



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:37 PM UTC

PDB ID : 2AVW / pdb_00002avw
Title : Crystal structure of monoclinic form of streptococcus Mac-1
Authors : Agniswamy, J.; Nagiec, M.J.; Liu, M.; Schuck, P.; Musser, J.M.; Sun, P.D.
Deposited on : 2005-08-30
Resolution : 2.00 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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

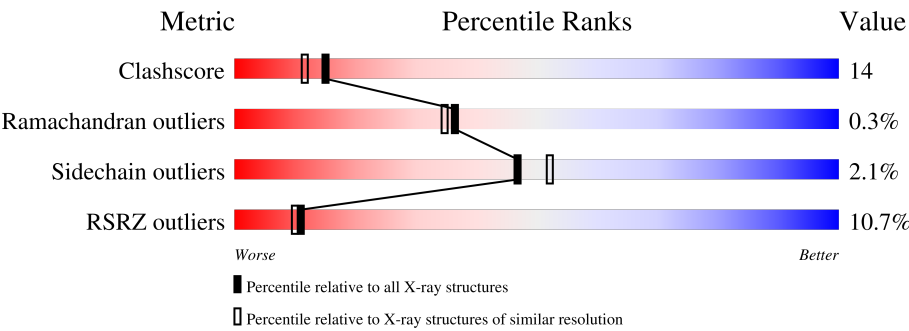
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	311	7% 71% 21% • 7%
1	B	311	11% 61% 29% • • 7%
1	C	311	9% 68% 23% • 7%
1	D	311	15% 65% 29% • 5%
1	E	311	13% 68% 25% • 5%
1	F	311	6% 67% 24% • 7%

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	GOL	F	1000	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14890 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 IgG-degrading protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2304	1468	393	439	4			
1	B	289	Total	C	N	O	S	5	0	0
			2295	1463	391	437	4			
1	C	289	Total	C	N	O	S	0	0	0
			2295	1463	391	437	4			
1	D	296	Total	C	N	O	S	0	0	0
			2353	1500	399	450	4			
1	E	296	Total	C	N	O	S	0	0	0
			2353	1500	399	450	4			
1	F	289	Total	C	N	O	S	7	0	0
			2295	1463	391	437	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MET	-	initiating methionine	GB 71910481
A	94	ALA	CYS	engineered mutation	GB 71910481
B	29	MET	-	initiating methionine	GB 71910481
B	94	ALA	CYS	engineered mutation	GB 71910481
C	29	MET	-	initiating methionine	GB 71910481
C	94	ALA	CYS	engineered mutation	GB 71910481
D	29	MET	-	initiating methionine	GB 71910481
D	94	ALA	CYS	engineered mutation	GB 71910481
E	29	MET	-	initiating methionine	GB 71910481
E	94	ALA	CYS	engineered mutation	GB 71910481
F	29	MET	-	initiating methionine	GB 71910481
F	94	ALA	CYS	engineered mutation	GB 71910481

- Molecule 2 is SULFATE ION (CCD ID: 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		
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	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			6	3	3		

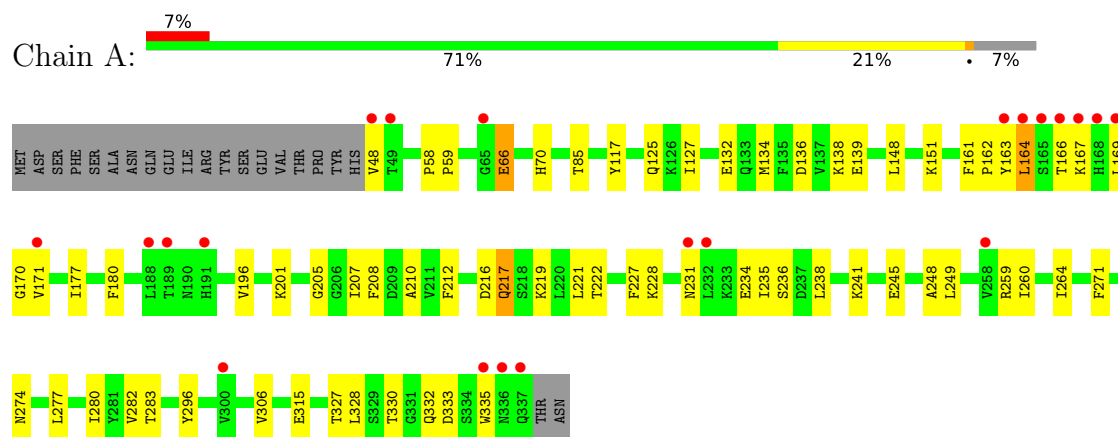
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	180	Total	O	0	0
			180	180		
4	B	146	Total	O	0	0
			146	146		
4	C	154	Total	O	0	0
			154	154		
4	D	138	Total	O	0	0
			138	138		
4	E	148	Total	O	0	0
			148	148		
4	F	193	Total	O	0	0
			193	193		

