



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:12 AM UTC

PDB ID : 2C4K / pdb_00002c4k
Title : Crystal structure of human phosphoribosylpyrophosphate synthetase- associated protein 39 (PAP39)
Authors : Kursula, P.; Stenmark, P.; Arrowsmith, C.; Berglund, H.; Edwards, A.; Ehn, M.; Flodin, S.; Graslund, S.; Hammarstrom, M.; Hallberg, B.M.; Holmberg Schiavone, L.; Kotenyova, T.; Nilsson-Ehle, P.; Ogg, D.; Persson, C.; Sage-mark, J.; Schuler, H.; Sundstrom, M.; Thorsell, A.G.; Van Den Berg, S.; Weigelt, J.; Nordlund, P.
Deposited on : 2005-10-20
Resolution : 2.65 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

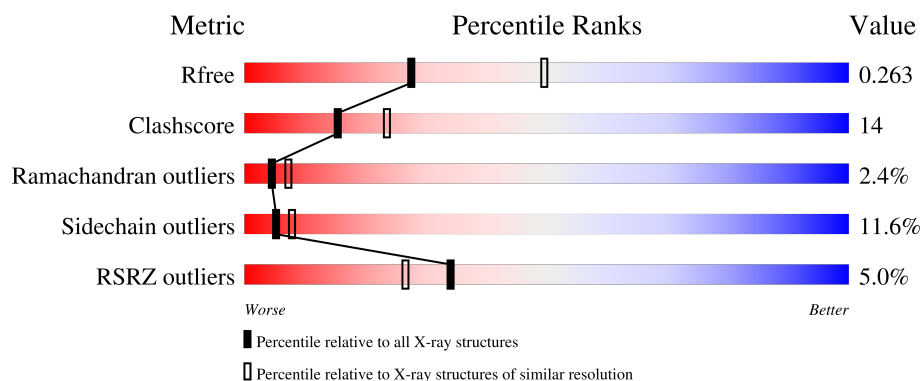
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	370	4% 53% 24% 5% 18%
1	B	370	4% 54% 23% 5% 18%
1	C	370	6% 54% 24% • 18%

Continued on next page...

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	D	370	
1	E	370	
1	F	370	

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
3	TAM	B	1353	-	-	X	-

2 Entry composition [i](#)

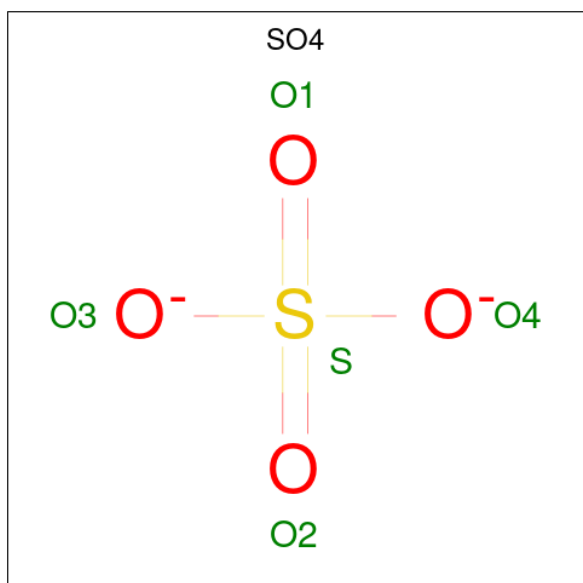
There are 4 unique types of molecules in this entry. The entry contains 14378 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHORIBOSYL PYROPHOSPHATE SYNTHETASE-ASSOCIATED PROTEIN 1.

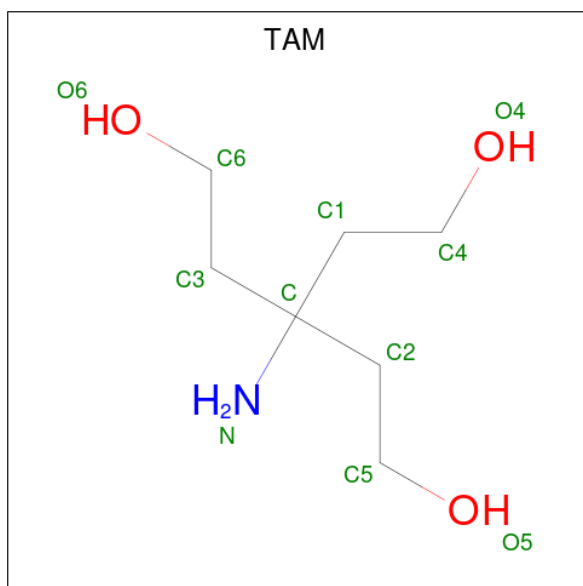
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2376	1513	414	438	11			
1	B	305	Total	C	N	O	S	0	0	0
			2376	1513	414	438	11			
1	C	305	Total	C	N	O	S	0	0	0
			2376	1513	414	438	11			
1	D	305	Total	C	N	O	S	0	0	0
			2376	1513	414	438	11			
1	E	305	Total	C	N	O	S	0	0	0
			2376	1513	414	438	11			
1	F	305	Total	C	N	O	S	0	0	0
			2376	1513	414	438	11			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is TRIS(HYDROXYETHYL)AMINOMETHANE (CCD ID: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			11	7	1	3		

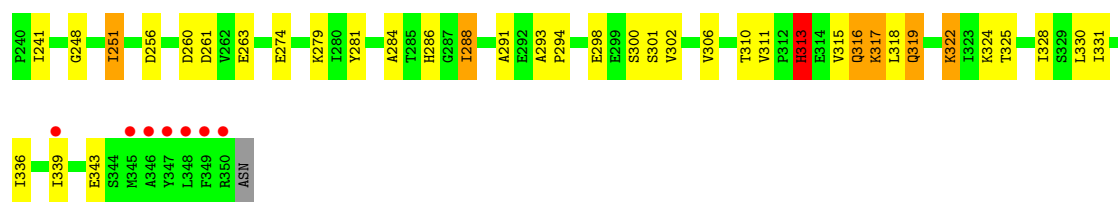
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		

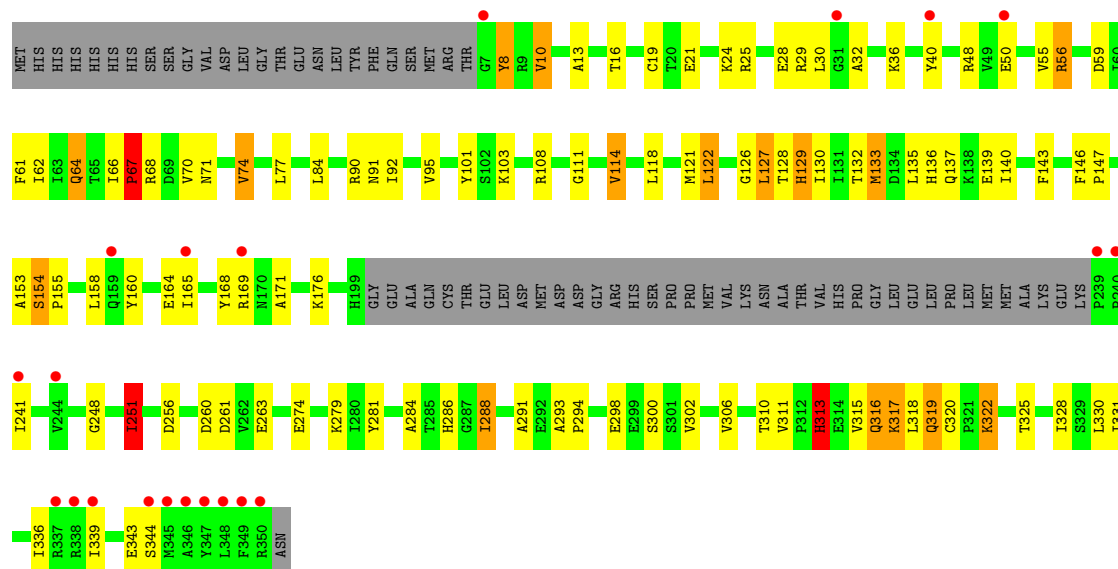
Continued on next page...

