



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 04:45 am BST

PDB ID : 3SY8  
Title : Crystal structure of the response regulator RocR  
Authors : Chen, M.W.; Kotaka, M.; Vonnrhein, C.; Bricogne, G.; Lescar, J.  
Deposited on : 2011-07-16  
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

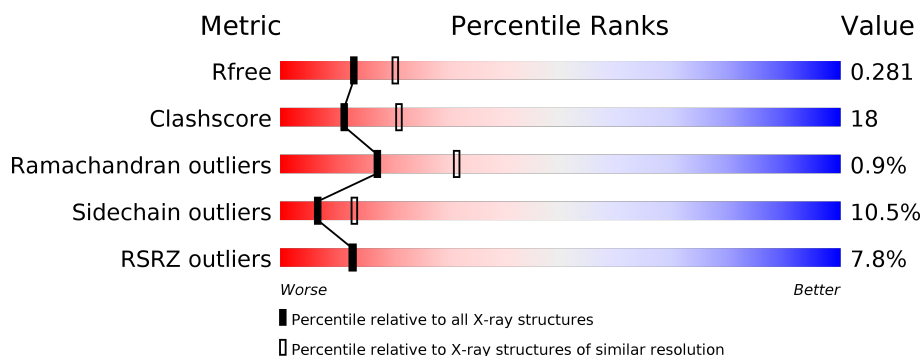
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 respectively. 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	400	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>27%</div> <div>• • •</div> </div> </div>
1	B	400	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>• • •</div> </div> </div>
1	C	400	<div> <div>6%</div> <div> <div></div> <div>62%</div> <div>29%</div> <div>• 5%</div> </div> </div>
1	D	400	<div> <div>14%</div> <div> <div></div> <div>59%</div> <div>28%</div> <div>6% 7%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11886 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 RocR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2979	1899	509	554	17			
1	B	392	Total	C	N	O	S	0	0	0
			3007	1918	513	558	18			
1	C	380	Total	C	N	O	S	0	0	0
			2906	1856	493	540	17			
1	D	371	Total	C	N	O	S	0	0	0
			2807	1792	477	522	16			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	TRP	ARG	CONFLICT	UNP Q9HX69
A	393	LEU	-	EXPRESSION TAG	UNP Q9HX69
A	394	GLU	-	EXPRESSION TAG	UNP Q9HX69
A	395	HIS	-	EXPRESSION TAG	UNP Q9HX69
A	396	HIS	-	EXPRESSION TAG	UNP Q9HX69
A	397	HIS	-	EXPRESSION TAG	UNP Q9HX69
A	398	HIS	-	EXPRESSION TAG	UNP Q9HX69
A	399	HIS	-	EXPRESSION TAG	UNP Q9HX69
A	400	HIS	-	EXPRESSION TAG	UNP Q9HX69
B	286	TRP	ARG	CONFLICT	UNP Q9HX69
B	393	LEU	-	EXPRESSION TAG	UNP Q9HX69
B	394	GLU	-	EXPRESSION TAG	UNP Q9HX69
B	395	HIS	-	EXPRESSION TAG	UNP Q9HX69
B	396	HIS	-	EXPRESSION TAG	UNP Q9HX69
B	397	HIS	-	EXPRESSION TAG	UNP Q9HX69
B	398	HIS	-	EXPRESSION TAG	UNP Q9HX69
B	399	HIS	-	EXPRESSION TAG	UNP Q9HX69
B	400	HIS	-	EXPRESSION TAG	UNP Q9HX69
C	286	TRP	ARG	CONFLICT	UNP Q9HX69
C	393	LEU	-	EXPRESSION TAG	UNP Q9HX69
C	394	GLU	-	EXPRESSION TAG	UNP Q9HX69

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	395	HIS	-	EXPRESSION TAG	UNP Q9HX69
C	396	HIS	-	EXPRESSION TAG	UNP Q9HX69
C	397	HIS	-	EXPRESSION TAG	UNP Q9HX69
C	398	HIS	-	EXPRESSION TAG	UNP Q9HX69
C	399	HIS	-	EXPRESSION TAG	UNP Q9HX69
C	400	HIS	-	EXPRESSION TAG	UNP Q9HX69
D	286	TRP	ARG	CONFLICT	UNP Q9HX69
D	393	LEU	-	EXPRESSION TAG	UNP Q9HX69
D	394	GLU	-	EXPRESSION TAG	UNP Q9HX69
D	395	HIS	-	EXPRESSION TAG	UNP Q9HX69
D	396	HIS	-	EXPRESSION TAG	UNP Q9HX69
D	397	HIS	-	EXPRESSION TAG	UNP Q9HX69
D	398	HIS	-	EXPRESSION TAG	UNP Q9HX69
D	399	HIS	-	EXPRESSION TAG	UNP Q9HX69
D	400	HIS	-	EXPRESSION TAG	UNP Q9HX69

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

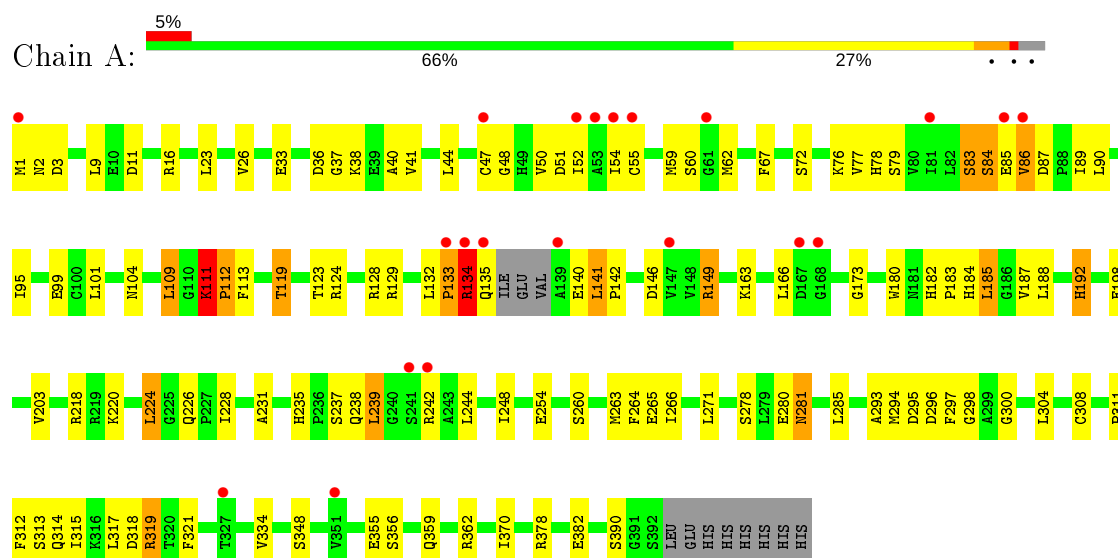
- Molecule 4 is water.