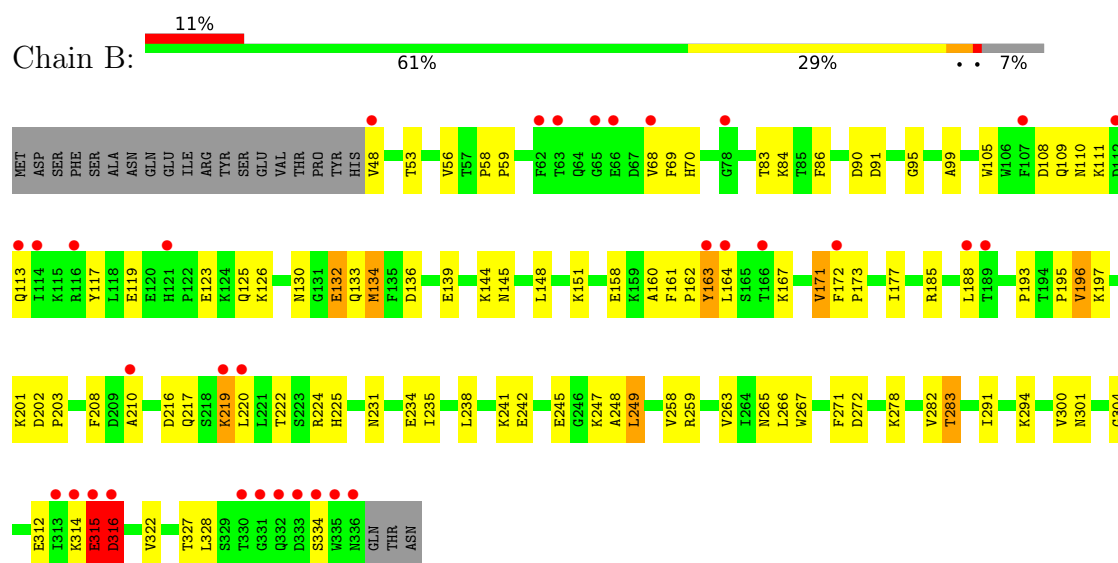
3 Residue-property plots

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: IgG-degrading protease



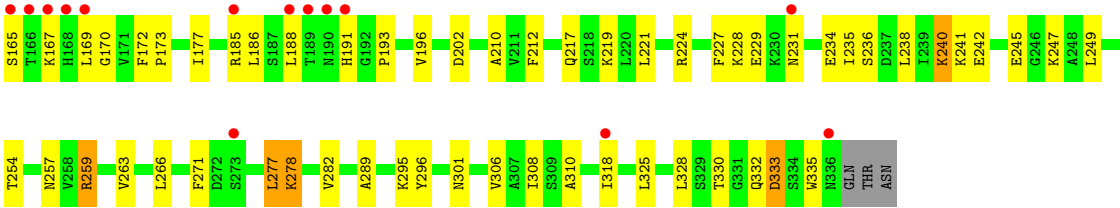
• Molecule 1: IgG-degrading protease



• Molecule 1: IgG-degrading protease







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.99Å 65.46Å 137.24Å 90.00° 105.81° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.00) 84.4 (50.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 1.95Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.267 0.236 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14890	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3218e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, GOL

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	0.39	0/2360	0.90	5/3190 (0.2%)
1	B	0.39	1/2351 (0.0%)	0.93	7/3178 (0.2%)
1	C	0.37	0/2351	0.91	7/3178 (0.2%)
1	D	0.35	0/2410	0.86	5/3259 (0.2%)
1	E	0.39	0/2410	0.90	10/3259 (0.3%)
1	F	0.39	0/2351	0.89	7/3178 (0.2%)
All	All	0.38	1/14233 (0.0%)	0.90	41/19242 (0.2%)

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	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	119	GLU	CB-CG	-5.85	1.34	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	GLU	N-CA-C	7.20	126.13	110.80
1	F	210	ALA	N-CA-C	-6.61	104.69	112.89
1	D	316	ASP	N-CA-C	-6.46	105.04	113.17
1	B	210	ALA	N-CA-C	-6.43	104.13	112.23
1	B	316	ASP	N-CA-C	-6.41	105.59	113.41
1	E	46	TYR	CA-CB-CG	-6.27	102.61	113.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	148	LEU	N-CA-C	6.24	121.02	113.41
1	A	210	ALA	N-CA-C	-6.01	105.44	112.89
1	A	85	THR	N-CA-C	-5.98	106.31	113.97
1	E	249	LEU	N-CA-C	5.95	119.09	109.40
1	B	282	VAL	N-CA-C	5.92	117.44	108.80
1	E	306	VAL	N-CA-C	-5.69	101.33	108.84
1	C	282	VAL	N-CA-C	5.62	116.80	108.65
1	C	278	LYS	N-CA-C	-5.62	107.42	114.56
1	C	172	PHE	CA-C-N	5.54	125.63	119.32
1	C	172	PHE	C-N-CA	5.54	125.63	119.32
1	E	148	LEU	N-CA-C	5.51	120.28	113.50
1	E	181	ILE	N-CA-C	5.50	115.74	110.74
1	B	249	LEU	N-CA-C	5.47	118.48	109.72
1	E	315	GLU	N-CA-C	-5.47	106.52	114.12
1	E	316	ASP	N-CA-C	-5.46	106.39	113.16
1	A	283	THR	N-CA-C	-5.44	101.02	109.72
1	D	172	PHE	CA-C-N	5.37	124.82	119.24
1	D	172	PHE	C-N-CA	5.37	124.82	119.24
1	F	172	PHE	CA-C-N	5.37	124.82	119.24
1	F	172	PHE	C-N-CA	5.37	124.82	119.24
1	B	119	GLU	CB-CG-CD	5.36	121.71	112.60
1	B	163	TYR	N-CA-C	5.32	119.77	113.28
1	C	315	GLU	N-CA-C	5.29	122.06	110.80
1	F	249	LEU	N-CA-C	5.25	118.13	109.72
1	A	164	LEU	N-CA-C	5.22	117.65	111.33
1	F	278	LYS	N-CA-C	-5.20	107.59	114.04
1	F	310	ALA	N-CA-C	-5.16	106.81	113.01
1	E	210	ALA	N-CA-C	-5.16	106.25	112.54
1	E	49	THR	N-CA-C	-5.15	107.16	113.50
1	C	210	ALA	N-CA-C	-5.15	105.75	111.36
1	D	282	VAL	N-CA-C	5.12	116.28	108.80
1	A	148	LEU	N-CA-C	5.12	119.60	112.90
1	E	282	VAL	N-CA-C	5.10	116.05	108.65
1	C	228	LYS	N-CA-C	5.06	117.18	111.11
1	D	99	ALA	N-CA-C	-5.03	105.88	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	46	TYR	Sidechain