Continued from previous page...

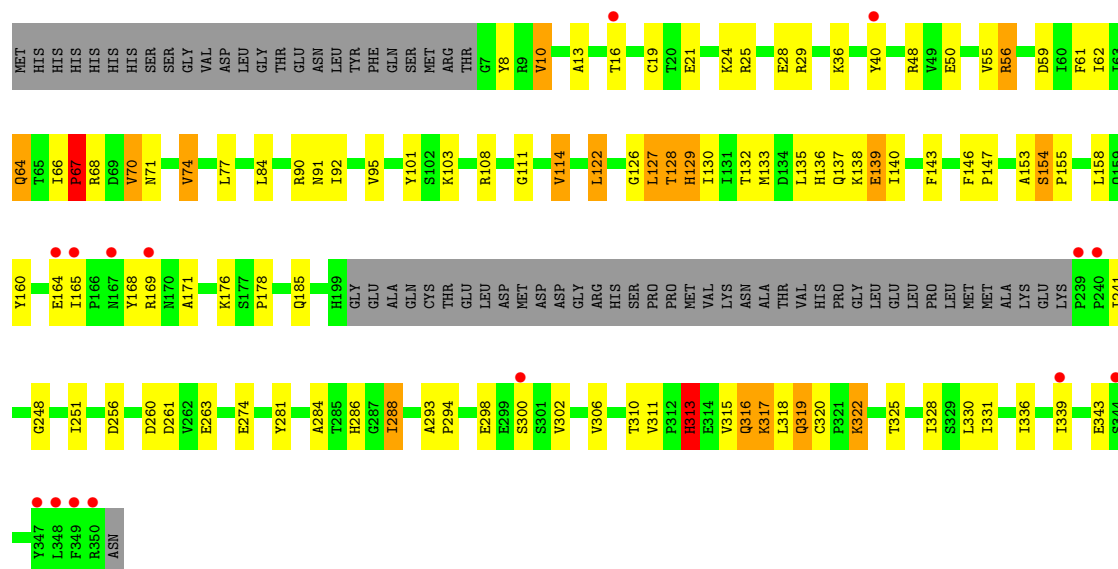
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	22	Total 22	O 22	0	0
4	C	10	Total 10	O 10	0	0
4	D	11	Total 11	O 11	0	0
4	E	17	Total 17	O 17	0	0
4	F	7	Total 7	O 7	0	0



• Molecule 1: PHOSPHORIBOSYL PYROPHOSPHATE SYNTHETASE-ASSOCIATED PROTEIN 1



• Molecule 1: PHOSPHORIBOSYL PYROPHOSPHATE SYNTHETASE-ASSOCIATED PROTEIN 1



Chain E:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	180.06Å 103.88Å 127.16Å 90.00° 97.63° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 20.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.65) 99.7 (20.00-2.65)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.67Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.269 , 0.299 (Not available) , 0.263	Depositor DCC
R_{free} test set	3370 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.791	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	14378	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, TAM

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	0.76	0/2412	1.00	2/3261 (0.1%)
1	B	0.77	0/2412	1.00	3/3261 (0.1%)
1	C	0.76	1/2412 (0.0%)	0.99	2/3261 (0.1%)
1	D	0.76	0/2412	0.99	2/3261 (0.1%)
1	E	0.76	0/2412	1.00	2/3261 (0.1%)
1	F	0.76	1/2412 (0.0%)	1.00	3/3261 (0.1%)
All	All	0.76	2/14472 (0.0%)	1.00	14/19566 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
All	All	0	12

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	251	ILE	CA-CB	5.22	1.60	1.53
1	C	251	ILE	CA-CB	5.00	1.59	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	313	HIS	CB-CA-C	-7.20	96.34	109.15
1	B	313	HIS	CB-CA-C	-7.06	96.59	109.15
1	F	313	HIS	CB-CA-C	-6.66	97.29	109.15
1	A	313	HIS	CB-CA-C	-6.63	97.35	109.15
1	D	313	HIS	CB-CA-C	-6.54	97.50	109.15
1	E	313	HIS	CB-CA-C	-6.51	97.56	109.15
1	B	133	MET	N-CA-C	5.60	118.52	109.40
1	B	70	VAL	N-CA-C	-5.52	105.15	110.72
1	F	133	MET	N-CA-C	5.40	118.25	109.24
1	F	70	VAL	N-CA-C	-5.36	105.31	110.72
1	C	133	MET	N-CA-C	5.31	118.10	109.24
1	A	133	MET	N-CA-C	5.29	118.08	109.24
1	E	133	MET	N-CA-C	5.27	118.00	109.40
1	D	70	VAL	N-CA-C	-5.09	105.58	110.72

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	GLU	Peptide
1	A	313	HIS	Peptide
1	B	164	GLU	Peptide
1	B	313	HIS	Peptide
1	C	164	GLU	Peptide
1	C	313	HIS	Peptide
1	D	164	GLU	Peptide
1	D	313	HIS	Peptide
1	E	164	GLU	Peptide
1	E	313	HIS	Peptide
1	F	164	GLU	Peptide
1	F	313	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2376	0	2464	69	0
1	B	2376	0	2464	77	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2376	0	2464	63	0
1	D	2376	0	2464	63	0
1	E	2376	0	2464	70	0
1	F	2376	0	2464	62	0
2	B	10	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	10	0	0	0	0
2	F	5	0	0	0	0
3	B	11	0	17	10	0
4	A	9	0	0	0	0
4	B	22	0	0	6	0
4	C	10	0	0	1	0
4	D	11	0	0	0	0
4	E	17	0	0	3	0
4	F	7	0	0	2	0
All	All	14378	0	14801	394	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 14.

