



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:31 AM GMT

PDB ID : 2DBR  
Title : Crystal Structure of Glyoxylate Reductase (PH0597) from *Pyrococcus horikoshii* OT3, Complexed with NADP (P1)  
Authors : Yoshikawa, S.; Arai, R.; Kinoshita, Y.; Uchikubo-Kamo, T.; Akasaka, R.; Terada, T.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2005-12-16  
Resolution : 2.61 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

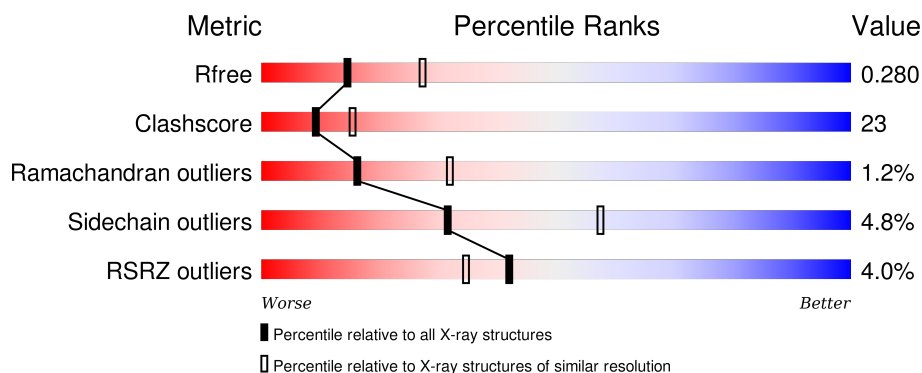
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>61%</span> <span>36%</span> </div> </div>
1	B	334	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>58%</span> <span>37%</span> </div> </div>
1	C	334	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>62%</span> <span>36%</span> </div> </div>
1	D	334	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>57%</span> <span>40%</span> </div> </div>
1	E	334	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>53%</span> <span>43%</span> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	334	

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
2	SO4	A	507	-	-	X	X
2	SO4	B	509	-	-	X	X
2	SO4	C	508	-	-	X	-
2	SO4	D	510	-	-	-	X
2	SO4	E	511	-	-	X	X
2	SO4	F	512	-	-	X	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16468 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 Glyoxylate reductase.

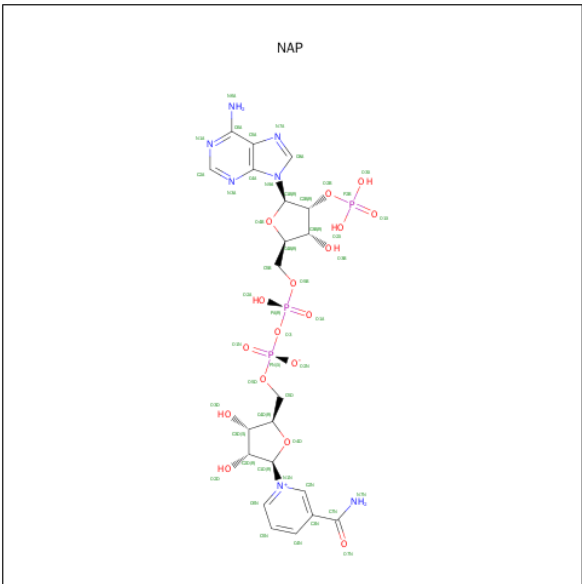
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2673	1725	459	483	6			
1	B	333	Total	C	N	O	S	0	0	0
			2673	1725	459	483	6			
1	C	333	Total	C	N	O	S	0	0	0
			2673	1725	459	483	6			
1	D	333	Total	C	N	O	S	0	0	0
			2673	1725	459	483	6			
1	E	333	Total	C	N	O	S	0	0	0
			2673	1725	459	483	6			
1	F	333	Total	C	N	O	S	0	0	0
			2673	1725	459	483	6			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

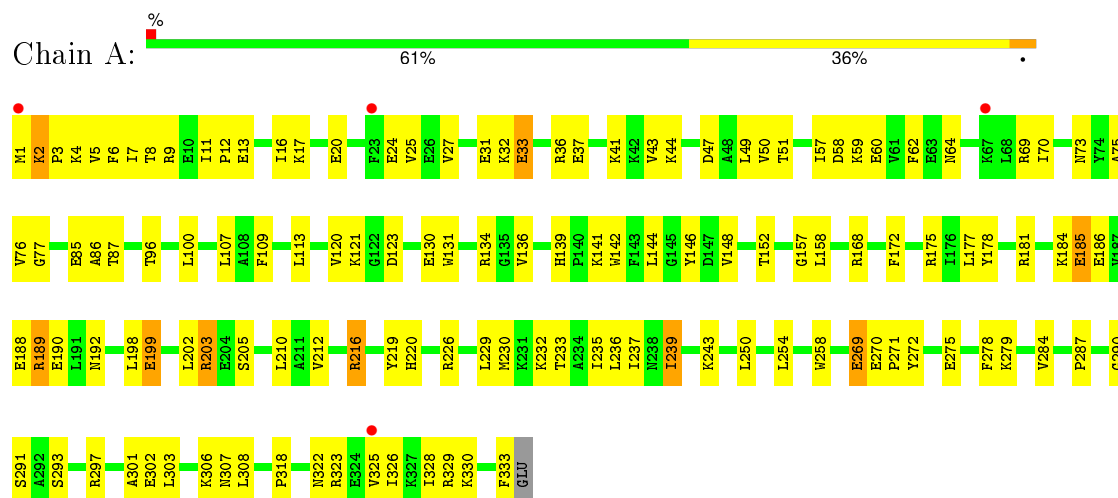
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	22	Total	O	0	0
			22	22		
4	C	18	Total	O	0	0
			18	18		
4	D	17	Total	O	0	0
			17	17		
4	E	6	Total	O	0	0
			6	6		
4	F	8	Total	O	0	0
			8	8		