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	2304	0	2239	51	0
1	B	2295	0	2231	78	0
1	C	2295	0	2231	66	0
1	D	2353	0	2283	81	0
1	E	2353	0	2283	62	0
1	F	2295	0	2231	61	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	F	6	0	4	1	0
4	A	180	0	0	9	0
4	B	146	0	0	8	0
4	C	154	0	0	3	0
4	D	138	0	0	6	0
4	E	148	0	0	3	0
4	F	193	0	0	2	0
All	All	14890	0	13502	376	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 (376) 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:A:161:PHE:HB3	1:A:164:LEU:HD12	1.34	1.08
1:C:167:LYS:HZ2	1:D:167:LYS:HE3	1.15	1.03
1:A:332:GLN:HA	1:A:335:TRP:HD1	1.28	0.99
1:F:259:ARG:H	1:F:259:ARG:HE	1.15	0.92
1:B:196:VAL:HG22	1:B:220:LEU:HD11	1.53	0.90
1:B:193:PRO:HG3	1:B:224:ARG:HD2	1.53	0.88
1:B:291:ILE:HG22	4:B:1078:HOH:O	1.75	0.86
1:B:265:ASN:HB2	1:B:283:THR:HG22	1.58	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:GLN:CD	1:F:318:ILE:HD11	2.01	0.85
1:A:167:LYS:HG2	1:B:167:LYS:HG2	1.59	0.85
1:B:201:LYS:HE3	4:B:1004:HOH:O	1.77	0.84
1:D:132:GLU:HG2	1:D:134:MET:HE3	1.60	0.83
1:C:167:LYS:NZ	1:D:167:LYS:HE3	1.94	0.83
1:E:132:GLU:HG2	1:E:134:MET:HE3	1.60	0.82
1:F:196:VAL:HG11	1:F:217:GLN:HG2	1.61	0.82
1:E:134:MET:HE2	1:E:134:MET:HA	1.63	0.81
1:E:95:GLY:HA2	1:E:263:VAL:HG11	1.64	0.79
1:B:267:TRP:HE1	1:B:283:THR:HB	1.48	0.79
1:F:236:SER:HA	1:F:277:LEU:HD23	1.64	0.79
1:B:134:MET:HE2	1:B:134:MET:HA	1.64	0.78
1:B:241:LYS:O	1:B:245:GLU:HG3	1.83	0.78
1:A:66:GLU:H	1:A:66:GLU:CD	1.87	0.78
1:E:48:VAL:CG2	1:E:240:LYS:HE3	2.14	0.77
1:F:332:GLN:HA	1:F:335:TRP:HD1	1.49	0.76
1:D:95:GLY:HA2	1:D:263:VAL:HG11	1.67	0.76
1:A:332:GLN:HA	1:A:335:TRP:CD1	2.17	0.76
1:E:48:VAL:HG21	1:E:240:LYS:HE3	1.68	0.74
1:E:228:LYS:HG2	1:E:229:GLU:HG3	1.69	0.74
1:C:269:ALA:HB1	1:C:277:LEU:HD11	1.70	0.73
1:D:134:MET:HA	1:D:134:MET:HE2	1.70	0.73
1:C:185:ARG:HG3	4:C:1098:HOH:O	1.89	0.72
1:C:113:GLN:NE2	1:C:332:GLN:HG3	2.05	0.72
1:B:196:VAL:CG2	1:B:220:LEU:HD11	2.20	0.71
1:F:92:LEU:HD12	1:F:165:SER:HA	1.71	0.71
1:D:301:ASN:HB2	1:D:318:ILE:HG13	1.73	0.70
1:B:83:THR:HB	1:B:148:LEU:HD23	1.72	0.70
1:C:166:THR:HB	1:D:167:LYS:HE2	1.73	0.70
1:B:315:GLU:HA	4:B:1088:HOH:O	1.92	0.70
1:D:226:ASP:CG	1:D:228:LYS:HG2	2.16	0.70
1:F:259:ARG:HE	1:F:259:ARG:N	1.90	0.70
1:C:92:LEU:HD12	1:C:165:SER:HA	1.73	0.69
1:D:269:ALA:HB1	1:D:277:LEU:HD11	1.73	0.69
1:F:134:MET:HA	1:F:134:MET:HE2	1.75	0.68
1:A:136:ASP:HB3	1:A:139:GLU:HG3	1.75	0.68
1:B:132:GLU:CG	1:B:134:MET:HE3	2.24	0.68
1:E:248:ALA:C	1:E:249:LEU:HD12	2.19	0.68
1:C:167:LYS:HE3	1:D:167:LYS:HG3	1.76	0.67
1:F:228:LYS:HG2	1:F:229:GLU:HG3	1.77	0.67
1:B:217:GLN:NE2	1:B:220:LEU:HD12	2.10	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:VAL:HG21	1:C:217:GLN:NE2	2.11	0.66
1:D:139:GLU:HB3	1:D:151:LYS:HG2	1.77	0.66
1:B:216:ASP:OD2	1:B:219:LYS:HD3	1.97	0.65
1:E:115:LYS:O	1:E:119:GLU:HG3	1.97	0.65
1:A:164:LEU:HD13	1:A:171:VAL:HG13	1.79	0.65
1:B:132:GLU:HG2	1:B:134:MET:HE3	1.79	0.64
1:A:134:MET:HA	1:A:134:MET:HE2	1.80	0.64
1:A:330:THR:OG1	1:A:332:GLN:HG2	1.98	0.64
1:B:95:GLY:HA2	1:B:263:VAL:HG11	1.81	0.63
1:C:117:TYR:CZ	1:C:208:PHE:HA	2.34	0.63
1:D:270:ASP:HB3	1:D:278:LYS:NZ	2.14	0.63
1:A:231:ASN:OD1	1:A:234:GLU:HG3	1.98	0.63
1:C:126:LYS:HD3	1:C:133:GLN:OE1	1.99	0.63
1:E:242:GLU:HG2	1:E:327:THR:HG21	1.80	0.63
1:E:161:PHE:HB3	1:E:164:LEU:HD12	1.81	0.62
1:E:249:LEU:HD23	1:E:325:LEU:HD11	1.80	0.62
1:D:332:GLN:HA	1:D:335:TRP:HD1	1.65	0.62
1:B:314:LYS:O	1:B:316:ASP:N	2.31	0.62
1:C:132:GLU:OE2	1:C:134:MET:HE1	2.00	0.61
1:F:257:ASN:HB2	1:F:259:ARG:NH2	2.15	0.61
1:A:227:PHE:HE2	1:A:238:LEU:HD23	1.66	0.61
1:B:258:VAL:HG23	1:B:259:ARG:HG3	1.82	0.61
1:E:242:GLU:CG	1:E:327:THR:HG21	2.31	0.61
1:C:241:LYS:O	1:C:245:GLU:HG3	2.01	0.60
1:B:53:THR:HB	1:B:56:VAL:HG21	1.83	0.60
1:E:161:PHE:N	1:E:162:PRO:HD3	2.15	0.59
1:E:95:GLY:HA3	1:E:171:VAL:O	2.02	0.59
1:A:163:TYR:HB2	4:A:1036:HOH:O	2.02	0.59
1:C:161:PHE:N	1:C:162:PRO:HD3	2.18	0.59
1:F:330:THR:OG1	1:F:332:GLN:HG2	2.03	0.59
1:D:270:ASP:HB3	1:D:278:LYS:HZ1	1.67	0.58
1:C:312:GLU:OE2	1:C:314:LYS:HE3	2.02	0.58
1:C:203:PRO:HG3	1:D:132:GLU:OE2	2.03	0.58
1:E:235:ILE:HD12	1:E:306:VAL:HG21	1.85	0.58
1:F:289:ALA:H	3:F:1000:GOL:C3	2.16	0.58
1:B:300:VAL:CG1	1:B:304:GLY:HA2	2.34	0.58
1:C:167:LYS:HZ3	1:D:163:TYR:HB3	1.68	0.58
1:F:301:ASN:HD22	1:F:318:ILE:CG2	2.17	0.58
1:D:255:TYR:HD1	1:D:257:ASN:HD22	1.51	0.57
1:F:227:PHE:HE2	1:F:238:LEU:HD23	1.68	0.57
1:E:241:LYS:O	1:E:245:GLU:HG3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:ARG:HG3	4:F:1034:HOH:O	2.05	0.57
1:B:70:HIS:HB2	4:B:1078:HOH:O	2.03	0.57
1:E:185:ARG:HA	1:E:202:ASP:HB2	1.86	0.57
1:C:127:ILE:HG23	1:D:130:ASN:HB2	1.86	0.57
1:B:231:ASN:OD1	1:B:234:GLU:HG3	2.04	0.57
1:B:294:LYS:HG3	4:B:1078:HOH:O	2.04	0.57
1:D:105:TRP:O	1:D:109:GLN:HG2	2.05	0.56
1:D:92:LEU:CD1	1:D:168:HIS:HA	2.36	0.56
1:E:279:ALA:HA	1:E:298:VAL:HG23	1.87	0.56
1:F:193:PRO:HG3	1:F:224:ARG:HD2	1.85	0.56
1:D:241:LYS:O	1:D:245:GLU:HG3	2.05	0.56
1:F:235:ILE:HD12	1:F:306:VAL:HG21	1.87	0.56
1:C:167:LYS:NZ	1:D:163:TYR:HB3	2.21	0.56
1:D:76:ASN:HD21	1:D:145:ASN:HD21	1.54	0.56
1:D:45:PRO:HD2	1:D:50:SER:OG	2.06	0.56
1:E:158:GLU:O	1:E:162:PRO:HG3	2.06	0.56
1:F:301:ASN:ND2	1:F:318:ILE:CG2	2.69	0.56
1:E:61:ASN:ND2	1:E:72:PRO:HD2	2.20	0.56
1:D:332:GLN:HA	1:D:335:TRP:CD1	2.41	0.55
1:C:50:SER:HB3	1:C:270:ASP:OD2	2.06	0.55
1:E:126:LYS:HE2	1:E:136:ASP:OD2	2.06	0.55
1:E:48:VAL:HG11	1:E:51:VAL:CG2	2.36	0.55
1:E:48:VAL:HG21	1:E:240:LYS:CE	2.37	0.55
1:E:263:VAL:HG12	4:E:1128:HOH:O	2.07	0.55
1:B:68:VAL:HG22	1:B:69:PHE:N	2.22	0.55
1:E:139:GLU:HB3	1:E:151:LYS:HG2	1.87	0.55
1:A:48:VAL:HB	1:A:271:PHE:O	2.06	0.55
1:D:201:LYS:HE3	4:D:1061:HOH:O	2.07	0.54
1:A:170:GLY:HA3	1:A:259:ARG:NH1	2.22	0.54
1:E:269:ALA:HB1	1:E:277:LEU:HD11	1.89	0.54
1:C:248:ALA:C	1:C:249:LEU:HD12	2.32	0.54
1:C:315:GLU:H	1:C:315:GLU:CD	2.16	0.54
1:D:160:ALA:C	1:D:162:PRO:HD3	2.32	0.54
1:A:151:LYS:HG3	4:A:1011:HOH:O	2.07	0.54
