.83
1:B:244:ARG:HH12	2:B:502:SVR:H18	1.44	0.83
1:B:2:CYS:HB2	1:B:25:TYR:O	1.79	0.82
2:B:502:SVR:N63	2:B:502:SVR:O78	2.12	0.82
1:A:42:GLN:HE22	1:A:43:LYS:HG3	1.43	0.82
1:B:12:LYS:HE3	1:B:60:ASN:HA	1.60	0.82
1:B:71:ARG:HE	1:B:120:GLU:CD	1.82	0.82
1:B:71:ARG:HE	1:B:120:GLU:CG	1.92	0.82
1:B:208:ASN:HB2	1:B:229:CYS:N	1.95	0.81
1:B:42:GLN:HB2	1:B:61:GLN:HB3	1.61	0.81
1:B:89:ILE:HB	1:B:105:SER:HB3	0.81	0.81
1:B:189:HIS:HB3	3:B:517:HOH:O	1.80	0.81
1:B:60:ASN:O	1:B:60:ASN:ND2	2.13	0.81
1:B:161:TYR:HE1	1:B:184:ILE:CG1	1.91	0.81
1:B:196:TYR:HE2	1:B:216:LYS:HB2	1.40	0.80
1:B:7:ARG:HA	3:B:573:HOH:O	1.80	0.80
1:B:5:PRO:HG3	3:B:714:HOH:O	1.81	0.80
1:B:40:ARG:HA	1:B:40:ARG:HE	1.45	0.80
1:B:78:LEU:CD1	1:B:91:TYR:HE1	1.94	0.80
1:A:45:GLY:HA2	1:A:58:LEU:HD22	1.62	0.80
1:B:57:THR:HB	1:B:59:PHE:CZ	2.16	0.80
1:B:70:PRO:HD2	1:B:80:ILE:HG13	1.63	0.80
1:A:118:ASN:HB3	1:A:119:PRO:HD3	1.64	0.80
1:A:89:ILE:CD1	1:A:117:TRP:HZ3	1.92	0.79
1:B:169:VAL:HG11	1:B:176:TRP:HZ3	1.48	0.79
1:B:45:GLY:O	1:B:111:SER:CA	2.26	0.79
1:B:78:LEU:CD1	1:B:91:TYR:CE1	2.66	0.79
1:B:220:LYS:HE3	1:B:221:LEU:N	1.98	0.78
1:B:169:VAL:HG22	1:B:178:ASP:OD2	1.83	0.78
1:A:42:GLN:HG2	1:A:63:ILE:HG13	1.65	0.78
1:A:118:ASN:HB3	1:A:119:PRO:CD	2.14	0.78
1:B:70:PRO:HB2	1:B:91:TYR:OH	1.83	0.78
1:B:169:VAL:HG13	1:B:178:ASP:HB3	1.64	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ASN:HB3	1:B:229:CYS:CA	2.14	0.77
1:A:241:LYS:HB2	3:A:534:HOH:O	1.84	0.77
1:A:233:ASN:HB2	3:A:598:HOH:O	1.83	0.77
1:B:89:ILE:CA	1:B:105:SER:HB2	2.13	0.77
1:B:133:PRO:HD3	1:B:176:TRP:CE2	2.19	0.77
1:B:71:ARG:HE	1:B:120:GLU:HG3	1.49	0.76
1:A:117:TRP:HB2	3:A:772:HOH:O	1.84	0.76
1:B:85:PHE:N	1:B:85:PHE:CD1	2.49	0.76
1:B:85:PHE:CG	1:B:86:GLY:N	2.51	0.76
1:A:208:ASN:CB	1:A:229:CYS:HB3	2.14	0.76
1:B:153:VAL:HG23	1:B:169:VAL:O	1.85	0.76
1:A:85:PHE:HB2	1:A:114:SER:HG	1.50	0.75
1:B:42:GLN:HA	1:B:42:GLN:OE1	1.85	0.75
1:B:127:VAL:HG12	1:B:127:VAL:O	1.85	0.75
1:A:181:THR:HG22	3:A:510:HOH:O	1.87	0.74
1:A:53:GLY:O	1:A:54:THR:OG1	2.05	0.74
1:B:39:TYR:CD1	1:B:62:CYS:SG	2.81	0.74
1:B:169:VAL:HG11	1:B:176:TRP:CZ3	2.22	0.73
1:B:43:LYS:HA	1:B:110:GLY:HA3	1.68	0.73
1:A:120:GLU:HG3	3:A:772:HOH:O	1.86	0.73
1:A:121:ALA:N	1:A:122:PRO:HD2	2.04	0.73
1:B:42:GLN:HG2	1:B:63:ILE:CD1	2.19	0.73
1:B:14:LYS:HE3	1:B:31:ILE:HG21	1.71	0.73
1:A:37:PRO:HG2	3:A:744:HOH:O	1.89	0.72
1:A:121:ALA:N	1:A:122:PRO:CD	2.53	0.72
1:A:42:GLN:HG3	1:A:63:ILE:CD1	2.20	0.72
1:B:241:LYS:HE3	1:B:242:CYS:N	2.05	0.72
1:B:208:ASN:CB	1:B:229:CYS:N	2.51	0.71
1:B:57:THR:HB	1:B:59:PHE:CE1	2.25	0.71
1:A:89:ILE:CD1	1:A:117:TRP:CZ3	2.69	0.71
1:B:89:ILE:HG13	1:B:117:TRP:HH2	1.55	0.71
1:A:24:ASN:HB3	1:A:29:ASP:CG	2.11	0.71
1:B:120:GLU:C	1:B:122:PRO:CD	2.58	0.71
1:B:14:LYS:HE3	1:B:31:ILE:CG2	2.20	0.71
1:B:132:PRO:HB2	1:B:140:HIS:HB3	1.73	0.71
1:A:45:GLY:CA	1:A:58:LEU:HD22	2.20	0.70
1:B:179:PRO:HG3	3:B:578:HOH:O	1.89	0.70
1:A:50:LYS:HZ3	1:B:88:SER:HB2	1.57	0.70
1:B:78:LEU:HD11	1:B:89:ILE:HG23	1.72	0.70
1:B:241:LYS:HE2	1:B:243:VAL:HG12	1.74	0.70
1:B:12:LYS:CE	1:B:60:ASN:CA	2.63	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ILE:O	1:B:49:ALA:HB3	1.92	0.69