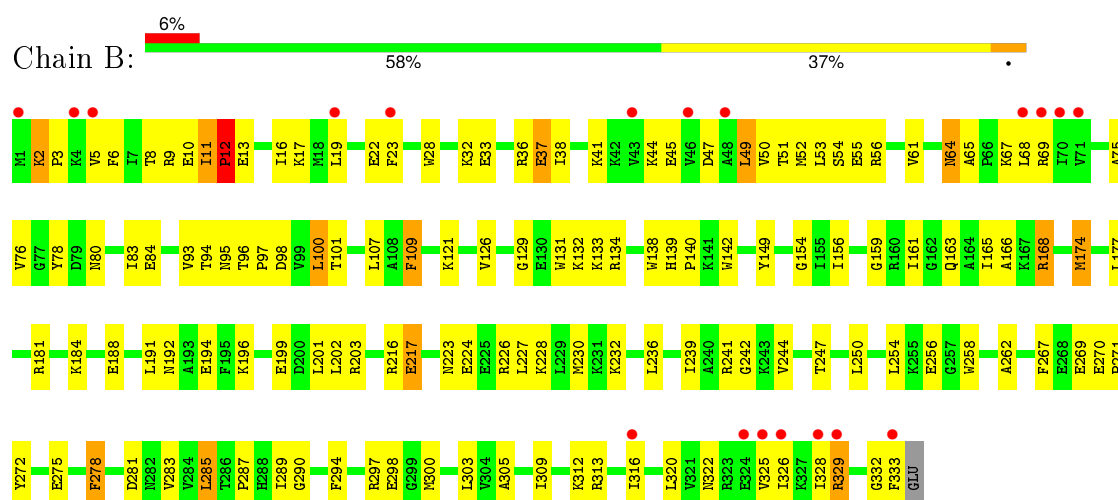
### 3 Residue-property plots

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: Glyoxylate reductase

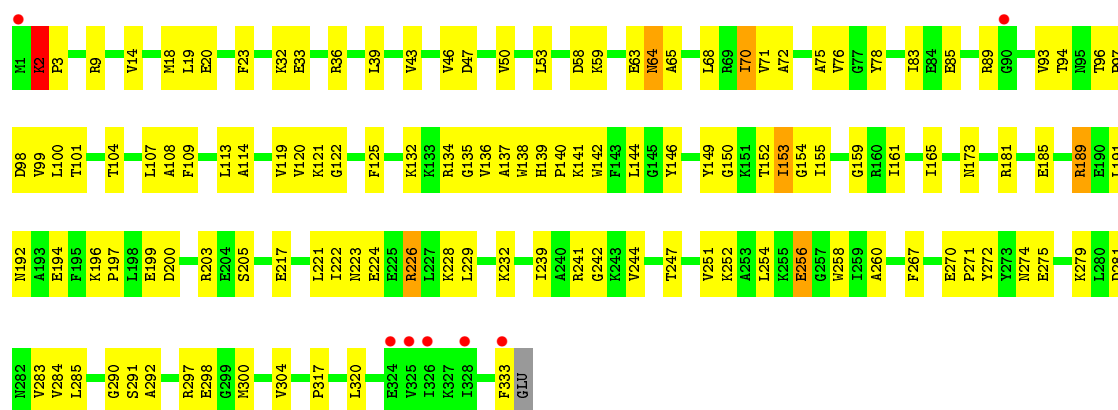


#### • Molecule 1: Glyoxylate reductase

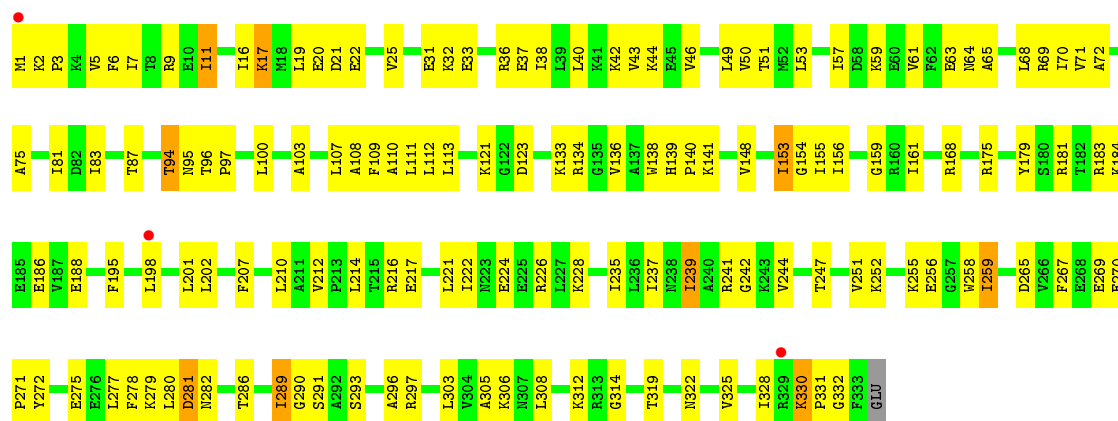


#### • Molecule 1: Glyoxylate reductase

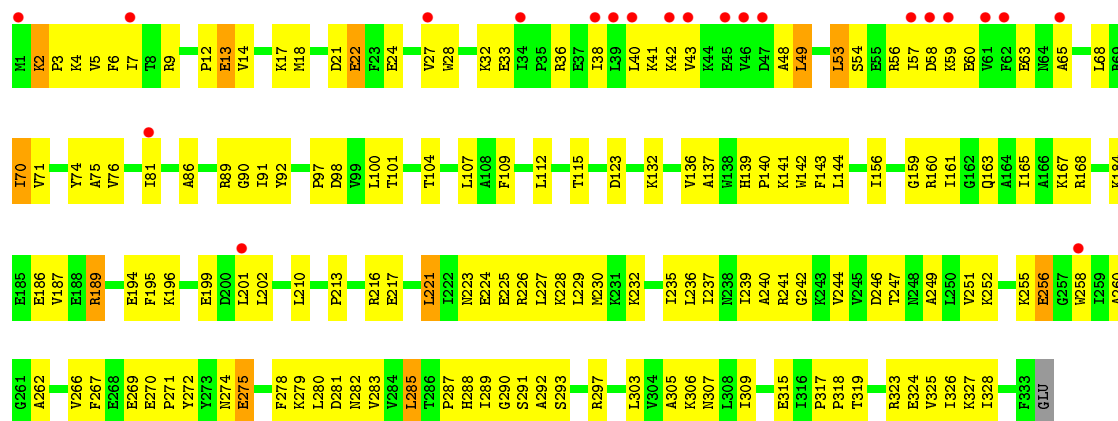




• Molecule 1: Glyoxylate reductase



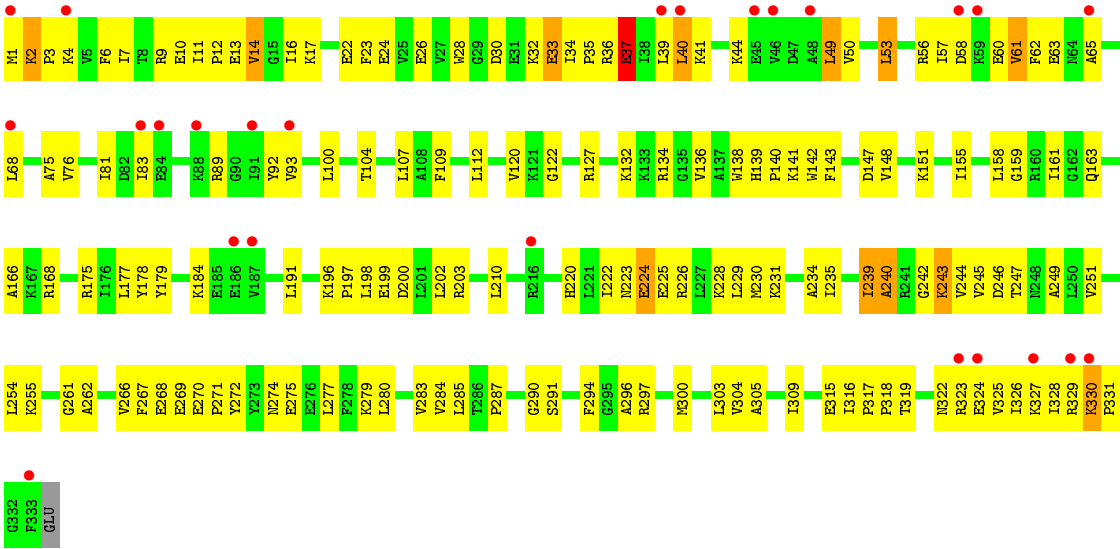
• Molecule 1: Glyoxylate reductase



• Molecule 1: Glyoxylate reductase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.05Å 85.44Å 107.13Å 113.76° 91.17° 94.00°	Depositor
Resolution (Å)	49.11 – 2.61 49.11 – 2.61	Depositor EDS
% Data completeness (in resolution range)	93.2 (49.11-2.61) 81.0 (49.11-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.64 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.218 , 0.284 0.215 , 0.280	Depositor DCC
$R_{free}$ test set	6279 reflections (10.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.9	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	0 of 62126 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16468	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 4.15% 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: NAP, SO4

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	0/2723	0.59	0/3675
1	B	0.33	0/2723	0.60	0/3675
1	C	0.34	0/2723	0.60	0/3675
1	D	0.33	0/2723	0.59	0/3675
1	E	0.30	0/2723	0.57	0/3675
1	F	0.31	0/2723	0.55	0/3675
All	All	0.33	0/16338	0.58	0/22050

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2673	0	2766	118	0
1	B	2673	0	2766	128	0
1	C	2673	0	2766	114	0
1	D	2673	0	2766	133	0
1	E	2673	0	2766	150	0
1	F	2673	0	2766	151	0
2	A	10	0	0	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	4	0
2	C	10	0	0	3	0
2	D	10	0	0	1	0
2	E	10	0	0	2	0
2	F	10	0	0	2	0
3	A	48	0	25	3	0
3	B	48	0	25	5	0
3	C	48	0	25	4	0
3	D	48	0	25	7	0
3	E	48	0	25	3	0
3	F	48	0	25	2	0
4	A	11	0	0	2	0
4	B	22	0	0	5	0
4	C	18	0	0	1	0
4	D	17	0	0	1	0
4	E	6	0	0	0	0
4	F	8	0	0	0	0
All	All	16468	0	16746	757	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 23.

