



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 09:17 PM EDT

PDB ID : 2YRF
Title : Crystal structure of 5-methylthioribose 1-phosphate isomerase from *Bacillus subtilis* complexed with sulfate ion
Authors : Tamura, H.; Inoue, T.; Kai, Y.; Matsumura, H.
Deposited on : 2007-04-02
Resolution : 2.70 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.36
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) : 2.36

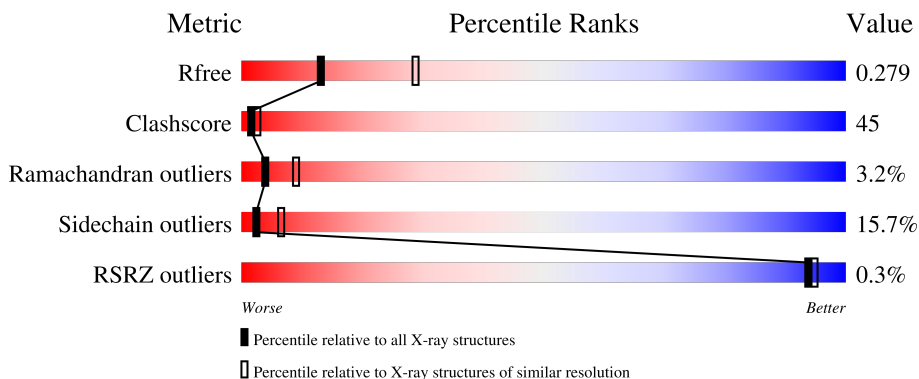
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	374	
1	B	374	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 5365 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 Methylthioribose-1-phosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	Total	C	N	O	S	0	0	0
			2625	1658	445	513	9			
1	B	341	Total	C	N	O	S	0	0	0
			2636	1664	449	514	9			

There are 42 discrepancies between the modelled and reference sequences:

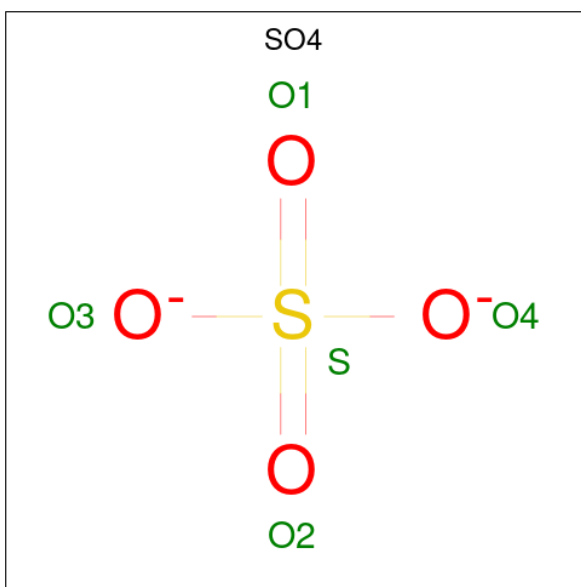
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP O31662
A	-19	GLY	-	expression tag	UNP O31662
A	-18	SER	-	expression tag	UNP O31662
A	-17	SER	-	expression tag	UNP O31662
A	-16	HIS	-	expression tag	UNP O31662
A	-15	HIS	-	expression tag	UNP O31662
A	-14	HIS	-	expression tag	UNP O31662
A	-13	HIS	-	expression tag	UNP O31662
A	-12	HIS	-	expression tag	UNP O31662
A	-11	HIS	-	expression tag	UNP O31662
A	-10	SER	-	expression tag	UNP O31662
A	-9	SER	-	expression tag	UNP O31662
A	-8	GLY	-	expression tag	UNP O31662
A	-7	LEU	-	expression tag	UNP O31662
A	-6	VAL	-	expression tag	UNP O31662
A	-5	PRO	-	expression tag	UNP O31662
A	-4	ARG	-	expression tag	UNP O31662
A	-3	GLY	-	expression tag	UNP O31662
A	-2	SER	-	expression tag	UNP O31662
A	-1	HIS	-	expression tag	UNP O31662
A	0	MET	-	expression tag	UNP O31662
B	-20	MET	-	expression tag	UNP O31662
B	-19	GLY	-	expression tag	UNP O31662
B	-18	SER	-	expression tag	UNP O31662
B	-17	SER	-	expression tag	UNP O31662

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP O31662
B	-15	HIS	-	expression tag	UNP O31662
B	-14	HIS	-	expression tag	UNP O31662
B	-13	HIS	-	expression tag	UNP O31662
B	-12	HIS	-	expression tag	UNP O31662
B	-11	HIS	-	expression tag	UNP O31662
B	-10	SER	-	expression tag	UNP O31662
B	-9	SER	-	expression tag	UNP O31662
B	-8	GLY	-	expression tag	UNP O31662
B	-7	LEU	-	expression tag	UNP O31662
B	-6	VAL	-	expression tag	UNP O31662
B	-5	PRO	-	expression tag	UNP O31662
B	-4	ARG	-	expression tag	UNP O31662
B	-3	GLY	-	expression tag	UNP O31662
B	-2	SER	-	expression tag	UNP O31662
B	-1	HIS	-	expression tag	UNP O31662
B	0	MET	-	expression tag	UNP O31662

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

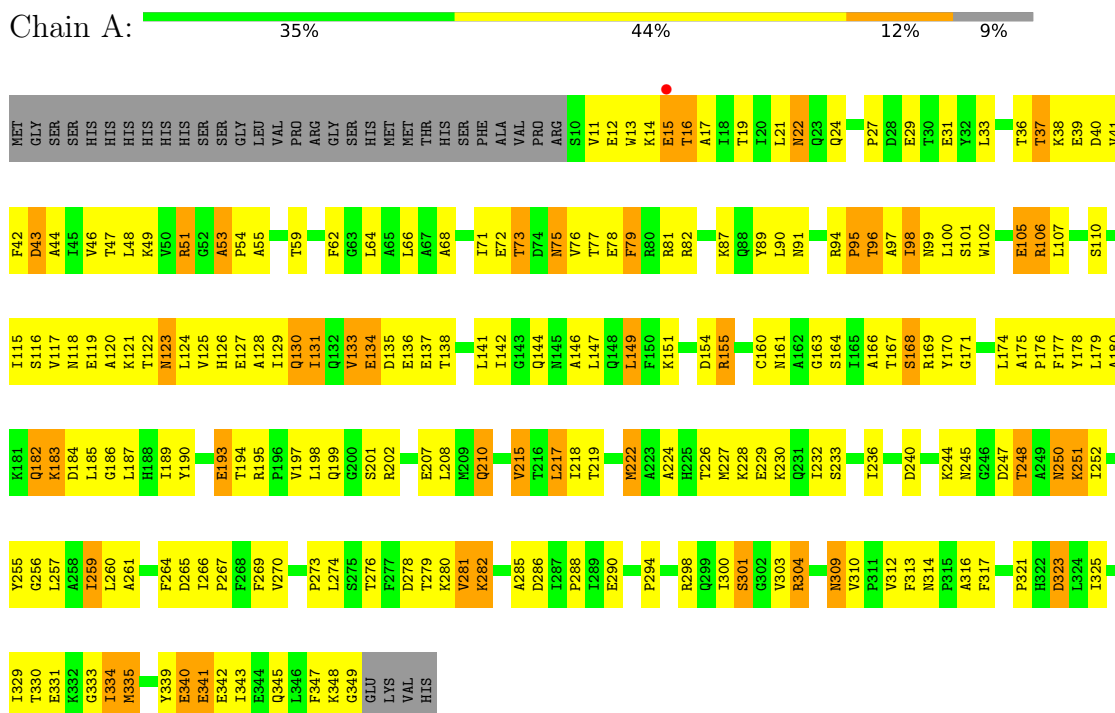
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total 52	O 52	0	0
3	B	42	Total 42	O 42	0	0