1:B:29:ASP:CB	1:B:51:CYS:HB3	1.86	0.68
1:B:109:LEU:HA	1:B:115:MET:N	2.09	0.68
1:B:2:CYS:SG	1:B:56:TRP:CE3	2.82	0.68
1:B:153:VAL:HB	1:B:169:VAL:HB	0.76	0.68
1:B:42:GLN:HG2	1:B:63:ILE:HG12	1.74	0.68
1:A:34:LEU:HD11	3:A:588:HOH:O	1.92	0.68
1:A:207:TYR:N	1:A:207:TYR:CD1	2.61	0.68
1:B:144:GLU:HG2	1:B:147:TYR:HE2	1.59	0.68
1:B:108:GLU:CA	1:B:115:MET:O	2.42	0.67
1:B:153:VAL:CG2	1:B:169:VAL:HB	2.24	0.67
1:A:43:LYS:HD3	1:A:115:MET:HG2	1.77	0.67
1:A:222:SER:HB2	2:A:501:SVR:H272	1.76	0.67
1:B:43:LYS:CA	1:B:110:GLY:CA	2.65	0.67
1:B:118:ASN:OD1	1:B:119:PRO:HD2	1.95	0.66
1:A:208:ASN:HB2	1:A:229:CYS:H	1.59	0.66
1:A:44:MET:O	1:A:59:PHE:HB2	1.95	0.66
1:B:64:LYS:HE2	1:B:66:ARG:NH1	2.09	0.66
1:B:12:LYS:HD2	1:B:33:TYR:CD1	2.30	0.66
1:A:50:LYS:HD3	1:B:88:SER:OG	1.96	0.66
1:A:127:VAL:HG21	3:A:708:HOH:O	1.96	0.65
1:A:194:ASN:O	1:A:242:CYS:HB3	1.95	0.65
1:A:242:CYS:O	1:A:243:VAL:HG22	1.95	0.65
1:B:78:LEU:HD11	1:B:89:ILE:HG21	1.78	0.65
1:B:131:SER:HB2	1:B:146:PHE:CD1	2.32	0.65
1:B:7:ARG:HB3	1:B:8:PRO:HD3	1.77	0.64
1:B:18:GLU:HG2	3:B:514:HOH:O	1.95	0.64
1:A:58:LEU:HD11	3:A:734:HOH:O	1.97	0.64
1:B:13:PHE:HB2	3:B:657:HOH:O	1.98	0.64
1:B:3:THR:HB	1:B:55:GLY:HA3	1.78	0.64
1:A:27:ILE:HD11	1:B:85:PHE:HD2	1.63	0.64
1:B:244:ARG:HH12	2:B:502:SVR:C18	2.11	0.64
1:B:89:ILE:HG13	1:B:117:TRP:CH2	2.33	0.63
2:A:501:SVR:O32	2:A:501:SVR:H8	1.98	0.63
1:B:12:LYS:HE2	1:B:60:ASN:HA	1.77	0.63
1:A:85:PHE:CD2	1:A:114:SER:OG	2.51	0.63
1:B:197:LEU:HD12	1:B:213:PHE:CD1	2.33	0.63
1:A:78:LEU:HG	1:A:89:ILE:HG21	1.80	0.63
1:B:41:LYS:HB2	1:B:113:GLY:H	1.64	0.63
1:B:109:LEU:N	1:B:115:MET:HB3	2.13	0.63
1:B:31:ILE:HB	1:B:49:ALA:HB1	1.80	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:PRO:CG	1:B:80:ILE:CD1	2.77	0.62
1:B:7:ARG:HD3	3:B:590:HOH:O	1.99	0.62
1:B:43:LYS:HB2	1:B:115:MET:CG	2.25	0.62
1:B:64:LYS:CE	1:B:66:ARG:HH12	2.11	0.62
1:B:56:TRP:CD1	1:B:56:TRP:O	2.52	0.62
1:B:109:LEU:HA	1:B:115:MET:HB2	1.80	0.62
1:B:161:TYR:CD2	1:B:182:CYS:HB3	2.34	0.62
2:B:502:SVR:O32	2:B:502:SVR:H8	1.98	0.62
1:B:78:LEU:HD22	1:B:79:ASP:N	2.16	0.61
1:B:243:VAL:HB	2:B:502:SVR:O25	2.00	0.61
1:A:79:ASP:HB2	3:A:719:HOH:O	2.00	0.61
1:A:12:LYS:HE2	1:A:61:GLN:H	1.65	0.61
1:B:120:GLU:C	1:B:122:PRO:N	2.52	0.61
1:B:78:LEU:HD21	1:B:89:ILE:HG23	1.81	0.61
1:A:73:ILE:HG12	1:A:123:ILE:CG2	2.30	0.61
1:A:66:ARG:HD3	3:A:655:HOH:O	2.00	0.61
1:B:164:ILE:HD11	1:B:183:GLN:CB	2.28	0.61
1:B:139:ARG:CD	1:B:158:ASN:HD21	2.13	0.61
1:A:50:LYS:HZ2	1:B:88:SER:HB2	1.64	0.61
1:A:85:PHE:HD2	1:A:114:SER:HG	1.43	0.61
1:B:241:LYS:HE2	1:B:243:VAL:CG1	2.30	0.61
1:A:242:CYS:C	1:A:243:VAL:HG22	2.20	0.61
1:A:208:ASN:HB3	1:A:229:CYS:CB	2.22	0.61
1:B:106:TYR:O	1:B:118:ASN:HB2	2.00	0.61
1:B:70:PRO:CD	1:B:80:ILE:HG13	2.31	0.60
1:A:45:GLY:O	1:A:111:SER:HB2	2.01	0.60
1:B:70:PRO:HG3	1:B:78:LEU:CD1	2.30	0.60
1:B:161:TYR:CE1	1:B:184:ILE:N	2.69	0.60
1:B:13:PHE:HB3	3:B:718:HOH:O	2.01	0.60
1:B:6:SER:HB2	1:B:11:MET:CE	2.30	0.60
1:A:85:PHE:CB	1:A:114:SER:HG	2.13	0.60
1:B:71:ARG:NE	1:B:120:GLU:CD	2.55	0.60
1:A:120:GLU:N	1:A:122:PRO:HD2	2.17	0.60
1:B:8:PRO:HG3	3:B:588:HOH:O	2.01	0.59