1:D:115:LYS:O	1:D:119:GLU:HG3	2.07	0.54
1:C:295:LYS:HE2	4:C:1066:HOH:O	2.08	0.54
1:F:115:LYS:O	1:F:119:GLU:HG3	2.07	0.54
1:A:161:PHE:N	1:A:162:PRO:HD3	2.23	0.53
1:F:266:LEU:HA	1:F:282:VAL:HG12	1.90	0.53
1:F:301:ASN:ND2	1:F:318:ILE:HG23	2.21	0.53
1:B:164:LEU:HD13	1:B:171:VAL:HG22	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:GLU:OE1	1:E:134:MET:HE1	2.09	0.53
1:F:164:LEU:HD21	1:F:188:LEU:HD11	1.90	0.53
1:D:84:LYS:HE3	1:D:90:ASP:O	2.09	0.53
1:E:73:TYR:HA	1:E:79:TRP:CH2	2.44	0.53
1:E:84:LYS:HE3	1:E:90:ASP:O	2.09	0.53
1:A:166:THR:HG22	1:A:166:THR:O	2.10	0.53
4:A:1160:HOH:O	1:B:132:GLU:HB2	2.09	0.53
1:C:189:THR:HG22	1:C:189:THR:O	2.09	0.52
1:F:259:ARG:H	1:F:259:ARG:NE	1.97	0.52
1:A:248:ALA:C	1:A:249:LEU:HD12	2.35	0.52
1:B:185:ARG:HA	1:B:202:ASP:HB2	1.90	0.52
1:F:241:LYS:HE2	1:F:245:GLU:OE2	2.08	0.52
1:C:314:LYS:O	1:C:316:ASP:N	2.41	0.52
1:B:160:ALA:C	1:B:162:PRO:HD3	2.34	0.52
1:B:161:PHE:N	1:B:162:PRO:HD3	2.25	0.52
1:A:161:PHE:HB3	1:A:164:LEU:CD1	2.24	0.52
1:A:236:SER:OG	1:A:277:LEU:HB2	2.09	0.52
1:D:248:ALA:C	1:D:249:LEU:HD12	2.35	0.51
1:D:126:LYS:HE2	1:D:136:ASP:OD2	2.10	0.51
1:F:132:GLU:HG2	1:F:134:MET:HE3	1.92	0.51
1:A:132:GLU:HG2	1:A:134:MET:HE3	1.92	0.51
1:D:180:PHE:CZ	1:D:207:ILE:HD12	2.45	0.51
1:B:95:GLY:HA2	1:B:263:VAL:CG1	2.40	0.51
1:C:158:GLU:C	1:C:162:PRO:HG3	2.35	0.51
1:D:95:GLY:HA2	1:D:263:VAL:CG1	2.40	0.51
1:B:219:LYS:NZ	1:B:334:SER:OG	2.43	0.51
1:F:169:LEU:HD23	1:F:170:GLY:N	2.26	0.51
1:B:248:ALA:C	1:B:249:LEU:HD12	2.35	0.51
1:B:139:GLU:OE2	1:B:151:LYS:HE3	2.11	0.51
1:C:330:THR:C	1:C:332:GLN:N	2.68	0.51
1:A:169:LEU:HB3	4:A:1101:HOH:O	2.10	0.51
1:C:117:TYR:HE1	1:C:210:ALA:HB3	1.77	0.50
1:F:212:PHE:HA	1:F:219:LYS:HG3	1.93	0.50
1:B:300:VAL:HG11	1:B:304:GLY:HA2	1.94	0.50
1:D:136:ASP:OD1	1:D:138:LYS:HB2	2.11	0.50
1:D:301:ASN:HB2	1:D:318:ILE:CG1	2.41	0.50
1:A:127:ILE:HG23	1:B:130:ASN:HB2	1.92	0.50
1:E:95:GLY:HA2	1:E:263:VAL:CG1	2.36	0.50
1:F:177:ILE:HG21	1:F:328:LEU:HD13	1.92	0.50
1:F:295:LYS:HD3	1:F:295:LYS:C	2.37	0.50
1:C:117:TYR:CE1	1:C:210:ALA:HB3	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:THR:CB	1:D:167:LYS:HE2	2.41	0.49
1:B:144:LYS:HG3	1:B:145:ASN:OD1	2.12	0.49
1:E:125:GLN:O	1:E:137:VAL:HG12	2.11	0.49
1:F:301:ASN:HD22	1:F:318:ILE:HG22	1.76	0.49
1:A:132:GLU:CD	1:A:134:MET:HE1	2.37	0.49
1:C:185:ARG:HA	1:C:202:ASP:HB2	1.94	0.49
1:E:92:LEU:CD1	1:E:168:HIS:HA	2.41	0.49
1:E:212:PHE:HA	1:E:219:LYS:HG3	1.94	0.49
1:A:274:ASN:HB3	4:A:1112:HOH:O	2.13	0.49
1:B:134:MET:HA	1:B:134:MET:CE	2.39	0.49
1:E:48:VAL:HG11	1:E:51:VAL:HG22	1.95	0.49
1:E:332:GLN:HA	1:E:335:TRP:HD1	1.78	0.49
1:F:156:PHE:HA	1:F:160:ALA:HB3	1.95	0.49
1:C:167:LYS:CE	1:D:167:LYS:HG3	2.43	0.49
1:E:312:GLU:HB2	1:E:314:LYS:HE3	1.94	0.48
1:B:193:PRO:HG3	1:B:224:ARG:CD	2.35	0.48
1:E:233:LYS:NZ	1:E:274:ASN:O	2.47	0.48
1:D:113:GLN:HG2	1:D:335:TRP:CD1	2.49	0.48
1:E:259:ARG:HG2	1:E:259:ARG:HH11	1.79	0.48
1:F:271:PHE:CE2	1:F:277:LEU:HD22	2.48	0.48
1:D:113:GLN:HG3	1:F:318:ILE:CD1	2.44	0.48
1:B:125:GLN:HG2	1:B:136:ASP:OD1	2.14	0.48
1:B:185:ARG:HG3	4:B:1053:HOH:O	2.14	0.48
1:D:73:TYR:HA	1:D:79:TRP:CH2	2.49	0.48
1:E:272:ASP:HB3	1:E:278:LYS:NZ	2.28	0.48
1:F:95:GLY:HA2	1:F:263:VAL:HG11	1.95	0.48
1:D:185:ARG:HA	1:D:202:ASP:HB2	1.95	0.47
1:E:158:GLU:C	1:E:162:PRO:HG3	2.38	0.47
1:A:235:ILE:HD12	1:A:306:VAL:HG21	1.95	0.47
1:D:53:THR:HB	1:D:56:VAL:HG21	1.96	0.47
1:A:201:LYS:HE3	4:A:1083:HOH:O	2.13	0.47
1:A:216:ASP:OD2	1:A:219:LYS:HD3	2.15	0.47
1:A:222:THR:HA	1:A:327:THR:O	2.15	0.47
1:C:255:TYR:O	1:C:260:ILE:HA	2.14	0.47
1:C:313:ILE:HG22	1:C:313:ILE:O	2.13	0.47
1:D:161:PHE:N	1:D:162:PRO:HD3	2.29	0.47
1:A:132:GLU:HG2	1:A:134:MET:CE	2.43	0.47
1:B:48:VAL:HB	1:B:271:PHE:O	2.14	0.47
1:E:166:THR:CG2	1:F:167:LYS:HE3	2.45	0.47
1:B:195:PRO:HB3	1:B:197:LYS:HE2	1.95	0.47
1:D:113:GLN:HG3	1:F:318:ILE:HD13	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LEU:HD21	1:B:188:LEU:CD2	2.45	0.47
1:E:161:PHE:HB3	1:E:164:LEU:CD1	2.45	0.47
1:C:217:GLN:NE2	4:C:1135:HOH:O	2.48	0.47
1:A:217:GLN:HB2	4:A:1088:HOH:O	2.14	0.46
1:B:117:TYR:CZ	1:B:208:PHE:HA	2.49	0.46
1:F:212:PHE:CE2	1:F:221:LEU:HD11	2.49	0.46
1:B:161:PHE:HB3	1:B:164:LEU:HD12	1.97	0.46
1:F:236:SER:OG	1:F:277:LEU:HB2	2.16	0.46
1:B:300:VAL:HG12	1:B:301:ASN:O	2.15	0.46
1:D:113:GLN:HB3	1:D:335:TRP:CD2	2.50	0.46
1:D:238:LEU:O	1:D:242:GLU:HG2	2.15	0.46
1:F:240:LYS:HB2	1:F:271:PHE:CE2	2.51	0.46
1:B:222:THR:HA	1:B:327:THR:O	2.16	0.46
1:B:315:GLU:N	4:B:1088:HOH:O	2.49	0.46
1:C:99:ALA:HB2	1:C:173:PRO:HA	1.98	0.46
1:C:255:TYR:CG	1:C:262:HIS:HB2	2.51	0.46
1:E:101:ASN:HB2	1:E:265:ASN:HD21	1.80	0.46
1:E:332:GLN:HA	1:E:335:TRP:CD1	2.51	0.46
1:A:117:TYR:CZ	1:A:208:PHE:HA	2.51	0.46
1:A:260:ILE:HG22	1:A:260:ILE:O	2.15	0.46
1:B:225:HIS:CG	1:B:238:LEU:HD21	2.51	0.46
1:C:113:GLN:HB3	1:C:335:TRP:CD2	2.51	0.46
1:C:185:ARG:NH2	1:D:132:GLU:OE2	2.49	0.46
1:D:256:ALA:N	4:D:1062:HOH:O	2.47	0.46
1:B:164:LEU:CD1	1:B:171:VAL:HG22	2.46	0.46
1:C:156:PHE:HA	1:C:160:ALA:HB3	1.97	0.46
1:C:196:VAL:HG22	1:C:220:LEU:HD22	1.98	0.46
1:B:105:TRP:O	1:B:109:GLN:HG2	2.16	0.46
1:F:227:PHE:CZ	1:F:325:LEU:HB2	2.51	0.46
1:B:113:GLN:H	1:B:113:GLN:CD	2.24	0.45
1:C:158:GLU:O	1:C:162:PRO:HG3	2.16	0.45
1:D:117:TYR:OH	1:D:208:PHE:HA	2.16	0.45
1:E:132:GLU:HG2	1:E:134:MET:CE	2.37	0.45
1:E:186:LEU:HD23	1:E:187:SER:N	2.31	0.45
1:C:117:TYR:OH	1:C:208:PHE:HA	2.17	0.45
1:F:185:ARG:HA	1:F:202:ASP:HB2	1.97	0.45
1:B:126:LYS:HD3	1:B:133:GLN:OE1	2.16	0.45
1:D:226:ASP:OD2	1:D:228:LYS:HG2	2.17	0.45
1:E:172:PHE:HD1	1:E:224:ARG:NH2	2.14	0.45
1:F:68:VAL:HG22	1:F:69:PHE:N	2.32	0.45
1:C:163:TYR:N	1:C:163:TYR:CD2	2.83	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:LYS:O	1:D:201:LYS:HG3	2.17	0.45
1:E:48:VAL:CG2	1:E:240:LYS:CE	2.89	0.45
1:E:160:ALA:C	1:E:162:PRO:HD3	2.42	0.45
1:E:180:PHE:CZ	1:E:207:ILE:HD12	2.52	0.45
1:F:126:LYS:HE2	1:F:136:ASP:OD2	2.17	0.45
1:F:169:LEU:HD23	1:F:170:GLY:H	1.82	0.45
