



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:29 AM UTC

PDB ID : 2YM9 / pdb_00002ym9
Title : SipD from Salmonella typhimurium
Authors : Lunelli, M.; Kolbe, M.
Deposited on : 2011-06-06
Resolution : 3.00 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

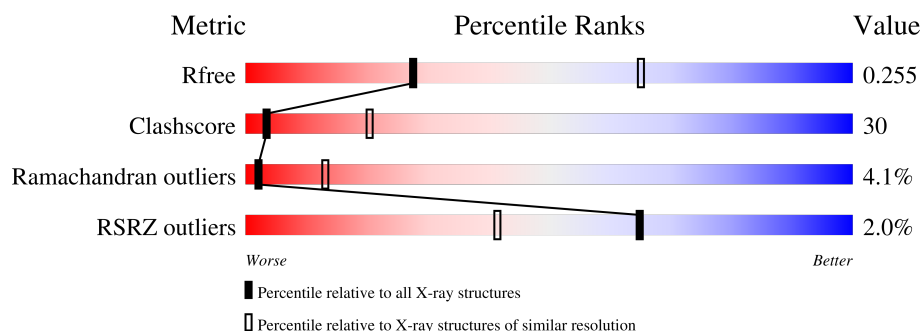
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	346	49% 34% • 13%
1	B	346	45% 32% 5% 18%
1	C	346	34% 26% •• 38%
1	D	346	11% 19% 5% 64%

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	A	1342	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7159 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 CELL INVASION PROTEIN SIPD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	1
			2288	1421	384	477	6			
1	B	285	Total	C	N	O	S	0	0	1
			2175	1349	366	454	6			
1	C	216	Total	C	N	O	S	0	0	0
			1659	1044	268	341	6			
1	D	124	Total	C	N	O	S	0	0	0
			972	616	150	202	4			

There are 12 discrepancies between the modelled and reference sequences:

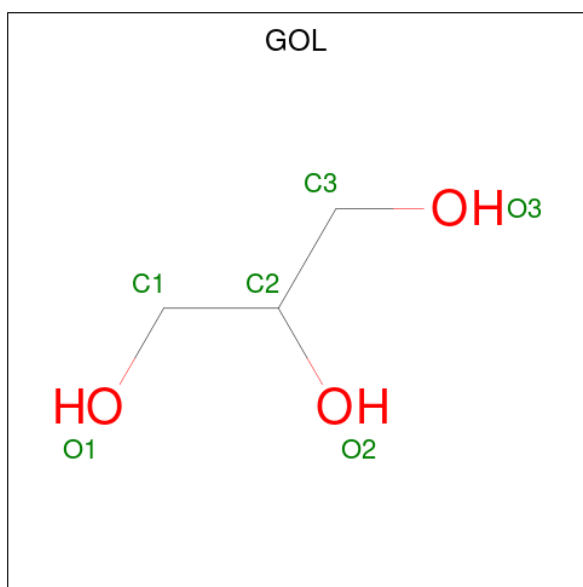
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q56026
A	-1	SER	-	expression tag	UNP Q56026
A	0	HIS	-	expression tag	UNP Q56026
B	-2	GLY	-	expression tag	UNP Q56026
B	-1	SER	-	expression tag	UNP Q56026
B	0	HIS	-	expression tag	UNP Q56026
C	-2	GLY	-	expression tag	UNP Q56026
C	-1	SER	-	expression tag	UNP Q56026
C	0	HIS	-	expression tag	UNP Q56026
D	-2	GLY	-	expression tag	UNP Q56026
D	-1	SER	-	expression tag	UNP Q56026
D	0	HIS	-	expression tag	UNP Q56026

- 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	A	1	Total	O	S	0	0
			5	4	1		
2	B	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	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

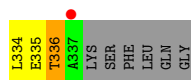
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