1:B:109:LEU:HA	1:B:115:MET:CB	2.33	0.59
1:A:133:PRO:HG3	3:A:526:HOH:O	2.01	0.59
1:B:89:ILE:O	1:B:105:SER:CB	2.43	0.59
1:A:27:ILE:HG12	1:B:86:GLY:HA2	1.85	0.59
1:A:79:ASP:O	1:A:80:ILE:HD13	2.03	0.59
1:A:170:LEU:HD22	3:B:628:HOH:O	2.01	0.59
1:A:214:LYS:HD3	3:A:641:HOH:O	2.03	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ARG:HB3	1:A:8:PRO:HD3	1.85	0.59
1:B:133:PRO:HD2	1:B:155:TYR:OH	2.03	0.59
1:A:46:PRO:HD3	1:A:58:LEU:HD13	1.80	0.58
1:B:96:GLY:C	1:B:127:VAL:HG12	2.23	0.58
1:A:85:PHE:HZ	1:A:109:LEU:HA	1.68	0.58
1:B:197:LEU:HD12	1:B:213:PHE:CE1	2.38	0.58
1:A:36:LEU:HG	3:A:634:HOH:O	2.03	0.58
1:B:42:GLN:HG2	1:B:63:ILE:CG1	2.33	0.58
1:A:220:LYS:CE	1:A:220:LYS:HA	2.33	0.58
1:B:43:LYS:CA	1:B:110:GLY:HA3	2.30	0.58
1:A:85:PHE:HD2	1:A:114:SER:OG	1.86	0.58
1:A:44:MET:O	1:A:59:PHE:CB	2.51	0.58
1:B:219:TYR:HD1	1:B:244:ARG:HA	1.69	0.58
1:B:31:ILE:O	1:B:49:ALA:N	2.34	0.57
1:B:144:GLU:HG2	1:B:147:TYR:CE2	2.38	0.57
1:A:115:MET:HA	3:A:631:HOH:O	2.04	0.57
1:A:24:ASN:HB3	1:A:29:ASP:OD1	2.05	0.57
1:B:230:SER:CB	1:B:234:THR:CB	2.70	0.57
1:A:120:GLU:C	1:A:122:PRO:HD2	2.25	0.57
1:A:136:SER:HB2	3:A:620:HOH:O	2.04	0.57
1:B:43:LYS:N	1:B:110:GLY:HA3	2.19	0.57
1:B:12:LYS:HD2	1:B:33:TYR:CB	2.35	0.57
1:B:241:LYS:HE3	1:B:243:VAL:HG12	1.84	0.57
1:B:184:ILE:HG12	3:B:713:HOH:O	2.04	0.57
1:A:11:MET:SD	1:A:60:ASN:ND2	2.78	0.57
1:B:8:PRO:O	1:B:11:MET:HE2	2.05	0.56
1:A:153:VAL:HG23	1:A:169:VAL:C	2.23	0.56
1:A:40:ARG:HH12	1:A:84:ASP:HB3	1.70	0.56
1:B:42:GLN:NE2	1:B:43:LYS:H	2.03	0.56
1:B:12:LYS:CE	1:B:60:ASN:HB2	2.33	0.56
1:A:42:GLN:CG	1:A:63:ILE:HG13	2.34	0.56
1:B:71:ARG:HD2	1:B:120:GLU:OE1	2.05	0.56
1:A:85:PHE:CE2	1:A:114:SER:HA	2.41	0.56
1:B:197:LEU:CD1	1:B:213:PHE:CE1	2.89	0.56
1:A:170:LEU:HD21	3:B:607:HOH:O	2.06	0.56
1:B:109:LEU:HB2	1:B:113:GLY:O	2.06	0.56
1:B:131:SER:HB2	1:B:146:PHE:CE1	2.41	0.56
1:B:139:ARG:HD3	1:B:158:ASN:ND2	2.21	0.56
1:B:134:SER:O	1:B:135:ILE:HG23	2.05	0.56
1:A:40:ARG:HB3	1:A:113:GLY:HA2	1.87	0.55
1:A:153:VAL:HB	1:A:169:VAL:CG2	2.36	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:LEU:HG	1:B:91:TYR:CD1	2.42	0.55
1:B:164:ILE:HD12	1:B:231:PRO:HB3	1.88	0.55
1:A:59:PHE:HZ	3:A:549:HOH:O	1.88	0.55
1:B:230:SER:HB3	3:B:603:HOH:O	2.06	0.55
1:B:6:SER:CB	1:B:11:MET:SD	2.92	0.55
1:B:78:LEU:CD1	1:B:89:ILE:CG2	2.83	0.55
1:B:220:LYS:HE3	1:B:220:LYS:C	2.26	0.55
1:B:127:VAL:CG1	1:B:127:VAL:O	2.54	0.55
1:B:241:LYS:HE3	1:B:242:CYS:H	1.69	0.55
1:B:14:LYS:CE	1:B:31:ILE:HG21	2.36	0.54
1:B:43:LYS:CA	1:B:110:GLY:HA2	2.21	0.54
1:A:135:ILE:HG21	1:A:180:PRO:HG2	1.88	0.54
1:B:109:LEU:CA	1:B:115:MET:CB	2.85	0.54
1:A:144:GLU:HB2	3:A:522:HOH:O	2.06	0.54
1:B:109:LEU:HA	1:B:114:SER:C	2.27	0.54
1:A:12:LYS:HE2	1:A:61:GLN:N	2.21	0.54
1:B:66:ARG:HB2	3:B:650:HOH:O	2.08	0.54
1:A:155:TYR:CE1	1:A:180:PRO:HG3	2.43	0.53
1:A:1:CYS:HA	1:A:26:ASN:HB3	1.89	0.53
1:B:208:ASN:CA	1:B:229:CYS:HB3	2.36	0.53
1:B:109:LEU:CA	1:B:115:MET:HB2	2.38	0.53
1:B:12:LYS:HE2	1:B:61:GLN:N	2.17	0.53
1:A:102:GLU:HG2	1:B:144:GLU:OE1	2.08	0.53
1:B:56:TRP:HD1	1:B:56:TRP:O	1.90	0.53
1:A:85:PHE:CD1	1:A:112:THR:O	2.62	0.53