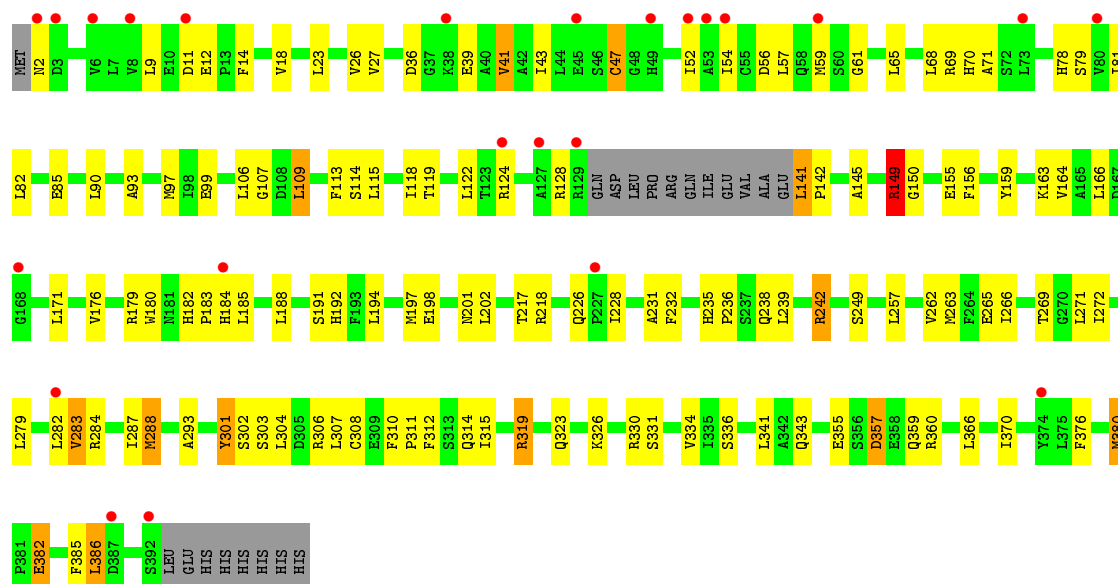
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	53	Total	O	0	0
			53	53		
4	C	33	Total	O	0	0
			33	33		
4	D	47	Total	O	0	0
			47	47		

### 3 Residue-property plots

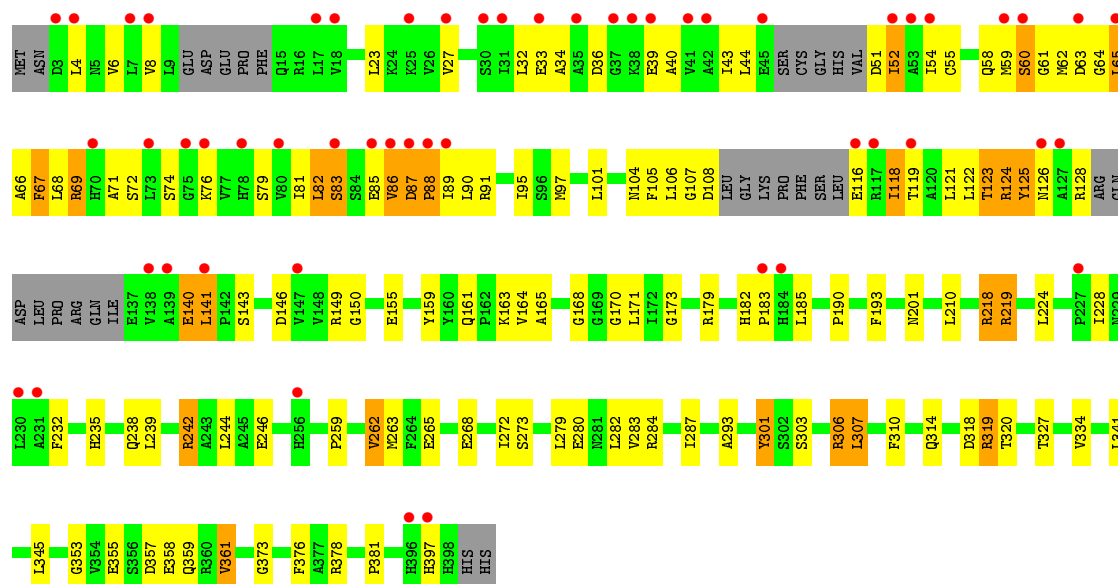
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: RocR





• Molecule 1: RocR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.80 Å   118.80 Å   495.10 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	19.96 – 2.50 19.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.96-2.50) 83.3 (19.96-2.50)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.73 (at 2.50 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.216   ,   0.285 0.211   ,   0.281	Depositor DCC
$R_{free}$ test set	3045 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.5	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11886	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

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

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	0.71	2/3036 (0.1%)	0.79	1/4118 (0.0%)
1	B	0.81	0/3065	0.85	2/4158 (0.0%)
1	C	0.68	2/2962 (0.1%)	0.75	3/4018 (0.1%)
1	D	0.73	0/2855	0.86	3/3871 (0.1%)
All	All	0.73	4/11918 (0.0%)	0.81	9/16165 (0.1%)

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
1	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	308	CYS	CB-SG	-7.81	1.69	1.82
1	A	55	CYS	CB-SG	-7.13	1.70	1.82
1	A	280	GLU	CG-CD	5.48	1.60	1.51
1	C	319	ARG	CG-CD	5.46	1.65	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	179	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	A	111	LYS	C-N-CD	-7.68	103.70	120.60
1	C	315	ILE	CB-CA-C	-6.98	97.64	111.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	306	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	61	GLY	N-CA-C	-5.73	98.78	113.10
1	D	179	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	149	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	266	ILE	CB-CA-C	-5.29	101.03	111.60
1	B	149	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	LYS	Peptide
1	C	141	LEU	Peptide

## 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	2979	0	3002	91	0
1	B	3007	0	3040	88	0
1	C	2906	0	2930	106	0
1	D	2807	0	2811	153	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	D	15	0	17	2	0
4	A	35	0	0	7	0
4	B	53	0	0	5	0
4	C	33	0	0	2	0
4	D	47	0	0	4	0
All	All	11886	0	11800	417	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 18.

All (417) 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:C:93:ALA:HB1	1:D:283:VAL:HG21	1.23	1.15
1:D:68:LEU:HG	1:D:69:ARG:NH1	1.70	1.07
1:D:66:ALA:N	1:D:69:ARG:HE	1.53	1.06
4:A:421:HOH:O	1:B:277:SER:HB3	1.50	1.06
1:D:125:TYR:HA	1:D:128:ARG:HB2	1.43	1.00
1:D:68:LEU:HG	1:D:69:ARG:HH12	1.22	0.98
1:A:104:ASN:HD21	1:A:128:ARG:HH21	1.03	0.97
1:C:69:ARG:CZ	1:D:246:GLU:OE1	2.13	0.96
1:A:84:SER:HB2	1:A:86:VAL:HG22	1.48	0.96
1:C:301:TYR:H	1:C:301:TYR:HD1	1.03	0.96
1:D:165:ALA:H	1:D:170:GLY:HA2	1.29	0.95
1:C:182:HIS:CD2	1:C:185:LEU:H	1.83	0.95
1:D:68:LEU:CB	1:D:69:ARG:HH11	1.80	0.94
1:A:59:MET:HE1	1:A:62:MET:HB3	1.45	0.94
1:D:279:LEU:O	1:D:283:VAL:HG23	1.70	0.92
1:D:69:ARG:HD3	1:D:69:ARG:N	1.81	0.92
1:D:68:LEU:CG	1:D:69:ARG:NH1	2.31	0.92
1:D:219:ARG:HH11	1:D:219:ARG:HG2	1.32	0.91
1:D:54:ILE:HA	1:D:81:ILE:O	1.70	0.91
1:D:68:LEU:HB2	1:D:69:ARG:HH11	1.33	0.91
1:D:65:LEU:C	1:D:69:ARG:HE	1.76	0.89
1:C:163:LYS:NZ	1:C:263:MET:HE1	1.88	0.89
1:C:141:LEU:HB2	4:C:421:HOH:O	1.71	0.89
1:D:355:GLU:H	1:D:359:GLN:HE21	1.19	0.88
1:D:318:ASP:OD2	1:D:320:THR:HG23	1.74	0.87
1:B:49:HIS:HD2	1:B:51:ASP:OD1	1.57	0.87
1:C:301:TYR:N	1:C:301:TYR:CD1	2.39	0.86
1:B:140:GLU:O	1:B:142:PRO:HD3	1.74	0.86
1:B:355:GLU:H	1:B:359:GLN:HE22	1.22	0.86
1:D:355:GLU:H	1:D:359:GLN:NE2	1.73	0.86
1:A:37:GLY:O	1:A:41:VAL:HG12	1.77	0.84
1:C:26:VAL:HG11	1:C:119:THR:HG22	1.58	0.84
1:B:327:THR:CG2	1:B:328:GLN:HE21	1.89	0.84
1:A:104:ASN:ND2	1:A:128:ARG:HH21	1.74	0.84
1:C:242:ARG:HA	1:C:242:ARG:NE	1.94	0.82
1:D:104:ASN:HD21	1:D:149:ARG:HH22	1.22	0.81
1:B:302:SER:HB2	4:B:431:HOH:O	1.78	0.81
1:D:67:PHE:HB3	1:D:69:ARG:NH2	1.95	0.81
1:C:357:ASP:OD1	1:C:360:ARG:NH2	2.15	0.80
1:C:182:HIS:HD2	1:C:184:HIS:H	1.29	0.80
1:B:11:ASP:HB2	1:B:59:MET:HG2	1.61	0.80
1:C:171:LEU:CD2	1:C:228:ILE:HD12	2.12	0.80