1:A:177:ILE:HG21	1:A:328:LEU:HD13	1.99	0.45
1:B:53:THR:HB	1:B:56:VAL:CG2	2.47	0.45
1:F:136:ASP:HB3	1:F:139:GLU:HG3	1.99	0.45
1:D:117:TYR:CZ	1:D:208:PHE:HA	2.52	0.44
1:F:161:PHE:N	1:F:162:PRO:HD3	2.31	0.44
1:A:241:LYS:O	1:A:245:GLU:HG3	2.17	0.44
1:C:74:VAL:O	1:C:77:GLN:HG2	2.17	0.44
1:D:195:PRO:HB3	1:D:197:LYS:HE2	2.00	0.44
1:A:167:LYS:HG2	1:B:167:LYS:HE3	1.99	0.44
1:C:68:VAL:HG22	1:C:69:PHE:N	2.32	0.44
1:C:266:LEU:HA	1:C:282:VAL:HG12	1.98	0.44
1:A:212:PHE:HA	1:A:219:LYS:HG3	1.99	0.44
1:C:53:THR:HB	1:C:56:VAL:HG21	1.99	0.44
1:C:193:PRO:HG3	1:C:224:ARG:HD2	2.00	0.44
1:C:163:TYR:N	1:C:163:TYR:HD2	2.14	0.44
1:C:330:THR:C	1:C:332:GLN:H	2.24	0.44
1:B:216:ASP:OD2	1:B:219:LYS:CD	2.66	0.44
1:B:235:ILE:HD13	1:B:322:VAL:HG21	1.99	0.44
1:F:240:LYS:HB2	1:F:271:PHE:CZ	2.53	0.44
1:F:333:ASP:HB3	4:F:1059:HOH:O	2.17	0.44
1:B:163:TYR:O	1:B:167:LYS:HG3	2.18	0.43
1:C:231:ASN:OD1	1:C:234:GLU:HG3	2.18	0.43
1:D:185:ARG:HG3	4:D:1039:HOH:O	2.17	0.43
1:E:272:ASP:OD2	1:E:278:LYS:NZ	2.51	0.43
1:E:297:PHE:O	1:E:308:ILE:HA	2.18	0.43
1:F:160:ALA:C	1:F:162:PRO:HD3	2.43	0.43
1:A:125:GLN:NE2	4:A:1073:HOH:O	2.50	0.43
1:B:99:ALA:HB2	1:B:173:PRO:HA	2.01	0.43
1:C:129:PHE:O	1:C:130:ASN:C	2.61	0.43
1:D:62:PHE:HB3	1:D:69:PHE:CZ	2.53	0.43
1:E:101:ASN:HB2	1:E:265:ASN:ND2	2.33	0.43
1:A:227:PHE:CE2	1:A:238:LEU:HD23	2.50	0.43
1:B:300:VAL:HG13	1:B:304:GLY:C	2.44	0.43
1:A:125:GLN:OE1	1:A:138:LYS:HD2	2.18	0.43
1:A:132:GLU:OE2	1:B:203:PRO:HG3	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:LEU:HD23	1:F:186:LEU:C	2.44	0.43
1:A:201:LYS:HE2	1:A:205:GLY:O	2.19	0.43
1:D:231:ASN:ND2	1:D:234:GLU:OE2	2.51	0.43
1:A:196:VAL:HG12	1:A:196:VAL:O	2.18	0.43
1:C:161:PHE:HB3	1:C:164:LEU:HD12	2.00	0.43
1:E:163:TYR:N	1:E:163:TYR:CD2	2.85	0.43
1:E:249:LEU:HD12	1:E:249:LEU:N	2.33	0.43
1:B:266:LEU:C	1:B:266:LEU:HD23	2.43	0.43
1:D:92:LEU:HD12	1:D:165:SER:HA	2.00	0.43
1:A:217:GLN:O	1:A:217:GLN:NE2	2.51	0.43
1:C:160:ALA:C	1:C:162:PRO:HD3	2.42	0.43
1:C:203:PRO:CG	1:D:132:GLU:OE2	2.65	0.43
1:F:242:GLU:OE1	1:F:247:LYS:HD2	2.19	0.43
1:A:136:ASP:CB	1:A:139:GLU:HG3	2.45	0.43
1:C:82:ILE:HG13	1:C:101:ASN:OD1	2.19	0.43
1:E:185:ARG:HG3	4:E:1095:HOH:O	2.19	0.43
1:D:58:PRO:HA	1:D:59:PRO:HD3	1.94	0.42
1:F:113:GLN:CD	1:F:113:GLN:H	2.27	0.42
1:A:58:PRO:HA	1:A:59:PRO:HD3	1.95	0.42
1:C:242:GLU:OE2	1:C:242:GLU:HA	2.19	0.42
1:E:132:GLU:CD	1:F:185:ARG:HH22	2.23	0.42
1:B:177:ILE:HG21	1:B:328:LEU:HD13	2.01	0.42
1:E:173:PRO:HG2	1:E:263:VAL:HG21	2.01	0.42
1:D:337:GLN:HB2	1:F:254:THR:HG21	2.01	0.42
1:B:110:ASN:HA	1:B:113:GLN:OE1	2.18	0.42
1:A:180:PHE:CZ	1:A:207:ILE:HD12	2.54	0.42
1:B:84:LYS:HE3	1:B:90:ASP:O	2.20	0.42
1:B:86:PHE:HA	1:B:91:ASP:OD2	2.19	0.42
1:C:300:VAL:HA	1:C:305:LYS:O	2.20	0.42
1:F:231:ASN:ND2	1:F:234:GLU:OE2	2.52	0.42
1:B:272:ASP:OD2	1:B:278:LYS:NZ	2.52	0.42
1:B:108:ASP:OD2	1:B:144:LYS:HE2	2.19	0.42
1:D:161:PHE:HB3	1:D:164:LEU:CD1	2.50	0.42
1:F:99:ALA:HB2	1:F:173:PRO:HA	2.01	0.42
1:B:258:VAL:HG11	4:B:1068:HOH:O	2.20	0.42
1:D:132:GLU:OE1	1:D:134:MET:HE1	2.19	0.42
1:C:193:PRO:HG3	1:C:224:ARG:HG2	2.01	0.41
1:D:318:ILE:O	1:D:318:ILE:HG12	2.20	0.41
1:E:68:VAL:HG22	1:E:69:PHE:N	2.35	0.41
1:B:258:VAL:HG23	1:B:259:ARG:N	2.35	0.41
1:D:99:ALA:HB2	1:D:173:PRO:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:GLN:NE2	4:D:1049:HOH:O	2.53	0.41
1:B:238:LEU:O	1:B:242:GLU:HG2	2.20	0.41
1:D:191:HIS:HA	4:D:1074:HOH:O	2.20	0.41
1:B:249:LEU:HD12	1:B:249:LEU:N	2.36	0.41
1:C:172:PHE:HA	1:C:173:PRO:HD3	1.92	0.41
1:D:50:SER:HA	1:D:269:ALA:O	2.20	0.41
1:D:123:GLU:O	1:D:123:GLU:HG2	2.18	0.41
1:D:184:TYR:HB3	4:D:1114:HOH:O	2.20	0.41
1:F:132:GLU:HG2	1:F:134:MET:CE	2.49	0.41
1:A:264:ILE:HD12	1:A:282:VAL:HG21	2.02	0.41
1:D:305:LYS:HB3	1:D:321:GLN:HG3	2.02	0.41
1:F:49:THR:HG23	1:F:271:PHE:HB2	2.02	0.41
1:E:139:GLU:CB	1:E:151:LYS:HG2	2.49	0.41
1:F:296:TYR:CD1	1:F:308:ILE:HD12	2.55	0.41
1:D:46:TYR:CD2	1:D:48:VAL:HG22	2.56	0.41
1:D:269:ALA:HB1	1:D:277:LEU:CD1	2.46	0.41
1:A:70:HIS:HE1	4:A:1128:HOH:O	2.03	0.41
1:B:58:PRO:HA	1:B:59:PRO:HD3	1.95	0.41
1:B:172:PHE:HA	1:B:173:PRO:HD3	1.97	0.41
1:B:242:GLU:OE1	1:B:247:LYS:HD2	2.21	0.41
1:C:193:PRO:HG3	1:C:224:ARG:CG	2.51	0.41
1:C:209:ASP:HA	1:C:212:PHE:O	2.21	0.41
1:D:62:PHE:CD1	1:D:71:ALA:HB2	2.56	0.41
1:D:110:ASN:O	1:D:114:ILE:HG13	2.21	0.41
1:D:125:GLN:HG3	1:D:138:LYS:HG2	2.02	0.41
1:D:255:TYR:HD1	1:D:257:ASN:ND2	2.18	0.41
1:F:125:GLN:HG3	1:F:137:VAL:HG12	2.03	0.41
1:A:212:PHE:CE2	1:A:221:LEU:HD11	2.56	0.40
1:A:280:ILE:HG13	1:A:296:TYR:HB2	2.03	0.40
1:B:158:GLU:O	1:B:162:PRO:HG3	2.22	0.40
1:C:191:HIS:ND1	1:C:191:HIS:N	2.68	0.40
1:D:95:GLY:HA3	1:D:171:VAL:O	2.21	0.40
1:E:64:GLN:HA	1:E:69:PHE:HD1	1.85	0.40
1:F:164:LEU:HD21	1:F:188:LEU:CD1	2.51	0.40
1:B:110:ASN:O	1:B:111:LYS:C	2.64	0.40
1:C:130:ASN:HB2	1:D:127:ILE:HG23	2.04	0.40
1:D:171:VAL:HG22	1:D:172:PHE:N	2.36	0.40
1:D:177:ILE:HG21	1:D:328:LEU:HD13	2.03	0.40
1:E:256:ALA:N	4:E:1030:HOH:O	2.48	0.40
1:C:272:ASP:OD1	1:C:272:ASP:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	288/311 (93%)	276 (96%)	12 (4%)	0	100	100
1	B	287/311 (92%)	270 (94%)	15 (5%)	2 (1%)	18	14
1	C	287/311 (92%)	270 (94%)	16 (6%)	1 (0%)	36	35
1	D	292/311 (94%)	274 (94%)	16 (6%)	2 (1%)	18	14
1	E	292/311 (94%)	280 (96%)	11 (4%)	1 (0%)	36	35
1	F	287/311 (92%)	279 (97%)	8 (3%)	0	100	100
All	All	1733/1866 (93%)	1649 (95%)	78 (4%)	6 (0%)	36	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	315	GLU
1	C	315	GLU
1	D	228	LYS
1	D	312	GLU
1	E	312	GLU
1	B	196	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	247/267 (92%)	242 (98%)	5 (2%)	48	54
1	B	246/267 (92%)	238 (97%)	8 (3%)	33	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	246/267 (92%)	241 (98%)	5 (2%)	48	54
1	D	253/267 (95%)	251 (99%)	2 (1%)	73	80
1	E	253/267 (95%)	248 (98%)	5 (2%)	48	54
1	F	246/267 (92%)	239 (97%)	7 (3%)	38	41
All	All	1491/1602 (93%)	1459 (98%)	32 (2%)	47	52