1:A:42:GLN:CG	1:A:63:ILE:CD1	2.86	0.53
1:B:125:GLU:O	1:B:126:SER:CB	2.56	0.53
1:B:108:GLU:O	1:B:109:LEU:HB3	2.08	0.53
1:B:161:TYR:CD1	1:B:184:ILE:HG23	2.44	0.52
1:B:196:TYR:CZ	1:B:216:LYS:HB2	2.42	0.52
1:B:120:GLU:CA	1:B:122:PRO:HD2	2.39	0.52
1:B:68:PRO:HG3	3:B:575:HOH:O	2.09	0.52
1:A:1:CYS:N	1:A:26:ASN:HB3	2.24	0.52
1:B:60:ASN:HD22	1:B:61:GLN:N	2.03	0.52
1:B:120:GLU:O	1:B:122:PRO:N	2.43	0.52
1:B:100:ILE:O	1:B:122:PRO:HA	2.09	0.52
1:B:31:ILE:C	1:B:49:ALA:HB3	2.29	0.52
1:B:89:ILE:N	1:B:105:SER:O	2.42	0.52
1:A:242:CYS:C	1:A:243:VAL:CG2	2.77	0.52
1:B:42:GLN:HB2	1:B:61:GLN:CB	2.38	0.52
1:B:69:SER:HB3	3:B:613:HOH:O	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ASN:HB3	1:A:29:ASP:OD2	2.10	0.51
1:B:166:ASN:OD1	1:B:210:ASN:ND2	2.44	0.51
1:B:220:LYS:CE	1:B:221:LEU:H	2.19	0.51
1:A:208:ASN:HA	1:A:229:CYS:HB2	1.93	0.51
1:A:126:SER:O	1:A:127:VAL:HB	2.11	0.51
1:A:11:MET:HA	1:A:62:CYS:HB3	1.93	0.51
1:B:71:ARG:NE	1:B:120:GLU:HG3	2.23	0.51
1:B:139:ARG:HD3	1:B:158:ASN:HD21	1.76	0.51
1:B:169:VAL:CG1	1:B:176:TRP:HZ3	2.20	0.51
1:B:132:PRO:HG2	1:B:140:HIS:HB2	1.93	0.51
1:B:169:VAL:CG1	1:B:176:TRP:CZ3	2.92	0.50
1:A:78:LEU:HG	1:A:89:ILE:CG2	2.42	0.50
1:B:14:LYS:CE	1:B:31:ILE:CG2	2.87	0.50
1:B:7:ARG:HB3	1:B:8:PRO:CD	2.42	0.50
1:A:202:LYS:HA	3:A:545:HOH:O	2.11	0.49
1:B:239:LEU:HD22	1:B:239:LEU:H	1.77	0.49
1:B:44:MET:H	1:B:110:GLY:HA2	1.76	0.49
1:A:220:LYS:HB2	1:A:244:ARG:O	2.12	0.49
1:B:31:ILE:O	1:B:49:ALA:CB	2.58	0.49
1:B:78:LEU:CG	1:B:91:TYR:CE1	2.96	0.49
1:B:208:ASN:OD1	1:B:228:THR:HG22	2.12	0.49
1:A:45:GLY:N	1:A:58:LEU:HD22	2.28	0.49
1:B:3:THR:HG23	1:B:4:ILE:N	2.27	0.49
1:B:118:ASN:CG	1:B:119:PRO:HD2	2.33	0.48
1:A:152:VAL:HA	3:A:672:HOH:O	2.13	0.48
1:B:238:GLU:HB2	3:B:690:HOH:O	2.11	0.48
1:B:51:CYS:HA	1:B:56:TRP:HA	1.96	0.48
1:B:169:VAL:HG13	1:B:178:ASP:CB	2.41	0.48
1:B:161:TYR:HD1	1:B:184:ILE:HG23	1.79	0.48
1:A:208:ASN:CB	1:A:229:CYS:H	2.27	0.48
1:A:1:CYS:CA	1:A:26:ASN:HB3	2.43	0.48
1:A:208:ASN:CB	1:A:229:CYS:CB	2.87	0.48
1:A:73:ILE:HB	3:A:553:HOH:O	2.14	0.48
1:B:14:LYS:HD3	1:B:31:ILE:HG23	1.96	0.47
1:B:119:PRO:O	1:B:122:PRO:HG2	2.14	0.47
1:A:135:ILE:CG2	1:A:180:PRO:HG2	2.44	0.47
1:B:171:CYS:CB	1:B:175:GLU:O	2.54	0.47
1:A:82:GLY:HA2	3:A:666:HOH:O	2.14	0.47
1:A:220:LYS:HE3	1:A:220:LYS:HA	1.97	0.47
1:B:71:ARG:H	1:B:71:ARG:HH11	1.61	0.47
1:B:31:ILE:CB	1:B:49:ALA:CB	2.72	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:HD23	1:A:58:LEU:HA	1.61	0.47
1:B:31:ILE:CA	1:B:49:ALA:HB3	2.43	0.47
1:A:40:ARG:NH1	1:A:84:ASP:HB3	2.30	0.47
1:B:51:CYS:HA	1:B:56:TRP:CB	2.45	0.47
1:A:176:TRP:HZ3	3:A:671:HOH:O	1.97	0.47
1:A:241:LYS:HB3	1:A:241:LYS:HE3	1.70	0.47
1:A:155:TYR:HE2	3:A:577:HOH:O	1.96	0.46
1:A:207:TYR:HD1	1:A:207:TYR:N	2.13	0.46
1:A:40:ARG:NH2	1:A:113:GLY:O	2.49	0.46
1:B:78:LEU:HG	1:B:90:THR:O	2.15	0.46
1:A:73:ILE:HG23	1:A:74:ASP:N	2.31	0.46
1:B:191:THR:HG21	3:B:656:HOH:O	2.14	0.46
1:B:153:VAL:H	1:B:169:VAL:H	1.64	0.46
1:A:220:LYS:NZ	2:A:501:SVR:C61	2.79	0.46
1:A:42:GLN:HB2	1:A:61:GLN:HB3	1.97	0.46
1:A:220:LYS:HZ3	2:A:501:SVR:C61	2.29	0.46
1:B:80:ILE:HG21	3:B:613:HOH:O	2.16	0.46