All (757) 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:159:GLY:HA3	3:B:402:NAP:H52A	1.28	1.12
1:D:2:LYS:HE2	1:D:2:LYS:HA	1.43	0.98
1:C:189:ARG:HH11	1:C:189:ARG:HB2	1.30	0.96
1:C:121:LYS:HD3	1:C:281:ASP:HB3	1.47	0.95
1:A:2:LYS:HA	1:A:2:LYS:NZ	1.86	0.90
1:B:2:LYS:NZ	1:B:2:LYS:HA	1.87	0.90
1:E:189:ARG:HB3	1:E:189:ARG:HH11	1.36	0.90
1:A:216:ARG:H	1:A:216:ARG:HD3	1.34	0.88
1:B:316:ILE:H	1:B:316:ILE:HD12	1.38	0.87
1:F:274:ASN:HD22	1:F:277:LEU:HB2	1.38	0.86
1:C:159:GLY:HA3	3:C:403:NAP:O2A	1.76	0.86
1:C:108:ALA:HB2	1:C:239:ILE:HD13	1.59	0.84
1:B:316:ILE:HG23	1:B:326:ILE:HD11	1.60	0.83
1:E:32:LYS:HA	1:F:136:VAL:HG22	1.60	0.83
1:E:53:LEU:HD12	1:E:53:LEU:H	1.44	0.82
1:D:7:ILE:HG21	1:D:11:ILE:HD12	1.62	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:LYS:HA	1:E:2:LYS:NZ	1.93	0.82
1:E:266:VAL:HG12	1:E:288:HIS:CD2	2.14	0.82
1:D:139:HIS:HD2	1:D:141:LYS:H	1.25	0.81
1:F:53:LEU:H	1:F:53:LEU:CD1	1.92	0.81
1:E:275:GLU:O	1:E:279:LYS:HG3	1.81	0.81
1:E:186:GLU:HA	1:E:189:ARG:HH12	1.47	0.79
1:F:134:ARG:HG2	1:F:142:TRP:HH2	1.48	0.79
1:F:202:LEU:O	1:F:230:MET:HA	1.83	0.79
1:C:139:HIS:CD2	1:C:141:LYS:H	2.02	0.77
1:B:69:ARG:HH12	1:B:329:ARG:HD3	1.49	0.77
1:C:2:LYS:HB2	1:C:3:PRO:HD3	1.65	0.77
1:A:107:LEU:HD22	1:A:290:GLY:HA2	1.66	0.77
1:D:224:GLU:HG2	1:D:228:LYS:HE3	1.67	0.76
1:B:156:ILE:HD11	1:B:201:LEU:HD22	1.66	0.76
1:E:136:VAL:HG22	1:F:32:LYS:HA	1.67	0.76
1:C:189:ARG:NH1	1:C:189:ARG:HB2	1.98	0.76
1:B:269:GLU:O	1:B:272:TYR:HB2	1.87	0.74
1:A:203:ARG:NH1	1:A:229:LEU:HD22	2.02	0.74
1:E:256:GLU:HB3	1:E:258:TRP:NE1	2.02	0.74
1:C:107:LEU:HD23	1:C:290:GLY:HA2	1.69	0.74
1:B:76:VAL:HG12	2:B:509:SO4:O3	1.88	0.74
1:A:47:ASP:HB3	1:A:333:PHE:CE2	2.23	0.74
1:B:2:LYS:HA	1:B:2:LYS:HZ3	1.51	0.73
1:F:53:LEU:H	1:F:53:LEU:HD12	1.51	0.73
1:B:216:ARG:HD2	4:B:518:HOH:O	1.88	0.73
1:D:139:HIS:CD2	1:D:141:LYS:H	2.06	0.73
1:A:243:LYS:HE2	1:F:225:GLU:OE2	1.89	0.73
1:A:2:LYS:HZ2	1:A:2:LYS:HA	1.52	0.73
1:E:246:ASP:HB3	1:E:249:ALA:HB3	1.70	0.73
1:E:168:ARG:HG3	1:E:168:ARG:HH11	1.54	0.73
1:A:189:ARG:HH11	1:A:189:ARG:HB3	1.52	0.73
1:E:189:ARG:HB3	1:E:189:ARG:NH1	2.02	0.73
1:E:247:THR:HG21	1:E:272:TYR:OH	1.89	0.72
1:A:199:GLU:HG2	1:A:229:LEU:HD13	1.71	0.72
1:E:104:THR:HA	1:E:290:GLY:O	1.89	0.72
1:D:107:LEU:HD22	1:D:290:GLY:HA2	1.72	0.72
1:D:286:THR:HB	1:D:289:ILE:CD1	2.20	0.71
1:B:96:THR:HA	1:B:303:LEU:HD23	1.71	0.71
1:F:251:VAL:O	1:F:255:LYS:HG3	1.92	0.70
1:C:185:GLU:CD	1:C:185:GLU:H	1.93	0.70
1:E:186:GLU:HA	1:E:189:ARG:NH1	2.07	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:ILE:HD11	1:D:201:LEU:HD22	1.74	0.70
1:A:203:ARG:HH12	1:A:229:LEU:HD22	1.56	0.70
1:E:75:ALA:HB1	2:E:511:SO4:O4	1.92	0.69
1:B:64:ASN:N	1:B:64:ASN:HD22	1.90	0.69
1:B:36:ARG:HD3	1:B:56:ARG:HH21	1.57	0.69
1:B:19:LEU:HD21	1:B:305:ALA:HA	1.74	0.69
1:C:194:GLU:OE2	1:C:196:LYS:HD3	1.93	0.69
1:E:2:LYS:HA	1:E:2:LYS:HZ3	1.57	0.69
1:B:41:LYS:O	1:B:44:LYS:HG2	1.91	0.69
1:A:2:LYS:HZ3	1:A:2:LYS:HA	1.58	0.69
1:D:70:ILE:HD13	1:D:308:LEU:HD23	1.73	0.69
1:B:19:LEU:HD23	1:B:309:ILE:HD11	1.75	0.68
1:C:139:HIS:HD2	1:C:141:LYS:H	1.39	0.68
1:C:135:GLY:O	1:D:32:LYS:HE3	1.93	0.68
1:F:269:GLU:O	1:F:272:TYR:HB2	1.93	0.68
1:F:177:LEU:HD22	1:F:196:LYS:HG3	1.75	0.68
1:F:159:GLY:HA3	3:F:406:NAP:O2A	1.93	0.68
1:F:275:GLU:HG2	1:F:279:LYS:HE3	1.76	0.68
1:B:202:LEU:O	1:B:230:MET:HA	1.94	0.68
1:A:226:ARG:HH11	1:A:226:ARG:HG3	1.59	0.68
1:E:107:LEU:HD23	1:E:290:GLY:HA2	1.75	0.67
1:D:65:ALA:HB1	1:D:68:LEU:HB2	1.75	0.67
1:D:11:ILE:H	1:D:11:ILE:HD13	1.59	0.67
1:E:240:ALA:O	1:E:266:VAL:HG11	1.94	0.67
1:E:247:THR:O	1:E:251:VAL:HG23	1.94	0.67
1:A:107:LEU:CD2	1:A:290:GLY:HA2	2.24	0.67
1:C:43:VAL:O	1:C:46:VAL:HG22	1.95	0.67
1:C:107:LEU:CD2	1:C:290:GLY:HA2	2.24	0.67
1:F:53:LEU:N	1:F:53:LEU:HD12	2.09	0.67
1:F:270:GLU:HA	1:F:271:PRO:C	2.15	0.67
1:C:152:THR:HG22	1:C:205:SER:HA	1.75	0.67
1:F:49:LEU:HB2	1:F:68:LEU:HD11	1.77	0.66
1:B:224:GLU:HG2	1:B:228:LYS:HE3	1.76	0.66
1:C:226:ARG:HH11	1:C:226:ARG:HG3	1.60	0.66
1:E:97:PRO:HD2	1:E:319:THR:HG21	1.77	0.66
1:F:316:ILE:HD12	1:F:316:ILE:N	2.10	0.66
1:B:2:LYS:HA	1:B:2:LYS:HZ2	1.59	0.66
1:E:256:GLU:HB3	1:E:258:TRP:HE1	1.61	0.66
1:A:322:ASN:O	1:A:325:VAL:HG12	1.96	0.66
1:B:159:GLY:CA	3:B:402:NAP:H52A	2.18	0.66
1:A:329:ARG:HG2	1:A:330:LYS:H	1.61	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:ILE:HD13	1:D:154:GLY:N	2.10	0.66
1:C:189:ARG:HH11	1:C:189:ARG:CB	2.08	0.66
1:C:224:GLU:HG3	1:C:258:TRP:CZ3	2.30	0.66
1:B:75:ALA:HB1	2:B:509:SO4:O1	1.95	0.66
1:D:184:LYS:HE2	1:D:186:GLU:HB3	1.78	0.66
1:E:7:ILE:HB	1:E:27:VAL:HG13	1.78	0.66
1:F:274:ASN:HD22	1:F:277:LEU:CB	2.08	0.65
1:A:75:ALA:HB1	2:A:507:SO4:O4	1.95	0.65
1:E:270:GLU:HA	1:E:271:PRO:C	2.15	0.65
1:B:139:HIS:HB3	1:B:142:TRP:CD1	2.30	0.65
1:F:2:LYS:H	1:F:3:PRO:CD	2.10	0.65
1:E:74:TYR:HE1	1:F:138:TRP:HH2	1.45	0.65
1:B:13:GLU:HG3	1:B:17:LYS:HE3	1.77	0.65
1:E:202:LEU:O	1:E:230:MET:HA	1.96	0.65
1:B:139:HIS:ND1	1:B:140:PRO:HD2	2.12	0.65
1:D:2:LYS:CE	1:D:2:LYS:HA	2.25	0.65
1:E:6:PHE:O	1:E:49:LEU:HD23	1.97	0.65
1:D:168:ARG:HG3	1:D:168:ARG:HH11	1.62	0.64
1:E:2:LYS:HB2	1:E:3:PRO:HD3	1.79	0.64
1:F:13:GLU:CG	1:F:17:LYS:HE3	2.27	0.64
1:D:217:GLU:HG3	3:D:404:NAP:H62A	1.62	0.64
1:B:294:PHE:O	1:B:298:GLU:HB2	1.98	0.64
1:A:37:GLU:CD	1:A:37:GLU:H	2.01	0.64
1:B:49:LEU:HD22	1:B:51:THR:HG23	1.79	0.64
1:D:306:LYS:HE2	1:D:306:LYS:HA	1.80	0.64
1:C:252:LYS:HE3	1:C:256:GLU:OE1	1.98	0.64
1:E:159:GLY:HA3	3:E:405:NAP:O2A	1.98	0.64
1:A:329:ARG:HG2	1:A:330:LYS:N	2.13	0.64
3:A:401:NAP:H3D	3:A:401:NAP:H6N	1.80	0.63
1:E:327:LYS:HD3	1:E:328:ILE:HD12	1.80	0.63
1:A:168:ARG:HH11	1:A:168:ARG:HG3	1.61	0.63
1:E:70:ILE:HD13	1:E:71:VAL:N	2.13	0.63
1:D:183:ARG:HG2	1:D:195:PHE:CD2	2.33	0.63
1:B:184:LYS:O	1:B:188:GLU:HG3	1.98	0.63
1:A:131:TRP:HB3	4:A:517:HOH:O	1.97	0.63
1:C:93:VAL:O	1:C:320:LEU:HD12	1.98	0.63
1:F:330:LYS:HB3	1:F:330:LYS:NZ	2.14	0.63
1:E:21:ASP:O	1:E:22:GLU:HG2	1.98	0.63
1:A:302:GLU:O	1:A:306:LYS:HG3	1.99	0.63
1:F:239:ILE:H	1:F:239:ILE:HD13	1.64	0.63
1:F:76:VAL:HG12	2:F:512:SO4:O1	1.98	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:ASN:ND2	1:F:277:LEU:HB2	2.12	0.62
1:A:307:ASN:OD1	1:A:318:PRO:HD2	1.99	0.62
1:A:136:VAL:HG22	1:B:32:LYS:HA	1.79	0.62
1:E:70:ILE:HG12	1:E:92:TYR:HB2	1.81	0.62
1:A:216:ARG:CD	1:A:216:ARG:H	2.10	0.62
1:D:256:GLU:HB3	1:D:258:TRP:NE1	2.14	0.62
1:B:226:ARG:HH11	1:B:226:ARG:HG3	1.63	0.62
1:D:121:LYS:HD3	1:D:281:ASP:HB3	1.81	0.62
1:A:2:LYS:HB2	1:A:3:PRO:HD3	1.82	0.62
1:F:322:ASN:O	1:F:325:VAL:HG12	1.99	0.62
1:C:153:ILE:HD12	1:C:155:ILE:HG13	1.82	0.62
1:A:96:THR:HA	1:A:303:LEU:HD23	1.81	0.62
1:F:138:TRP:HZ3	1:F:140:PRO:HG3	1.64	0.61
1:D:322:ASN:O	1:D:325:VAL:HG12	2.01	0.61
1:C:153:ILE:HD13	1:C:154:GLY:N	2.14	0.61
1:A:189:ARG:CZ	1:C:20:GLU:HG2	2.30	0.61
1:F:58:ASP:O	1:F:61:VAL:HG23	2.00	0.61
1:D:202:LEU:HD13	1:D:226:ARG:HB3	1.83	0.61
1:B:159:GLY:O	1:B:163:GLN:HG3	2.01	0.60
1:E:74:TYR:CE1	1:F:138:TRP:HH2	2.19	0.60
1:A:120:VAL:HG21	1:A:284:VAL:HG13	1.83	0.60
1:D:270:GLU:HA	1:D:271:PRO:C	2.22	0.60
1:D:226:ARG:HG3	1:D:226:ARG:HH11	1.65	0.60
1:E:36:ARG:NH2	1:E:58:ASP:OD2	2.35	0.60
1:E:76:VAL:HG12	2:E:511:SO4:O3	2.01	0.60
1:E:280:LEU:HB2	1:E:283:VAL:CG2	2.32	0.60
1:A:13:GLU:HG3	1:A:17:LYS:HE2	1.83	0.60
1:E:40:LEU:HD11	1:E:60:GLU:OE1	2.00	0.60
1:F:197:PRO:HD2	1:F:200:ASP:HB2	1.84	0.60
1:F:57:ILE:HD12	1:F:57:ILE:N	2.16	0.60
1:C:64:ASN:HD22	1:C:64:ASN:N	1.98	0.60
1:B:216:ARG:HB3	1:B:216:ARG:NH1	2.17	0.60
1:E:115:THR:HG22	1:E:235:ILE:HD13	1.84	0.60
1:E:221:LEU:O	1:E:226:ARG:HG3	2.01	0.60
1:F:202:LEU:HD13	1:F:226:ARG:HB3	1.84	0.59
1:A:158:LEU:HD22	1:A:178:TYR:CG	2.37	0.59
1:A:232:LYS:HA	1:A:258:TRP:O	2.01	0.59
1:E:307:ASN:OD1	1:E:318:PRO:HD2	2.03	0.59
1:B:239:ILE:HD12	1:B:239:ILE:C	2.23	0.59
1:F:93:VAL:HB	1:F:322:ASN:ND2	2.18	0.59
1:C:104:THR:HB	1:C:161:ILE:HD12	1.84	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:LEU:HD13	3:D:404:NAP:H5N	1.86	0.58
1:E:132:LYS:HA	1:F:271:PRO:HB2	1.84	0.58
1:E:86:ALA:HB1	1:E:91:ILE:HB	1.85	0.58
1:D:291:SER:OG	1:D:297:ARG:NH1	2.37	0.58
1:A:189:ARG:HG2	1:A:190:GLU:N	2.18	0.58
1:E:65:ALA:HB1	1:E:68:LEU:HB2	1.85	0.58
1:D:269:GLU:O	1:D:272:TYR:HB2	2.04	0.58
1:D:216:ARG:HG2	1:D:216:ARG:NH1	2.19	0.58
1:B:305:ALA:O	1:B:309:ILE:HG12	2.04	0.58
1:F:28:TRP:CZ3	1:F:34:ILE:HG13	2.38	0.58
1:B:12:PRO:HG2	1:B:297:ARG:O	2.03	0.57
1:B:65:ALA:HB1	1:B:68:LEU:HB2	1.85	0.57
1:E:112:LEU:C	1:E:112:LEU:HD23	2.25	0.57
1:D:216:ARG:HH11	1:D:216:ARG:HG2	1.69	0.57
1:B:322:ASN:O	1:B:325:VAL:HG12	2.04	0.57
1:A:87:THR:HG23	1:A:325:VAL:HB	1.86	0.57
1:A:69:ARG:HH21	1:A:329:ARG:NE	2.03	0.57
1:A:62:PHE:CZ	1:A:86:ALA:HB2	2.40	0.57
1:E:161:ILE:O	1:E:165:ILE:HG13	2.05	0.56
1:F:13:GLU:HG3	1:F:17:LYS:HE3	1.87	0.56
1:C:224:GLU:HG3	1:C:258:TRP:HZ3	1.70	0.56
1:D:252:LYS:O	1:D:256:GLU:HB2	2.05	0.56
1:C:223:ASN:HD21	1:E:315:GLU:HG2	1.69	0.56
1:B:216:ARG:HH11	1:B:216:ARG:HB3	1.69	0.56
1:A:12:PRO:HD2	1:A:301:ALA:HB2	1.87	0.56
1:A:269:GLU:O	1:A:272:TYR:HB2	2.05	0.56
1:C:14:VAL:HG11	1:C:298:GLU:OE2	2.05	0.56
1:B:312:LYS:HA	1:B:333:PHE:HE1	1.68	0.56
1:C:223:ASN:ND2	1:E:315:GLU:HG2	2.21	0.56
1:C:78:TYR:CD1	1:C:83:ILE:HD11	2.41	0.56
1:C:9:ARG:NH2	1:C:33:GLU:HG3	2.20	0.56
1:C:104:THR:HG22	1:C:239:ILE:HD12	1.87	0.56
1:D:159:GLY:HA3	3:D:404:NAP:O5B	2.06	0.56
1:E:291:SER:OG	1:E:297:ARG:NH1	2.39	0.56
1:C:19:LEU:O	1:C:23:PHE:HB2	2.04	0.56
1:F:226:ARG:HG3	1:F:226:ARG:HH11	1.71	0.56
1:D:96:THR:HA	1:D:303:LEU:HD23	1.88	0.56
1:D:17:LYS:O	1:D:20:GLU:HG2	2.05	0.56
1:F:328:ILE:H	1:F:328:ILE:HD12	1.71	0.55
1:A:328:ILE:N	1:A:328:ILE:HD12	2.20	0.55
1:C:59:LYS:HE2	1:C:63:GLU:OE1	2.05	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:ILE:HD11	1:D:16:ILE:HD11	1.88	0.55
1:E:303:LEU:HA	1:E:306:LYS:HE2	1.87	0.55
1:F:163:GLN:HB3	1:F:191:LEU:HD11	1.87	0.55
1:E:53:LEU:HD23	1:E:241:ARG:NH2	2.22	0.55
1:B:109:PHE:HZ	1:B:174:MET:HE2	1.71	0.55
1:E:307:ASN:HA	1:E:318:PRO:HD2	1.88	0.55
1:F:328:ILE:N	1:F:328:ILE:HD12	2.22	0.55
1:A:185:GLU:HB3	1:C:20:GLU:OE2	2.06	0.55
4:A:510:HOH:O	1:C:20:GLU:HB3	2.06	0.55
1:B:166:ALA:HB3	1:B:191:LEU:HD13	1.88	0.55
1:D:259:ILE:H	1:D:259:ILE:HD13	1.71	0.55
1:D:259:ILE:N	1:D:259:ILE:HD13	2.21	0.55
1:F:139:HIS:CD2	1:F:141:LYS:H	2.25	0.55
1:F:13:GLU:HG2	1:F:17:LYS:HE3	1.88	0.55
1:E:123:ASP:HA	1:F:285:LEU:O	2.07	0.55
1:C:199:GLU:O	1:C:203:ARG:HG3	2.06	0.55
1:D:57:ILE:O	1:D:57:ILE:HG22	2.06	0.55
1:D:9:ARG:NH2	1:D:33:GLU:HG3	2.22	0.55
1:D:138:TRP:HZ3	1:D:140:PRO:HG3	1.71	0.55
1:D:156:ILE:O	1:D:212:VAL:HG13	2.06	0.55
1:D:214:LEU:HB2	1:D:241:ARG:HG3	1.88	0.55
1:D:256:GLU:HB3	1:D:258:TRP:CD1	2.42	0.55
1:E:280:LEU:HB2	1:E:283:VAL:HG23	1.89	0.55
1:D:7:ILE:HG12	1:D:50:VAL:HB	1.89	0.54
1:A:270:GLU:HA	1:A:271:PRO:C	2.25	0.54
1:D:11:ILE:H	1:D:11:ILE:CD1	2.20	0.54
1:C:120:VAL:HB	4:C:510:HOH:O	2.07	0.54
1:A:189:ARG:HH11	1:A:189:ARG:CB	2.19	0.54
1:E:107:LEU:CD2	1:E:290:GLY:HA2	2.37	0.54
1:C:70:ILE:HD13	1:C:71:VAL:N	2.22	0.54
1:A:59:LYS:HG3	1:A:85:GLU:OE2	2.07	0.54
1:E:242:GLY:HA3	1:E:267:PHE:C	2.27	0.54