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:TYR:N	1:C:301:TYR:HD1	1.75	0.80
1:D:82:LEU:CD1	1:D:108:ASP:HA	2.12	0.80
1:A:235:HIS:H	1:A:238:GLN:HE21	1.30	0.79
1:C:171:LEU:HD22	1:C:228:ILE:HD12	1.64	0.79
1:D:182:HIS:HD2	1:D:185:LEU:H	1.29	0.78
1:D:68:LEU:CB	1:D:69:ARG:NH1	2.46	0.78
1:B:118:ILE:O	1:B:122:LEU:HD12	1.83	0.77
1:C:93:ALA:CB	1:D:283:VAL:HG21	2.10	0.77
1:D:242:ARG:HE	1:D:242:ARG:HA	1.50	0.77
1:D:68:LEU:H	1:D:69:ARG:NH1	1.82	0.77
1:D:66:ALA:N	1:D:69:ARG:NE	2.33	0.76
1:C:355:GLU:H	1:C:359:GLN:HE22	1.31	0.76
1:A:235:HIS:H	1:A:238:GLN:NE2	1.84	0.76
1:B:89:ILE:HG21	1:D:306:ARG:HG3	1.67	0.76
1:D:163:LYS:NZ	1:D:263:MET:HE1	2.01	0.75
1:D:219:ARG:CG	1:D:219:ARG:HH11	1.98	0.75
1:C:355:GLU:H	1:C:359:GLN:NE2	1.85	0.75
1:C:171:LEU:HD21	1:C:228:ILE:HG23	1.68	0.75
1:D:52:ILE:HB	1:D:125:TYR:OH	1.86	0.75
1:A:355:GLU:H	1:A:359:GLN:HE21	1.35	0.74
1:D:125:TYR:HA	1:D:128:ARG:CB	2.16	0.74
1:D:242:ARG:NE	1:D:242:ARG:HA	2.02	0.74
1:C:182:HIS:HD2	1:C:185:LEU:H	1.33	0.74
1:B:9:LEU:HD22	1:B:62:MET:HE3	1.69	0.73
1:C:163:LYS:HZ2	1:C:263:MET:HE1	1.52	0.73
1:C:93:ALA:HB1	1:D:283:VAL:CG2	2.11	0.73
1:D:66:ALA:H	1:D:69:ARG:HH21	1.36	0.73
1:A:59:MET:CE	1:A:62:MET:HB3	2.18	0.73
1:D:65:LEU:C	1:D:69:ARG:NE	2.41	0.73
1:D:219:ARG:NH1	1:D:219:ARG:HG2	1.98	0.73
1:A:188:LEU:HD22	1:A:192:HIS:CD2	2.23	0.73
1:B:9:LEU:HD22	1:B:62:MET:CE	2.19	0.73
1:C:235:HIS:H	1:C:238:GLN:HE21	1.35	0.73
1:C:242:ARG:HE	1:C:242:ARG:HA	1.50	0.73
1:A:271:LEU:HD22	1:A:294:MET:HE1	1.70	0.72
1:B:218:ARG:HH12	1:B:229:ASN:ND2	1.87	0.72
1:D:68:LEU:CG	1:D:69:ARG:HH11	1.99	0.72
1:B:277:SER:OG	4:B:432:HOH:O	2.07	0.71
1:C:163:LYS:NZ	1:C:263:MET:CE	2.53	0.71
1:B:218:ARG:NH1	1:B:229:ASN:ND2	2.39	0.70
1:D:55:CYS:C	1:D:83:SER:H	1.93	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ASN:HD21	1:A:128:ARG:NH2	1.84	0.70
1:D:69:ARG:H	1:D:69:ARG:HD3	1.56	0.70
1:D:171:LEU:CD2	1:D:228:ILE:HD11	2.21	0.69
1:C:307:LEU:HD12	1:C:341:LEU:HD21	1.73	0.69
1:B:274:ALA:O	1:B:306:ARG:NH2	2.26	0.69
1:D:55:CYS:O	1:D:83:SER:N	2.25	0.69
1:A:83:SER:CB	1:A:111:LYS:HE3	2.22	0.69
1:C:26:VAL:CG1	1:C:119:THR:HG22	2.22	0.69
1:B:218:ARG:NH1	1:B:229:ASN:HD22	1.90	0.68
1:C:171:LEU:HD22	1:C:228:ILE:CD1	2.23	0.68
1:A:112:PRO:HG2	1:D:273:SER:HB3	1.76	0.68
1:B:49:HIS:CD2	1:B:51:ASP:OD1	2.46	0.68
1:C:97:MET:HE2	1:D:284:ARG:HG3	1.76	0.68
1:B:355:GLU:H	1:B:359:GLN:NE2	1.92	0.67
1:A:146:ASP:OD2	1:A:182:HIS:HE1	1.77	0.67
1:D:69:ARG:CD	1:D:69:ARG:N	2.57	0.67
1:B:138:VAL:CG1	1:B:140:GLU:HG2	2.24	0.67
1:A:239:LEU:HB3	1:A:278:SER:HB3	1.77	0.67
1:A:271:LEU:HD22	1:A:294:MET:CE	2.24	0.67
1:B:138:VAL:HG13	1:B:140:GLU:HG2	1.77	0.67
1:C:182:HIS:CD2	1:C:184:HIS:H	2.10	0.67
1:D:108:ASP:OD1	4:D:414:HOH:O	2.13	0.67
1:D:182:HIS:CD2	1:D:185:LEU:H	2.13	0.67
1:D:89:ILE:O	1:D:90:LEU:HD12	1.95	0.66
1:B:27:VAL:HG22	1:B:122:LEU:HD21	1.77	0.66
1:C:109:LEU:HD11	1:C:113:PHE:HB3	1.77	0.66
1:A:198:GLU:HG2	1:A:235:HIS:CE1	2.31	0.66
1:D:82:LEU:H	1:D:82:LEU:HD12	1.61	0.65
1:B:327:THR:HG23	1:B:328:GLN:HE21	1.60	0.65
1:B:84:SER:HB2	1:B:86:VAL:HG22	1.78	0.65
1:C:382:GLU:O	1:C:386:LEU:HD23	1.96	0.65
1:A:235:HIS:HD2	1:A:237:SER:H	1.44	0.65
1:A:59:MET:HE1	1:A:62:MET:CB	2.25	0.64
1:D:163:LYS:HZ3	1:D:263:MET:HE1	1.61	0.64
1:B:219:ARG:HD2	1:B:255:PHE:O	1.98	0.64
1:D:81:ILE:HG13	1:D:106:LEU:HD13	1.80	0.64
1:C:279:LEU:O	1:C:283:VAL:HG22	1.98	0.64
1:C:57:LEU:HG	1:C:82:LEU:HD22	1.80	0.63
1:A:265:GLU:HG2	1:A:293:ALA:HB3	1.79	0.63
1:B:161:GLN:HE21	1:B:372:GLN:HE21	1.47	0.63
1:D:218:ARG:NH1	1:D:228:ILE:O	2.32	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ARG:CD	1:D:69:ARG:H	2.12	0.63
1:A:9:LEU:HD11	1:A:67:PHE:CD2	2.34	0.62
1:D:171:LEU:HD23	1:D:228:ILE:HD11	1.80	0.62
1:A:319:ARG:NH2	4:A:409:HOH:O	2.31	0.62
1:C:69:ARG:NH1	1:D:246:GLU:OE1	2.32	0.62
1:B:155:GLU:HA	4:B:412:HOH:O	1.98	0.62
1:A:242:ARG:HA	1:A:281:ASN:HD21	1.65	0.62
1:D:173:GLY:HA2	1:D:228:ILE:HG23	1.82	0.61
1:A:318:ASP:N	4:A:405:HOH:O	2.31	0.61
1:C:149:ARG:CG	1:C:149:ARG:HH11	2.13	0.61
1:A:87:ASP:CG	1:C:306:ARG:HH12	2.04	0.61
1:C:141:LEU:N	1:C:142:PRO:HD3	2.15	0.61
1:C:272:ILE:HG12	1:C:306:ARG:NH2	2.15	0.61