1:B:125:GLU:O	1:B:126:SER:HB3	2.15	0.45
1:A:70:PRO:HD3	3:A:666:HOH:O	2.15	0.45
1:B:72:ASP:HB2	3:B:663:HOH:O	2.16	0.45
1:B:73:ILE:HG22	3:B:619:HOH:O	2.16	0.45
1:B:33:TYR:HB3	1:B:41:LYS:HZ1	1.82	0.45
1:A:220:LYS:CE	2:A:501:SVR:O78	2.64	0.45
1:B:131:SER:HB2	1:B:146:PHE:HD1	1.76	0.45
1:B:41:LYS:H	1:B:113:GLY:HA3	1.82	0.45
1:A:43:LYS:HD3	1:A:115:MET:SD	2.57	0.45
1:B:11:MET:HE2	1:B:11:MET:HB2	1.86	0.45
1:A:12:LYS:HB2	1:A:33:TYR:HB3	1.97	0.45
1:A:14:LYS:HD3	1:A:31:ILE:HD13	1.99	0.45
1:A:44:MET:O	1:A:59:PHE:CG	2.70	0.45
1:B:85:PHE:CD2	1:B:86:GLY:N	2.81	0.45
1:B:96:GLY:CA	1:B:127:VAL:O	2.65	0.44
1:A:42:GLN:HG2	1:A:63:ILE:CG1	2.44	0.44
1:A:23:ALA:HB1	3:A:536:HOH:O	2.17	0.44
1:A:208:ASN:HA	1:A:229:CYS:CB	2.47	0.44
1:B:148:THR:HG22	1:B:151:SER:OG	2.18	0.44
1:A:64:LYS:HB2	3:A:563:HOH:O	2.16	0.44
1:B:33:TYR:HB2	1:B:41:LYS:HE3	1.99	0.44
1:B:155:TYR:CZ	1:B:180:PRO:HB3	2.53	0.44
1:B:9:ILE:HD13	3:B:515:HOH:O	2.17	0.44
1:B:50:LYS:O	1:B:56:TRP:HB2	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:SER:CB	1:B:146:PHE:CE1	3.00	0.44
1:B:161:TYR:CE1	1:B:183:GLN:C	2.91	0.44
1:B:244:ARG:NH1	2:B:502:SVR:H18	2.23	0.44
2:A:501:SVR:C2	2:A:501:SVR:O24	2.65	0.44
1:A:102:GLU:HG3	3:A:715:HOH:O	2.17	0.44
1:B:31:ILE:CG2	1:B:49:ALA:HB3	2.47	0.44
1:B:164:ILE:HG21	1:B:231:PRO:HG3	2.00	0.43
1:A:61:GLN:OE1	1:A:63:ILE:HD11	2.18	0.43
1:A:16:SER:O	1:A:17:VAL:C	2.56	0.43
1:A:4:ILE:HB	1:A:5:PRO:HD2	2.01	0.43
1:A:208:ASN:CA	1:A:229:CYS:HB3	2.48	0.43
1:A:7:ARG:HB3	1:A:8:PRO:CD	2.49	0.43
1:A:40:ARG:HG3	1:A:65:ARG:H	1.83	0.43
1:B:134:SER:O	1:B:135:ILE:CG2	2.66	0.43
1:A:99:LEU:HD23	1:A:124:CYS:HB2	2.01	0.43
1:A:120:GLU:H	1:A:122:PRO:HD2	1.84	0.43
1:A:42:GLN:CG	1:A:63:ILE:CG1	2.97	0.43
1:B:209:ASP:O	1:B:228:THR:HG23	2.19	0.43
1:B:78:LEU:HD22	1:B:79:ASP:H	1.84	0.42
1:B:109:LEU:N	1:B:115:MET:CB	2.79	0.42
1:A:244:ARG:HB3	3:A:565:HOH:O	2.19	0.42
1:A:44:MET:HG3	3:A:638:HOH:O	2.18	0.42
1:B:208:ASN:HB3	1:B:229:CYS:N	2.24	0.42
1:B:222:SER:HB3	2:B:502:SVR:H272	2.00	0.42
1:A:127:VAL:O	1:A:127:VAL:HG12	2.19	0.42
1:A:85:PHE:HE2	1:A:108:GLU:O	2.02	0.42
1:A:79:ASP:C	1:A:80:ILE:HD13	2.39	0.42
2:A:501:SVR:C2	2:A:501:SVR:S17	3.07	0.42
1:B:242:CYS:C	1:B:243:VAL:HG12	2.40	0.42
1:B:197:LEU:HB3	1:B:213:PHE:HA	2.01	0.42
1:B:31:ILE:CD1	1:B:56:TRP:CD2	3.03	0.42
1:B:241:LYS:HE2	2:B:502:SVR:O24	2.19	0.42
1:B:70:PRO:CG	1:B:78:LEU:CD1	2.97	0.42
1:B:108:GLU:N	1:B:115:MET:O	2.53	0.42
1:B:89:ILE:O	1:B:105:SER:N	2.53	0.41
1:A:243:VAL:HB	2:A:501:SVR:O23	2.19	0.41
1:A:11:MET:HE1	1:A:60:ASN:ND2	2.35	0.41
1:B:152:VAL:HG13	1:B:168:GLY:HA2	2.02	0.41
1:B:78:LEU:CD2	1:B:79:ASP:N	2.83	0.41
1:A:153:VAL:HG22	3:A:671:HOH:O	2.20	0.41
1:B:166:ASN:ND2	1:B:167:SER:H	2.17	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ASN:CA	1:B:229:CYS:CB	2.98	0.41
1:B:161:TYR:CD1	1:B:183:GLN:C	2.94	0.41
1:B:71:ARG:N	1:B:71:ARG:HH11	2.17	0.41
1:B:39:TYR:HD1	1:B:62:CYS:SG	2.41	0.41
1:B:196:TYR:OH	1:B:216:LYS:CB	2.69	0.41
1:B:78:LEU:CD1	1:B:89:ILE:HG23	2.48	0.41
1:B:3:THR:O	1:B:56:TRP:CZ3	2.74	0.41
1:B:45:GLY:C	1:B:110:GLY:O	2.59	0.41
1:B:109:LEU:CB	1:B:113:GLY:O	2.69	0.41