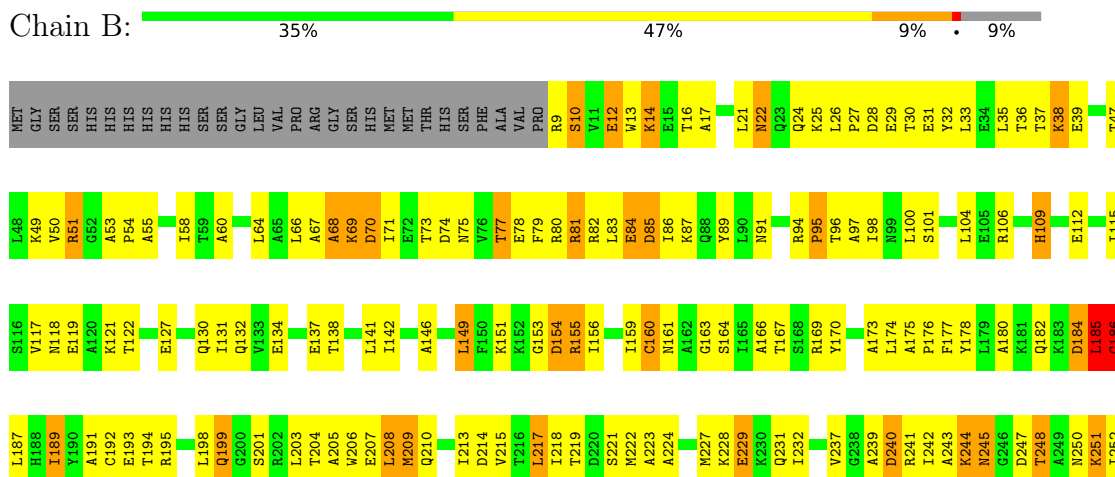
3 Residue-property plots

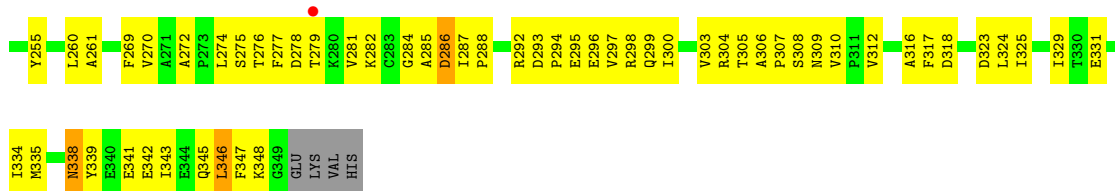
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Methylthioribose-1-phosphate isomerase



- Molecule 1: Methylthioribose-1-phosphate isomerase





4 Data and refinement statistics i

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	69.27Å 69.27Å 154.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.36 – 2.70 41.36 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.5 (41.36-2.70) 93.7 (41.36-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.69Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.284 0.222 , 0.279	Depositor DCC
R_{free} test set	915 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtrriage
Anisotropy	0.018	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 17.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.076 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5365	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.53	1/2667 (0.0%)	0.77	1/3619 (0.0%)
1	B	0.49	0/2678	0.79	3/3633 (0.1%)
All	All	0.51	1/5345 (0.0%)	0.78	4/7252 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	GLY	CA-C	6.03	1.61	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	LEU	CA-CB-CG	13.56	146.49	115.30
1	A	349	GLY	N-CA-C	8.71	134.87	113.10
1	B	14	LYS	N-CA-C	-6.17	94.34	111.00
1	B	186	GLY	N-CA-C	5.11	125.87	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	2625	0	2643	250	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2636	0	2656	244	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
3	A	52	0	0	1	0
3	B	42	0	0	2	0
All	All	5365	0	5299	480	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 45.