1:C:115:LEU:O	1:C:119:THR:HG23	2.01	0.61
1:C:81:ILE:HA	1:C:107:GLY:O	2.01	0.61
1:D:66:ALA:CA	1:D:69:ARG:HE	2.14	0.60
1:D:68:LEU:N	1:D:69:ARG:NH1	2.49	0.60
1:A:83:SER:HB3	1:A:111:LYS:HE3	1.83	0.60
1:D:65:LEU:HA	1:D:69:ARG:CZ	2.32	0.60
1:D:307:LEU:HD12	1:D:341:LEU:HD21	1.84	0.60
1:C:149:ARG:NH1	1:C:149:ARG:HG3	2.17	0.59
1:D:104:ASN:ND2	1:D:149:ARG:HH22	1.97	0.59
1:A:231:ALA:HA	1:A:263:MET:O	2.02	0.59
1:D:95:ILE:HG12	1:D:105:PHE:CE2	2.38	0.59
1:B:59:MET:HE1	1:B:62:MET:SD	2.43	0.58
1:B:84:SER:HB2	1:B:86:VAL:CG2	2.33	0.58
1:D:82:LEU:HD13	1:D:108:ASP:HA	1.85	0.58
1:C:36:ASP:OD1	1:C:39:GLU:HG3	2.04	0.58
1:D:82:LEU:HD12	1:D:107:GLY:O	2.04	0.58
1:D:171:LEU:HD21	1:D:228:ILE:CD1	2.33	0.58
1:D:44:LEU:HD22	1:D:76:LYS:HE3	1.84	0.58
1:C:149:ARG:HG3	1:C:150:GLY:N	2.19	0.57
1:A:220:LYS:HE2	1:A:382:GLU:OE2	2.05	0.57
1:C:149:ARG:HG3	1:C:149:ARG:HH11	1.68	0.57
1:B:179:ARG:NH2	4:B:409:HOH:O	2.37	0.57
1:C:171:LEU:HD23	1:C:171:LEU:C	2.25	0.57
1:A:119:THR:O	1:A:123:THR:HG23	2.03	0.57
1:D:91:ARG:NH2	4:D:414:HOH:O	2.38	0.57
1:C:310:PHE:CE2	1:D:90:LEU:HD21	2.39	0.57
1:A:182:HIS:HD2	1:A:184:HIS:H	1.53	0.56
1:B:266:ILE:HD11	1:B:312:PHE:CE1	2.40	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:LYS:N	1:B:112:PRO:HD2	2.20	0.56
1:B:327:THR:CG2	1:B:328:GLN:NE2	2.66	0.56
1:D:150:GLY:HA2	1:D:155:GLU:HG3	1.88	0.56
1:C:97:MET:HE3	1:D:287:ILE:HD12	1.86	0.56
1:C:54:ILE:HG12	1:C:81:ILE:HB	1.87	0.56
1:A:235:HIS:CD2	1:A:237:SER:H	2.22	0.56
1:B:5:ASN:HB3	1:B:51:ASP:H	1.70	0.56
1:B:325:MET:HE2	1:B:362:ARG:HG2	1.87	0.55
1:D:268:GLU:OE2	1:D:303:SER:OG	2.21	0.55
1:D:61:GLY:O	1:D:65:LEU:N	2.39	0.55
1:D:86:VAL:O	1:D:88:PRO:HD3	2.06	0.55
1:A:185:LEU:CD1	1:A:188:LEU:HD11	2.37	0.55
1:B:9:LEU:HD23	1:B:34:ALA:HB3	1.88	0.55
1:C:171:LEU:HD21	1:C:228:ILE:HD12	1.88	0.55
1:C:236:PRO:O	1:C:239:LEU:HB2	2.06	0.55
1:B:89:ILE:CG2	1:D:306:ARG:HG3	2.37	0.55
1:D:171:LEU:CD2	1:D:228:ILE:CD1	2.85	0.55
1:D:159:TYR:CE2	1:D:381:PRO:HD3	2.42	0.55
1:D:59:MET:HB3	1:D:61:GLY:HA2	1.89	0.55
1:B:72:SER:HB2	1:B:101:LEU:O	2.08	0.55
1:B:148:VAL:HG22	1:B:202:LEU:HD11	1.88	0.54
1:C:302:SER:O	1:C:306:ARG:HG2	2.07	0.54
1:D:235:HIS:H	1:D:238:GLN:HE21	1.54	0.54
1:A:318:ASP:HB2	4:A:405:HOH:O	2.07	0.54
1:C:182:HIS:CD2	1:C:185:LEU:N	2.67	0.54
1:A:83:SER:O	1:A:111:LYS:HB2	2.07	0.54
1:A:83:SER:HB2	1:A:111:LYS:HE3	1.90	0.54
1:A:356:SER:O	1:A:359:GLN:HG2	2.07	0.54
1:D:82:LEU:HD12	1:D:108:ASP:HA	1.88	0.54
1:D:66:ALA:N	1:D:69:ARG:HH21	2.04	0.54
1:D:235:HIS:H	1:D:238:GLN:NE2	2.06	0.54
1:D:52:ILE:HD11	1:D:81:ILE:HD12	1.91	0.53
1:D:122:LEU:O	1:D:126:ASN:HB2	2.08	0.53
1:B:173:GLY:HA2	1:B:228:ILE:HG23	1.91	0.53
1:D:58:GLN:C	1:D:60:SER:N	2.59	0.53
1:B:161:GLN:NE2	1:B:372:GLN:HE21	2.07	0.53
1:B:182:HIS:CD2	1:B:185:LEU:HB2	2.44	0.53
1:D:116:GLU:HB3	1:D:118:ILE:HD12	1.91	0.53
1:A:317:LEU:HD22	1:A:321:PHE:CE2	2.43	0.53
1:A:87:ASP:OD2	1:C:306:ARG:NH1	2.42	0.52
1:D:293:ALA:HA	1:D:314:GLN:O	2.08	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:VAL:HG22	1:D:54:ILE:HB	1.90	0.52
1:A:11:ASP:HB2	1:A:59:MET:HG2	1.90	0.52
1:A:355:GLU:H	1:A:359:GLN:NE2	2.05	0.52
1:B:112:PRO:O	1:B:113:PHE:HB2	2.09	0.52
1:D:64:GLY:C	1:D:69:ARG:NH2	2.63	0.52
1:D:263:MET:HE3	1:D:314:GLN:NE2	2.25	0.52
1:D:65:LEU:HA	1:D:69:ARG:NE	2.25	0.52
1:A:318:ASP:CB	4:A:405:HOH:O	2.57	0.52
1:D:34:ALA:HB3	1:D:40:ALA:HB2	1.91	0.51
1:A:9:LEU:HD13	1:A:62:MET:HE2	1.92	0.51
1:D:106:LEU:HD21	1:D:125:TYR:CD1	2.46	0.51
1:B:147:VAL:HA	1:B:180:TRP:CH2	2.46	0.51
1:C:194:LEU:O	1:C:198:GLU:HB2	2.10	0.51
1:C:265:GLU:HG2	1:C:293:ALA:HB3	1.92	0.51
1:C:310:PHE:HB3	1:C:312:PHE:CE1	2.46	0.51
1:D:140:GLU:CD	1:D:141:LEU:H	2.14	0.51
1:A:111:LYS:HG3	1:A:111:LYS:O	2.11	0.51
1:B:310:PHE:CE2	1:B:312:PHE:HB2	2.46	0.51
1:C:283:VAL:HG13	1:D:90:LEU:HD23	1.92	0.51
1:A:173:GLY:HA2	1:A:228:ILE:HG23	1.93	0.51
1:B:163:LYS:NZ	1:B:263:MET:HE1	2.25	0.51
1:C:266:ILE:HG21	1:C:271:LEU:HD13	1.93	0.51
1:D:60:SER:N	1:D:61:GLY:CA	2.73	0.51
1:D:71:ALA:O	1:D:74:SER:OG	2.25	0.51
1:A:95:ILE:O	1:A:99:GLU:HG3	2.11	0.51
1:D:54:ILE:HG12	1:D:81:ILE:HB	1.93	0.51
1:D:259:PRO:HD2	4:D:435:HOH:O	2.10	0.51