All (394) 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:136:HIS:CD2	1:B:137:GLN:HE21	2.02	0.78
1:A:8:TYR:OH	1:A:337:ARG:HG3	1.85	0.77
1:B:324:LYS:NZ	3:B:1353:TAM:H32	2.00	0.76
1:C:315:VAL:O	1:C:319:GLN:NE2	2.21	0.74
1:D:129:HIS:HA	1:D:146:PHE:CD1	2.23	0.73
1:A:129:HIS:HA	1:A:146:PHE:CD1	2.23	0.73
1:C:129:HIS:HA	1:C:146:PHE:CD1	2.24	0.73
1:B:315:VAL:O	1:B:319:GLN:NE2	2.21	0.73
1:C:136:HIS:CD2	1:C:137:GLN:HE21	2.07	0.73
1:F:315:VAL:O	1:F:319:GLN:NE2	2.21	0.73
1:E:129:HIS:HA	1:E:146:PHE:CD1	2.24	0.72
1:F:136:HIS:CD2	1:F:137:GLN:HE21	2.07	0.72
1:A:139:GLU:HG3	1:E:139:GLU:HG3	1.70	0.72
1:E:315:VAL:O	1:E:319:GLN:NE2	2.22	0.72
1:B:129:HIS:HA	1:B:146:PHE:CD1	2.25	0.72
1:A:315:VAL:O	1:A:319:GLN:NE2	2.23	0.72
1:F:129:HIS:HA	1:F:146:PHE:CD1	2.23	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:MET:HE1	1:F:328:ILE:HG12	1.72	0.71
1:D:315:VAL:O	1:D:319:GLN:NE2	2.24	0.70
1:D:136:HIS:CD2	1:D:137:GLN:HE21	2.10	0.70
1:E:136:HIS:CD2	1:E:137:GLN:HE21	2.09	0.69
1:A:133:MET:HE1	1:A:328:ILE:HG12	1.74	0.69
1:E:133:MET:HE1	1:E:328:ILE:HG12	1.73	0.69
1:B:133:MET:HE1	1:B:328:ILE:HG12	1.75	0.68
1:D:133:MET:HE1	1:D:328:ILE:HG12	1.74	0.68
1:C:133:MET:HE1	1:C:328:ILE:HG12	1.75	0.68
1:D:40:TYR:HB2	1:D:48:ARG:HB2	1.76	0.67
1:D:139:GLU:HG3	1:F:139:GLU:HG3	1.75	0.67
1:D:129:HIS:HB2	1:D:147:PRO:O	1.95	0.66
1:E:40:TYR:HB2	1:E:48:ARG:HB2	1.78	0.66
1:E:152:ARG:HG2	4:E:2010:HOH:O	1.95	0.66
1:C:19:CYS:SG	1:C:67:PRO:HG3	2.36	0.66
1:B:40:TYR:HB2	1:B:48:ARG:HB2	1.78	0.65
1:A:40:TYR:HB2	1:A:48:ARG:HB2	1.79	0.65
1:B:301:SER:HA	4:B:2017:HOH:O	1.96	0.65
1:F:140:ILE:HG23	1:F:143:PHE:CD2	2.32	0.65
1:A:92:ILE:HD12	1:A:126:GLY:O	1.97	0.64
1:B:140:ILE:HG23	1:B:143:PHE:CD2	2.33	0.64
1:C:40:TYR:HB2	1:C:48:ARG:HB2	1.80	0.64
1:C:129:HIS:HB2	1:C:147:PRO:O	1.98	0.64
1:F:40:TYR:HB2	1:F:48:ARG:HB2	1.80	0.64
1:A:136:HIS:CD2	1:A:137:GLN:HE21	2.14	0.64
1:F:19:CYS:SG	1:F:67:PRO:HG3	2.38	0.64
1:A:129:HIS:HB2	1:A:147:PRO:O	1.97	0.63
1:C:140:ILE:HG23	1:C:143:PHE:CD2	2.34	0.63
1:E:19:CYS:SG	1:E:67:PRO:HG3	2.39	0.63
1:B:324:LYS:HE3	3:B:1353:TAM:H31	1.80	0.63
1:A:19:CYS:SG	1:A:67:PRO:HG3	2.39	0.62
1:A:140:ILE:HG23	1:A:143:PHE:CD2	2.34	0.62
1:D:19:CYS:SG	1:D:67:PRO:HG3	2.39	0.62
1:E:92:ILE:HD12	1:E:126:GLY:O	1.99	0.62
1:E:140:ILE:HG23	1:E:143:PHE:CD2	2.35	0.62
1:E:300:SER:OG	1:E:302:VAL:HG12	2.00	0.62
1:F:92:ILE:HD12	1:F:126:GLY:O	2.00	0.62
1:F:129:HIS:HB2	1:F:147:PRO:O	1.98	0.62
1:B:92:ILE:HD12	1:B:126:GLY:O	2.00	0.61
1:B:324:LYS:HZ1	3:B:1353:TAM:H32	1.66	0.61
1:B:19:CYS:SG	1:B:67:PRO:HG3	2.41	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:ILE:HG23	1:D:143:PHE:CD2	2.35	0.61
1:E:59:ASP:OD1	1:E:91:ASN:HB2	2.00	0.61
1:D:300:SER:OG	1:D:302:VAL:HG12	2.01	0.60
1:B:64:GLN:HA	1:B:64:GLN:NE2	2.17	0.60
1:D:24:LYS:O	1:D:28:GLU:HG2	2.02	0.60
1:A:59:ASP:OD1	1:A:91:ASN:HB2	2.02	0.60
1:D:313:HIS:HA	1:D:316:GLN:HE21	1.67	0.60
1:F:24:LYS:O	1:F:28:GLU:HG2	2.02	0.60
1:C:300:SER:OG	1:C:302:VAL:HG12	2.02	0.59
1:E:24:LYS:O	1:E:28:GLU:HG2	2.02	0.59
1:C:64:GLN:HA	1:C:64:GLN:NE2	2.18	0.59
1:E:129:HIS:HB2	1:E:147:PRO:O	2.02	0.58
1:F:59:ASP:OD1	1:F:91:ASN:HB2	2.03	0.58
1:B:129:HIS:HB2	1:B:147:PRO:O	2.04	0.58
1:B:328:ILE:O	1:B:331:ILE:HG22	2.03	0.58
1:D:328:ILE:O	1:D:331:ILE:HG22	2.04	0.58
1:F:300:SER:OG	1:F:302:VAL:HG12	2.03	0.58
1:B:324:LYS:NZ	3:B:1353:TAM:C3	2.67	0.58
1:B:300:SER:OG	1:B:302:VAL:HG12	2.04	0.57
1:D:59:ASP:OD1	1:D:91:ASN:HB2	2.03	0.57
1:D:92:ILE:HD12	1:D:126:GLY:O	2.04	0.57
1:A:24:LYS:O	1:A:28:GLU:HG2	2.04	0.57
1:F:107:MET:HE2	4:F:2005:HOH:O	2.04	0.57
1:E:328:ILE:O	1:E:331:ILE:HG22	2.04	0.57
1:B:140:ILE:HG23	1:B:143:PHE:CE2	2.40	0.57
1:C:92:ILE:HD12	1:C:126:GLY:O	2.04	0.57
1:A:300:SER:OG	1:A:302:VAL:HG12	2.04	0.56
1:A:313:HIS:HA	1:A:316:GLN:HE21	1.69	0.56
1:F:328:ILE:O	1:F:331:ILE:HG22	2.04	0.56
1:E:8:TYR:OH	1:E:337:ARG:HG3	2.04	0.56
1:F:90:ARG:C	1:F:91:ASN:HD22	2.13	0.56
1:C:313:HIS:HA	1:C:316:GLN:HE21	1.70	0.56
1:C:24:LYS:O	1:C:28:GLU:HG2	2.05	0.56
1:B:24:LYS:O	1:B:28:GLU:HG2	2.06	0.56
1:C:328:ILE:O	1:C:331:ILE:HG22	2.05	0.56
1:F:313:HIS:HA	1:F:316:GLN:HE21	1.71	0.56
1:A:64:GLN:HA	1:A:64:GLN:NE2	2.22	0.55
1:B:313:HIS:HA	1:B:316:GLN:HE21	1.71	0.55
1:C:59:ASP:OD1	1:C:91:ASN:HB2	2.07	0.55
1:C:61:PHE:HE2	1:C:339:ILE:HD11	1.72	0.55
1:D:64:GLN:HA	1:D:64:GLN:NE2	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:TYR:CE2	1:C:306:VAL:HG21	2.43	0.54
1:E:313:HIS:O	1:E:316:GLN:HG3	2.07	0.54
1:B:95:VAL:HG21	1:B:336:ILE:HD11	1.89	0.54
1:E:140:ILE:HG23	1:E:143:PHE:CE2	2.43	0.54
1:C:90:ARG:C	1:C:91:ASN:HD22	2.16	0.54
1:A:328:ILE:O	1:A:331:ILE:HG22	2.06	0.54
1:D:160:TYR:CE2	1:D:306:VAL:HG21	2.43	0.54
1:B:61:PHE:HE2	1:B:339:ILE:HD11	1.73	0.54
1:A:140:ILE:HG23	1:A:143:PHE:CE2	2.43	0.54
1:D:313:HIS:O	1:D:316:GLN:HG3	2.08	0.53
1:E:154:SER:O	1:E:155:PRO:C	2.49	0.53
1:B:59:ASP:OD1	1:B:91:ASN:HB2	2.08	0.53
1:C:16:THR:HB	1:C:19:CYS:HB2	1.89	0.53
1:A:160:TYR:CE2	1:A:306:VAL:HG21	2.43	0.53
1:E:313:HIS:HA	1:E:316:GLN:HE21	1.73	0.53
1:E:61:PHE:HE2	1:E:339:ILE:HD11	1.73	0.53
1:B:64:GLN:HA	1:B:64:GLN:HE21	1.74	0.53
1:F:313:HIS:O	1:F:316:GLN:HG3	2.09	0.53
1:A:168:TYR:O	1:A:171:ALA:HB3	2.09	0.53
1:B:133:MET:CE	1:B:153:ALA:HB2	2.39	0.53
1:C:140:ILE:HG23	1:C:143:PHE:CE2	2.44	0.53
1:D:90:ARG:C	1:D:91:ASN:HD22	2.17	0.53
1:D:95:VAL:HG21	1:D:336:ILE:HD11	1.91	0.53
1:D:185:GLN:HG3	1:F:178:PRO:HG2	1.91	0.53
1:F:61:PHE:HE2	1:F:339:ILE:HD11	1.74	0.53
1:F:160:TYR:CE2	1:F:306:VAL:HG21	2.44	0.53
1:A:95:VAL:HG21	1:A:336:ILE:HD11	1.90	0.53
1:B:90:ARG:C	1:B:91:ASN:HD22	2.17	0.53
1:D:140:ILE:HG23	1:D:143:PHE:CE2	2.43	0.53
1:F:140:ILE:HG23	1:F:143:PHE:CE2	2.43	0.53
1:A:313:HIS:O	1:A:316:GLN:HG3	2.09	0.52
1:E:64:GLN:HA	1:E:64:GLN:NE2	2.25	0.52
1:E:95:VAL:HG21	1:E:336:ILE:HD11	1.91	0.52
1:A:90:ARG:C	1:A:91:ASN:HD22	2.16	0.52