All (480) 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:80:ARG:NH2	1:B:112:GLU:HA	1.40	1.33
1:B:80:ARG:HH22	1:B:112:GLU:CA	1.57	1.16
1:A:71:ILE:HD11	1:A:79:PHE:CD2	1.93	1.04
1:B:169:ARG:HD2	1:B:170:TYR:H	1.24	1.02
1:B:37:THR:HG22	1:B:39:GLU:H	1.25	1.02
1:A:71:ILE:HD11	1:A:79:PHE:CE2	1.97	0.99
1:A:22:ASN:HB2	1:A:33:LEU:HD21	1.39	0.98
1:B:338:ASN:ND2	1:B:341:GLU:HG2	1.78	0.97
1:A:183:LYS:NZ	1:A:183:LYS:H	1.62	0.94
1:A:183:LYS:HZ1	1:A:183:LYS:N	1.63	0.94
1:A:194:THR:HG21	1:A:251:LYS:HG2	1.48	0.93
1:B:308:SER:O	1:B:309:ASN:HB3	1.72	0.90
1:B:68:ALA:HB1	1:B:79:PHE:HZ	1.35	0.88
1:B:53:ALA:HB3	1:B:54:PRO:HD3	1.56	0.88
1:A:37:THR:HG23	1:A:39:GLU:OE1	1.74	0.87
1:A:183:LYS:H	1:A:183:LYS:HZ1	1.14	0.87
1:A:68:ALA:O	1:A:71:ILE:HG12	1.75	0.86
1:A:248:THR:HG22	1:A:325:ILE:HD11	1.57	0.86
1:B:278:ASP:OD1	1:B:281:VAL:HG13	1.76	0.86
1:B:22:ASN:HD21	1:B:24:GLN:HG2	1.38	0.86
1:B:169:ARG:HG3	1:B:170:TYR:CD1	2.11	0.86
1:A:183:LYS:HB3	1:A:185:LEU:HD13	1.56	0.86
1:B:80:ARG:HH22	1:B:112:GLU:HA	0.71	0.85
1:A:304:ARG:HH11	1:B:28:ASP:HB3	1.40	0.85
1:B:134:GLU:O	1:B:138:THR:HG23	1.75	0.85
1:B:300:ILE:HG13	1:B:305:THR:HG21	1.59	0.85
1:A:304:ARG:NH1	1:B:28:ASP:HB3	1.92	0.84
1:B:73:THR:HG21	1:B:78:GLU:HB3	1.58	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ASN:ND2	1:B:341:GLU:H	1.75	0.83
1:B:193:GLU:HG2	1:B:219:THR:HA	1.60	0.82
1:B:83:LEU:HD13	1:B:83:LEU:O	1.80	0.81
1:A:343:ILE:HG23	1:A:347:PHE:HD1	1.45	0.81
1:A:37:THR:HG23	1:A:39:GLU:H	1.46	0.81
1:B:22:ASN:ND2	1:B:24:GLN:HG2	1.95	0.81
1:B:80:ARG:NH2	1:B:112:GLU:CA	2.28	0.81
1:B:205:ALA:O	1:B:209:MET:HG3	1.82	0.80
1:A:136:GLU:HG2	1:A:169:ARG:HD3	1.64	0.79
1:A:134:GLU:O	1:A:138:THR:HG23	1.82	0.79
1:A:259:ILE:HD12	1:B:260:LEU:HD12	1.64	0.79
1:A:24:GLN:OE1	1:A:47:THR:HG22	1.83	0.79
1:A:202:ARG:HG2	1:B:305:THR:O	1.83	0.78
1:B:248:THR:HG21	1:B:270:VAL:HG11	1.64	0.78
1:A:248:THR:CG2	1:A:325:ILE:HD11	2.14	0.77
1:A:168:SER:O	1:A:169:ARG:HG3	1.85	0.77
1:A:227:MET:HA	1:A:232:ILE:HG12	1.65	0.77
1:B:244:LYS:HB3	1:B:281:VAL:O	1.85	0.77
1:A:347:PHE:O	1:A:348:LYS:HG3	1.84	0.76
1:A:343:ILE:HG23	1:A:347:PHE:CD1	2.21	0.76
1:B:137:GLU:O	1:B:141:LEU:HD23	1.86	0.76
1:B:201:SER:HB2	1:B:217:LEU:HD11	1.66	0.76
1:B:345:GLN:O	1:B:345:GLN:HG3	1.86	0.76
1:B:9:ARG:HG2	1:B:10:SER:N	2.00	0.75
1:A:98:ILE:HD11	1:A:276:THR:O	1.87	0.75
1:A:125:VAL:O	1:A:129:ILE:HG13	1.87	0.75
1:B:194:THR:O	1:B:198:LEU:HA	1.85	0.75
1:A:129:ILE:O	1:A:133:VAL:HG22	1.87	0.75
1:A:130:GLN:HA	1:A:133:VAL:CG2	2.16	0.74
1:A:183:LYS:HB3	1:A:185:LEU:CD1	2.17	0.74
1:B:208:LEU:HB3	1:B:215:VAL:HG21	1.69	0.73
1:A:224:ALA:HB2	1:A:260:LEU:HD21	1.70	0.73
1:B:169:ARG:HD2	1:B:170:TYR:N	2.01	0.73
1:B:338:ASN:HD22	1:B:341:GLU:HG2	1.49	0.73
1:B:80:ARG:NH1	1:B:112:GLU:O	2.22	0.73
1:B:68:ALA:HB1	1:B:79:PHE:CZ	2.21	0.73
1:A:37:THR:HG22	1:A:40:ASP:H	1.52	0.73
1:B:191:ALA:O	1:B:217:LEU:HD23	1.88	0.72
1:A:22:ASN:HB2	1:A:33:LEU:CD2	2.18	0.72
1:A:130:GLN:O	1:A:133:VAL:HG23	1.90	0.72
1:B:189:ILE:HD11	1:B:208:LEU:CD2	2.20	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ARG:HG2	1:B:198:LEU:HD21	1.72	0.71
1:B:77:THR:O	1:B:81:ARG:HB2	1.91	0.71
1:B:106:ARG:HD2	1:B:131:ILE:HD11	1.73	0.71
1:A:71:ILE:HG13	1:A:71:ILE:O	1.89	0.71
1:B:201:SER:CB	1:B:217:LEU:HD11	2.21	0.70
1:A:91:ASN:HD21	1:A:101:SER:HB3	1.56	0.70
1:B:32:TYR:C	1:B:33:LEU:HD22	2.13	0.70
1:B:223:ALA:O	1:B:227:MET:HG3	1.90	0.70
1:A:71:ILE:CD1	1:A:79:PHE:CD2	2.74	0.69
1:A:255:TYR:O	1:A:259:ILE:HG22	1.92	0.69
1:A:128:ALA:O	1:A:131:ILE:HG22	1.93	0.69
1:B:169:ARG:CD	1:B:170:TYR:H	2.03	0.68
1:A:163:GLY:HA3	1:A:174:LEU:HD12	1.76	0.68
1:A:274:LEU:HD13	1:A:331:GLU:OE1	1.94	0.68
1:A:217:LEU:HD13	1:B:297:VAL:HG12	1.76	0.68
1:B:117:VAL:O	1:B:121:LYS:HB2	1.94	0.68
1:A:300:ILE:O	1:A:303:VAL:HG22	1.93	0.67
1:B:245:ASN:ND2	1:B:247:ASP:H	1.91	0.67
1:A:183:LYS:NZ	1:A:183:LYS:N	2.32	0.67
1:B:37:THR:CG2	1:B:39:GLU:HB2	2.24	0.67
1:B:25:LYS:HG3	1:B:31:GLU:HG2	1.77	0.67
1:B:242:ILE:HG13	1:B:248:THR:HG22	1.76	0.67
1:A:14:LYS:O	1:A:16:THR:N	2.27	0.67
1:A:309:ASN:HD22	1:A:309:ASN:H	1.43	0.66
1:B:293:ASP:O	1:B:296:GLU:HB2	1.95	0.66
1:A:259:ILE:HD13	1:A:259:ILE:C	2.15	0.66