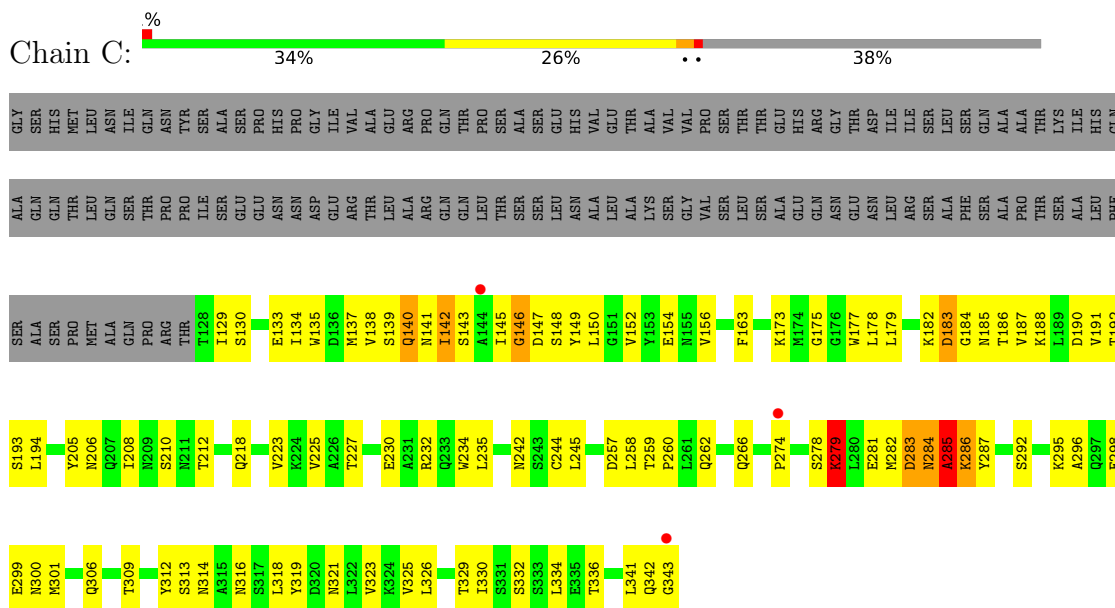
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	10	Total	O	0	0
			10	10		
4	C	11	Total	O	0	0
			11	11		
4	D	2	Total	O	0	0
			2	2		

- Molecule 1: CELL INVASION PROTEIN SIPD

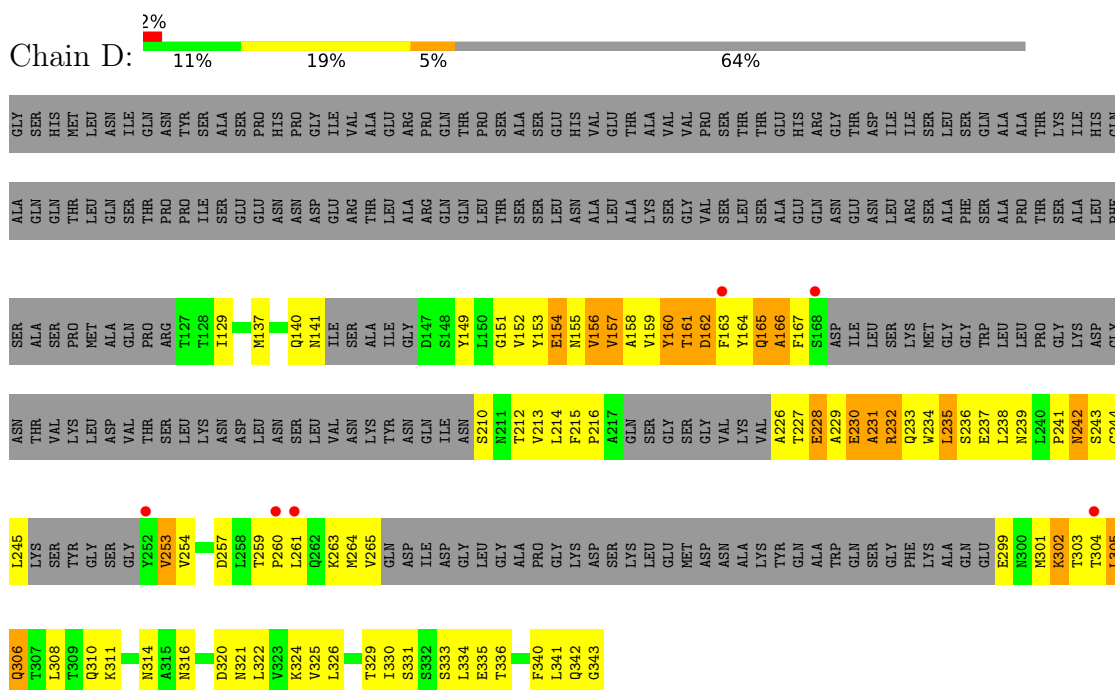




- Molecule 1: CELL INVASION PROTEIN SIPD



- Molecule 1: CELL INVASION PROTEIN SIPD



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	128.37Å 128.37Å 350.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 3.00 19.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (19.94-3.00) 96.9 (19.94-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.98Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.229 , 0.258 0.228 , 0.255	Depositor DCC
R_{free} test set	1635 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	74.2	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7159	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: GOL, 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	0.56	1/2321 (0.0%)	0.97	7/3153 (0.2%)
1	B	0.50	1/2206 (0.0%)	1.05	18/2993 (0.6%)
1	C	0.50	0/1686	1.02	11/2286 (0.5%)
1	D	0.56	0/984	1.14	11/1335 (0.8%)
All	All	0.53	2/7197 (0.0%)	1.03	47/9767 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	336	THR	C-N	-5.56	1.25	1.33
1	A	338	LYS	C-N	-5.33	1.25	1.33