1:D:128:THR:O	1:D:146:PHE:HB2	2.09	0.52
1:B:286:HIS:HA	1:B:310:THR:CG2	2.40	0.52
1:D:61:PHE:HE2	1:D:339:ILE:HD11	1.75	0.52
1:C:133:MET:CE	1:C:153:ALA:HB2	2.40	0.52
1:E:160:TYR:CE2	1:E:306:VAL:HG21	2.44	0.52
1:B:324:LYS:HE3	3:B:1353:TAM:C3	2.40	0.52
1:B:160:TYR:CE2	1:B:306:VAL:HG21	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ALA:HB3	1:C:64:GLN:CD	2.34	0.52
1:F:154:SER:O	1:F:155:PRO:C	2.52	0.52
1:C:286:HIS:HA	1:C:310:THR:CG2	2.40	0.52
1:A:154:SER:O	1:A:155:PRO:C	2.50	0.52
1:C:64:GLN:HA	1:C:64:GLN:HE21	1.75	0.52
1:D:16:THR:HB	1:D:19:CYS:HB2	1.90	0.51
1:B:286:HIS:HA	1:B:310:THR:HG21	1.92	0.51
1:E:13:ALA:HB3	1:E:64:GLN:CD	2.35	0.51
1:B:139:GLU:HB2	4:B:2008:HOH:O	2.10	0.51
1:D:165:ILE:HG12	1:D:281:TYR:CE2	2.46	0.51
1:B:165:ILE:HG12	1:B:281:TYR:CE2	2.46	0.51
1:B:128:THR:O	1:B:146:PHE:HB2	2.09	0.51
1:D:168:TYR:O	1:D:171:ALA:HB3	2.10	0.51
1:E:13:ALA:HB3	1:E:64:GLN:NE2	2.25	0.51
1:E:16:THR:HB	1:E:19:CYS:HB2	1.91	0.51
1:A:92:ILE:CD1	1:A:126:GLY:O	2.59	0.51
1:A:244:VAL:HG12	1:E:244:VAL:HG12	1.92	0.51
1:C:95:VAL:HG21	1:C:336:ILE:HD11	1.93	0.50
1:C:317:LYS:HE3	1:C:325:THR:HG22	1.92	0.50
1:F:95:VAL:HG21	1:F:336:ILE:HD11	1.92	0.50
1:C:154:SER:O	1:C:155:PRO:C	2.53	0.50
1:E:133:MET:CE	1:E:153:ALA:HB2	2.42	0.50
1:F:317:LYS:HE3	1:F:325:THR:HG22	1.92	0.50
1:A:133:MET:CE	1:A:153:ALA:HB2	2.42	0.50
1:C:165:ILE:HG12	1:C:281:TYR:CE2	2.47	0.50
1:E:317:LYS:HE3	1:E:325:THR:HG22	1.93	0.50
1:B:16:THR:HB	1:B:19:CYS:HB2	1.93	0.50
1:E:101:TYR:CD1	1:E:114:VAL:HG21	2.46	0.50
1:E:168:TYR:O	1:E:171:ALA:HB3	2.12	0.50
1:A:61:PHE:HE2	1:A:339:ILE:HD11	1.75	0.50
1:B:13:ALA:HB3	1:B:64:GLN:CD	2.37	0.50
1:E:92:ILE:CD1	1:E:126:GLY:O	2.60	0.50
1:E:286:HIS:HA	1:E:310:THR:CG2	2.42	0.50
1:A:286:HIS:HA	1:A:310:THR:CG2	2.42	0.50
1:F:168:TYR:O	1:F:171:ALA:HB3	2.12	0.50
1:B:168:TYR:O	1:B:171:ALA:HB3	2.12	0.49
1:F:13:ALA:HB3	1:F:64:GLN:NE2	2.27	0.49
1:D:133:MET:CE	1:D:153:ALA:HB2	2.41	0.49
1:A:165:ILE:HG12	1:A:281:TYR:CE2	2.47	0.49
1:C:286:HIS:HA	1:C:310:THR:HG21	1.94	0.49
1:D:101:TYR:CD1	1:D:114:VAL:HG21	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:HIS:HA	1:D:310:THR:CG2	2.42	0.49
1:B:138:LYS:HB2	4:B:2007:HOH:O	2.11	0.49
1:D:154:SER:O	1:D:155:PRO:C	2.55	0.49
1:B:324:LYS:CE	3:B:1353:TAM:C3	2.90	0.49
1:D:176:LYS:NZ	1:D:256:ASP:OD2	2.45	0.49
1:E:165:ILE:HG12	1:E:281:TYR:CE2	2.47	0.49
1:E:286:HIS:HA	1:E:310:THR:HG21	1.94	0.49
1:F:260:ASP:HA	1:F:288:ILE:HG12	1.94	0.49
1:B:154:SER:O	1:B:155:PRO:C	2.54	0.49
1:D:317:LYS:HE3	1:D:325:THR:HG22	1.94	0.49
1:E:90:ARG:C	1:E:91:ASN:HD22	2.20	0.49
1:F:16:THR:HB	1:F:19:CYS:HB2	1.95	0.49
1:F:64:GLN:NE2	1:F:64:GLN:HA	2.27	0.49
1:F:133:MET:CE	1:F:153:ALA:HB2	2.42	0.49
1:F:286:HIS:HA	1:F:310:THR:CG2	2.43	0.49
1:F:165:ILE:HG12	1:F:281:TYR:CE2	2.48	0.49
1:A:13:ALA:HB3	1:A:64:GLN:CD	2.38	0.49
1:C:168:TYR:O	1:C:171:ALA:HB3	2.13	0.49
1:B:92:ILE:CD1	1:B:126:GLY:O	2.61	0.49
1:B:317:LYS:HE3	1:B:325:THR:HG22	1.94	0.49
1:A:317:LYS:HE3	1:A:325:THR:HG22	1.94	0.48
1:F:13:ALA:HB3	1:F:64:GLN:CD	2.37	0.48
1:F:128:THR:O	1:F:146:PHE:HB2	2.14	0.48
1:A:13:ALA:HB3	1:A:64:GLN:NE2	2.29	0.48
1:A:260:ASP:HA	1:A:288:ILE:HG12	1.96	0.48
1:C:128:THR:O	1:C:146:PHE:HB2	2.12	0.48
1:A:132:THR:HG21	1:A:135:LEU:HD21	1.96	0.48
1:A:286:HIS:HA	1:A:310:THR:HG21	1.95	0.48
1:C:313:HIS:O	1:C:316:GLN:HG3	2.13	0.48
1:D:286:HIS:HA	1:D:310:THR:HG21	1.95	0.48
1:F:25:ARG:O	1:F:29:ARG:HG3	2.13	0.48
1:A:16:THR:HB	1:A:19:CYS:HB2	1.94	0.48
1:E:128:THR:O	1:E:146:PHE:HB2	2.12	0.48
1:A:256:ASP:O	1:A:284:ALA:HA	2.14	0.48
1:B:313:HIS:O	1:B:316:GLN:HG3	2.13	0.48
1:D:320:CYS:SG	1:D:322:LYS:HB3	2.54	0.48
1:C:64:GLN:HG3	1:C:77:LEU:HB2	1.96	0.48
1:E:260:ASP:HA	1:E:288:ILE:HG12	1.95	0.48
1:C:260:ASP:HA	1:C:288:ILE:HG12	1.95	0.47
1:D:260:ASP:HA	1:D:288:ILE:HG12	1.95	0.47
1:F:92:ILE:CD1	1:F:126:GLY:O	2.61	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:TYR:CD1	1:B:114:VAL:HG21	2.49	0.47
1:B:260:ASP:HA	1:B:288:ILE:HG12	1.95	0.47
1:A:101:TYR:CD1	1:A:114:VAL:HG21	2.50	0.47
1:B:61:PHE:CE2	1:B:339:ILE:HD11	2.49	0.47
1:B:112:SER:HB3	1:E:83:ALA:HA	1.96	0.47
1:B:176:LYS:NZ	1:B:256:ASP:OD2	2.47	0.47
1:D:67:PRO:O	1:D:68:ARG:HB3	2.15	0.47
1:D:330:LEU:HD23	1:D:330:LEU:O	2.15	0.47
1:E:25:ARG:O	1:E:29:ARG:HG3	2.15	0.47
1:C:68:ARG:HD2	1:C:68:ARG:O	2.15	0.47
1:A:122:LEU:O	1:A:127:LEU:HB2	2.15	0.47
1:D:256:ASP:O	1:D:284:ALA:HA	2.15	0.47
1:A:320:CYS:SG	1:A:322:LYS:HB3	2.55	0.47
1:B:25:ARG:O	1:B:29:ARG:HG3	2.15	0.47
1:E:137:GLN:HB3	4:E:2008:HOH:O	2.16	0.46
1:F:256:ASP:O	1:F:284:ALA:HA	2.14	0.46
1:B:330:LEU:HD23	1:B:330:LEU:O	2.15	0.46
1:C:61:PHE:CE2	1:C:339:ILE:HD11	2.50	0.46
1:C:101:TYR:CD1	1:C:114:VAL:HG21	2.50	0.46
1:D:92:ILE:CD1	1:D:126:GLY:O	2.63	0.46
1:E:55:VAL:O	1:E:56:ARG:C	2.58	0.46
1:D:13:ALA:HB3	1:D:64:GLN:CD	2.40	0.46
1:B:64:GLN:HG3	1:B:77:LEU:HB2	1.98	0.46
1:F:101:TYR:CD1	1:F:114:VAL:HG21	2.50	0.46
1:A:64:GLN:HA	1:A:64:GLN:HE21	1.79	0.46
1:B:132:THR:HG21	1:B:135:LEU:HD21	1.98	0.46
1:F:286:HIS:HA	1:F:310:THR:HG21	1.97	0.46
1:A:68:ARG:HD2	1:A:68:ARG:O	2.15	0.46
1:E:132:THR:HG21	1:E:135:LEU:HD21	1.98	0.46
1:F:61:PHE:CE2	1:F:339:ILE:HD11	2.50	0.46
1:A:25:ARG:O	1:A:29:ARG:HG3	2.16	0.46
1:A:330:LEU:O	1:A:330:LEU:HD23	2.17	0.46
1:C:132:THR:HG21	1:C:135:LEU:HD21	1.98	0.46
1:E:286:HIS:ND1	1:E:310:THR:HG21	2.32	0.45
1:D:64:GLN:HA	1:D:64:GLN:HE21	1.81	0.45
1:F:261:ASP:C	1:F:261:ASP:OD1	2.59	0.45
1:B:55:VAL:O	1:B:56:ARG:C	2.59	0.45
4:B:2004:HOH:O	1:E:109:LYS:HG2	2.16	0.45
1:C:55:VAL:O	1:C:56:ARG:C	2.59	0.45
1:E:101:TYR:CD1	1:E:114:VAL:CG2	3.00	0.45
1:F:286:HIS:ND1	1:F:310:THR:HG21	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:VAL:O	1:E:74:VAL:HG13	2.17	0.45
1:A:176:LYS:NZ	1:A:256:ASP:OD2	2.46	0.45
1:B:324:LYS:HD2	4:B:2021:HOH:O	2.16	0.45
1:B:330:LEU:HB2	4:B:2002:HOH:O	2.15	0.45