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	GLU
1	A	217	GLN
1	A	228	LYS
1	A	315	GLU
1	A	333	ASP
1	B	123	GLU
1	B	132	GLU
1	B	134	MET
1	B	171	VAL
1	B	219	LYS
1	B	283	THR
1	B	312	GLU
1	B	316	ASP
1	C	72	PRO
1	C	119	GLU
1	C	163	TYR
1	C	166	THR
1	C	316	ASP
1	D	66	GLU
1	D	315	GLU
1	E	48	VAL
1	E	66	GLU
1	E	189	THR
1	E	242	GLU
1	E	315	GLU
1	F	128	ASN
1	F	191	HIS
1	F	240	LYS
1	F	259	ARG
1	F	277	LEU
1	F	278	LYS
1	F	333	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	121	HIS
1	A	217	GLN
1	B	109	GLN
1	B	190	ASN
1	B	191	HIS
1	B	276	ASN
1	C	76	ASN
1	C	104	HIS
1	C	121	HIS
1	C	190	ASN
1	C	332	GLN
1	D	76	ASN
1	D	77	GLN
1	D	125	GLN
1	D	130	ASN
1	D	133	GLN
1	D	190	ASN
1	D	276	ASN
1	D	288	ASN
1	D	337	GLN
1	E	125	GLN
1	E	130	ASN
1	E	175	HIS
1	E	190	ASN
1	E	317	ASN
1	E	336	ASN
1	E	337	GLN
1	F	77	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](#)