1:D:116:GLU:HB3	1:D:118:ILE:CD1	2.41	0.50
1:D:68:LEU:H	1:D:69:ARG:CZ	2.23	0.50
1:C:176:VAL:HG21	1:C:232:PHE:CE2	2.46	0.50
1:A:248:ILE:HD13	1:A:264:PHE:CZ	2.46	0.50
1:D:165:ALA:N	1:D:170:GLY:HA2	2.12	0.50
1:D:67:PHE:HB3	1:D:69:ARG:HH22	1.75	0.50
1:A:26:VAL:CG1	1:A:119:THR:HG22	2.42	0.50
1:B:59:MET:CE	1:B:62:MET:HB3	2.41	0.50
1:B:266:ILE:HD11	1:B:312:PHE:HE1	1.76	0.50
1:D:168:GLY:HA3	4:D:428:HOH:O	2.11	0.49
1:B:275:PRO:HG2	1:B:278:SER:OG	2.12	0.49
1:D:119:THR:O	1:D:123:THR:HG23	2.13	0.49
1:B:163:LYS:NZ	1:B:263:MET:CE	2.75	0.49
1:C:307:LEU:CD1	1:C:341:LEU:HD21	2.40	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LEU:HD13	1:B:228:ILE:HG12	1.93	0.49
1:B:9:LEU:HD22	1:B:62:MET:HE1	1.94	0.49
1:D:272:ILE:HD11	1:D:306:ARG:NH2	2.28	0.49
1:C:282:LEU:HB3	1:C:310:PHE:CZ	2.48	0.49
1:C:56:ASP:C	1:C:56:ASP:OD1	2.51	0.49
1:D:164:VAL:HG21	1:D:376:PHE:CG	2.48	0.49
1:D:60:SER:N	1:D:61:GLY:HA3	2.28	0.49
1:D:67:PHE:HB3	1:D:69:ARG:CZ	2.42	0.49
1:C:149:ARG:CG	1:C:149:ARG:NH1	2.74	0.48
1:C:284:ARG:HA	1:D:97:MET:HE2	1.94	0.48
1:C:182:HIS:HD2	1:C:185:LEU:N	2.08	0.48
1:D:171:LEU:HD21	1:D:228:ILE:HD13	1.95	0.48
1:A:112:PRO:HD2	4:A:415:HOH:O	2.14	0.48
1:C:182:HIS:HD2	1:C:184:HIS:N	2.05	0.48
1:D:121:LEU:HA	1:D:124:ARG:HB2	1.94	0.48
1:D:4:LEU:HD23	1:D:27:VAL:HG13	1.95	0.48
1:D:79:SER:HB3	1:D:106:LEU:HD11	1.94	0.48
1:C:99:GLU:HG2	1:C:145:ALA:HB2	1.95	0.48
1:A:72:SER:OG	1:A:101:LEU:O	2.32	0.47
1:B:109:LEU:HD23	1:B:113:PHE:CE2	2.49	0.47
1:B:226:GLN:HB3	1:B:228:ILE:HD13	1.95	0.47
1:C:23:LEU:O	1:C:27:VAL:HB	2.14	0.47
1:B:182:HIS:HD2	1:B:184:HIS:H	1.61	0.47
1:C:263:MET:CE	1:C:314:GLN:NE2	2.78	0.47
1:D:43:ILE:CG2	1:D:43:ILE:O	2.62	0.47
1:B:106:LEU:HD11	1:B:125:TYR:HB2	1.96	0.47
1:C:11:ASP:C	1:C:11:ASP:OD1	2.53	0.47
1:C:269:THR:O	1:C:272:ILE:HB	2.14	0.47
1:A:26:VAL:HG13	1:A:119:THR:HG22	1.97	0.47
1:A:1:MET:O	1:A:2:ASN:HB3	2.15	0.47
1:C:231:ALA:HA	1:C:263:MET:O	2.15	0.47
1:D:282:LEU:HB3	1:D:310:PHE:CZ	2.50	0.47
1:D:66:ALA:HA	1:D:69:ARG:HG2	1.97	0.47
1:A:111:LYS:CG	1:A:111:LYS:O	2.62	0.47
1:A:48:GLY:CA	1:A:76:LYS:HE2	2.45	0.47
1:A:248:ILE:HD12	1:A:285:LEU:HD21	1.96	0.47
1:D:232:PHE:HE1	1:D:262:VAL:CG2	2.28	0.47
1:A:40:ALA:HB1	1:A:67:PHE:CE1	2.50	0.46
1:B:163:LYS:HZ1	1:B:263:MET:HE1	1.79	0.46
1:D:165:ALA:H	1:D:170:GLY:CA	2.12	0.46
1:D:40:ALA:HA	1:D:43:ILE:HB	1.96	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:GLY:O	1:B:227:PRO:HD3	2.15	0.46
1:B:235:HIS:CD2	1:B:237:SER:H	2.33	0.46
1:C:303:SER:HA	1:C:306:ARG:HG3	1.96	0.46
1:D:307:LEU:HD13	1:D:345:LEU:CD1	2.45	0.46
1:A:78:HIS:HD2	1:A:79:SER:OG	1.98	0.46
1:C:263:MET:HE3	1:C:314:GLN:NE2	2.31	0.46
1:D:52:ILE:CD1	1:D:54:ILE:HG13	2.46	0.46
1:A:146:ASP:O	1:A:149:ARG:HG3	2.16	0.46
1:C:14:PHE:O	1:C:18:VAL:HG23	2.15	0.46
1:C:217:THR:HG23	1:C:386:LEU:HD21	1.98	0.46
1:B:118:ILE:HG22	1:B:122:LEU:HD11	1.98	0.46
1:D:68:LEU:N	1:D:69:ARG:CZ	2.79	0.46
1:A:109:LEU:HD23	1:A:113:PHE:CE2	2.51	0.45
1:A:185:LEU:HD13	1:A:188:LEU:HD11	1.97	0.45
1:B:50:VAL:O	1:B:77:VAL:HA	2.16	0.45
1:D:122:LEU:HD23	1:D:125:TYR:HE1	1.80	0.45
1:D:4:LEU:HD13	1:D:126:ASN:OD1	2.16	0.45
1:A:48:GLY:HA2	1:A:76:LYS:HE2	1.98	0.45
1:B:2:ASN:HB3	1:B:3:ASP:H	1.45	0.45
1:D:190:PRO:HA	1:D:193:PHE:CE2	2.51	0.45
1:A:134:ARG:HB3	1:A:135:GLN:H	1.62	0.45
1:A:242:ARG:HA	1:A:281:ASN:ND2	2.29	0.45
1:C:287:ILE:O	1:C:288:MET:C	2.55	0.45
1:B:182:HIS:HD2	1:B:185:LEU:H	1.64	0.45
1:C:164:VAL:HG21	1:C:376:PHE:CD1	2.52	0.45
1:D:65:LEU:CA	1:D:69:ARG:NE	2.80	0.45
1:A:180:TRP:HB3	1:A:188:LEU:HB2	1.97	0.45
1:B:106:LEU:HD21	1:B:125:TYR:HA	1.98	0.45
1:B:163:LYS:HZ1	1:B:263:MET:CE	2.30	0.45
1:C:159:TYR:CG	1:C:179:ARG:HG3	2.52	0.45
1:C:163:LYS:NZ	1:C:314:GLN:HE22	2.15	0.45
1:D:72:SER:HB2	1:D:101:LEU:O	2.17	0.45
1:C:191:SER:OG	4:C:413:HOH:O	2.21	0.45
1:A:109:LEU:HA	1:A:109:LEU:HD12	1.79	0.45
1:A:163:LYS:NZ	1:A:314:GLN:HE22	2.15	0.45
1:C:90:LEU:HD21	1:D:310:PHE:CD1	2.52	0.45
1:B:182:HIS:CD2	1:B:185:LEU:H	2.35	0.44
1:B:326:LYS:HB2	4:B:410:HOH:O	2.17	0.44
1:A:182:HIS:CD2	1:A:183:PRO:HD2	2.52	0.44
1:A:146:ASP:OD2	1:A:182:HIS:CE1	2.64	0.44