1:D:210:LEU:O	1:D:239:ILE:HD13	2.08	0.54
1:B:13:GLU:CG	1:B:17:LYS:HE3	2.38	0.54
1:A:139:HIS:CD2	1:A:141:LYS:H	2.25	0.54
1:D:31:GLU:HG2	4:D:519:HOH:O	2.06	0.54
1:F:23:PHE:HE1	1:F:309:ILE:HD13	1.71	0.54
1:B:53:LEU:HD21	2:B:509:SO4:O1	2.08	0.54
1:F:49:LEU:HB2	1:F:68:LEU:CD1	2.38	0.54
1:F:93:VAL:HB	1:F:322:ASN:HD21	1.72	0.54
1:D:239:ILE:O	1:D:239:ILE:HG12	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:GLY:HA3	1:D:267:PHE:C	2.28	0.54
1:B:247:THR:HG21	1:B:272:TYR:OH	2.08	0.53
1:A:186:GLU:HA	1:A:189:ARG:HD3	1.88	0.53
1:A:69:ARG:HH21	1:A:329:ARG:CZ	2.20	0.53
1:D:258:TRP:CD1	1:D:258:TRP:N	2.75	0.53
1:D:11:ILE:N	1:D:11:ILE:HD13	2.23	0.53
1:D:81:ILE:O	1:D:83:ILE:HD12	2.08	0.53
1:C:272:TYR:CE2	1:C:274:ASN:HB2	2.43	0.53
1:B:52:MET:HB2	1:B:55:GLU:OE1	2.08	0.53
1:B:216:ARG:HH11	1:B:216:ARG:CB	2.21	0.53
1:C:256:GLU:HB3	1:C:258:TRP:CD1	2.43	0.53
1:F:104:THR:HG21	1:F:161:ILE:HD13	1.89	0.53
1:A:203:ARG:HG3	1:A:203:ARG:HH11	1.74	0.53
1:D:43:VAL:O	1:D:46:VAL:HG22	2.09	0.53
1:F:243:LYS:HA	1:F:268:GLU:HG2	1.90	0.53
1:A:181:ARG:HG3	3:A:401:NAP:C4A	2.38	0.53
1:D:226:ARG:NH1	1:D:226:ARG:HG3	2.24	0.53
1:E:36:ARG:NH2	1:E:56:ARG:HE	2.07	0.53
1:A:31:GLU:HG3	1:A:32:LYS:N	2.22	0.53
1:B:224:GLU:O	1:B:228:LYS:HG3	2.08	0.53
1:E:141:LYS:HE3	1:F:10:GLU:HG2	1.91	0.53
1:B:328:ILE:O	1:B:328:ILE:HG22	2.09	0.53
1:B:98:ASP:HA	1:B:101:THR:OG1	2.09	0.53
1:C:270:GLU:HA	1:C:271:PRO:C	2.29	0.53
1:A:9:ARG:NH2	1:A:33:GLU:HG3	2.24	0.53
1:D:280:LEU:HB3	1:D:282:ASN:OD1	2.09	0.53
1:E:68:LEU:O	1:E:91:ILE:HD12	2.09	0.52
1:B:11:ILE:HD13	1:B:16:ILE:HD11	1.91	0.52
1:F:240:ALA:O	1:F:266:VAL:HG11	2.09	0.52
1:F:179:TYR:CD2	1:F:198:LEU:HD13	2.44	0.52
1:D:202:LEU:CD1	1:D:226:ARG:HB3	2.38	0.52
1:D:83:ILE:HD12	1:D:83:ILE:H	1.74	0.52
1:E:33:GLU:CG	1:E:54:SER:HB3	2.39	0.52
1:E:269:GLU:O	1:E:272:TYR:HB2	2.10	0.52
1:A:236:LEU:C	1:A:237:ILE:HD12	2.30	0.52
1:B:134:ARG:HB3	4:B:525:HOH:O	2.08	0.52
1:D:113:LEU:HD23	1:D:148:VAL:HG21	1.91	0.52
1:B:194:GLU:OE2	1:B:196:LYS:NZ	2.43	0.52
1:C:50:VAL:HA	1:C:72:ALA:O	2.09	0.52
1:A:172:PHE:CZ	1:B:168:ARG:HG2	2.44	0.52
1:C:152:THR:CG2	1:C:205:SER:HA	2.39	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:LYS:HE2	1:D:20:GLU:OE1	2.10	0.52
1:B:5:VAL:HG12	1:B:23:PHE:HB3	1.91	0.52
1:C:136:VAL:HG22	1:D:32:LYS:HA	1.91	0.52
1:A:41:LYS:O	1:A:44:LYS:HG2	2.10	0.52
1:D:11:ILE:HD11	1:D:16:ILE:CD1	2.40	0.51
1:E:199:GLU:HG3	1:E:229:LEU:CD1	2.40	0.51
1:A:121:LYS:HB3	1:A:121:LYS:HZ3	1.75	0.51
1:B:107:LEU:HD22	1:B:290:GLY:HA2	1.92	0.51
1:A:188:GLU:O	1:A:192:ASN:N	2.43	0.51
1:C:94:THR:HG22	1:C:320:LEU:HA	1.90	0.51
1:C:141:LYS:C	1:C:144:LEU:HD21	2.29	0.51
1:F:275:GLU:O	1:F:279:LYS:HG3	2.11	0.51
1:D:168:ARG:HG3	1:D:168:ARG:NH1	2.25	0.51
1:A:7:ILE:HB	1:A:27:VAL:HG22	1.91	0.51
1:B:2:LYS:HB2	1:B:3:PRO:HD3	1.92	0.51
1:D:75:ALA:O	1:D:95:ASN:HB2	2.10	0.51
1:B:232:LYS:HA	1:B:258:TRP:O	2.10	0.51
1:D:244:VAL:O	1:D:244:VAL:HG12	2.11	0.51
1:A:69:ARG:HE	1:A:329:ARG:NH1	2.09	0.51
1:F:329:ARG:HG2	1:F:330:LYS:N	2.25	0.51
1:F:220:HIS:CE1	1:F:246:ASP:HA	2.45	0.51
1:D:7:ILE:HG22	1:D:9:ARG:O	2.11	0.50
1:E:251:VAL:O	1:E:255:LYS:HG3	2.11	0.50
1:F:247:THR:O	1:F:251:VAL:HG23	2.11	0.50
1:F:175:ARG:NH1	1:F:177:LEU:HD21	2.26	0.50
1:A:275:GLU:CG	1:A:279:LYS:HE3	2.41	0.50
1:B:270:GLU:HA	1:B:271:PRO:C	2.30	0.50
1:F:112:LEU:C	1:F:112:LEU:HD23	2.31	0.50
1:A:328:ILE:HG22	1:A:328:ILE:O	2.11	0.50
1:B:309:ILE:O	1:B:313:ARG:HG3	2.10	0.50
1:B:49:LEU:HD23	1:B:50:VAL:N	2.27	0.50
1:F:323:ARG:O	1:F:326:ILE:HG13	2.11	0.50
1:F:328:ILE:H	1:F:328:ILE:CD1	2.24	0.50
1:E:139:HIS:CD2	1:E:141:LYS:H	2.29	0.50
1:D:36:ARG:NH2	1:D:61:VAL:HG23	2.27	0.50
1:A:323:ARG:O	1:A:326:ILE:HG12	2.10	0.50
1:B:216:ARG:HB2	1:B:217:GLU:OE1	2.12	0.50
1:E:144:LEU:HB3	1:F:294:PHE:CE1	2.46	0.50
1:B:78:TYR:C	1:B:80:ASN:H	2.14	0.50
1:E:53:LEU:H	1:E:53:LEU:CD1	2.20	0.50
1:E:266:VAL:HG12	1:E:288:HIS:HD2	1.72	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:256:GLU:HB3	1:E:258:TRP:CD1	2.46	0.50
1:E:36:ARG:CZ	1:E:56:ARG:HH21	2.24	0.50
1:B:94:THR:HG22	1:B:320:LEU:HA	1.94	0.50
1:A:123:ASP:HA	1:B:285:LEU:O	2.12	0.50
1:B:36:ARG:HH22	1:B:61:VAL:HG23	1.77	0.50
1:B:328:ILE:O	1:B:329:ARG:HB2	2.11	0.50
1:A:219:TYR:HD2	1:F:199:GLU:HG3	1.76	0.50
1:A:189:ARG:HG2	1:A:190:GLU:H	1.76	0.50
1:B:161:ILE:O	1:B:165:ILE:HG13	2.11	0.50
1:D:314:GLY:HA2	1:D:331:PRO:O	2.12	0.50
1:F:231:LYS:HB2	1:F:234:ALA:HB2	1.93	0.49
1:F:168:ARG:HH11	1:F:168:ARG:HG3	1.77	0.49
1:B:138:TRP:CZ3	1:B:140:PRO:HG3	2.47	0.49
1:A:60:GLU:O	1:A:64:ASN:ND2	2.40	0.49
1:C:76:VAL:HG12	2:C:508:SO4:O3	2.12	0.49
1:F:247:THR:HG21	1:F:272:TYR:OH	2.12	0.49
1:A:235:ILE:HG22	1:A:237:ILE:CD1	2.43	0.49
1:A:57:ILE:HD12	1:A:57:ILE:N	2.27	0.49
1:C:256:GLU:HB3	1:C:258:TRP:NE1	2.27	0.49
1:E:38:ILE:O	1:E:42:LYS:HG2	2.12	0.49
1:F:303:LEU:HD21	1:F:319:THR:HG21	1.94	0.49
1:D:138:TRP:CZ3	1:D:140:PRO:HG3	2.48	0.49
1:A:73:ASN:ND2	1:A:77:GLY:O	2.45	0.49
1:E:168:ARG:NH1	1:E:168:ARG:HG3	2.24	0.49
1:E:6:PHE:HD2	1:E:49:LEU:HD21	1.77	0.49
1:B:8:THR:OG1	1:B:51:THR:HA	2.12	0.49
1:E:278:PHE:CD2	1:F:127:ARG:HA	2.47	0.49
1:A:203:ARG:HH12	1:A:229:LEU:CD2	2.26	0.49
1:E:217:GLU:N	1:E:217:GLU:OE1	2.45	0.49
1:B:287:PRO:HG2	1:B:289:ILE:CG2	2.43	0.49
1:E:260:ALA:O	1:E:282:ASN:HB2	2.12	0.49
1:C:221:LEU:HG	1:C:222:ILE:HD12	1.95	0.49
1:D:241:ARG:HB2	1:D:244:VAL:HG23	1.94	0.49
1:E:199:GLU:HA	1:E:229:LEU:HD13	1.94	0.49
1:F:40:LEU:HD11	1:F:60:GLU:OE1	2.13	0.49
1:F:107:LEU:HD22	1:F:290:GLY:HA2	1.94	0.49
1:F:7:ILE:HG23	1:F:50:VAL:HB	1.93	0.49
1:E:235:ILE:HG22	1:E:237:ILE:CD1	2.42	0.49
1:F:41:LYS:O	1:F:44:LYS:HG2	2.13	0.49
1:B:154:GLY:HA2	1:B:177:LEU:O	2.13	0.49
1:E:305:ALA:O	1:E:309:ILE:HG13	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:VAL:O	1:F:151:LYS:HB2	2.13	0.49
1:B:242:GLY:HA3	1:B:267:PHE:C	2.32	0.49
1:B:181:ARG:HG3	3:B:402:NAP:C4A	2.43	0.48
1:E:271:PRO:HB2	1:F:132:LYS:HA	1.95	0.48
1:A:271:PRO:HB2	1:B:132:LYS:HA	1.95	0.48
1:C:139:HIS:HB3	1:C:142:TRP:CG	2.47	0.48
1:B:312:LYS:HA	1:B:333:PHE:CE1	2.48	0.48
1:A:47:ASP:HB3	1:A:333:PHE:CD2	2.48	0.48
1:A:136:VAL:HG22	1:B:32:LYS:CA	2.43	0.48
1:E:90:GLY:HA2	1:E:325:VAL:HG23	1.95	0.48
1:E:163:GLN:O	1:E:167:LYS:HG3	2.13	0.48
1:F:53:LEU:HD11	1:F:75:ALA:HB2	1.94	0.48
1:E:101:THR:HA	1:E:161:ILE:HD13	1.96	0.48
1:A:237:ILE:N	1:A:237:ILE:HD12	2.28	0.48
1:C:254:LEU:HD13	1:C:283:VAL:CG2	2.43	0.48
1:A:216:ARG:N	1:A:216:ARG:HD3	2.16	0.48
1:A:37:GLU:CD	1:A:37:GLU:N	2.67	0.48
1:C:9:ARG:HH21	1:C:33:GLU:HA	1.79	0.48
1:D:111:LEU:HD11	1:D:265:ASP:HB2	1.94	0.48
1:C:101:THR:HA	1:C:161:ILE:CD1	2.43	0.48
1:F:316:ILE:HD12	1:F:316:ILE:H	1.78	0.48
1:C:32:LYS:HA	1:D:136:VAL:HG22	1.95	0.48
1:E:33:GLU:HG3	1:E:54:SER:HB3	1.96	0.48
1:F:35:PRO:C	1:F:37:GLU:N	2.63	0.48
1:B:290:GLY:HA3	3:B:402:NAP:O7N	2.14	0.48
1:C:181:ARG:CZ	3:C:403:NAP:O1X	2.62	0.48
1:E:184:LYS:HD3	1:E:187:VAL:HG21	1.96	0.48
1:E:32:LYS:CA	1:F:136:VAL:HG22	2.36	0.48
1:E:232:LYS:HA	1:E:258:TRP:O	2.13	0.48
3:F:406:NAP:H4B	3:F:406:NAP:O2A	2.14	0.48
1:E:280:LEU:HB2	1:E:283:VAL:HG21	1.96	0.48
1:A:7:ILE:HG12	1:A:50:VAL:HB	1.96	0.48
1:E:195:PHE:CD1	1:E:196:LYS:N	2.82	0.48
1:C:113:LEU:HB3	1:D:110:ALA:HB2	1.96	0.48
1:A:199:GLU:HG2	1:A:229:LEU:CD1	2.41	0.47
1:A:76:VAL:HG12	2:A:507:SO4:O3	2.14	0.47
1:D:175:ARG:HH11	1:D:175:ARG:HG2	1.78	0.47
1:B:69:ARG:CD	1:B:333:PHE:HA	2.44	0.47
1:A:219:TYR:OH	1:F:225:GLU:OE1	2.33	0.47
1:D:289:ILE:H	1:D:289:ILE:HD13	1.78	0.47
1:F:22:GLU:OE1	1:F:22:GLU:HA	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:ARG:HD2	1:F:56:ARG:HH22	1.79	0.47
1:B:107:LEU:CD2	1:B:290:GLY:HA2	2.45	0.47
1:E:104:THR:HB	1:E:161:ILE:HD12	1.94	0.47
1:C:226:ARG:HA	1:C:229:LEU:HD12	1.95	0.47
1:E:235:ILE:HG22	1:E:237:ILE:HD12	1.95	0.47
1:B:69:ARG:NH1	1:B:329:ARG:HD3	2.25	0.47
1:D:2:LYS:HE2	1:D:2:LYS:CA	2.29	0.47
1:D:139:HIS:HD2	1:D:141:LYS:N	2.05	0.47
1:D:133:LYS:NZ	1:F:175:ARG:HE	2.11	0.47
1:A:168:ARG:NH1	1:A:168:ARG:HG3	2.29	0.47
1:D:87:THR:HG23	1:D:325:VAL:HB	1.97	0.47
1:A:9:ARG:NH2	1:A:33:GLU:HA	2.29	0.47
1:D:207:PHE:HE1	1:D:235:ILE:HD12	1.79	0.47
1:A:186:GLU:HA	1:A:189:ARG:CD	2.44	0.47
1:B:22:GLU:CB	1:B:309:ILE:HD12	2.45	0.47
1:B:22:GLU:HG3	1:B:309:ILE:HD12	1.96	0.47
1:B:47:ASP:HB3	1:B:333:PHE:CD2	2.49	0.47
1:B:139:HIS:ND1	1:B:140:PRO:CD	2.77	0.47
3:A:401:NAP:C3D	3:A:401:NAP:H6N	2.44	0.47
1:E:216:ARG:HB2	1:E:217:GLU:OE1	2.15	0.47
1:E:63:GLU:HG3	1:E:89:ARG:HH22	1.80	0.47
1:A:291:SER:OG	1:A:297:ARG:NH1	2.47	0.47
1:D:255:LYS:HB3	1:D:255:LYS:HE2	1.81	0.47
1:C:85:GLU:O	1:C:89:ARG:HG3	2.14	0.47
1:B:278:PHE:CD1	1:B:278:PHE:N	2.82	0.47
1:A:57:ILE:O	1:A:57:ILE:HG22	2.15	0.47
1:E:28:TRP:CE3	1:E:28:TRP:HA	2.49	0.47
1:C:2:LYS:CB	1:C:3:PRO:HD3	2.40	0.47
1:F:83:ILE:CG2	1:F:322:ASN:HB3	2.45	0.47
1:E:285:LEU:HD12	1:F:127:ARG:HB2	1.96	0.47
1:C:150:GLY:HA2	1:C:173:ASN:O	2.15	0.47
1:F:305:ALA:O	1:F:309:ILE:HG12	2.14	0.47
1:E:4:LYS:HA	1:E:24:GLU:HB3	1.97	0.47
1:B:9:ARG:HH21	1:B:33:GLU:HA	1.79	0.47
1:D:184:LYS:O	1:D:188:GLU:HG3	2.15	0.46
1:A:70:ILE:HD13	1:A:308:LEU:HD23	1.98	0.46
1:C:139:HIS:HA	1:C:140:PRO:HD3	1.83	0.46
1:C:224:GLU:HG2	1:C:228:LYS:HE2	1.98	0.46
1:C:47:ASP:HB3	1:C:333:PHE:CD2	2.49	0.46
1:B:37:GLU:CD	1:B:37:GLU:N	2.68	0.46
1:B:224:GLU:CG	1:B:228:LYS:HE3	2.44	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:PRO:O	1:B:98:ASP:HB2	2.15	0.46
1:C:244:VAL:HG12	1:C:244:VAL:O	2.14	0.46
1:A:239:ILE:H	1:A:239:ILE:HD13	1.80	0.46
1:F:39:LEU:C	1:F:41:LYS:H	2.18	0.46
1:A:226:ARG:HH11	1:A:226:ARG:CG	2.28	0.46
1:F:138:TRP:CZ3	1:F:140:PRO:HG3	2.49	0.46
1:F:83:ILE:HG23	1:F:322:ASN:HB3	1.97	0.46
1:E:13:GLU:HG3	1:E:17:LYS:HE3	1.97	0.46
1:F:13:GLU:O	1:F:16:ILE:N	2.48	0.46
1:D:275:GLU:HG2	1:D:279:LYS:HE3	1.97	0.46
3:B:402:NAP:H51A	4:B:511:HOH:O	2.16	0.46
1:D:108:ALA:HA	1:D:239:ILE:HG21	1.97	0.46
1:E:98:ASP:OD1	1:E:160:ARG:HD2	2.16	0.46
1:A:202:LEU:O	1:A:230:MET:HA	2.16	0.46
1:C:146:TYR:CE2	1:C:260:ALA:HB1	2.50	0.46
1:B:236:LEU:O	1:B:262:ALA:HA	2.16	0.46
1:C:72:ALA:HB1	1:C:304:VAL:HG13	1.98	0.46
1:E:143:PHE:CE2	1:F:287:PRO:HG3	2.50	0.46
1:B:283:VAL:HG12	1:B:285:LEU:CD2	2.45	0.46
1:C:285:LEU:O	1:D:123:ASP:HA	2.16	0.46
1:D:38:ILE:O	1:D:42:LYS:HG2	2.16	0.46
1:D:256:GLU:HG2	1:D:258:TRP:HE1	1.81	0.45
1:F:4:LYS:HE3	1:F:24:GLU:OE2	2.16	0.45
1:C:53:LEU:HD21	1:C:75:ALA:HB1	1.98	0.45
1:D:75:ALA:HB1	2:D:510:SO4:O1	2.17	0.45
1:C:138:TRP:HZ3	1:C:140:PRO:HG3	1.81	0.45
1:E:224:GLU:O	1:E:228:LYS:HG3	2.17	0.45
1:B:49:LEU:HD23	1:B:50:VAL:H	1.81	0.45
1:F:93:VAL:CB	1:F:322:ASN:HD21	2.29	0.45
1:E:36:ARG:NH1	1:E:36:ARG:HG3	2.32	0.45
1:E:59:LYS:HE3	1:E:63:GLU:OE1	2.16	0.45
1:B:28:TRP:CZ3	1:B:38:ILE:HG21	2.51	0.45
1:B:36:ARG:CD	1:B:56:ARG:HH21	2.25	0.45
1:F:291:SER:OG	1:F:297:ARG:NH1	2.50	0.45
1:B:5:VAL:HB	1:B:23:PHE:CD2	2.52	0.45
1:D:112:LEU:HD23	1:D:112:LEU:C	2.37	0.45
1:D:153:ILE:HD12	1:D:155:ILE:HG13	1.99	0.45
1:C:232:LYS:HA	1:C:258:TRP:O	2.17	0.45
1:F:34:ILE:HD13	1:F:39:LEU:HD13	1.99	0.45
1:F:107:LEU:CD2	1:F:290:GLY:HA2	2.46	0.45
1:D:21:ASP:OD2	1:D:22:GLU:HG2	2.16	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:GLU:HG3	1:E:258:TRP:CH2	2.52	0.45