7 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	1001	-	4,4,4	0.34	0	6,6,6	0.14	0
2	SO4	C	1003	-	4,4,4	0.33	0	6,6,6	0.13	0
2	SO4	D	1004	-	4,4,4	0.33	0	6,6,6	0.12	0
3	GOL	F	1000	-	5,5,5	4.83	5 (100%)	5,5,5	6.16	3 (60%)
2	SO4	F	1006	-	4,4,4	0.31	0	6,6,6	0.24	0
2	SO4	B	1002	-	4,4,4	0.32	0	6,6,6	0.14	0
2	SO4	E	1005	-	4,4,4	0.41	0	6,6,6	0.09	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	GOL	F	1000	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1000	GOL	C3-C2	-8.16	1.20	1.51
3	F	1000	GOL	O1-C1	4.77	1.62	1.42
3	F	1000	GOL	O3-C3	3.20	1.55	1.42
3	F	1000	GOL	C1-C2	-2.96	1.40	1.51
3	F	1000	GOL	O2-C2	-2.87	1.35	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1000	GOL	O3-C3-C2	11.38	161.61	110.38
3	F	1000	GOL	O2-C2-C3	6.92	137.82	109.18
3	F	1000	GOL	O1-C1-C2	3.44	125.85	110.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1000	GOL	O1-C1-C2-C3
3	F	1000	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1000	GOL	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	290/311 (93%)	0.45	21 (7%)	21 20	14, 29, 58, 81	0
1	B	289/311 (92%)	0.87	33 (11%)	10 9	17, 35, 61, 83	1 (0%)
1	C	289/311 (92%)	0.70	29 (10%)	12 11	16, 33, 58, 80	0
1	D	296/311 (95%)	0.97	46 (15%)	5 4	20, 37, 71, 88	0
1	E	296/311 (95%)	0.80	40 (13%)	7 6	17, 34, 66, 83	0
1	F	288/311 (92%)	0.41	18 (6%)	26 24	13, 28, 58, 81	0
All	All	1748/1866 (93%)	0.70	187 (10%)	11 10	13, 33, 63, 88	1 (0%)