1:A:36:ASP:HA	1:A:62:MET:SD	2.57	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:HIS:H	1:B:238:GLN:NE2	2.16	0.44
1:D:182:HIS:HA	1:D:183:PRO:HD3	1.89	0.44
1:A:132:LEU:HD12	1:A:133:PRO:HD2	1.99	0.44
1:A:300:GLY:HA2	1:C:304:LEU:HD12	1.99	0.44
1:A:308:CYS:O	1:C:330:ARG:NH2	2.51	0.44
1:D:143:SER:O	1:D:146:ASP:HB2	2.17	0.44
1:D:319:ARG:HB2	1:D:353:GLY:HA3	2.00	0.44
1:C:52:ILE:HG21	1:C:81:ILE:HD12	1.99	0.44
1:B:182:HIS:CG	1:B:185:LEU:HB2	2.53	0.44
1:A:51:ASP:C	1:A:52:ILE:HG13	2.37	0.44
1:C:149:ARG:NH2	1:C:183:PRO:HG3	2.33	0.44
1:D:66:ALA:O	1:D:69:ARG:HG2	2.17	0.44
1:D:39:GLU:O	1:D:43:ILE:HG12	2.18	0.44
1:D:89:ILE:C	1:D:90:LEU:HD12	2.38	0.44
1:B:317:LEU:HA	1:B:317:LEU:HD23	1.70	0.43
1:D:85:GLU:HG3	1:D:108:ASP:HB3	1.99	0.43
1:D:373:GLY:HA2	3:D:3380:EPE:O3S	2.18	0.43
1:D:52:ILE:CD1	1:D:81:ILE:HD12	2.48	0.43
1:D:357:ASP:O	1:D:361:VAL:HG13	2.19	0.43
1:A:50:VAL:HB	1:A:77:VAL:HG22	2.00	0.43
1:B:166:LEU:HD21	1:B:371:ALA:HB2	2.00	0.43
1:C:166:LEU:O	1:C:360:ARG:HD3	2.19	0.43
1:D:88:PRO:HA	1:D:91:ARG:HB2	2.00	0.43
1:A:9:LEU:HD13	1:A:62:MET:CE	2.47	0.43
1:C:150:GLY:HA2	1:C:155:GLU:OE1	2.17	0.43
1:B:356:SER:H	1:B:359:GLN:NE2	2.16	0.43
1:D:6:VAL:HG11	1:D:23:LEU:HD13	2.01	0.43
1:A:180:TRP:O	1:A:187:VAL:HA	2.19	0.43
1:C:97:MET:HE2	1:D:284:ARG:CG	2.47	0.43
1:A:182:HIS:CG	1:A:183:PRO:HD2	2.54	0.43
1:A:266:ILE:O	1:A:294:MET:HA	2.18	0.43
1:B:51:ASP:O	1:B:78:HIS:HB2	2.18	0.43
1:C:188:LEU:HD22	1:C:192:HIS:CG	2.54	0.43
1:D:61:GLY:O	1:D:65:LEU:HB2	2.19	0.43
1:B:276:ALA:O	1:B:277:SER:C	2.55	0.42
1:B:59:MET:HE1	1:B:62:MET:HB3	2.01	0.42
1:C:156:PHE:CE2	1:C:180:TRP:HB2	2.53	0.42
1:C:171:LEU:CD2	1:C:228:ILE:HG23	2.43	0.42
1:D:263:MET:CE	1:D:314:GLN:NE2	2.82	0.42
1:A:311:PRO:HD2	1:A:312:PHE:CD2	2.54	0.42
1:D:161:GLN:HE22	3:D:3380:EPE:H102	1.83	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ILE:HD13	1:A:315:ILE:HA	1.80	0.42
1:A:16:ARG:HD3	1:A:33:GLU:HB3	2.01	0.42
1:B:4:LEU:HA	1:B:4:LEU:HD12	1.38	0.42
1:D:265:GLU:HG2	1:D:293:ALA:HB3	2.02	0.42
1:C:43:ILE:O	1:C:47:CYS:HB2	2.19	0.42
1:D:87:ASP:HA	1:D:88:PRO:HD2	1.83	0.42
1:C:249:SER:HB3	1:C:288:MET:CE	2.49	0.42
1:A:297:PHE:CD2	1:A:298:GLY:N	2.87	0.42
1:B:235:HIS:HD2	1:B:237:SER:OG	2.03	0.42
1:C:113:PHE:HB2	1:C:118:ILE:HD11	2.02	0.42
1:C:68:LEU:O	1:C:71:ALA:HB3	2.19	0.42
1:A:266:ILE:O	1:A:295:ASP:N	2.44	0.42
1:B:263:MET:HE3	1:B:314:GLN:OE1	2.20	0.42
1:D:66:ALA:CA	1:D:69:ARG:HG2	2.50	0.42
1:A:141:LEU:HA	1:A:142:PRO:HD3	1.91	0.42
1:A:182:HIS:CG	1:A:185:LEU:CD1	3.03	0.42
1:A:87:ASP:OD1	1:C:306:ARG:NH1	2.53	0.42
1:C:310:PHE:CG	1:C:311:PRO:HD2	2.55	0.41
1:C:336:SER:OG	1:C:366:LEU:HD22	2.19	0.41
1:C:78:HIS:HD2	1:C:79:SER:OG	2.03	0.41
1:D:55:CYS:SG	1:D:67:PHE:CE2	3.13	0.41
1:B:232:PHE:HE1	1:B:262:VAL:HG22	1.85	0.41
1:B:95:ILE:HD13	1:B:95:ILE:N	2.36	0.41
1:C:218:ARG:HG3	1:C:257:LEU:HD22	2.02	0.41
1:A:166:LEU:N	4:A:407:HOH:O	2.53	0.41
1:B:359:GLN:HB2	1:B:359:GLN:HE21	1.66	0.41
1:C:41:VAL:HG23	1:C:70:HIS:HB3	2.02	0.41
1:A:224:LEU:HD12	1:A:224:LEU:HA	1.89	0.41
1:B:4:LEU:HD11	1:B:125:TYR:CE2	2.56	0.41
1:C:380:MET:HE3	1:C:385:PHE:HA	2.03	0.41
1:D:232:PHE:HE1	1:D:262:VAL:HG22	1.85	0.41
1:A:348:SER:HB2	1:A:370:ILE:HD12	2.03	0.41
1:B:161:GLN:HA	1:B:162:PRO:HD3	1.86	0.40
1:C:197:MET:HG2	1:C:202:LEU:HB2	2.02	0.40
1:D:163:LYS:NZ	1:D:314:GLN:HE22	2.19	0.40
1:B:109:LEU:HG	1:B:113:PHE:CD2	2.56	0.40
1:B:118:ILE:HG22	1:B:122:LEU:CD1	2.51	0.40
1:B:194:LEU:O	1:B:198:GLU:HG3	2.20	0.40
1:B:326:LYS:HD3	1:B:326:LYS:HA	1.70	0.40
1:C:226:GLN:HB3	1:C:228:ILE:HG12	2.03	0.40
1:B:161:GLN:O	1:B:174:ALA:HA	2.21	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ARG:HD2	1:D:218:ARG:HA	1.82	0.40
1:D:66:ALA:N	1:D:69:ARG:NH2	2.68	0.40
1:A:112:PRO:HG2	1:D:273:SER:CB	2.49	0.40
1:C:124:ARG:HD3	1:C:128:ARG:NH2	2.36	0.40
1:A:23:LEU:HD11	1:A:54:ILE:HD12	2.03	0.40
1:B:57:LEU:HA	1:B:57:LEU:HD23	1.71	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	385/400 (96%)	356 (92%)	24 (6%)	5 (1%)	12	21
1	B	390/400 (98%)	370 (95%)	18 (5%)	2 (0%)	29	48
1	C	376/400 (94%)	349 (93%)	25 (7%)	2 (0%)	29	48
1	D	361/400 (90%)	338 (94%)	18 (5%)	5 (1%)	11	20
All	All	1512/1600 (94%)	1413 (94%)	85 (6%)	14 (1%)	17	31