1:C:92:ILE:CD1	1:C:126:GLY:O	2.65	0.45
1:C:344:SER:HA	2:C:1351:SO4:O4	2.17	0.45
1:D:13:ALA:HB3	1:D:64:GLN:NE2	2.31	0.45
1:A:128:THR:O	1:A:146:PHE:HB2	2.16	0.45
1:C:256:ASP:O	1:C:284:ALA:HA	2.17	0.45
1:D:61:PHE:CE2	1:D:339:ILE:HD11	2.51	0.45
1:D:178:PRO:HG2	1:F:185:GLN:HG3	1.97	0.45
1:B:324:LYS:CE	3:B:1353:TAM:O6	2.65	0.45
1:C:310:THR:HG22	4:C:2010:HOH:O	2.16	0.45
1:D:25:ARG:O	1:D:29:ARG:HG3	2.17	0.45
1:D:64:GLN:HG3	1:D:77:LEU:HB2	1.98	0.45
1:E:256:ASP:O	1:E:284:ALA:HA	2.17	0.45
1:F:320:CYS:SG	1:F:322:LYS:HB3	2.57	0.45
1:E:61:PHE:CE2	1:E:339:ILE:HD11	2.50	0.45
1:F:330:LEU:O	1:F:330:LEU:HD23	2.17	0.45
1:A:286:HIS:ND1	1:A:310:THR:HG21	2.32	0.44
1:E:137:GLN:HB2	1:E:140:ILE:HG13	1.99	0.44
1:A:64:GLN:HG3	1:A:77:LEU:HB2	1.98	0.44
1:B:286:HIS:ND1	1:B:310:THR:HG21	2.32	0.44
1:F:260:ASP:N	4:F:2007:HOH:O	2.50	0.44
1:A:137:GLN:HB2	1:A:140:ILE:HG13	1.99	0.44
1:B:62:ILE:HD11	1:B:84:LEU:HD12	1.99	0.44
1:B:288:ILE:HD11	1:E:44:ASN:HB3	1.99	0.44
1:D:71:ASN:OD1	1:D:101:TYR:OH	2.30	0.44
1:D:122:LEU:O	1:D:127:LEU:HB2	2.17	0.44
1:F:64:GLN:HG3	1:F:77:LEU:HB2	1.99	0.44
1:D:286:HIS:ND1	1:D:310:THR:HG21	2.33	0.44
1:F:62:ILE:HD11	1:F:84:LEU:HD12	1.99	0.44
1:C:330:LEU:O	1:C:330:LEU:HD23	2.17	0.44
1:D:138:LYS:HD2	1:F:106:LYS:NZ	2.32	0.44
1:D:101:TYR:CD1	1:D:114:VAL:CG2	3.01	0.44
1:C:13:ALA:HB3	1:C:64:GLN:NE2	2.32	0.44
1:C:293:ALA:N	1:C:294:PRO:CD	2.81	0.44
1:D:55:VAL:O	1:D:56:ARG:C	2.60	0.44
1:D:261:ASP:C	1:D:261:ASP:OD1	2.61	0.44
1:B:293:ALA:N	1:B:294:PRO:CD	2.81	0.44
1:A:61:PHE:CE2	1:A:339:ILE:HD11	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:VAL:O	1:A:74:VAL:HG13	2.18	0.43
1:F:67:PRO:O	1:F:68:ARG:HB3	2.17	0.43
1:F:122:LEU:O	1:F:127:LEU:HB2	2.17	0.43
1:D:132:THR:HG21	1:D:135:LEU:HD21	2.00	0.43
1:E:64:GLN:HG3	1:E:77:LEU:HB2	1.99	0.43
1:E:293:ALA:N	1:E:294:PRO:CD	2.81	0.43
1:F:55:VAL:O	1:F:56:ARG:C	2.61	0.43
1:C:122:LEU:O	1:C:127:LEU:HB2	2.18	0.43
1:D:70:VAL:O	1:D:74:VAL:HG13	2.18	0.43
1:E:62:ILE:HD11	1:E:84:LEU:HD12	1.99	0.43
1:F:132:THR:HG21	1:F:135:LEU:HD21	2.00	0.43
1:D:293:ALA:N	1:D:294:PRO:CD	2.82	0.43
1:B:324:LYS:CE	3:B:1353:TAM:H31	2.47	0.43
1:C:67:PRO:O	1:C:68:ARG:HB3	2.18	0.43
1:C:118:LEU:HA	1:C:121:MET:HE2	2.00	0.43
1:E:67:PRO:O	1:E:68:ARG:HB3	2.19	0.43
1:E:158:LEU:CD1	1:E:187:TYR:CD2	3.01	0.43
1:E:261:ASP:OD1	1:E:261:ASP:C	2.60	0.43
1:A:55:VAL:O	1:A:56:ARG:C	2.61	0.43
1:C:71:ASN:OD1	1:C:101:TYR:OH	2.33	0.43
1:B:13:ALA:HB3	1:B:64:GLN:NE2	2.33	0.43
1:C:70:VAL:O	1:C:74:VAL:HG13	2.19	0.43
1:E:298:GLU:HA	1:E:322:LYS:HE2	2.00	0.43
1:C:176:LYS:NZ	1:C:256:ASP:OD2	2.51	0.43
1:C:286:HIS:ND1	1:C:310:THR:HG21	2.34	0.43
1:D:62:ILE:HD11	1:D:84:LEU:HD12	2.00	0.43
1:D:68:ARG:HD2	1:D:68:ARG:O	2.18	0.43
1:F:10:VAL:HA	1:F:61:PHE:O	2.19	0.43
1:B:118:LEU:HA	1:B:121:MET:HE2	2.01	0.43
1:D:137:GLN:HB2	1:D:140:ILE:HG13	2.01	0.43
1:E:64:GLN:HA	1:E:64:GLN:HE21	1.83	0.43
1:B:68:ARG:HD2	1:B:68:ARG:O	2.19	0.42
1:B:261:ASP:OD1	1:B:261:ASP:C	2.62	0.42
1:C:62:ILE:HD11	1:C:84:LEU:HD12	2.00	0.42
1:A:71:ASN:OD1	1:A:101:TYR:OH	2.31	0.42
1:E:182:LYS:NZ	4:E:2006:HOH:O	2.43	0.42
1:A:261:ASP:C	1:A:261:ASP:OD1	2.61	0.42
1:C:10:VAL:HA	1:C:61:PHE:O	2.19	0.42
1:B:101:TYR:CD1	1:B:114:VAL:CG2	3.03	0.42
1:C:25:ARG:O	1:C:29:ARG:HG3	2.19	0.42
1:A:298:GLU:HA	1:A:322:LYS:HE2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:VAL:HA	1:D:61:PHE:O	2.20	0.42
1:A:138:LYS:HD2	1:E:106:LYS:HZ2	1.85	0.42
1:B:256:ASP:O	1:B:284:ALA:HA	2.19	0.42
1:B:324:LYS:HE2	3:B:1353:TAM:O6	2.20	0.42
1:C:101:TYR:CD1	1:C:114:VAL:CG2	3.03	0.42
1:A:178:PRO:HG2	1:E:185:GLN:HG3	2.02	0.42
1:B:70:VAL:O	1:B:74:VAL:HG13	2.20	0.42
1:F:101:TYR:CD1	1:F:114:VAL:CG2	3.03	0.42
1:F:293:ALA:N	1:F:294:PRO:CD	2.82	0.42
1:F:298:GLU:HA	1:F:322:LYS:HE2	2.01	0.42
1:A:67:PRO:O	1:A:68:ARG:HB3	2.18	0.42
1:A:101:TYR:CD1	1:A:114:VAL:CG2	3.03	0.42
1:B:67:PRO:O	1:B:68:ARG:HB3	2.20	0.42
1:B:134:ASP:OD1	1:B:152:ARG:HA	2.19	0.42
1:B:324:LYS:HZ2	3:B:1353:TAM:C3	2.33	0.42
1:C:261:ASP:OD1	1:C:261:ASP:C	2.63	0.42
1:E:122:LEU:O	1:E:127:LEU:HB2	2.18	0.42
1:F:137:GLN:HB2	1:F:140:ILE:HG13	2.01	0.42
1:F:176:LYS:NZ	1:F:256:ASP:OD2	2.51	0.42
1:A:62:ILE:HD11	1:A:84:LEU:HD12	2.02	0.41
1:A:128:THR:O	1:A:129:HIS:HB3	2.20	0.41
1:C:298:GLU:HA	1:C:322:LYS:HE2	2.01	0.41
1:F:71:ASN:OD1	1:F:101:TYR:OH	2.30	0.41
1:E:10:VAL:HA	1:E:61:PHE:O	2.20	0.41
1:B:10:VAL:HA	1:B:61:PHE:O	2.20	0.41
1:B:251:ILE:HB	1:B:279:LYS:HB2	2.03	0.41
1:C:251:ILE:HB	1:C:279:LYS:HB2	2.02	0.41
1:E:320:CYS:SG	1:E:322:LYS:HB3	2.60	0.41
1:A:257:ASP:CG	1:A:258:ILE:HG13	2.45	0.41
1:D:298:GLU:HA	1:D:322:LYS:HE2	2.02	0.41
1:A:10:VAL:HA	1:A:61:PHE:O	2.20	0.41
1:A:293:ALA:N	1:A:294:PRO:CD	2.83	0.41
1:B:122:LEU:O	1:B:127:LEU:HB2	2.20	0.41
1:B:152:ARG:HD2	1:B:154:SER:OG	2.21	0.41
1:E:71:ASN:OD1	1:E:101:TYR:OH	2.34	0.41
1:F:64:GLN:HA	1:F:64:GLN:HE21	1.85	0.41
1:B:298:GLU:HA	1:B:322:LYS:HE2	2.02	0.41
1:C:320:CYS:SG	1:C:322:LYS:HB3	2.61	0.41
1:C:137:GLN:HB2	1:C:140:ILE:HG13	2.03	0.41
1:C:30:LEU:C	1:C:32:ALA:H	2.28	0.40
1:A:308:THR:C	1:A:310:THR:H	2.30	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:ARG:HB2	1:E:109:LYS:H	1.78	0.40
1:A:85:LYS:HD3	1:A:126:GLY:HA3	2.04	0.40
1:A:152:ARG:HD2	1:A:154:SER:OG	2.21	0.40
1:A:251:ILE:HB	1:A:279:LYS:HB2	2.03	0.40
1:B:137:GLN:HB2	1:B:140:ILE:HG13	2.04	0.40
1:E:257:ASP:CG	1:E:258:ILE:HG13	2.46	0.40
1:D:313:HIS:O	1:D:315:VAL:N	2.55	0.40
1:E:313:HIS:O	1:E:315:VAL:N	2.54	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	301/370 (81%)	270 (90%)	24 (8%)	7 (2%)	5	8
1	B	301/370 (81%)	270 (90%)	23 (8%)	8 (3%)	4	6
1	C	301/370 (81%)	271 (90%)	22 (7%)	8 (3%)	4	6
1	D	301/370 (81%)	272 (90%)	22 (7%)	7 (2%)	5	8
1	E	301/370 (81%)	272 (90%)	21 (7%)	8 (3%)	4	6
1	F	301/370 (81%)	271 (90%)	24 (8%)	6 (2%)	6	10
All	All	1806/2220 (81%)	1626 (90%)	136 (8%)	44 (2%)	4	7