1:B:45:GLY:O	1:B:111:SER:CB	2.67	0.41
1:A:43:LYS:HA	1:A:110:GLY:HA3	2.02	0.41
1:B:57:THR:CB	1:B:59:PHE:CZ	2.97	0.40
1:B:241:LYS:HA	1:B:241:LYS:HD2	1.87	0.40
1:B:109:LEU:H	1:B:115:MET:HB3	1.83	0.40
1:B:70:PRO:HG3	1:B:80:ILE:CD1	2.49	0.40
1:A:73:ILE:HG12	1:A:123:ILE:HG21	2.01	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:582:HOH:O	3:A:582:HOH:O[2_555]	1.42	0.78

## 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	242/244 (99%)	169 (70%)	49 (20%)	24 (10%)	1	0
1	B	241/244 (99%)	173 (72%)	46 (19%)	22 (9%)	1	0
All	All	483/488 (99%)	342 (71%)	95 (20%)	46 (10%)	1	0

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	54	THR
1	A	59	PHE
1	A	126	SER
1	A	127	VAL
1	A	159	SER
1	A	210	ASN
1	B	17	VAL
1	B	54	THR
1	B	58	LEU
1	B	59	PHE
1	B	85	PHE
1	B	117	TRP
1	B	159	SER
1	B	210	ASN
1	A	18	GLU
1	A	28	GLY
1	A	60	ASN
1	A	81	GLY
1	A	104	LYS
1	A	113	GLY
1	A	114	SER
1	B	44	MET
1	B	109	LEU
1	A	44	MET
1	A	111	SER
1	A	118	ASN
1	B	95	SER
1	B	126	SER
1	A	37	PRO
1	A	166	ASN
1	B	37	PRO
1	B	86	GLY
1	B	132	PRO
1	A	86	GLY
1	A	178	ASP
1	B	121	ALA
1	B	8	PRO
1	B	116	VAL
1	B	127	VAL
1	A	8	PRO
1	B	160	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	73	ILE
1	B	28	GLY
1	B	73	ILE
1	A	27	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	214/214 (100%)	175 (82%)	39 (18%)	2	1
1	B	212/214 (99%)	168 (79%)	44 (21%)	1	1
All	All	426/428 (100%)	343 (80%)	83 (20%)	2	1

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	CYS
1	A	3	THR
1	A	11	MET
1	A	18	GLU
1	A	24	ASN
1	A	26	ASN
1	A	31	ILE
1	A	37	PRO
1	A	42	GLN
1	A	43	LYS
1	A	57	THR
1	A	58	LEU
1	A	59	PHE
1	A	60	ASN
1	A	61	GLN
1	A	63	ILE
1	A	71	ARG
1	A	78	LEU
1	A	89	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	116	VAL
1	A	123	ILE
1	A	126	SER
1	A	127	VAL
1	A	128	LYS
1	A	146	PHE
1	A	147	TYR
1	A	171	CYS
1	A	181	THR
1	A	187	CYS
1	A	197	LEU
1	A	207	TYR
1	A	209	ASP
1	A	214	LYS
1	A	220	LYS
1	A	222	SER
1	A	228	THR
1	A	234	THR
1	A	243	VAL
1	A	244	ARG
1	B	2	CYS
1	B	3	THR
1	B	6	SER
1	B	11	MET
1	B	29	ASP
1	B	31	ILE
1	B	37	PRO
1	B	39	TYR
1	B	40	ARG
1	B	42	GLN
1	B	44	MET
1	B	52	THR
1	B	58	LEU
1	B	60	ASN
1	B	61	GLN
1	B	71	ARG
1	B	78	LEU
1	B	80	ILE
1	B	85	PHE
1	B	88	SER
1	B	97	TYR
1	B	109	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	115	MET
1	B	118	ASN
1	B	120	GLU
1	B	123	ILE
1	B	128	LYS
1	B	132	PRO
1	B	139	ARG
1	B	146	PHE
1	B	148	THR
1	B	154	THR
1	B	161	TYR
1	B	171	CYS
1	B	181	THR
1	B	184	ILE
1	B	187	CYS
1	B	197	LEU
1	B	209	ASP
1	B	212	ASP
1	B	220	LYS
1	B	228	THR
1	B	234	THR
1	B	241	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	42	GLN
1	B	60	ASN
1	B	158	ASN
1	B	166	ASN
1	B	210	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SVR	A	501	-	93,93,93	1.95	31 (33%)	133,145,145	2.42	39 (29%)
2	SVR	B	502	-	93,93,93	1.91	29 (31%)	133,145,145	2.40	38 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SVR	A	501	-	-	0/76/76/76	0/8/8/8
2	SVR	B	502	-	-	0/76/76/76	0/8/8/8

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	SVR	C15-S21	-3.04	1.74	1.78
2	B	502	SVR	C15-S21	-2.84	1.74	1.78
2	A	501	SVR	C71-S75	-2.69	1.74	1.78
2	B	502	SVR	C71-S75	-2.49	1.75	1.78