1:A:54:PRO:HG3	1:A:167:THR:HG22	1.76	0.66
1:B:195:ARG:HG2	1:B:198:LEU:CD2	2.25	0.66
1:B:51:ARG:NH2	1:B:166:ALA:HB2	2.11	0.66
1:A:185:LEU:HB3	1:A:187:LEU:HD13	1.76	0.66
1:A:118:ASN:H	1:A:118:ASN:ND2	1.94	0.66
1:A:130:GLN:O	1:A:134:GLU:HG3	1.96	0.66
1:A:178:TYR:OH	1:A:207:GLU:HG3	1.96	0.65
1:B:294:PRO:HB3	1:B:312:VAL:HG22	1.78	0.65
1:A:95:PRO:O	1:A:97:ALA:N	2.29	0.65
1:A:72:GLU:O	1:A:73:THR:HB	1.96	0.65
1:A:137:GLU:O	1:A:141:LEU:HD23	1.97	0.65
1:A:130:GLN:HA	1:A:133:VAL:HG23	1.79	0.65
1:B:153:GLY:HA2	1:B:186:GLY:O	1.97	0.65
1:A:102:TRP:CZ3	1:A:131:ILE:HD11	2.32	0.64
1:B:51:ARG:HB2	2:B:502:SO4:O3	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ALA:HB3	1:B:176:PRO:HD3	1.80	0.64
1:B:244:LYS:O	1:B:244:LYS:HG3	1.97	0.64
1:A:21:LEU:HD12	1:A:31:GLU:O	1.96	0.64
1:B:208:LEU:CB	1:B:215:VAL:HG21	2.28	0.64
1:B:250:ASN:ND2	1:B:251:LYS:H	1.94	0.64
1:B:307:PRO:O	1:B:310:VAL:HG12	1.97	0.64
1:A:149:LEU:CD2	1:A:329:ILE:HD11	2.29	0.63
1:A:119:GLU:HG3	1:A:120:ALA:N	2.12	0.63
1:B:299:GLN:HA	1:B:305:THR:HG23	1.80	0.63
1:A:248:THR:HG21	1:A:270:VAL:HG21	1.80	0.63
1:B:189:ILE:HD11	1:B:208:LEU:HD23	1.81	0.63
1:A:106:ARG:NH2	1:A:134:GLU:OE1	2.31	0.63
1:A:37:THR:CG2	1:A:39:GLU:OE1	2.46	0.62
1:B:9:ARG:HD2	1:B:12:GLU:OE1	1.99	0.62
1:B:37:THR:HG21	1:B:39:GLU:HB2	1.81	0.62
1:A:72:GLU:HG2	3:A:552:HOH:O	1.98	0.62
1:A:96:THR:CG2	1:A:290:GLU:H	2.12	0.62
1:B:316:ALA:HB3	1:B:317:PHE:CE2	2.34	0.62
1:A:149:LEU:HD21	1:A:329:ILE:HD11	1.82	0.62
1:A:245:ASN:ND2	1:A:247:ASP:CG	2.53	0.62
1:A:282:LYS:CD	1:A:282:LYS:H	2.12	0.62
1:A:31:GLU:OE2	1:A:33:LEU:HD11	2.00	0.62
1:A:37:THR:HG22	1:A:40:ASP:N	2.15	0.61
1:B:159:ILE:HG22	1:B:237:VAL:HG12	1.81	0.61
1:B:274:LEU:HG	1:B:347:PHE:CZ	2.35	0.61
1:A:193:GLU:HG2	1:A:219:THR:HA	1.82	0.61
1:B:73:THR:CG2	1:B:78:GLU:HB3	2.30	0.61
1:A:79:PHE:CD1	1:A:79:PHE:C	2.72	0.61
1:A:264:PHE:O	1:A:266:ILE:HG13	2.01	0.61
1:B:31:GLU:OE2	1:B:33:LEU:HD21	2.01	0.61
1:A:247:ASP:OD1	1:A:321:PRO:HA	2.01	0.60
1:B:228:LYS:HE2	1:B:229:GLU:OE1	2.01	0.60
1:A:195:ARG:HG2	1:A:198:LEU:HD21	1.82	0.60
1:A:201:SER:HB2	1:B:306:ALA:HB2	1.81	0.60
1:B:284:GLY:O	1:B:286:ASP:N	2.35	0.60
1:B:98:ILE:HB	1:B:241:ARG:HG3	1.82	0.60
1:B:208:LEU:HB3	1:B:215:VAL:CG2	2.32	0.60
1:A:97:ALA:HA	1:A:240:ASP:O	2.00	0.60
1:A:210:GLN:HG3	1:A:210:GLN:O	2.00	0.60
1:B:84:GLU:O	1:B:86:ILE:N	2.35	0.60
1:A:183:LYS:HB2	1:A:183:LYS:HZ2	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:N	1:A:33:LEU:HD22	2.16	0.60
1:A:193:GLU:OE1	1:B:195:ARG:NH1	2.27	0.59
1:B:67:ALA:C	1:B:69:LYS:H	2.05	0.59
1:A:14:LYS:C	1:A:16:THR:H	2.05	0.59
1:A:54:PRO:HG2	1:A:166:ALA:O	2.02	0.59
1:A:276:THR:O	1:A:276:THR:HG22	2.02	0.59
1:B:169:ARG:HG3	1:B:170:TYR:CE1	2.35	0.59
1:B:84:GLU:O	1:B:87:LYS:N	2.35	0.59
1:A:245:ASN:HD22	1:A:247:ASP:CG	2.04	0.59
1:A:91:ASN:HD22	1:A:100:LEU:HG	1.67	0.59
1:B:118:ASN:HA	1:B:121:LYS:HE2	1.85	0.59
1:A:96:THR:HG21	1:A:290:GLU:H	1.67	0.59
1:A:309:ASN:H	1:A:309:ASN:ND2	2.01	0.59
1:B:180:ALA:HB1	1:B:185:LEU:HD22	1.84	0.59
1:A:38:LYS:NZ	1:A:39:GLU:OE2	2.35	0.58
1:A:179:LEU:O	1:A:183:LYS:NZ	2.36	0.58
1:A:96:THR:HG22	1:A:288:PRO:O	2.03	0.58
1:B:185:LEU:HD23	1:B:187:LEU:HD13	1.85	0.58
1:A:282:LYS:HE2	1:A:286:ASP:OD2	2.04	0.58
1:A:24:GLN:OE1	1:A:47:THR:CG2	2.51	0.57
1:B:299:GLN:HG3	1:B:303:VAL:O	2.05	0.57
1:A:183:LYS:H	1:A:183:LYS:HZ2	1.52	0.57
1:A:341:GLU:CA	1:A:341:GLU:OE1	2.53	0.57
1:B:64:LEU:O	1:B:67:ALA:HB3	2.05	0.57
1:B:338:ASN:HD21	1:B:341:GLU:H	1.52	0.57
1:A:208:LEU:HD12	1:A:215:VAL:CG1	2.35	0.57
1:A:278:ASP:CG	1:A:281:VAL:HG12	2.24	0.57
1:A:180:ALA:CB	1:A:187:LEU:HD22	2.34	0.57
1:B:184:ASP:OD2	1:B:184:ASP:C	2.43	0.57
1:A:147:LEU:HD23	1:A:179:LEU:HD23	1.86	0.56
1:B:231:GLN:HB3	3:B:516:HOH:O	2.06	0.56
1:A:37:THR:CG2	1:A:39:GLU:H	2.16	0.56
1:A:329:ILE:HG12	1:A:334:ILE:HD13	1.88	0.56
1:B:338:ASN:HB3	1:B:341:GLU:OE1	2.06	0.56
1:A:47:THR:HG22	1:A:47:THR:O	2.06	0.56
1:A:75:ASN:HB3	1:A:78:GLU:HB2	1.87	0.56
1:A:126:HIS:O	1:A:130:GLN:HB3	2.04	0.56
1:A:208:LEU:CD1	1:A:215:VAL:HG13	2.35	0.56
1:B:13:TRP:CE2	1:B:14:LYS:O	2.58	0.56
1:A:341:GLU:OE1	1:A:341:GLU:HA	2.05	0.56
1:B:84:GLU:O	1:B:85:ASP:C	2.44	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:THR:O	1:A:142:ILE:HG13	2.06	0.55