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	ILE
1	B	241	ILE
1	C	241	ILE
1	D	241	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	241	ILE
1	F	241	ILE
1	A	67	PRO
1	A	111	GLY
1	B	8	TYR
1	B	67	PRO
1	B	111	GLY
1	C	8	TYR
1	C	67	PRO
1	C	111	GLY
1	D	8	TYR
1	D	67	PRO
1	D	111	GLY
1	E	8	TYR
1	E	67	PRO
1	E	111	GLY
1	F	67	PRO
1	F	111	GLY
1	A	56	ARG
1	A	108	ARG
1	B	56	ARG
1	B	108	ARG
1	C	56	ARG
1	C	108	ARG
1	D	56	ARG
1	D	108	ARG
1	E	56	ARG
1	E	108	ARG
1	F	56	ARG
1	F	108	ARG
1	B	291	ALA
1	F	291	ALA
1	A	248	GLY
1	A	291	ALA
1	C	291	ALA
1	E	291	ALA
1	C	248	GLY
1	D	248	GLY
1	B	248	GLY
1	E	248	GLY

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	258/315 (82%)	228 (88%)	30 (12%)	5	8
1	B	258/315 (82%)	229 (89%)	29 (11%)	6	8
1	C	258/315 (82%)	228 (88%)	30 (12%)	5	8
1	D	258/315 (82%)	228 (88%)	30 (12%)	5	8
1	E	258/315 (82%)	228 (88%)	30 (12%)	5	8
1	F	258/315 (82%)	227 (88%)	31 (12%)	5	7
All	All	1548/1890 (82%)	1368 (88%)	180 (12%)	5	8