2	A	501	SVR	C69-S73	-2.26	1.75	1.78
2	A	501	SVR	C11-S17	-2.04	1.75	1.78
2	A	501	SVR	C68-C66	2.03	1.46	1.42
2	A	501	SVR	O23-S17	2.09	1.53	1.43
2	B	502	SVR	C48-C46	2.11	1.42	1.39
2	B	502	SVR	C65-C66	2.13	1.46	1.42
2	B	502	SVR	C43-N44	2.13	1.41	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	SVR	O23-S17	2.15	1.54	1.43
2	B	502	SVR	O80-S75	2.17	1.54	1.43
2	A	501	SVR	C48-C46	2.18	1.42	1.39
2	B	502	SVR	O77-S73	2.18	1.54	1.43
2	B	502	SVR	O86-S83	2.19	1.54	1.43
2	A	501	SVR	C65-C66	2.20	1.46	1.42
2	B	502	SVR	O29-S21	2.21	1.54	1.43
2	B	502	SVR	O35-S31	2.22	1.54	1.43
2	A	501	SVR	O86-S83	2.22	1.54	1.43
2	A	501	SVR	O36-S31	2.23	1.54	1.43
2	A	501	SVR	O35-S31	2.23	1.54	1.43
2	A	501	SVR	O77-S73	2.24	1.54	1.43
2	A	501	SVR	O80-S75	2.25	1.54	1.43
2	B	502	SVR	O78-S73	2.27	1.54	1.43
2	B	502	SVR	O36-S31	2.27	1.54	1.43
2	A	501	SVR	O78-S73	2.27	1.54	1.43
2	A	501	SVR	O29-S21	2.29	1.54	1.43
2	B	502	SVR	O81-S75	2.29	1.54	1.43
2	B	502	SVR	O28-S21	2.31	1.54	1.43
2	A	501	SVR	O81-S75	2.34	1.54	1.43
2	A	501	SVR	O28-S21	2.35	1.55	1.43
2	B	502	SVR	C69-C66	2.50	1.47	1.43
2	A	501	SVR	C69-C66	2.54	1.47	1.43
2	B	502	SVR	C43-N41	2.62	1.42	1.37
2	A	501	SVR	C43-N41	2.69	1.42	1.37
2	B	502	SVR	C2-N1	2.75	1.42	1.35
2	A	501	SVR	C2-N1	2.76	1.42	1.35
2	B	502	SVR	C51-N53	2.80	1.42	1.35
2	A	501	SVR	C51-N53	2.88	1.43	1.35
2	B	502	SVR	C26-N19	3.13	1.43	1.35
2	B	502	SVR	C3-C6	3.24	1.47	1.42
2	A	501	SVR	C61-N63	3.29	1.44	1.35
2	A	501	SVR	C26-N19	3.30	1.44	1.35
2	B	502	SVR	C61-N63	3.30	1.44	1.35
2	A	501	SVR	C3-C6	3.34	1.47	1.42
2	A	501	SVR	O79-S73	3.36	1.63	1.44
2	A	501	SVR	O30-S21	3.36	1.63	1.44
2	B	502	SVR	O30-S21	3.39	1.63	1.44
2	B	502	SVR	O82-S75	3.42	1.63	1.44
2	B	502	SVR	O79-S73	3.43	1.63	1.44
2	A	501	SVR	O34-S31	3.44	1.63	1.44
2	A	501	SVR	O82-S75	3.48	1.63	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	SVR	O34-S31	3.54	1.64	1.44
2	A	501	SVR	O84-S83	4.09	1.63	1.43
2	B	502	SVR	O84-S83	4.09	1.63	1.43
2	A	501	SVR	O24-S17	4.10	1.63	1.43
2	B	502	SVR	O24-S17	4.11	1.63	1.43
2	B	502	SVR	C11-C6	4.57	1.50	1.43
2	A	501	SVR	C11-C6	4.94	1.50	1.43

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	SVR	C16-C10-C15	-4.01	118.61	123.23
2	B	502	SVR	C70-C71-C68	-3.90	117.57	121.04
2	A	501	SVR	C70-C71-C68	-3.85	117.61	121.04
2	A	501	SVR	C3-N1-C2	-3.75	117.05	128.87
2	B	502	SVR	C3-N1-C2	-3.72	117.15	128.87
2	A	501	SVR	C16-C10-C15	-3.67	119.00	123.23
2	A	501	SVR	C12-C15-C10	-3.50	117.92	121.04
2	B	502	SVR	C12-C15-C10	-3.33	118.08	121.04
2	B	502	SVR	C18-C11-S17	-3.23	112.21	117.82
2	A	501	SVR	C18-C11-S17	-3.21	112.24	117.82
2	B	502	SVR	C72-C68-C71	-3.06	119.71	123.23
2	A	501	SVR	C72-C68-C71	-2.93	119.86	123.23
2	B	502	SVR	O4-C2-C5	-2.81	116.17	120.97
2	B	502	SVR	C7-C3-N1	-2.76	115.29	123.10
2	A	501	SVR	O4-C2-C5	-2.76	116.26	120.97
2	A	501	SVR	C7-C3-N1	-2.70	115.48	123.10
2	B	502	SVR	O45-C43-N41	-2.46	119.85	123.58
2	A	501	SVR	O45-C43-N41	-2.40	119.94	123.58
2	A	501	SVR	C62-C58-C56	-2.39	116.35	119.24
2	A	501	SVR	C18-C11-C6	-2.32	117.56	120.80
2	B	502	SVR	C67-C65-N63	-2.25	116.75	123.10
2	B	502	SVR	C18-C11-C6	-2.23	117.69	120.80