1:B:310:VAL:O	1:B:310:VAL:HG13	2.06	0.55
1:A:193:GLU:CG	1:A:219:THR:HA	2.36	0.55
1:A:347:PHE:O	1:A:348:LYS:CG	2.52	0.55
1:B:21:LEU:HD11	1:B:30:THR:HG23	1.88	0.55
1:B:294:PRO:C	1:B:296:GLU:H	2.10	0.55
1:A:155:ARG:H	1:A:155:ARG:HE	1.55	0.55
1:A:195:ARG:HD3	1:B:193:GLU:OE2	2.07	0.55
1:A:183:LYS:CB	1:A:185:LEU:HD13	2.32	0.55
1:B:250:ASN:HD22	1:B:251:LYS:H	1.55	0.55
1:B:160:CYS:SG	1:B:251:LYS:HD2	2.47	0.54
1:A:294:PRO:HB2	1:A:298:ARG:NH2	2.21	0.54
1:B:60:ALA:CB	1:B:100:LEU:HD12	2.38	0.54
1:A:14:LYS:HB2	1:A:17:ALA:O	2.08	0.54
1:A:117:VAL:CG1	1:A:121:LYS:HE3	2.37	0.54
1:B:51:ARG:HH22	1:B:166:ALA:HB2	1.73	0.54
1:A:163:GLY:CA	1:A:174:LEU:HD12	2.36	0.54
1:A:314:ASN:HA	1:B:222:MET:HE1	1.90	0.54
1:A:131:ILE:HD13	1:A:131:ILE:O	2.08	0.54
1:A:161:ASN:HB2	1:A:199:GLN:O	2.08	0.54
1:B:98:ILE:O	1:B:98:ILE:HG13	2.06	0.54
1:B:185:LEU:O	1:B:187:LEU:N	2.35	0.54
1:B:308:SER:O	1:B:309:ASN:CB	2.48	0.54
1:A:194:THR:HG21	1:A:251:LYS:CG	2.31	0.54
1:A:37:THR:O	1:A:41:VAL:HG23	2.07	0.53
1:B:297:VAL:HG12	1:B:297:VAL:O	2.07	0.53
1:B:67:ALA:O	1:B:69:LYS:N	2.41	0.53
1:B:224:ALA:HB2	1:B:260:LEU:HD21	1.90	0.53
1:A:217:LEU:HD22	1:A:218:ILE:N	2.24	0.53
1:B:25:LYS:HD2	1:B:29:GLU:OE2	2.07	0.53
1:B:232:ILE:HG13	1:B:232:ILE:O	2.08	0.53
1:B:245:ASN:C	1:B:245:ASN:HD22	2.11	0.53
1:B:58:ILE:CD1	1:B:132:GLN:HA	2.38	0.53
1:A:190:TYR:OH	1:A:230:LYS:HD2	2.09	0.53
1:A:195:ARG:HG2	1:A:198:LEU:CD2	2.39	0.53
1:B:180:ALA:CB	1:B:187:LEU:HD22	2.39	0.53
1:B:345:GLN:O	1:B:345:GLN:CG	2.57	0.52
1:A:107:LEU:HD22	1:A:127:GLU:HB3	1.90	0.52
1:B:81:ARG:C	1:B:81:ARG:CD	2.78	0.52
1:B:13:TRP:CD2	1:B:14:LYS:O	2.62	0.52
1:B:307:PRO:HG2	1:B:310:VAL:HB	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LYS:HA	1:A:251:LYS:HE3	1.91	0.52
1:A:72:GLU:OE1	1:A:72:GLU:HA	2.09	0.52
1:B:156:ILE:N	1:B:156:ILE:HD13	2.24	0.52
1:B:75:ASN:HB3	1:B:78:GLU:HB3	1.92	0.52
1:A:335:MET:HE2	1:A:339:TYR:HD2	1.75	0.52
1:B:14:LYS:HG2	1:B:17:ALA:O	2.10	0.52
1:A:147:LEU:HD11	1:A:185:LEU:HD22	1.91	0.52
1:A:36:THR:HG22	1:A:36:THR:O	2.09	0.52
1:B:91:ASN:HA	1:B:100:LEU:HD21	1.92	0.52
1:B:169:ARG:CD	1:B:170:TYR:N	2.69	0.52
1:B:339:TYR:O	1:B:343:ILE:HG13	2.10	0.52
1:B:173:ALA:O	1:B:176:PRO:HD2	2.10	0.51
1:A:244:LYS:HG3	1:A:279:THR:O	2.11	0.51
1:A:226:THR:HG23	1:A:230:LYS:HG3	1.92	0.51
1:A:228:LYS:HD3	1:A:229:GLU:OE2	2.09	0.51
1:B:169:ARG:O	1:B:170:TYR:HB2	2.09	0.51
1:A:330:THR:HB	1:A:331:GLU:OE1	2.11	0.51
1:B:160:CYS:SG	1:B:199:GLN:HG3	2.51	0.51
1:A:130:GLN:C	1:A:133:VAL:HG23	2.30	0.51
1:A:313:PHE:HB3	1:B:218:ILE:HG22	1.93	0.51
1:A:309:ASN:HD22	1:A:309:ASN:N	2.03	0.51
1:B:96:THR:HG21	1:B:317:PHE:CD1	2.46	0.51
1:A:197:VAL:O	1:A:197:VAL:HG12	2.10	0.50
1:B:53:ALA:CB	1:B:54:PRO:HD3	2.36	0.50
1:A:208:LEU:HD13	1:A:215:VAL:HG13	1.92	0.50
1:A:102:TRP:HZ3	1:A:131:ILE:HD11	1.74	0.50
1:B:155:ARG:H	1:B:155:ARG:HE	1.59	0.50
1:B:252:ILE:N	1:B:317:PHE:HA	2.27	0.50
1:A:91:ASN:ND2	1:A:101:SER:HB3	2.25	0.50
1:A:91:ASN:ND2	1:A:100:LEU:HG	2.25	0.50
1:A:185:LEU:O	1:A:187:LEU:N	2.37	0.50
1:B:284:GLY:C	1:B:286:ASP:N	2.64	0.50
1:A:51:ARG:HB2	2:A:501:SO4:O3	2.12	0.50
1:A:282:LYS:CE	1:A:286:ASP:OD2	2.59	0.50
1:A:115:ILE:HG23	1:A:116:SER:N	2.26	0.50
1:A:94:ARG:O	1:A:100:LEU:HD23	2.10	0.50
1:A:79:PHE:C	1:A:79:PHE:HD1	2.15	0.50
1:A:169:ARG:NH2	1:A:170:TYR:OH	2.45	0.50
1:B:243:ALA:O	1:B:245:ASN:N	2.45	0.50
1:A:102:TRP:CH2	1:A:131:ILE:HD11	2.47	0.49
1:A:106:ARG:NH1	1:A:127:GLU:OE2	2.38	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLY:O	1:A:260:LEU:HB2	2.12	0.49
1:A:13:TRP:CE3	1:A:62:PHE:HB3	2.47	0.49
1:B:67:ALA:HB1	1:B:86:ILE:HD13	1.94	0.49
1:A:179:LEU:O	1:A:182:GLN:HG2	2.12	0.49
1:B:98:ILE:HD13	1:B:241:ARG:NH1	2.27	0.49
1:A:171:GLY:O	1:A:175:ALA:HB2	2.13	0.49
1:B:155:ARG:HE	1:B:155:ARG:N	2.10	0.49
1:B:245:ASN:ND2	1:B:245:ASN:C	2.64	0.49
1:A:167:THR:OG1	1:A:168:SER:N	2.45	0.49
1:B:329:ILE:N	1:B:329:ILE:HD12	2.27	0.49
1:B:149:LEU:HG	1:B:269:PHE:CZ	2.47	0.49
1:B:66:LEU:O	1:B:69:LYS:HB2	2.12	0.49
1:B:195:ARG:NH2	1:B:299:GLN:O	2.45	0.49
1:B:341:GLU:HG3	1:B:342:GLU:N	2.27	0.49
1:A:53:ALA:HB3	1:A:54:PRO:CD	2.42	0.49
1:A:120:ALA:O	1:A:124:LEU:HG	2.13	0.49