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	21	GLU
1	A	36	LYS
1	A	50	GLU
1	A	64	GLN
1	A	66	ILE
1	A	67	PRO
1	A	74	VAL
1	A	103	LYS
1	A	114	VAL
1	A	122	LEU
1	A	127	LEU
1	A	128	THR
1	A	129	HIS
1	A	130	ILE
1	A	139	GLU
1	A	154	SER
1	A	158	LEU
1	A	169	ARG
1	A	251	ILE
1	A	263	GLU
1	A	274	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	288	ILE
1	A	311	VAL
1	A	316	GLN
1	A	317	LYS
1	A	318	LEU
1	A	319	GLN
1	A	322	LYS
1	A	343	GLU
1	B	8	TYR
1	B	10	VAL
1	B	21	GLU
1	B	36	LYS
1	B	50	GLU
1	B	64	GLN
1	B	66	ILE
1	B	67	PRO
1	B	74	VAL
1	B	103	LYS
1	B	114	VAL
1	B	122	LEU
1	B	127	LEU
1	B	129	HIS
1	B	139	GLU
1	B	154	SER
1	B	158	LEU
1	B	169	ARG
1	B	251	ILE
1	B	263	GLU
1	B	274	GLU
1	B	288	ILE
1	B	311	VAL
1	B	316	GLN
1	B	317	LYS
1	B	318	LEU
1	B	319	GLN
1	B	322	LYS
1	B	343	GLU
1	C	8	TYR
1	C	10	VAL
1	C	21	GLU
1	C	36	LYS
1	C	50	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	64	GLN
1	C	66	ILE
1	C	67	PRO
1	C	74	VAL
1	C	103	LYS
1	C	114	VAL
1	C	122	LEU
1	C	127	LEU
1	C	129	HIS
1	C	130	ILE
1	C	139	GLU
1	C	154	SER
1	C	158	LEU
1	C	169	ARG
1	C	251	ILE
1	C	263	GLU
1	C	274	GLU
1	C	288	ILE
1	C	311	VAL
1	C	316	GLN
1	C	317	LYS
1	C	318	LEU
1	C	319	GLN
1	C	322	LYS
1	C	343	GLU
1	D	10	VAL
1	D	21	GLU
1	D	36	LYS
1	D	50	GLU
1	D	64	GLN
1	D	66	ILE
1	D	67	PRO
1	D	74	VAL
1	D	103	LYS
1	D	114	VAL
1	D	122	LEU
1	D	127	LEU
1	D	128	THR
1	D	129	HIS
1	D	130	ILE
1	D	139	GLU
1	D	154	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	158	LEU
1	D	169	ARG
1	D	251	ILE
1	D	263	GLU
1	D	274	GLU
1	D	288	ILE
1	D	311	VAL
1	D	316	GLN
1	D	317	LYS
1	D	318	LEU
1	D	319	GLN
1	D	322	LYS
1	D	343	GLU
1	E	10	VAL
1	E	19	CYS
1	E	21	GLU
1	E	36	LYS
1	E	50	GLU
1	E	64	GLN
1	E	66	ILE
1	E	67	PRO
1	E	74	VAL
1	E	103	LYS
1	E	114	VAL
1	E	122	LEU
1	E	127	LEU
1	E	128	THR
1	E	129	HIS
1	E	139	GLU
1	E	154	SER
1	E	158	LEU
1	E	169	ARG
1	E	251	ILE
1	E	263	GLU
1	E	274	GLU
1	E	288	ILE
1	E	311	VAL
1	E	316	GLN
1	E	317	LYS
1	E	318	LEU
1	E	319	GLN
1	E	322	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	343	GLU
1	F	8	TYR
1	F	10	VAL
1	F	21	GLU
1	F	36	LYS
1	F	50	GLU
1	F	64	GLN
1	F	66	ILE
1	F	67	PRO
1	F	74	VAL
1	F	103	LYS
1	F	114	VAL
1	F	122	LEU
1	F	127	LEU
1	F	128	THR
1	F	129	HIS
1	F	130	ILE
1	F	139	GLU
1	F	154	SER
1	F	158	LEU
1	F	169	ARG
1	F	251	ILE
1	F	263	GLU
1	F	274	GLU
1	F	288	ILE
1	F	311	VAL
1	F	316	GLN
1	F	317	LYS
1	F	318	LEU
1	F	319	GLN
1	F	322	LYS
1	F	343	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	91	ASN
1	A	137	GLN
1	A	170	ASN
1	A	185	GLN
1	A	316	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	319	GLN
1	B	64	GLN
1	B	91	ASN
1	B	137	GLN
1	B	170	ASN
1	B	316	GLN
1	B	319	GLN
1	C	64	GLN
1	C	91	ASN
1	C	137	GLN
1	C	159	GLN
1	C	170	ASN
1	C	185	GLN
1	C	316	GLN
1	C	319	GLN
1	D	14	ASN
1	D	64	GLN
1	D	91	ASN
1	D	137	GLN
1	D	316	GLN
1	D	319	GLN
1	E	64	GLN
1	E	91	ASN
1	E	137	GLN
1	E	316	GLN
1	E	319	GLN
1	F	14	ASN
1	F	64	GLN
1	F	91	ASN
1	F	137	GLN
1	F	185	GLN
1	F	316	GLN
1	F	319	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	B	1352	-	4,4,4	0.31	0	6,6,6	0.42	0
2	SO4	E	1351	-	4,4,4	0.32	0	6,6,6	0.25	0
2	SO4	B	1351	-	4,4,4	0.40	0	6,6,6	0.29	0
2	SO4	F	1351	-	4,4,4	0.35	0	6,6,6	0.23	0
3	TAM	B	1353	-	10,10,10	0.59	0	12,12,12	1.71	2 (16%)
2	SO4	E	1352	-	4,4,4	0.24	0	6,6,6	0.26	0
2	SO4	C	1351	-	4,4,4	0.30	0	6,6,6	0.25	0
2	SO4	D	1351	-	4,4,4	0.31	0	6,6,6	0.58	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	TAM	B	1353	-	-	6/12/12/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1353	TAM	C6-C3-C	4.88	121.72	115.97
3	B	1353	TAM	C3-C-C2	-2.13	106.75	110.50