1:E:7:ILE:HB	1:E:27:VAL:HG22	1.99	0.45
1:B:11:ILE:HB	1:B:12:PRO:HD2	1.98	0.45
1:E:194:GLU:OE2	1:E:196:LYS:HE3	2.15	0.45
1:F:296:ALA:O	1:F:300:MET:HG3	2.16	0.45
1:F:255:LYS:HG2	1:F:280:LEU:HD21	1.99	0.45
1:C:221:LEU:O	1:C:226:ARG:NH1	2.50	0.45
1:E:38:ILE:HA	1:E:41:LYS:HE2	1.99	0.45
1:E:5:VAL:HG23	1:E:48:ALA:C	2.38	0.45
1:E:186:GLU:N	1:E:186:GLU:OE2	2.50	0.45
1:F:75:ALA:HB1	2:F:512:SO4:O2	2.17	0.45
1:A:185:GLU:HB3	1:C:20:GLU:CD	2.38	0.45
1:D:286:THR:HB	1:D:289:ILE:HD12	1.95	0.45
1:F:22:GLU:HG3	1:F:309:ILE:HD12	1.99	0.45
1:B:6:PHE:O	1:B:49:LEU:HD23	2.16	0.45
1:C:14:VAL:O	1:C:18:MET:HG3	2.17	0.45
1:A:5:VAL:CG1	1:A:25:VAL:HG22	2.46	0.45
1:E:323:ARG:O	1:E:326:ILE:HG12	2.16	0.45
1:B:316:ILE:N	1:B:316:ILE:HD12	2.19	0.45
1:C:53:LEU:HD22	1:C:241:ARG:NH2	2.31	0.45
1:F:316:ILE:N	1:F:316:ILE:CD1	2.80	0.45
1:B:8:THR:HG1	1:B:51:THR:HA	1.81	0.45
1:F:210:LEU:O	1:F:239:ILE:HD13	2.17	0.45
1:D:330:LYS:NZ	1:D:330:LYS:HB2	2.32	0.45
1:D:5:VAL:CG1	1:D:25:VAL:HG22	2.47	0.45
1:F:246:ASP:HB3	1:F:249:ALA:HB3	1.99	0.44
1:D:94:THR:HG22	1:D:319:THR:O	2.17	0.44
1:F:6:PHE:O	1:F:49:LEU:HD23	2.17	0.44
1:C:226:ARG:NH1	1:C:226:ARG:HG3	2.28	0.44
1:F:3:PRO:HB2	1:F:23:PHE:CD2	2.52	0.44
1:F:35:PRO:O	1:F:37:GLU:N	2.51	0.44
1:E:184:LYS:CD	1:E:187:VAL:HG21	2.47	0.44
1:E:63:GLU:N	1:E:89:ARG:HH12	2.15	0.44
1:B:149:TYR:HE2	4:B:522:HOH:O	2.00	0.44
1:B:64:ASN:H	1:B:64:ASN:HD22	1.60	0.44
1:C:149:TYR:CD2	1:D:168:ARG:NH2	2.85	0.44
1:A:152:THR:HG22	1:A:205:SER:HA	1.99	0.44
1:E:281:ASP:C	1:E:283:VAL:H	2.21	0.44
1:E:112:LEU:O	1:E:112:LEU:HD23	2.18	0.44
1:E:28:TRP:HE3	1:E:28:TRP:HA	1.82	0.44
1:F:222:ILE:HB	1:F:245:VAL:HG22	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:TYR:CE1	1:A:233:THR:HB	2.53	0.44
1:C:75:ALA:O	1:C:96:THR:N	2.46	0.44
1:F:57:ILE:HD13	1:F:81:ILE:HG12	2.00	0.44
1:A:184:LYS:O	1:A:188:GLU:HG3	2.17	0.44
1:A:275:GLU:O	1:A:279:LYS:HG3	2.17	0.44
1:A:157:GLY:HA3	1:A:212:VAL:HG12	1.99	0.44
1:A:8:THR:OG1	1:A:51:THR:HA	2.17	0.44
1:F:63:GLU:HG2	1:F:89:ARG:NH2	2.32	0.44
1:C:36:ARG:HH22	1:C:58:ASP:CG	2.20	0.44
1:C:291:SER:C	1:C:297:ARG:NH1	2.71	0.44
1:B:156:ILE:CD1	1:B:201:LEU:HD22	2.41	0.44
1:D:6:PHE:HB3	1:D:49:LEU:HD23	2.00	0.44
1:B:69:ARG:HD3	1:B:332:GLY:O	2.17	0.44
1:B:188:GLU:O	1:B:192:ASN:N	2.51	0.44
1:B:256:GLU:HG2	1:B:258:TRP:NE1	2.32	0.44
1:F:147:ASP:O	1:F:151:LYS:HG3	2.17	0.44
1:D:19:LEU:HD21	1:D:305:ALA:HA	1.98	0.44
1:F:330:LYS:HB3	1:F:330:LYS:HZ2	1.81	0.44
1:B:93:VAL:HB	1:B:322:ASN:ND2	2.33	0.44
1:D:235:ILE:HG22	1:D:237:ILE:HD12	2.00	0.44
1:E:252:LYS:O	1:E:256:GLU:HB2	2.18	0.44
1:B:5:VAL:HG13	1:B:5:VAL:O	2.18	0.44
1:F:92:TYR:OH	1:F:331:PRO:HD3	2.18	0.44
1:F:158:LEU:HD22	1:F:178:TYR:CG	2.53	0.44
1:B:75:ALA:O	1:B:95:ASN:HB2	2.18	0.43
1:B:241:ARG:NH2	2:B:509:SO4:O2	2.46	0.43
1:C:252:LYS:O	1:C:256:GLU:HB2	2.18	0.43
1:C:247:THR:HG21	1:C:272:TYR:OH	2.17	0.43
1:E:9:ARG:NH2	1:E:33:GLU:HA	2.33	0.43
1:C:291:SER:OG	1:C:297:ARG:NH1	2.51	0.43
1:B:250:LEU:O	1:B:254:LEU:HG	2.18	0.43
1:E:201:LEU:HD23	1:E:201:LEU:C	2.39	0.43
1:F:242:GLY:HA3	1:F:267:PHE:C	2.39	0.43
1:D:2:LYS:N	1:D:3:PRO:HD2	2.33	0.43
1:F:226:ARG:HA	1:F:229:LEU:HD12	2.00	0.43
1:E:168:ARG:CG	1:E:168:ARG:HH11	2.27	0.43
1:F:6:PHE:HD1	1:F:26:GLU:HB3	1.84	0.43
1:A:139:HIS:HB3	1:A:142:TRP:CD1	2.53	0.43
1:C:161:ILE:O	1:C:165:ILE:HG12	2.18	0.43
1:D:9:ARG:HH21	1:D:33:GLU:HG3	1.83	0.43
1:C:144:LEU:HD22	1:C:144:LEU:N	2.34	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:323:ARG:C	1:F:325:VAL:H	2.22	0.43
1:E:317:PRO:HA	1:E:318:PRO:HD3	1.86	0.43
1:E:139:HIS:HB3	1:E:142:TRP:CG	2.53	0.43
1:D:275:GLU:O	1:D:279:LYS:HG3	2.19	0.43
1:B:100:LEU:HD23	1:B:300:MET:SD	2.57	0.43
1:C:65:ALA:HB1	1:C:68:LEU:HB2	2.00	0.43
1:F:65:ALA:HB1	1:F:68:LEU:HB2	1.99	0.43
1:D:184:LYS:HE2	1:D:186:GLU:CB	2.47	0.43
1:E:36:ARG:HH11	1:E:36:ARG:HG3	1.83	0.43
1:A:210:LEU:O	1:A:239:ILE:HD13	2.19	0.43
1:A:6:PHE:HB3	1:A:49:LEU:HD23	2.01	0.43
1:F:223:ASN:OD1	1:F:226:ARG:HG2	2.18	0.43
1:A:16:ILE:O	1:A:20:GLU:HG2	2.19	0.43
1:F:7:ILE:HA	1:F:50:VAL:HB	2.01	0.43
1:F:315:GLU:O	1:F:331:PRO:HB2	2.18	0.43
1:D:251:VAL:HG22	1:D:277:LEU:HD13	2.00	0.43
1:D:11:ILE:CD1	1:D:16:ILE:HD11	2.49	0.43
1:E:239:ILE:C	1:E:239:ILE:HD12	2.39	0.43
1:C:141:LYS:HA	1:C:144:LEU:HD21	1.99	0.43
1:A:59:LYS:HE2	1:A:85:GLU:OE2	2.19	0.43
1:E:140:PRO:O	1:E:144:LEU:HD11	2.19	0.43
1:E:292:ALA:HB1	1:F:143:PHE:O	2.19	0.43
1:F:9:ARG:NH2	1:F:33:GLU:HG3	2.34	0.43
1:B:47:ASP:OD1	1:B:67:LYS:HE2	2.18	0.43
1:E:224:GLU:HG3	1:E:258:TRP:HH2	1.84	0.43
1:F:2:LYS:N	1:F:3:PRO:CD	2.78	0.43
1:F:317:PRO:HA	1:F:318:PRO:HD3	1.85	0.43
1:F:224:GLU:O	1:F:228:LYS:HG3	2.19	0.43
1:D:50:VAL:HA	1:D:72:ALA:O	2.18	0.43
1:E:213:PRO:HD2	3:E:405:NAP:H8A	2.01	0.43
1:A:13:GLU:OE2	1:A:16:ILE:HB	2.19	0.43
1:E:40:LEU:HD11	1:E:60:GLU:CD	2.38	0.43
1:D:69:ARG:HD2	1:D:332:GLY:O	2.19	0.43
1:B:223:ASN:O	1:B:227:LEU:HG	2.19	0.43
1:D:312:LYS:C	1:D:314:GLY:H	2.22	0.42
1:A:175:ARG:CZ	1:A:177:LEU:HD21	2.49	0.42
1:C:108:ALA:HA	1:C:239:ILE:HG21	2.00	0.42
1:F:202:LEU:CD1	1:F:226:ARG:HB3	2.47	0.42
1:C:222:ILE:HD12	1:C:222:ILE:N	2.34	0.42
1:B:283:VAL:HG12	1:B:285:LEU:HD21	2.01	0.42
1:A:239:ILE:HG12	1:A:239:ILE:O	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:VAL:CG2	1:F:32:LYS:HG2	2.49	0.42
1:C:94:THR:HG21	1:C:317:PRO:HB3	2.00	0.42
1:D:44:LYS:HD2	1:D:64:ASN:O	2.19	0.42
1:D:290:GLY:HA3	3:D:404:NAP:O7N	2.20	0.42
1:E:137:ALA:HB2	1:F:270:GLU:O	2.19	0.42
1:D:195:PHE:C	1:D:195:PHE:CD1	2.91	0.42
1:F:34:ILE:HD11	1:F:39:LEU:HA	2.00	0.42
1:D:175:ARG:HG2	1:D:175:ARG:NH1	2.34	0.42
1:F:262:ALA:O	1:F:283:VAL:HA	2.19	0.42
1:F:120:VAL:HG21	1:F:284:VAL:HG13	2.01	0.42
1:E:272:TYR:CE2	1:E:274:ASN:HB2	2.54	0.42
1:B:139:HIS:HB3	1:B:142:TRP:CG	2.55	0.42
1:F:327:LYS:HG2	1:F:328:ILE:N	2.33	0.42
1:F:166:ALA:HB3	1:F:191:LEU:HD13	2.01	0.42
1:A:250:LEU:O	1:A:254:LEU:HG	2.19	0.42
1:C:114:ALA:HA	1:C:119:VAL:HG23	2.01	0.42
2:C:508:SO4:O3	3:C:403:NAP:C5N	2.67	0.42
1:A:144:LEU:HB3	1:B:294:PHE:CE1	2.55	0.42
1:E:327:LYS:HD3	1:E:328:ILE:CD1	2.46	0.42
1:F:39:LEU:O	1:F:41:LYS:N	2.52	0.42
1:D:36:ARG:O	1:D:40:LEU:HG	2.20	0.42
1:E:324:GLU:O	1:E:324:GLU:HG2	2.20	0.42
1:C:181:ARG:NH2	3:C:403:NAP:O1X	2.53	0.42
1:C:39:LEU:O	1:C:43:VAL:HG22	2.20	0.42
1:F:1:MET:HA	1:F:22:GLU:C	2.40	0.42
1:F:235:ILE:HA	1:F:261:GLY:O	2.20	0.42
1:B:201:LEU:HD23	1:B:201:LEU:C	2.40	0.42
1:F:175:ARG:HH12	1:F:177:LEU:HD21	1.84	0.42
1:D:59:LYS:HG2	1:D:63:GLU:OE1	2.20	0.42
1:D:328:ILE:HD12	1:D:328:ILE:N	2.35	0.42
1:F:53:LEU:CD1	1:F:75:ALA:HB2	2.49	0.42
1:C:185:GLU:N	1:C:185:GLU:OE2	2.39	0.42
1:F:35:PRO:C	1:F:37:GLU:H	2.22	0.42
1:C:242:GLY:HA3	1:C:267:PHE:C	2.40	0.42
1:E:236:LEU:O	1:E:262:ALA:HA	2.20	0.42
1:C:53:LEU:HD21	1:C:75:ALA:CB	2.50	0.42
1:B:8:THR:HG21	1:B:51:THR:HG22	2.02	0.42
1:D:221:LEU:O	1:D:221:LEU:HD23	2.20	0.42
1:D:179:TYR:HD2	1:D:198:LEU:HD13	1.85	0.41
1:B:64:ASN:N	1:B:64:ASN:ND2	2.61	0.41
1:A:307:ASN:HA	1:A:318:PRO:HD2	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ARG:NH2	1:C:33:GLU:HA	2.35	0.41
1:F:62:PHE:O	1:F:89:ARG:NH1	2.53	0.41
1:C:97:PRO:O	1:C:99:VAL:N	2.42	0.41
1:B:199:GLU:OE1	1:B:203:ARG:CZ	2.68	0.41
1:E:256:GLU:CB	1:E:258:TRP:HE1	2.31	0.41
1:D:161:ILE:HG13	3:D:404:NAP:O2N	2.20	0.41
1:D:70:ILE:HG12	1:D:71:VAL:N	2.35	0.41
1:D:221:LEU:HD22	1:D:222:ILE:HD12	2.02	0.41
1:C:134:ARG:HD2	1:C:142:TRP:HH2	1.85	0.41
1:F:275:GLU:CG	1:F:279:LYS:HE3	2.48	0.41
1:F:139:HIS:HA	1:F:140:PRO:HD3	1.91	0.41
1:E:33:GLU:HG2	1:E:54:SER:HB3	2.02	0.41
1:D:103:ALA:HB2	1:D:296:ALA:HB2	2.02	0.41
1:C:191:LEU:O	1:C:192:ASN:HB3	2.20	0.41
1:C:197:PRO:HD2	1:C:200:ASP:OD2	2.20	0.41
1:E:12:PRO:O	1:E:14:VAL:N	2.54	0.41
1:C:138:TRP:CZ2	1:D:297:ARG:CZ	3.04	0.41
1:A:17:LYS:HA	1:A:20:GLU:HG3	2.02	0.41
1:D:51:THR:HG21	1:D:57:ILE:HG12	2.02	0.41
1:A:9:ARG:HH21	1:A:33:GLU:HA	1.85	0.41
1:E:195:PHE:CD1	1:E:195:PHE:C	2.93	0.41
1:F:63:GLU:HG2	1:F:89:ARG:HH22	1.85	0.41
1:D:247:THR:O	1:D:251:VAL:HG23	2.20	0.41
1:D:53:LEU:C	1:D:53:LEU:HD12	2.40	0.41
1:B:47:ASP:HB3	1:B:333:PHE:HD2	1.84	0.41
1:E:70:ILE:O	1:E:70:ILE:HG23	2.20	0.41
1:A:141:LYS:HD2	1:B:10:GLU:HG2	2.01	0.41
1:E:57:ILE:HB	1:E:81:ILE:HG12	2.03	0.41
1:B:244:VAL:O	1:B:244:VAL:HG12	2.21	0.41
1:A:278:PHE:N	1:A:278:PHE:CD1	2.88	0.41
1:A:87:THR:HG23	1:A:325:VAL:CB	2.50	0.41
1:C:247:THR:O	1:C:251:VAL:HG23	2.20	0.41
1:E:278:PHE:CD1	1:E:278:PHE:N	2.88	0.41
1:D:278:PHE:N	1:D:278:PHE:CD1	2.88	0.41
1:E:36:ARG:NE	1:E:56:ARG:HH21	2.19	0.41
1:F:197:PRO:HD2	1:F:200:ASP:OD2	2.21	0.41
1:B:126:VAL:HG22	1:B:131:TRP:CE3	2.55	0.41
1:A:107:LEU:HD22	1:A:290:GLY:CA	2.43	0.41
1:D:217:GLU:HG3	3:D:404:NAP:N6A	2.34	0.41
1:F:57:ILE:CD1	1:F:57:ILE:N	2.84	0.41
1:C:75:ALA:HB1	2:C:508:SO4:O2	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:ASN:O	1:E:275:GLU:C	2.59	0.41
1:F:13:GLU:O	1:F:14:VAL:C	2.59	0.41
1:E:139:HIS:CD2	1:E:141:LYS:HB2	2.56	0.41
1:C:300:MET:O	1:C:304:VAL:HG23	2.21	0.41
1:D:95:ASN:OD1	1:D:97:PRO:HD3	2.21	0.41
1:B:9:ARG:NH2	1:B:33:GLU:HA	2.36	0.41
1:B:33:GLU:H	1:B:33:GLU:CD	2.24	0.41
1:F:254:LEU:HD13	1:F:283:VAL:CG2	2.51	0.41
1:E:14:VAL:O	1:E:18:MET:HG3	2.21	0.41
1:E:156:ILE:HD12	1:E:210:LEU:HD23	2.03	0.41
1:F:93:VAL:CG2	1:F:322:ASN:HD21	2.34	0.41
1:C:120:VAL:HG21	1:C:284:VAL:HG13	2.03	0.41
1:D:210:LEU:O	1:D:239:ILE:CD1	2.70	0.41
1:F:62:PHE:HB3	1:F:89:ARG:HD2	2.02	0.41
1:F:155:ILE:O	1:F:178:TYR:HA	2.21	0.41
1:C:122:GLY:O	1:C:125:PHE:HB3	2.21	0.41
1:E:223:ASN:O	1:E:227:LEU:HG	2.21	0.41
1:F:244:VAL:O	1:F:244:VAL:HG12	2.21	0.41
1:D:139:HIS:HA	1:D:140:PRO:HD3	1.97	0.40
1:D:57:ILE:HD12	1:D:57:ILE:N	2.36	0.40
1:C:275:GLU:O	1:C:279:LYS:HG3	2.21	0.40
1:B:121:LYS:HD3	1:B:281:ASP:HB3	2.03	0.40
1:E:240:ALA:HA	3:E:405:NAP:H1D	2.04	0.40
1:E:107:LEU:CD2	1:E:289:ILE:HG13	2.52	0.40
1:C:64:ASN:ND2	1:C:64:ASN:N	2.68	0.40
1:A:32:LYS:O	1:A:33:GLU:O	2.39	0.40
1:C:244:VAL:CG1	1:C:244:VAL:O	2.69	0.40
1:C:36:ARG:NH2	1:C:58:ASP:OD1	2.46	0.40
1:A:4:LYS:HG2	1:A:24:GLU:OE2	2.20	0.40
1:C:2:LYS:HZ2	1:C:2:LYS:HB3	1.87	0.40
1:D:181:ARG:HB3	3:D:404:NAP:O3X	2.21	0.40
1:A:158:LEU:HD22	1:A:178:TYR:CD2	2.56	0.40
1:C:292:ALA:N	1:C:297:ARG:NH1	2.69	0.40
1:E:244:VAL:HG12	1:E:244:VAL:O	2.21	0.40
1:B:129:GLY:HA2	4:B:514:HOH:O	2.22	0.40
1:A:113:LEU:HD23	1:A:148:VAL:HG21	2.04	0.40
1:C:132:LYS:HA	1:D:271:PRO:HB2	2.02	0.40
1:E:199:GLU:HG3	1:E:229:LEU:HD11	2.04	0.40
1:F:9:ARG:HG2	1:F:9:ARG:HH11	1.87	0.40
1:A:287:PRO:HD3	1:B:126:VAL:HG23	2.03	0.40
1:E:287:PRO:HD3	1:F:122:GLY:O	2.22	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ARG:HH22	1:A:58:ASP:CG	2.24	0.40
1:D:156:ILE:HD12	1:D:198:LEU:CD1	2.51	0.40
1:A:11:ILE:HB	1:A:12:PRO:CD	2.51	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	331/334 (99%)	299 (90%)	29 (9%)	3 (1%)	21	41
1	B	331/334 (99%)	299 (90%)	28 (8%)	4 (1%)	16	32
1	C	331/334 (99%)	303 (92%)	25 (8%)	3 (1%)	21	41
1	D	331/334 (99%)	306 (92%)	24 (7%)	1 (0%)	46	70
1	E	331/334 (99%)	297 (90%)	30 (9%)	4 (1%)	16	32
1	F	331/334 (99%)	292 (88%)	30 (9%)	9 (3%)	6	10
All	All	1986/2004 (99%)	1796 (90%)	166 (8%)	24 (1%)	16	32