1:A:54:PRO:CG	1:A:167:THR:HG22	2.42	0.48
1:A:178:TYR:OH	1:A:207:GLU:CG	2.60	0.48
1:B:206:TRP:O	1:B:210:GLN:HG2	2.13	0.48
1:B:316:ALA:HB3	1:B:317:PHE:CD2	2.48	0.48
1:A:169:ARG:HB3	1:A:170:TYR:CD1	2.48	0.48
1:B:276:THR:HG22	1:B:276:THR:O	2.13	0.48
1:B:282:LYS:HG3	3:B:508:HOH:O	2.13	0.48
1:B:294:PRO:HB3	1:B:312:VAL:CG2	2.42	0.48
1:A:98:ILE:CD1	1:A:276:THR:C	2.82	0.48
1:A:217:LEU:HD13	1:B:297:VAL:CG1	2.43	0.48
1:B:96:THR:HG21	1:B:317:PHE:CG	2.49	0.48
1:B:146:ALA:HB3	1:B:176:PRO:HG3	1.94	0.48
1:B:60:ALA:HB2	1:B:100:LEU:CD1	2.44	0.48
1:B:185:LEU:CD2	1:B:187:LEU:HD13	2.43	0.48
1:A:96:THR:HG21	1:A:317:PHE:CD2	2.48	0.48
1:A:182:GLN:C	1:A:184:ASP:N	2.67	0.48
1:A:14:LYS:O	1:A:17:ALA:N	2.46	0.48
1:B:275:SER:C	1:B:277:PHE:H	2.17	0.48
1:B:35:LEU:N	1:B:35:LEU:HD12	2.29	0.48
1:A:144:GLN:HG2	1:A:179:LEU:CD2	2.44	0.48
1:A:119:GLU:CG	1:A:120:ALA:N	2.76	0.47
1:A:208:LEU:HD12	1:A:215:VAL:HG11	1.95	0.47
1:B:67:ALA:C	1:B:69:LYS:N	2.68	0.47
1:A:12:GLU:OE1	1:A:12:GLU:HA	2.12	0.47
1:A:87:LYS:O	1:A:91:ASN:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ASP:HB3	1:A:168:SER:OG	2.14	0.47
1:A:182:GLN:C	1:A:184:ASP:H	2.17	0.47
1:B:338:ASN:HD22	1:B:341:GLU:H	1.55	0.47
1:A:14:LYS:C	1:A:16:THR:N	2.66	0.47
1:A:130:GLN:CA	1:A:133:VAL:HG23	2.43	0.47
1:B:94:ARG:HA	1:B:95:PRO:HD3	1.63	0.47
1:B:300:ILE:HG13	1:B:305:THR:CG2	2.38	0.47
1:A:222:MET:HA	1:B:252:ILE:HD11	1.97	0.47
1:A:274:LEU:HD13	1:A:331:GLU:CD	2.34	0.47
1:B:73:THR:HG22	1:B:75:ASN:N	2.30	0.47
1:B:160:CYS:HA	1:B:194:THR:HG21	1.95	0.47
1:B:284:GLY:C	1:B:286:ASP:H	2.18	0.47
1:B:299:GLN:HB2	1:B:304:ARG:HA	1.95	0.47
1:A:198:LEU:HD13	1:B:305:THR:HB	1.97	0.47
1:A:335:MET:O	1:A:339:TYR:HE2	1.97	0.47
1:A:333:GLY:C	1:A:334:ILE:HG12	2.35	0.47
1:B:36:THR:O	1:B:66:LEU:HD21	2.14	0.47
1:B:79:PHE:O	1:B:83:LEU:HB2	2.13	0.47
1:B:274:LEU:HG	1:B:347:PHE:CE2	2.50	0.47
1:B:299:GLN:HG3	1:B:303:VAL:C	2.36	0.47
1:B:84:GLU:C	1:B:86:ILE:N	2.68	0.47
1:B:307:PRO:C	1:B:308:SER:O	2.51	0.46
1:A:72:GLU:O	1:A:73:THR:CB	2.64	0.46
1:A:107:LEU:CD2	1:A:127:GLU:HB3	2.45	0.46
1:B:177:PHE:CD1	1:B:189:ILE:HG21	2.50	0.46
1:A:79:PHE:CD2	1:A:117:VAL:HG13	2.50	0.46
1:A:177:PHE:CE1	1:A:189:ILE:HG12	2.50	0.46
1:B:73:THR:HG22	1:B:75:ASN:O	2.15	0.46
1:B:178:TYR:OH	1:B:207:GLU:OE2	2.28	0.46
1:B:154:ASP:OD1	1:B:154:ASP:N	2.48	0.46
1:B:248:THR:OG1	1:B:325:ILE:HD11	2.15	0.46
1:B:294:PRO:C	1:B:296:GLU:N	2.69	0.46
1:A:44:ALA:HA	1:A:49:LYS:HG3	1.98	0.46
1:B:208:LEU:HD12	1:B:213:ILE:HG13	1.98	0.46
1:B:242:ILE:HD12	1:B:276:THR:O	2.15	0.46
1:A:89:TYR:HD2	1:A:90:LEU:HD12	1.79	0.46
1:A:185:LEU:C	1:A:187:LEU:H	2.18	0.46
1:A:19:THR:HA	1:A:33:LEU:O	2.16	0.45
1:A:197:VAL:O	1:A:197:VAL:CG1	2.64	0.45
1:B:38:LYS:HG2	1:B:89:TYR:CE2	2.51	0.45
1:B:272:ALA:HB1	1:B:276:THR:HB	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ALA:CB	1:B:100:LEU:CD1	2.95	0.45
1:B:81:ARG:C	1:B:81:ARG:HD2	2.36	0.45
1:B:250:ASN:ND2	1:B:251:LYS:N	2.62	0.45
1:B:98:ILE:CB	1:B:241:ARG:HG3	2.47	0.45
1:A:129:ILE:O	1:A:133:VAL:CG2	2.62	0.45
1:A:130:GLN:HA	1:A:133:VAL:HG21	1.98	0.45
1:B:298:ARG:HH11	1:B:312:VAL:HG13	1.81	0.45
1:A:146:ALA:CB	1:A:329:ILE:HD13	2.46	0.45
1:A:193:GLU:OE2	1:A:195:ARG:HG3	2.16	0.45
1:B:138:THR:O	1:B:142:ILE:HG13	2.16	0.45
1:A:340:GLU:CA	1:A:340:GLU:OE2	2.64	0.45
1:A:154:ASP:HB2	1:A:233:SER:CB	2.47	0.45
1:B:255:TYR:HB2	1:B:318:ASP:OD1	2.17	0.45
1:A:245:ASN:HB2	1:A:282:LYS:O	2.16	0.45
1:B:292:ARG:HH21	1:B:292:ARG:HG2	1.80	0.45
1:A:278:ASP:HB3	1:A:281:VAL:CG1	2.47	0.45
1:B:47:THR:OG1	1:B:49:LYS:NZ	2.46	0.45
1:B:64:LEU:HD12	1:B:86:ILE:HG21	1.99	0.45
1:A:298:ARG:NH1	1:A:310:VAL:O	2.47	0.44
1:A:251:LYS:HE3	1:A:316:ALA:O	2.17	0.44
1:A:257:LEU:O	1:A:261:ALA:N	2.49	0.44
1:A:43:ASP:O	1:A:47:THR:HB	2.18	0.44
1:A:98:ILE:O	1:A:100:LEU:N	2.50	0.44
1:B:109:HIS:HA	1:B:112:GLU:HG3	1.99	0.44
1:B:155:ARG:C	1:B:156:ILE:HD13	2.38	0.44
1:B:164:SER:O	1:B:167:THR:O	2.36	0.44
1:A:47:THR:CG2	1:A:47:THR:O	2.64	0.44
1:A:98:ILE:H	1:A:98:ILE:HG13	1.58	0.44
1:B:155:ARG:HB2	1:B:232:ILE:HA	1.99	0.44
1:B:284:GLY:O	1:B:287:ILE:N	2.34	0.44
1:A:123:ASN:HD22	1:A:123:ASN:HA	1.53	0.44
1:B:50:VAL:O	1:B:50:VAL:HG13	2.17	0.44