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	LYS
1	A	112	PRO
1	A	133	PRO
1	A	134	ARG
1	D	67	PHE
1	C	319	ARG
1	D	397	HIS
1	B	2	ASN
1	B	193	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	288	MET
1	D	88	PRO
1	D	301	TYR
1	A	141	LEU
1	D	118	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	324/337 (96%)	286 (88%)	38 (12%)	5	10
1	B	328/337 (97%)	298 (91%)	30 (9%)	9	18
1	C	317/337 (94%)	289 (91%)	28 (9%)	10	19
1	D	300/337 (89%)	263 (88%)	37 (12%)	4	9
All	All	1269/1348 (94%)	1136 (90%)	133 (10%)	7	13

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	38	LYS
1	A	44	LEU
1	A	47	CYS
1	A	60	SER
1	A	83	SER
1	A	84	SER
1	A	85	GLU
1	A	86	VAL
1	A	89	ILE
1	A	90	LEU
1	A	109	LEU
1	A	111	LYS
1	A	119	THR
1	A	124	ARG
1	A	129	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	134	ARG
1	A	140	GLU
1	A	149	ARG
1	A	185	LEU
1	A	192	HIS
1	A	203	VAL
1	A	218	ARG
1	A	224	LEU
1	A	226	GLN
1	A	239	LEU
1	A	244	LEU
1	A	254	GLU
1	A	260	SER
1	A	281	ASN
1	A	296	ASP
1	A	304	LEU
1	A	313	SER
1	A	319	ARG
1	A	334	VAL
1	A	362	ARG
1	A	378	ARG
1	A	390	SER
1	B	2	ASN
1	B	4	LEU
1	B	26	VAL
1	B	41	VAL
1	B	60	SER
1	B	83	SER
1	B	84	SER
1	B	86	VAL
1	B	90	LEU
1	B	108	ASP
1	B	109	LEU
1	B	116	GLU
1	B	119	THR
1	B	122	LEU
1	B	130	GLN
1	B	136	ILE
1	B	140	GLU
1	B	149	ARG
1	B	152	ASP
1	B	171	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	218	ARG
1	B	219	ARG
1	B	224	LEU
1	B	241	SER
1	B	251	LEU
1	B	262	VAL
1	B	266	ILE
1	B	326	LYS
1	B	327	THR
1	B	358	GLU
1	C	2	ASN
1	C	9	LEU
1	C	12	GLU
1	C	41	VAL
1	C	47	CYS
1	C	59	MET
1	C	65	LEU
1	C	85	GLU
1	C	106	LEU
1	C	109	LEU
1	C	114	SER
1	C	122	LEU
1	C	149	ARG
1	C	201	ASN
1	C	242	ARG
1	C	262	VAL
1	C	283	VAL
1	C	301	TYR
1	C	323	GLN
1	C	326	LYS
1	C	331	SER
1	C	334	VAL
1	C	343	GLN
1	C	357	ASP
1	C	370	ILE
1	C	380	MET
1	C	382	GLU
1	C	386	LEU
1	D	32	LEU
1	D	33	GLU
1	D	36	ASP
1	D	51	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	52	ILE
1	D	60	SER
1	D	62	MET
1	D	63	ASP
1	D	65	LEU
1	D	69	ARG
1	D	82	LEU
1	D	83	SER
1	D	86	VAL
1	D	87	ASP
1	D	123	THR
1	D	124	ARG
1	D	125	TYR
1	D	140	GLU
1	D	141	LEU
1	D	201	ASN
1	D	210	LEU
1	D	218	ARG
1	D	219	ARG
1	D	224	LEU
1	D	239	LEU
1	D	242	ARG
1	D	244	LEU
1	D	262	VAL
1	D	280	GLU
1	D	301	TYR
1	D	307	LEU
1	D	319	ARG
1	D	327	THR
1	D	334	VAL
1	D	358	GLU
1	D	361	VAL
1	D	378	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	15	GLN
1	A	78	HIS
1	A	104	ASN
1	A	161	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	182	HIS
1	A	229	ASN
1	A	235	HIS
1	A	238	GLN
1	A	281	ASN
1	A	314	GLN
1	A	359	GLN
1	A	383	GLN
1	B	15	GLN
1	B	49	HIS
1	B	70	HIS
1	B	135	GLN
1	B	161	GLN
1	B	182	HIS
1	B	209	GLN
1	B	229	ASN
1	B	235	HIS
1	B	238	GLN
1	B	328	GLN
1	B	359	GLN
1	C	78	HIS
1	C	104	ASN
1	C	161	GLN
1	C	182	HIS
1	C	201	ASN
1	C	209	GLN
1	C	235	HIS
1	C	238	GLN
1	C	314	GLN
1	C	359	GLN
1	D	5	ASN
1	D	104	ASN
1	D	161	GLN
1	D	182	HIS
1	D	235	HIS
1	D	238	GLN
1	D	314	GLN
1	D	359	GLN