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	GLU
1	F	240	ALA
1	B	329	ARG
1	C	98	ASP
1	C	137	ALA
1	E	13	GLU
1	F	243	LYS
1	A	198	LEU
1	B	54	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	278	PHE
1	E	22	GLU
1	E	275	GLU
1	F	37	GLU
1	F	40	LEU
1	B	12	PRO
1	E	43	VAL
1	F	2	LYS
1	F	224	GLU
1	C	2	LYS
1	D	37	GLU
1	F	33	GLU
1	F	14	VAL
1	F	12	PRO
1	A	43	VAL

### 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	282/283 (100%)	267 (95%)	15 (5%)	28	52	
1	B	282/283 (100%)	265 (94%)	17 (6%)	24	45	
1	C	282/283 (100%)	272 (96%)	10 (4%)	43	70	
1	D	282/283 (100%)	269 (95%)	13 (5%)	33	60	
1	E	282/283 (100%)	270 (96%)	12 (4%)	35	63	
1	F	282/283 (100%)	268 (95%)	14 (5%)	30	55	
All	All	1692/1698 (100%)	1611 (95%)	81 (5%)	31	57	

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	100	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	109	PHE
1	A	130	GLU
1	A	134	ARG
1	A	185	GLU
1	A	189	ARG
1	A	199	GLU
1	A	203	ARG
1	A	216	ARG
1	A	220	HIS
1	A	239	ILE
1	A	269	GLU
1	A	293	SER
1	B	2	LYS
1	B	11	ILE
1	B	12	PRO
1	B	37	GLU
1	B	45	GLU
1	B	49	LEU
1	B	64	ASN
1	B	83	ILE
1	B	84	GLU
1	B	100	LEU
1	B	109	PHE
1	B	133	LYS
1	B	168	ARG
1	B	174	MET
1	B	217	GLU
1	B	275	GLU
1	B	285	LEU
1	C	2	LYS
1	C	64	ASN
1	C	70	ILE
1	C	100	LEU
1	C	109	PHE
1	C	153	ILE
1	C	189	ARG
1	C	217	GLU
1	C	226	ARG
1	C	256	GLU
1	D	1	MET
1	D	11	ILE
1	D	17	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	94	THR
1	D	109	PHE
1	D	134	ARG
1	D	153	ILE
1	D	239	ILE
1	D	259	ILE
1	D	281	ASP
1	D	289	ILE
1	D	293	SER
1	D	330	LYS
1	E	2	LYS
1	E	49	LEU
1	E	53	LEU
1	E	70	ILE
1	E	100	LEU
1	E	109	PHE
1	E	189	ARG
1	E	221	LEU
1	E	225	GLU
1	E	256	GLU
1	E	285	LEU
1	E	293	SER
1	F	11	ILE
1	F	30	ASP
1	F	37	GLU
1	F	49	LEU
1	F	53	LEU
1	F	61	VAL
1	F	100	LEU
1	F	109	PHE
1	F	184	LYS
1	F	203	ARG
1	F	239	ILE
1	F	304	VAL
1	F	324	GLU
1	F	330	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	139	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	64	ASN
1	B	248	ASN
1	B	322	ASN
1	C	64	ASN
1	C	139	HIS
1	C	223	ASN
1	D	139	HIS
1	E	139	HIS
1	F	64	ASN
1	F	139	HIS
1	F	220	HIS
1	F	274	ASN
1	F	322	ASN