1:B:87:LYS:HG3	1:B:104:LEU:HB3	1.99	0.44
1:B:189:ILE:HG12	1:B:215:VAL:HG22	2.00	0.44
1:B:316:ALA:CB	1:B:317:PHE:CE2	3.01	0.44
1:B:37:THR:HG22	1:B:38:LYS:N	2.31	0.44
1:B:163:GLY:HA3	1:B:174:LEU:HD12	1.99	0.44
1:A:11:VAL:HG13	1:A:59:THR:HG22	1.98	0.44
1:A:169:ARG:C	1:A:170:TYR:HD1	2.20	0.44
1:B:161:ASN:ND2	1:B:203:LEU:HB3	2.32	0.44
1:B:334:ILE:HG22	1:B:335:MET:N	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ILE:CG2	1:A:190:TYR:N	2.80	0.43
1:B:146:ALA:HB2	1:B:329:ILE:HG21	1.99	0.43
1:B:317:PHE:CD2	1:B:317:PHE:N	2.86	0.43
1:A:125:VAL:HG12	1:A:129:ILE:HD11	2.00	0.43
1:A:105:GLU:O	1:A:106:ARG:C	2.55	0.43
1:B:127:GLU:O	1:B:130:GLN:HB3	2.17	0.43
1:B:251:LYS:HE2	1:B:316:ALA:O	2.17	0.43
1:A:252:ILE:O	1:A:252:ILE:HG23	2.18	0.43
1:B:346:LEU:C	1:B:348:LYS:H	2.21	0.43
1:A:144:GLN:HG2	1:A:179:LEU:HD21	2.00	0.43
1:A:244:LYS:HD3	1:A:279:THR:HG23	2.00	0.43
1:A:266:ILE:HA	1:A:267:PRO:HD3	1.80	0.43
1:A:301:SER:OG	1:B:303:VAL:HG11	2.18	0.43
1:B:25:LYS:HE3	1:B:31:GLU:OE1	2.19	0.43
1:A:75:ASN:C	1:A:75:ASN:HD22	2.21	0.43
1:A:98:ILE:HD11	1:A:276:THR:C	2.39	0.43
1:A:168:SER:O	1:A:169:ARG:CG	2.63	0.43
1:A:316:ALA:HB3	1:A:317:PHE:CD2	2.54	0.43
1:B:78:GLU:O	1:B:82:ARG:HG2	2.19	0.43
1:B:204:THR:HG23	1:B:208:LEU:HD22	2.00	0.43
1:B:294:PRO:O	1:B:296:GLU:N	2.52	0.43
1:B:294:PRO:HA	1:B:312:VAL:HG21	2.00	0.43
1:A:72:GLU:OE1	1:A:72:GLU:CA	2.66	0.43
1:B:37:THR:HG22	1:B:39:GLU:N	2.10	0.43
1:B:205:ALA:O	1:B:209:MET:CG	2.60	0.43
1:A:125:VAL:HG12	1:A:129:ILE:CD1	2.49	0.42
1:A:183:LYS:NZ	1:A:183:LYS:CB	2.82	0.42
1:A:115:ILE:CG2	1:A:116:SER:N	2.82	0.42
1:B:242:ILE:CG1	1:B:248:THR:HG22	2.46	0.42
1:B:299:GLN:HG2	1:B:300:ILE:N	2.34	0.42
1:A:250:ASN:HD22	1:A:250:ASN:HA	1.66	0.42
1:A:169:ARG:C	1:A:170:TYR:CD1	2.92	0.42
1:B:26:LEU:HB3	1:B:27:PRO:HA	2.01	0.42
1:B:98:ILE:CG2	1:B:241:ARG:HG3	2.49	0.42
1:A:42:PHE:O	1:A:46:VAL:HG23	2.19	0.42
1:A:273:PRO:HG2	1:A:276:THR:OG1	2.20	0.42
1:B:115:ILE:N	1:B:119:GLU:OE2	2.45	0.42
1:A:248:THR:HG22	1:A:325:ILE:CD1	2.40	0.42
1:A:147:LEU:HD11	1:A:185:LEU:CD2	2.50	0.42
1:A:274:LEU:HB2	1:A:331:GLU:OE2	2.20	0.42
1:B:127:GLU:O	1:B:131:ILE:HG13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ILE:HA	1:A:269:PHE:O	2.20	0.42
1:A:341:GLU:O	1:A:342:GLU:C	2.58	0.42
1:B:199:GLN:O	1:B:203:LEU:HB2	2.20	0.42
1:A:160:CYS:SG	1:A:161:ASN:N	2.91	0.42
1:A:177:PHE:CD1	1:A:189:ILE:HG12	2.55	0.41
1:B:97:ALA:HA	1:B:240:ASP:O	2.19	0.41
1:B:245:ASN:HD22	1:B:247:ASP:H	1.64	0.41
1:B:245:ASN:HD21	1:B:247:ASP:CG	2.22	0.41
1:A:164:SER:N	1:A:207:GLU:OE2	2.53	0.41
1:A:189:ILE:N	1:A:189:ILE:HD12	2.35	0.41
1:B:32:TYR:O	1:B:33:LEU:HD22	2.20	0.41
1:B:245:ASN:HD21	1:B:247:ASP:CB	2.34	0.41
1:A:264:PHE:O	1:A:265:ASP:C	2.59	0.41
1:A:54:PRO:O	1:A:55:ALA:C	2.59	0.41
1:A:76:VAL:CG1	1:A:77:THR:N	2.84	0.41
1:A:335:MET:O	1:A:339:TYR:CE2	2.73	0.41
1:B:174:LEU:HD22	1:B:208:LEU:HD21	2.02	0.41
1:B:307:PRO:O	1:B:308:SER:C	2.58	0.41
1:A:62:PHE:HE1	1:A:129:ILE:HG12	1.85	0.41
1:B:274:LEU:HD12	1:B:274:LEU:HA	1.81	0.41
1:A:98:ILE:C	1:A:100:LEU:N	2.73	0.41
1:A:175:ALA:HB3	1:A:176:PRO:HD3	2.02	0.41
1:A:95:PRO:HG2	1:A:96:THR:H	1.85	0.41
1:A:294:PRO:HB3	1:A:312:VAL:HG22	2.02	0.41
1:B:184:ASP:OD2	1:B:184:ASP:O	2.38	0.41
1:B:274:LEU:O	1:B:277:PHE:HB2	2.21	0.41
1:B:306:ALA:HB1	1:B:307:PRO:HD2	2.02	0.41
1:A:189:ILE:HG22	1:A:190:TYR:N	2.36	0.41
1:A:197:VAL:HG12	1:A:199:GLN:HG3	2.02	0.41
1:A:64:LEU:HD12	1:A:64:LEU:HA	1.86	0.40
1:A:323:ASP:OD2	1:A:323:ASP:N	2.53	0.40
1:B:106:ARG:HH12	1:B:130:GLN:HG3	1.86	0.40
1:B:174:LEU:O	1:B:175:ALA:C	2.58	0.40
1:B:24:GLN:OE1	1:B:49:LYS:HG2	2.21	0.40
1:B:274:LEU:HD11	1:B:346:LEU:HD23	2.03	0.40
1:B:55:ALA:HB2	1:B:166:ALA:O	2.21	0.40
1:B:192:CYS:HA	1:B:218:ILE:O	2.22	0.40
1:B:204:THR:HG23	1:B:208:LEU:CD2	2.52	0.40
1:B:260:LEU:O	1:B:261:ALA:C	2.60	0.40
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.84	0.40
1:A:193:GLU:HG3	1:A:193:GLU:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:THR:HG22	1:B:97:ALA:N	2.35	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	338/374 (90%)	297 (88%)	32 (10%)	9 (3%)	5	12
1	B	339/374 (91%)	280 (83%)	46 (14%)	13 (4%)	3	7
All	All	677/748 (90%)	577 (85%)	78 (12%)	22 (3%)	4	9