### 5.3.3 RNA ⓘ

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](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EPE	D	3380	2	15,15,15	0.74	1 (6%)	18,20,20	2.54	7 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	D	3380	2	-	3/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3380	EPE	C10-S	2.18	1.80	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3380	EPE	C5-N4-C3	5.12	120.36	108.83
3	D	3380	EPE	O2S-S-C10	4.90	112.81	106.92
3	D	3380	EPE	C9-N1-C6	-3.87	101.33	111.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3380	EPE	C6-C5-N4	3.67	118.18	110.64
3	D	3380	EPE	C6-N1-C2	3.60	116.93	108.83
3	D	3380	EPE	C9-N1-C2	-2.58	104.65	111.23
3	D	3380	EPE	C5-C6-N1	2.03	114.80	110.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	3380	EPE	C10-C9-N1-C2
3	D	3380	EPE	C10-C9-N1-C6
3	D	3380	EPE	C8-C7-N4-C5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3380	EPE	2	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

### 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	389/400 (97%)	0.06	21 (5%) 25 27	37, 63, 85, 98	0
1	B	392/400 (98%)	-0.05	21 (5%) 25 27	34, 54, 79, 96	0
1	C	380/400 (95%)	0.21	24 (6%) 20 21	53, 74, 100, 109	0
1	D	371/400 (92%)	0.36	54 (14%) 2 2	35, 60, 141, 146	0
All	All	1532/1600 (95%)	0.14	120 (7%) 13 13	34, 63, 104, 146	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	73	LEU	7.5
1	D	139	ALA	7.1
1	B	1	MET	6.1
1	C	227	PRO	5.9
1	C	392	SER	5.5
1	D	25	LYS	5.2
1	D	75	GLY	4.8
1	D	18	VAL	4.7
1	D	86	VAL	4.6
1	B	392	SER	4.5
1	D	41	VAL	4.5
1	B	391	GLY	4.3
1	D	138	VAL	4.3
1	C	53	ALA	4.2
1	A	134	ARG	4.2
1	A	61	GLY	4.1
1	A	53	ALA	4.0
1	D	17	LEU	4.0
1	C	54	ILE	3.9
1	C	3	ASP	3.9
1	C	52	ILE	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	4	LEU	3.8
1	B	168	GLY	3.7
1	C	282	LEU	3.7
1	B	242	ARG	3.7
1	D	33	GLU	3.7
1	D	53	ALA	3.7
1	D	88	PRO	3.6
1	C	2	ASN	3.6
1	D	76	LYS	3.6
1	A	241	SER	3.5
1	D	39	GLU	3.5
1	B	52	ILE	3.5
1	C	38	LYS	3.5
1	A	86	VAL	3.4
1	A	327	THR	3.4
1	B	145	ALA	3.4
1	D	37	GLY	3.4
1	A	54	ILE	3.4
1	D	126	ASN	3.4
1	B	130	GLN	3.3
1	A	85	GLU	3.3
1	B	53	ALA	3.3
1	A	242	ARG	3.3
1	D	396	HIS	3.3
1	C	387	ASP	3.3
1	D	38	LYS	3.2
1	C	127	ALA	3.2
1	C	8	VAL	3.2
1	D	119	THR	3.1
1	D	54	ILE	3.1
1	A	168	GLY	3.1
1	A	52	ILE	3.0
1	B	137	GLU	3.0
1	D	42	ALA	3.0
1	A	133	PRO	3.0
1	C	49	HIS	2.9
1	C	168	GLY	2.9
1	C	45	GLU	2.9
1	C	59	MET	2.8
1	D	59	MET	2.8
1	A	139	ALA	2.8
1	A	351	VAL	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	27	VAL	2.7
1	D	70	HIS	2.7
1	C	73	LEU	2.7
1	A	135	GLN	2.7
1	C	184	HIS	2.7
1	D	116	GLU	2.6
1	B	7	LEU	2.6
1	D	60	SER	2.6
1	D	78	HIS	2.6
1	D	184	HIS	2.6
1	B	54	ILE	2.6
1	B	240	GLY	2.6
1	A	81	ILE	2.6
1	D	8	VAL	2.6
1	D	89	ILE	2.6
1	D	256	HIS	2.6
1	A	147	VAL	2.5
1	B	112	PRO	2.5
1	D	85	GLU	2.5
1	A	167	ASP	2.5
1	B	3	ASP	2.5
1	D	63	ASP	2.5
1	D	3	ASP	2.4
1	D	141	LEU	2.4
1	D	80	VAL	2.4
1	A	47	CYS	2.4
1	D	45	GLU	2.4
1	B	131	ASP	2.4
1	C	129	ARG	2.4
1	B	77	VAL	2.4
1	B	79	SER	2.4
1	D	30	SER	2.4
1	B	50	VAL	2.3
1	D	7	LEU	2.3
1	C	374	TYR	2.3
1	D	87	ASP	2.3
1	D	127	ALA	2.3
1	B	113	PHE	2.2
1	D	183	PRO	2.2
1	D	83	SER	2.2
1	D	31	ILE	2.2
1	B	111	LYS	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	227	PRO	2.2
1	D	52	ILE	2.2
1	D	397	HIS	2.1
1	C	80	VAL	2.1
1	D	231	ALA	2.1
1	C	11	ASP	2.1
1	D	147	VAL	2.1
1	A	55	CYS	2.1
1	D	230	LEU	2.1
1	C	6	VAL	2.1
1	C	124	ARG	2.1
1	D	35	ALA	2.1
1	D	117	ARG	2.0
1	D	65	LEU	2.0
1	A	1	MET	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	D	401	1/1	0.91	0.06	50,50,50,50	0
2	MG	C	401	1/1	0.94	0.06	90,90,90,90	0
3	EPE	D	3380	15/15	0.94	0.15	56,61,69,70	0
2	MG	A	401	1/1	0.95	0.05	49,49,49,49	0
2	MG	B	401	1/1	0.98	0.19	49,49,49,49	0



## 6.5 Other polymers

There are no such residues in this entry.