### 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](#)

18 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	$\# Z  > 2$
3	NAP	A	401	-	42,52,52	1.09	3 (7%)	54,80,80	1.78	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	501	-	4,4,4	0.91	0	6,6,6	0.09	0
2	SO4	A	507	-	4,4,4	0.90	0	6,6,6	0.07	0
3	NAP	B	402	-	42,52,52	1.08	3 (7%)	54,80,80	2.08	8 (14%)
2	SO4	B	503	-	4,4,4	0.91	0	6,6,6	0.08	0
2	SO4	B	509	-	4,4,4	0.91	0	6,6,6	0.11	0
3	NAP	C	403	-	42,52,52	1.11	3 (7%)	54,80,80	1.79	7 (12%)
2	SO4	C	502	-	4,4,4	0.91	0	6,6,6	0.09	0
2	SO4	C	508	-	4,4,4	0.90	0	6,6,6	0.06	0
3	NAP	D	404	-	42,52,52	1.07	3 (7%)	54,80,80	1.93	9 (16%)
2	SO4	D	504	-	4,4,4	0.91	0	6,6,6	0.07	0
2	SO4	D	510	-	4,4,4	0.91	0	6,6,6	0.08	0
3	NAP	E	405	-	42,52,52	1.11	5 (11%)	54,80,80	1.82	6 (11%)
2	SO4	E	505	-	4,4,4	0.91	0	6,6,6	0.07	0
2	SO4	E	511	-	4,4,4	0.91	0	6,6,6	0.08	0
3	NAP	F	406	-	42,52,52	1.10	3 (7%)	54,80,80	1.90	6 (11%)
2	SO4	F	506	-	4,4,4	0.91	0	6,6,6	0.08	0
2	SO4	F	512	-	4,4,4	0.91	0	6,6,6	0.08	0