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	THR
1	A	95	PRO
1	A	96	THR
1	B	68	ALA
1	B	186	GLY
1	B	239	ALA
1	B	244	LYS
1	A	15	GLU
1	B	85	ASP
1	B	251	LYS
1	B	285	ALA
1	A	99	ASN
1	A	222	MET
1	B	160	CYS
1	B	184	ASP
1	A	285	ALA
1	B	288	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	295	GLU
1	B	70	ASP
1	A	186	GLY
1	B	95	PRO
1	A	53	ALA

5.3.2 Protein sidechains [i](#)

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	283/313 (90%)	233 (82%)	50 (18%)	2 4
1	B	284/313 (91%)	245 (86%)	39 (14%)	3 8
All	All	567/626 (91%)	478 (84%)	89 (16%)	2 6

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	16	THR
1	A	22	ASN
1	A	27	PRO
1	A	29	GLU
1	A	37	THR
1	A	43	ASP
1	A	48	LEU
1	A	51	ARG
1	A	66	LEU
1	A	75	ASN
1	A	79	PHE
1	A	81	ARG
1	A	82	ARG
1	A	98	ILE
1	A	105	GLU
1	A	106	ARG
1	A	110	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	122	THR
1	A	123	ASN
1	A	130	GLN
1	A	131	ILE
1	A	133	VAL
1	A	134	GLU
1	A	149	LEU
1	A	151	LYS
1	A	155	ARG
1	A	168	SER
1	A	182	GLN
1	A	183	LYS
1	A	193	GLU
1	A	210	GLN
1	A	215	VAL
1	A	217	LEU
1	A	248	THR
1	A	250	ASN
1	A	251	LYS
1	A	259	ILE
1	A	280	LYS
1	A	281	VAL
1	A	282	LYS
1	A	301	SER
1	A	304	ARG
1	A	309	ASN
1	A	323	ASP
1	A	334	ILE
1	A	335	MET
1	A	340	GLU
1	A	341	GLU
1	A	345	GLN
1	B	10	SER
1	B	12	GLU
1	B	16	THR
1	B	22	ASN
1	B	38	LYS
1	B	51	ARG
1	B	69	LYS
1	B	70	ASP
1	B	71	ILE
1	B	74	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	77	THR
1	B	81	ARG
1	B	84	GLU
1	B	101	SER
1	B	109	HIS
1	B	122	THR
1	B	149	LEU
1	B	151	LYS
1	B	154	ASP
1	B	155	ARG
1	B	182	GLN
1	B	185	LEU
1	B	189	ILE
1	B	199	GLN
1	B	208	LEU
1	B	209	MET
1	B	214	ASP
1	B	217	LEU
1	B	221	SER
1	B	229	GLU
1	B	240	ASP
1	B	245	ASN
1	B	248	THR
1	B	279	THR
1	B	286	ASP
1	B	323	ASP
1	B	331	GLU
1	B	338	ASN
1	B	346	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	75	ASN
1	A	91	ASN
1	A	99	ASN
1	A	118	ASN
1	A	123	ASN
1	A	130	GLN
1	A	144	GLN
1	A	231	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	245	ASN
1	A	250	ASN
1	A	309	ASN
1	A	322	HIS
1	B	22	ASN
1	B	123	ASN
1	B	132	GLN
1	B	161	ASN
1	B	245	ASN
1	B	250	ASN
1	B	322	HIS
1	B	338	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	501	-	4,4,4	0.21	0	6,6,6	0.26	0
2	SO4	B	502	-	4,4,4	0.23	0	6,6,6	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SO4	1	0
2	B	502	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	340/374 (90%)	-0.35	1 (0%) 94 95	7, 30, 54, 71	0
1	B	341/374 (91%)	-0.29	1 (0%) 94 95	10, 33, 61, 75	0
All	All	681/748 (91%)	-0.32	2 (0%) 94 95	7, 31, 58, 75	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	GLU	2.9
1	B	279	THR	2.6

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 monosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	501	5/5	0.98	0.16	34,34,36,37	0
2	SO4	B	502	5/5	0.99	0.13	31,32,33,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.