2	A	501	SVR	O25-S17-O23	-2.18	100.08	111.64
2	B	502	SVR	O25-S17-O23	-2.17	100.10	111.64
2	A	501	SVR	C67-C65-N63	-2.15	117.02	123.10
2	B	502	SVR	C62-C58-C56	-2.12	116.68	119.24
2	A	501	SVR	C9-C5-C8	-2.11	116.69	119.24
2	B	502	SVR	C9-C5-C8	-2.09	116.71	119.24
2	A	501	SVR	C72-C76-C74	-2.08	117.35	120.25
2	A	501	SVR	C69-C66-C68	2.02	118.34	116.31
2	B	502	SVR	C27-C20-C13	2.04	123.49	121.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	SVR	C9-C5-C2	2.32	127.97	120.60
2	B	502	SVR	C20-C13-N19	2.33	122.34	118.71
2	A	501	SVR	C9-C5-C2	2.33	127.98	120.60
2	A	501	SVR	C20-C13-N19	2.43	122.50	118.71
2	B	502	SVR	C46-N44-C43	2.44	131.36	126.65
2	B	502	SVR	O34-S31-C22	2.49	113.97	106.94
2	A	501	SVR	O34-S31-C22	2.57	114.17	106.94
2	A	501	SVR	C46-N44-C43	2.65	131.76	126.65
2	B	502	SVR	O36-S31-C22	2.66	113.16	106.63
2	A	501	SVR	C66-C65-N63	2.68	124.73	120.58
2	A	501	SVR	O36-S31-C22	2.69	113.24	106.63
2	B	502	SVR	C66-C65-N63	2.87	125.03	120.58
2	B	502	SVR	C71-C68-C66	2.98	121.72	118.11
2	A	501	SVR	C71-C68-C66	3.07	121.83	118.11
2	B	502	SVR	O85-S83-C76	3.10	115.67	106.94
2	A	501	SVR	C15-C10-C6	3.13	121.90	118.11
2	A	501	SVR	O85-S83-C76	3.17	115.89	106.94
2	B	502	SVR	C5-C8-C13	3.19	125.80	119.75
2	B	502	SVR	C15-C10-C6	3.27	122.06	118.11
2	A	501	SVR	C5-C8-C13	3.27	125.95	119.75
2	A	501	SVR	C6-C3-N1	3.34	125.75	120.58
2	B	502	SVR	C6-C3-N1	3.52	126.03	120.58
2	B	502	SVR	N44-C43-N41	3.52	118.06	112.53
2	A	501	SVR	N44-C43-N41	3.60	118.19	112.53
2	A	501	SVR	C5-C2-N1	4.02	123.80	115.94
2	B	502	SVR	C76-C74-C69	4.05	124.35	120.09
2	B	502	SVR	C5-C2-N1	4.06	123.87	115.94
2	A	501	SVR	C76-C74-C69	4.18	124.50	120.09
2	A	501	SVR	C22-C18-C11	4.56	124.89	120.09
2	B	502	SVR	C22-C18-C11	4.61	124.95	120.09
2	A	501	SVR	O77-S73-C69	4.96	111.83	106.20
2	B	502	SVR	O77-S73-C69	5.10	111.99	106.20
2	B	502	SVR	O80-S75-C71	5.28	112.18	106.20
2	A	501	SVR	O80-S75-C71	5.29	112.20	106.20
2	A	501	SVR	O29-S21-C15	6.02	113.03	106.20
2	B	502	SVR	O29-S21-C15	6.19	113.22	106.20
2	B	502	SVR	O81-S75-C71	7.06	114.20	106.20
2	B	502	SVR	O23-S17-C11	7.19	114.35	106.20
2	A	501	SVR	O81-S75-C71	7.22	114.39	106.20
2	B	502	SVR	O28-S21-C15	7.31	114.49	106.20
2	B	502	SVR	O24-S17-C11	7.33	114.51	106.20
2	A	501	SVR	O23-S17-C11	7.39	114.58	106.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	SVR	O28-S21-C15	7.40	114.59	106.20
2	A	501	SVR	O24-S17-C11	7.62	114.84	106.20
2	B	502	SVR	O78-S73-C69	8.78	116.16	106.20
2	A	501	SVR	O78-S73-C69	8.81	116.19	106.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SVR	8	0
2	B	502	SVR	8	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	244/244 (100%)	-0.37	3 (1%) 81 80	23, 31, 35, 37	0
1	B	243/244 (99%)	-0.36	1 (0%) 93 93	23, 31, 35, 38	0
All	All	487/488 (99%)	-0.37	4 (0%) 87 87	23, 31, 35, 38	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	240	PRO	2.7
1	A	59	PHE	2.3
1	A	147	TYR	2.1
1	B	36	LEU	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SVR	A	501	86/86	0.95	0.12	0.42	33,41,46,50	0
2	SVR	B	502	86/86	0.92	0.11	0.08	34,41,49,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.