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	164	LEU	5.5
1	C	335	TRP	5.2
1	B	331	GLY	5.0
1	B	220	LEU	5.0
1	A	167	LYS	4.9
1	E	163	TYR	4.9
1	F	166	THR	4.8
1	A	166	THR	4.7
1	B	335	TRP	4.7
1	D	188	LEU	4.7
1	C	313	ILE	4.5
1	D	45	PRO	4.3
1	B	48	VAL	4.1
1	B	166	THR	4.1
1	F	169	LEU	4.0
1	D	163	TYR	4.0
1	E	46	TYR	4.0
1	D	169	LEU	4.0
1	D	317	ASN	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	210	ALA	4.0
1	E	165	SER	4.0
1	C	334	SER	3.9
1	D	44	THR	3.9
1	E	188	LEU	3.8
1	C	331	GLY	3.8
1	D	318	ILE	3.8
1	E	164	LEU	3.8
1	F	164	LEU	3.8
1	E	45	PRO	3.8
1	D	46	TYR	3.8
1	F	168	HIS	3.8
1	F	336	ASN	3.7
1	D	65	GLY	3.7
1	C	165	SER	3.7
1	B	315	GLU	3.7
1	B	332	GLN	3.7
1	A	336	ASN	3.6
1	B	116	ARG	3.6
1	B	188	LEU	3.6
1	C	163	TYR	3.6
1	F	163	TYR	3.6
1	B	163	TYR	3.5
1	A	165	SER	3.5
1	D	316	ASP	3.5
1	E	172	PHE	3.5
1	D	43	VAL	3.5
1	D	189	THR	3.5
1	C	186	LEU	3.4
1	F	273	SER	3.4
1	A	163	TYR	3.4
1	A	48	VAL	3.4
1	D	165	SER	3.4
1	E	169	LEU	3.4
1	B	314	LYS	3.4
1	C	336	ASN	3.4
1	D	258	VAL	3.4
1	F	318	ILE	3.4
1	E	48	VAL	3.3
1	D	166	THR	3.3
1	C	188	LEU	3.2
1	B	334	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	313	ILE	3.1
1	E	317	ASN	3.1
1	C	332	GLN	3.1
1	C	333	ASP	3.1
1	E	316	ASP	3.1
1	D	310	ALA	3.1
1	A	189	THR	3.0
1	D	48	VAL	3.0
1	D	232	LEU	3.0
1	D	260	ILE	3.0
1	D	193	PRO	3.0
1	E	171	VAL	3.0
1	C	315	GLU	3.0
1	E	43	VAL	3.0
1	D	42	GLU	3.0
1	E	313	ILE	3.0
1	C	65	GLY	2.9
1	B	333	ASP	2.9
1	B	114	ILE	2.9
1	E	166	THR	2.9
1	D	228	LYS	2.9
1	A	188	LEU	2.8
1	B	164	LEU	2.8
1	B	66	GLU	2.8
1	F	165	SER	2.8
1	A	337	GLN	2.8
1	D	168	HIS	2.8
1	E	168	HIS	2.8
1	B	172	PHE	2.8
1	E	67	ASP	2.8
1	C	66	GLU	2.8
1	D	137	VAL	2.8
1	B	313	ILE	2.8
1	E	167	LYS	2.8
1	E	259	ARG	2.8
1	D	191	HIS	2.8
1	D	62	PHE	2.8
1	D	289	ALA	2.8
1	F	188	LEU	2.8
1	B	330	THR	2.8
1	A	258	VAL	2.8
1	A	191	HIS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	162	PRO	2.7
1	A	168	HIS	2.7
1	E	65	GLY	2.7
1	D	315	GLU	2.7
1	C	112	ASP	2.7
1	D	314	LYS	2.7
1	A	164	LEU	2.7
1	E	315	GLU	2.6
1	B	336	ASN	2.6
1	F	190	ASN	2.6
1	E	162	PRO	2.6
1	E	318	ILE	2.6
1	C	197	LYS	2.6
1	D	167	LYS	2.6
1	E	300	VAL	2.5
1	F	185	ARG	2.5
1	F	49	THR	2.5
1	F	231	ASN	2.5
1	D	194	THR	2.5
1	E	191	HIS	2.5
1	A	231	ASN	2.5
1	B	316	ASP	2.5
1	E	44	THR	2.5
1	D	162	PRO	2.5
1	D	187	SER	2.4
1	D	279	ALA	2.4
1	A	169	LEU	2.4
1	C	48	VAL	2.4
1	B	63	THR	2.4
1	E	189	THR	2.4
1	C	210	ALA	2.4
1	F	167	LYS	2.4
1	D	192	GLY	2.4
1	C	119	GLU	2.4
1	C	63	THR	2.4
1	D	227	PHE	2.4
1	A	49	THR	2.4
1	D	68	VAL	2.3
1	F	189	THR	2.3
1	E	42	GLU	2.3
1	D	190	ASN	2.3
1	C	111	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	335	TRP	2.3
1	C	116	ARG	2.3
1	E	62	PHE	2.3
1	C	114	ILE	2.3
1	A	300	VAL	2.3
1	B	68	VAL	2.3
1	B	112	ASP	2.3
1	E	60	ALA	2.3
1	E	230	LYS	2.3
1	A	171	VAL	2.2
1	B	189	THR	2.2
1	A	232	LEU	2.2
1	E	258	VAL	2.2
1	B	65	GLY	2.2
1	D	66	GLU	2.2
1	C	146	HIS	2.2
1	A	65	GLY	2.2
1	E	210	ALA	2.2
1	C	166	THR	2.2
1	B	107	PHE	2.1
1	E	66	GLU	2.1
1	E	275	GLY	2.1
1	C	191	HIS	2.1
1	E	190	ASN	2.1
1	A	335	TRP	2.1
1	B	62	PHE	2.1
1	B	78	GLY	2.1
1	B	121	HIS	2.1
1	E	289	ALA	2.1
1	B	219	LYS	2.1
1	C	167	LYS	2.1
1	D	172	PHE	2.1
1	C	68	VAL	2.1
1	E	312	GLU	2.1
1	D	67	ASP	2.1
1	E	278	LYS	2.0
1	E	192	GLY	2.0
1	B	113	GLN	2.0
1	D	186	LEU	2.0
1	C	316	ASP	2.0
1	F	191	HIS	2.0
1	D	278	LYS	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	GOL	F	1000	6/6	0.80	0.15	43,49,49,50	0
2	SO4	D	1004	5/5	0.94	0.10	39,41,42,45	0
2	SO4	E	1005	5/5	0.95	0.10	29,31,33,35	0
2	SO4	C	1003	5/5	0.97	0.07	26,26,27,31	0
2	SO4	B	1002	5/5	0.97	0.07	30,32,32,32	0
2	SO4	F	1006	5/5	0.98	0.05	16,23,25,25	0
2	SO4	A	1001	5/5	0.98	0.06	21,23,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.