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1353	TAM	C1-C-C3-C6
3	B	1353	TAM	C2-C-C3-C6
3	B	1353	TAM	N-C-C3-C6
3	B	1353	TAM	C-C1-C4-O4
3	B	1353	TAM	C-C2-C5-O5
3	B	1353	TAM	C3-C-C2-C5

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1353	TAM	10	0
2	C	1351	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

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, 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	305/370 (82%)	0.54	13 (4%) 40 32	6, 36, 55, 82	0
1	B	305/370 (82%)	0.48	15 (4%) 35 27	7, 33, 52, 81	0
1	C	305/370 (82%)	0.57	21 (6%) 23 17	7, 35, 53, 83	0
1	D	305/370 (82%)	0.59	15 (4%) 35 27	4, 37, 56, 86	0
1	E	305/370 (82%)	0.54	10 (3%) 49 40	5, 36, 57, 84	0
1	F	305/370 (82%)	0.53	18 (5%) 28 21	9, 36, 54, 81	0
All	All	1830/2220 (82%)	0.54	92 (5%) 34 26	4, 36, 55, 86	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	239	PRO	4.8
1	C	347	TYR	4.4
1	A	347	TYR	4.3
1	D	40	TYR	4.0
1	D	347	TYR	4.0
1	E	348	LEU	4.0
1	D	239	PRO	3.9
1	F	347	TYR	3.9
1	B	349	PHE	3.7
1	F	239	PRO	3.7
1	B	348	LEU	3.6
1	C	348	LEU	3.5
1	A	349	PHE	3.4
1	E	350	ARG	3.3
1	C	349	PHE	3.3
1	D	350	ARG	3.2
1	A	339	ILE	3.2
1	D	349	PHE	3.2
1	A	167	ASN	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	239	PRO	3.0
1	E	349	PHE	3.0
1	F	346	ALA	2.9
1	B	346	ALA	2.8
1	D	164	GLU	2.8
1	F	68	ARG	2.8
1	C	346	ALA	2.8
1	E	347	TYR	2.8
1	F	166	PRO	2.8
1	D	344	SER	2.8
1	D	348	LEU	2.8
1	B	347	TYR	2.8
1	E	346	ALA	2.8
1	F	240	PRO	2.8
1	F	246	ASP	2.8
1	C	40	TYR	2.8
1	D	167	ASN	2.7
1	A	240	PRO	2.7
1	D	300	SER	2.7
1	E	239	PRO	2.7
1	F	348	LEU	2.6
1	F	350	ARG	2.6
1	E	240	PRO	2.5
1	C	159	GLN	2.5
1	D	169	ARG	2.5
1	F	159	GLN	2.5
1	F	349	PHE	2.5
1	B	163	GLU	2.5
1	F	7	GLY	2.5
1	D	339	ILE	2.4
1	C	337	ARG	2.4
1	B	339	ILE	2.4
1	F	344	SER	2.4
1	E	50	GLU	2.4
1	F	185	GLN	2.4
1	B	40	TYR	2.3
1	C	240	PRO	2.3
1	E	164	GLU	2.3
1	B	350	ARG	2.3
1	A	40	TYR	2.3
1	D	16	THR	2.3
1	A	163	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	240	PRO	2.3
1	B	38	VAL	2.3
1	B	8	TYR	2.3
1	B	169	ARG	2.3
1	A	169	ARG	2.2
1	C	241	ILE	2.2
1	C	339	ILE	2.2
1	C	345	MET	2.2
1	C	50	GLU	2.2
1	C	344	SER	2.2
1	E	342	GLY	2.2
1	C	338	ARG	2.2
1	B	239	PRO	2.2
1	C	7	GLY	2.2
1	C	31	GLY	2.2
1	A	301	SER	2.2
1	A	241	ILE	2.2
1	C	244	VAL	2.2
1	F	313	HIS	2.2
1	B	50	GLU	2.1
1	B	345	MET	2.1
1	F	290	SER	2.1
1	A	32	ALA	2.1
1	C	169	ARG	2.1
1	C	165	ILE	2.1
1	D	165	ILE	2.1
1	C	350	ARG	2.1
1	B	18	ALA	2.1
1	F	277	ALA	2.1
1	A	246	ASP	2.0
1	F	326	VAL	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	TAM	B	1353	11/11	0.85	0.12	30,31,32,32	0
2	SO4	E	1352	5/5	0.87	0.12	65,65,66,66	0
2	SO4	C	1351	5/5	0.87	0.12	69,69,70,70	0
2	SO4	F	1351	5/5	0.91	0.11	49,50,51,51	0
2	SO4	B	1351	5/5	0.91	0.12	40,42,42,42	0
2	SO4	E	1351	5/5	0.92	0.10	55,55,56,57	0
2	SO4	B	1352	5/5	0.94	0.08	46,47,48,48	0
2	SO4	D	1351	5/5	0.96	0.08	38,38,39,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.