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	NAP	A	401	-	-	0/27/67/67	0/5/5/5
2	SO4	A	501	-	-	0/0/0/0	0/0/0/0
2	SO4	A	507	-	-	0/0/0/0	0/0/0/0
3	NAP	B	402	-	-	0/27/67/67	0/5/5/5
2	SO4	B	503	-	-	0/0/0/0	0/0/0/0
2	SO4	B	509	-	-	0/0/0/0	0/0/0/0
3	NAP	C	403	-	-	0/27/67/67	0/5/5/5
2	SO4	C	502	-	-	0/0/0/0	0/0/0/0
2	SO4	C	508	-	-	0/0/0/0	0/0/0/0
3	NAP	D	404	-	-	0/27/67/67	0/5/5/5
2	SO4	D	504	-	-	0/0/0/0	0/0/0/0
2	SO4	D	510	-	-	0/0/0/0	0/0/0/0
3	NAP	E	405	-	-	0/27/67/67	0/5/5/5
2	SO4	E	505	-	-	0/0/0/0	0/0/0/0
2	SO4	E	511	-	-	0/0/0/0	0/0/0/0
3	NAP	F	406	-	-	0/27/67/67	0/5/5/5
2	SO4	F	506	-	-	0/0/0/0	0/0/0/0
2	SO4	F	512	-	-	0/0/0/0	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	405	NAP	C6N-N1N	2.02	1.40	1.35
3	E	405	NAP	C3N-C7N	2.04	1.53	1.50
3	B	402	NAP	O4B-C1B	2.24	1.44	1.41
3	A	401	NAP	O4B-C1B	2.28	1.44	1.41
3	D	404	NAP	O4D-C1D	2.35	1.44	1.41
3	D	404	NAP	O4B-C1B	2.35	1.44	1.41
3	F	406	NAP	O4D-C1D	2.43	1.44	1.41
3	F	406	NAP	O4B-C1B	2.46	1.44	1.41
3	A	401	NAP	O4D-C1D	2.47	1.44	1.41
3	E	405	NAP	O4B-C1B	2.53	1.44	1.41
3	E	405	NAP	O4D-C1D	2.59	1.44	1.41
3	B	402	NAP	O4D-C1D	2.62	1.44	1.41
3	C	403	NAP	O4B-C1B	2.62	1.44	1.41
3	C	403	NAP	O4D-C1D	2.64	1.44	1.41
3	C	403	NAP	P2B-O1X	3.08	1.61	1.51
3	E	405	NAP	P2B-O1X	3.08	1.61	1.51
3	A	401	NAP	P2B-O1X	3.13	1.61	1.51
3	B	402	NAP	P2B-O1X	3.14	1.61	1.51
3	F	406	NAP	P2B-O1X	3.16	1.61	1.51
3	D	404	NAP	P2B-O1X	3.16	1.61	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NAP	N3A-C2A-N1A	-10.25	121.04	128.89
3	D	404	NAP	N3A-C2A-N1A	-10.24	121.05	128.89
3	E	405	NAP	N3A-C2A-N1A	-10.19	121.09	128.89
3	A	401	NAP	N3A-C2A-N1A	-10.15	121.13	128.89
3	C	403	NAP	N3A-C2A-N1A	-10.11	121.15	128.89
3	F	406	NAP	N3A-C2A-N1A	-9.98	121.26	128.89
3	B	402	NAP	C4B-O4B-C1B	-6.60	102.47	109.72
3	F	406	NAP	C4D-O4D-C1D	-4.95	104.28	109.72
3	D	404	NAP	C4D-O4D-C1D	-4.62	104.64	109.72
3	E	405	NAP	PN-O3-PA	-4.28	120.70	132.73
3	C	403	NAP	PN-O3-PA	-4.24	120.81	132.73
3	F	406	NAP	PN-O3-PA	-4.04	121.38	132.73
3	B	402	NAP	O4B-C1B-C2B	-3.96	99.44	106.60
3	B	402	NAP	PN-O3-PA	-3.81	122.04	132.73
3	D	404	NAP	PN-O3-PA	-3.60	122.61	132.73
3	A	401	NAP	PN-O3-PA	-3.37	123.26	132.73
3	E	405	NAP	C4D-O4D-C1D	-2.88	106.56	109.72
3	D	404	NAP	C4B-O4B-C1B	-2.82	106.62	109.72

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NAP	C4D-O4D-C1D	-2.80	106.65	109.72
3	D	404	NAP	C3B-C2B-C1B	-2.78	97.35	102.73
3	A	401	NAP	C3B-C2B-C1B	-2.65	97.60	102.73
3	E	405	NAP	C3B-C2B-C1B	-2.63	97.64	102.73
3	A	401	NAP	C3N-C7N-N7N	-2.60	114.97	117.82
3	F	406	NAP	C3B-C2B-C1B	-2.56	97.78	102.73
3	A	401	NAP	C4B-O4B-C1B	-2.53	106.93	109.72
3	C	403	NAP	C4D-O4D-C1D	-2.39	107.09	109.72
3	D	404	NAP	O4B-C1B-C2B	-2.39	102.28	106.60
3	B	402	NAP	C4A-C5A-N7A	-2.33	107.33	109.48
3	F	406	NAP	C3N-C7N-N7N	-2.33	115.26	117.82
3	A	401	NAP	O4B-C1B-C2B	-2.32	102.41	106.60
3	C	403	NAP	C3B-C2B-C1B	-2.27	98.33	102.73
3	C	403	NAP	C3N-C7N-N7N	-2.26	115.34	117.82
3	E	405	NAP	C3N-C7N-N7N	-2.17	115.45	117.82
3	E	405	NAP	C4A-C5A-N7A	-2.12	107.53	109.48
3	C	403	NAP	C4A-C5A-N7A	-2.12	107.53	109.48
3	B	402	NAP	C3N-C7N-N7N	-2.12	115.50	117.82
3	D	404	NAP	C4A-C5A-N7A	-2.11	107.54	109.48
3	D	404	NAP	C3N-C7N-N7N	-2.07	115.55	117.82
3	F	406	NAP	O4D-C1D-N1N	2.41	110.78	108.13
3	D	404	NAP	O4D-C1D-N1N	2.44	110.81	108.13
3	C	403	NAP	O4B-C1B-N9A	2.47	113.27	108.10
3	B	402	NAP	O4B-C1B-N9A	2.50	113.33	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAP	3	0
2	A	507	SO4	2	0
3	B	402	NAP	5	0
2	B	509	SO4	4	0
3	C	403	NAP	4	0
2	C	508	SO4	3	0
3	D	404	NAP	7	0
2	D	510	SO4	1	0
3	E	405	NAP	3	0
2	E	511	SO4	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	406	NAP	2	0
2	F	512	SO4	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	333/334 (99%)	-0.12	4 (1%) 81 77	16, 41, 73, 99	0
1	B	333/334 (99%)	0.10	19 (5%) 27 20	16, 47, 97, 107	0
1	C	333/334 (99%)	-0.17	7 (2%) 67 61	19, 42, 75, 91	0
1	D	333/334 (99%)	-0.23	3 (0%) 85 83	21, 46, 77, 98	0
1	E	333/334 (99%)	0.24	21 (6%) 23 17	25, 62, 95, 120	0
1	F	333/334 (99%)	0.32	25 (7%) 17 12	24, 63, 118, 129	0
All	All	1998/2004 (99%)	0.02	79 (3%) 42 35	16, 49, 97, 129	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	8.3
1	E	1	MET	7.2
1	B	328	ILE	6.8
1	A	1	MET	6.7
1	F	1	MET	5.8
1	D	1	MET	4.7
1	E	38	ILE	4.4
1	C	1	MET	4.3
1	F	68	LEU	4.2
1	B	333	PHE	3.6
1	E	45	GLU	3.5
1	E	201	LEU	3.4
1	E	46	VAL	3.4
1	F	48	ALA	3.3
1	B	324	GLU	3.2
1	C	325	VAL	3.2
1	F	324	GLU	3.2
1	B	326	ILE	3.0
1	B	70	ILE	3.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	5	VAL	3.0
1	E	39	LEU	2.9
1	E	65	ALA	2.9
1	B	4	LYS	2.9
1	B	48	ALA	2.8
1	C	328	ILE	2.8
1	E	81	ILE	2.8
1	F	84	GLU	2.8
1	E	34	ILE	2.8
1	B	23	PHE	2.8
1	F	323	ARG	2.8
1	B	325	VAL	2.7
1	B	68	LEU	2.7
1	F	216	ARG	2.7
1	F	186	GLU	2.7
1	F	88	LYS	2.6
1	F	83	ILE	2.6
1	F	327	LYS	2.5
1	A	23	PHE	2.5
1	F	46	VAL	2.5
1	F	93	VAL	2.5
1	B	329	ARG	2.5
1	E	61	VAL	2.5
1	F	329	ARG	2.5
1	F	4	LYS	2.5
1	B	316	ILE	2.5
1	D	198	LEU	2.5
1	E	27	VAL	2.5
1	F	58	ASP	2.5
1	F	45	GLU	2.4
1	E	42	LYS	2.4
1	F	39	LEU	2.4
1	F	65	ALA	2.4
1	B	19	LEU	2.4
1	E	57	ILE	2.4
1	B	43	VAL	2.4
1	B	46	VAL	2.4
1	E	43	VAL	2.3
1	B	69	ARG	2.3
1	B	71	VAL	2.3
1	E	40	LEU	2.3
1	E	58	ASP	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	325	VAL	2.3
1	F	59	LYS	2.2
1	E	62	PHE	2.2
1	E	59	LYS	2.2
1	C	90	GLY	2.2
1	F	333	PHE	2.2
1	E	258	TRP	2.1
1	F	40	LEU	2.1
1	C	333	PHE	2.1
1	E	7	ILE	2.1
1	E	47	ASP	2.1
1	C	324	GLU	2.1
1	F	187	VAL	2.1
1	C	326	ILE	2.1
1	A	67	LYS	2.1
1	F	91	ILE	2.1
1	F	330	LYS	2.0
1	D	329	ARG	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	SO4	E	511	5/5	0.91	0.63	12.44	119,119,120,122	5
2	SO4	D	510	5/5	0.89	0.34	8.82	127,127,128,129	0
2	SO4	A	507	5/5	0.95	0.22	5.07	82,84,89,89	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	509	5/5	0.90	0.33	3.74	92,94,97,97	0
2	SO4	F	512	5/5	0.93	0.26	3.54	114,114,115,115	0
2	SO4	C	508	5/5	0.92	0.19	1.36	92,92,95,95	5
3	NAP	D	404	48/48	0.92	0.17	0.37	54,68,77,82	0
3	NAP	F	406	48/48	0.89	0.19	0.36	64,86,99,102	0
3	NAP	E	405	48/48	0.91	0.18	0.23	65,73,95,96	0
3	NAP	B	402	48/48	0.97	0.16	0.06	23,35,45,48	0
3	NAP	C	403	48/48	0.94	0.15	-0.07	43,53,63,69	0
3	NAP	A	401	48/48	0.96	0.14	-0.07	20,41,55,63	0
2	SO4	D	504	5/5	0.95	0.15	-0.59	72,72,73,77	0
2	SO4	E	505	5/5	0.94	0.14	-0.72	76,76,78,79	0
2	SO4	A	501	5/5	0.98	0.12	-0.86	54,54,55,59	0
2	SO4	C	502	5/5	0.96	0.13	-1.31	49,51,59,60	0
2	SO4	B	503	5/5	0.98	0.09	-2.85	45,53,56,59	0
2	SO4	F	506	5/5	0.96	0.13	-	81,83,84,84	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.