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	ILE	N-CA-C	-14.19	99.62	113.53
1	D	155	ASN	N-CA-C	-9.70	100.71	111.28
1	C	286	LYS	N-CA-C	-9.37	100.42	112.23
1	D	232	ARG	N-CA-C	-9.33	101.16	112.54
1	B	38	THR	N-CA-C	8.94	119.73	108.19
1	C	142	ILE	N-CA-C	-8.69	101.70	113.00
1	A	117	PHE	N-CA-C	-8.41	97.44	109.29
1	C	147	ASP	N-CA-C	-8.33	102.16	111.82
1	D	161	THR	N-CA-C	-7.90	104.24	114.04
1	D	231	ALA	N-CA-C	-7.76	105.77	114.62
1	D	302	LYS	N-CA-C	-7.72	102.55	110.97
1	D	305	LEU	N-CA-C	-7.45	101.45	111.96
1	B	141	ASN	N-CA-C	7.36	120.23	111.33
1	B	198	LEU	N-CA-C	-7.30	103.40	111.36
1	B	137	MET	N-CA-C	-7.22	101.65	112.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	242	ASN	N-CA-C	-7.02	102.76	111.75
1	D	235	LEU	N-CA-C	-6.99	103.72	111.82
1	C	285	ALA	N-CA-C	-6.91	96.09	110.80
1	C	279	LYS	N-CA-C	6.88	125.45	110.80
1	B	88	ASN	N-CA-C	-6.55	103.35	112.45
1	D	154	GLU	N-CA-C	-6.11	106.46	114.04
1	B	235	LEU	N-CA-C	-6.10	104.71	111.36
1	B	51	ALA	N-CA-C	-6.05	104.01	111.33
1	C	283	ASP	N-CA-C	5.99	123.55	110.80
1	C	206	ASN	N-CA-C	-5.95	105.99	113.72
1	D	331	SER	N-CA-C	-5.89	104.85	111.28
1	B	81	GLN	N-CA-C	-5.88	104.78	111.14
1	A	113	THR	N-CA-C	5.87	119.52	111.54
1	A	263	LYS	N-CA-C	-5.75	105.09	111.36
1	C	225	VAL	N-CA-C	5.69	117.31	109.46
1	A	110	SER	N-CA-C	5.67	118.87	110.48
1	A	185	ASN	N-CA-C	5.65	118.46	108.24
1	B	240	LEU	CA-C-N	5.63	125.62	120.21
1	B	240	LEU	C-N-CA	5.63	125.62	120.21
1	B	312	TYR	N-CA-C	-5.61	104.86	110.97
1	D	162	ASP	N-CA-C	-5.56	104.85	111.03
1	B	208	ILE	N-CA-C	5.50	115.17	106.32
1	C	146	GLY	N-CA-C	-5.45	106.06	113.37
1	A	218	GLN	N-CA-C	5.45	118.26	110.68
1	A	277	ASP	N-CA-C	-5.45	106.10	114.16
1	B	278	SER	N-CA-C	5.36	116.42	108.86
1	B	310	GLN	N-CA-C	-5.26	105.55	111.28
1	B	133	GLU	N-CA-C	-5.25	106.14	112.54
1	C	173	LYS	N-CA-C	-5.14	105.07	113.19
1	B	187	VAL	N-CA-C	5.09	115.98	108.45
1	B	136	ASP	N-CA-C	-5.08	106.86	113.16
1	C	186	THR	N-CA-C	-5.08	101.82	109.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2288	0	2253	117	0
1	B	2175	0	2135	130	0
1	C	1659	0	1633	107	0
1	D	972	0	943	107	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	6	0	8	4	0
3	B	6	0	8	0	0
4	A	15	0	0	0	0
4	B	10	0	0	0	0
4	C	11	0	0	0	0
4	D	2	0	0	0	0
All	All	7159	0	6980	422	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 30.

All (422) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:ILE:HG13	1:C:146:GLY:N	1.66	1.07
1:B:40:HIS:HB3	1:B:45:ILE:HG13	1.38	1.04
1:D:234:TRP:O	1:D:238:LEU:HB2	1.54	1.04
1:C:282:MET:HE2	1:C:287:TYR:HA	1.44	0.96
1:A:105:LEU:HB3	1:A:134:ILE:HD11	1.48	0.95
1:B:87:LEU:HD13	1:B:138:VAL:HG12	1.46	0.94
1:C:138:VAL:HG13	1:C:330:ILE:HG21	1.49	0.94
1:A:37:THR:HG23	1:A:336:THR:HG23	1.52	0.92
1:D:260:PRO:HG3	1:D:301:MET:HE3	1.49	0.91
1:A:117:PHE:HD1	1:A:118:SER:H	1.18	0.90
1:C:145:ILE:HG13	1:C:146:GLY:H	1.32	0.90
1:B:130:SER:HB2	1:B:134:ILE:HG12	1.54	0.89
1:B:188:LYS:HG2	1:B:281:GLU:HG2	1.57	0.86
1:B:91:ALA:HB2	1:B:135:TRP:HB2	1.60	0.83
1:C:292:SER:HA	1:C:295:LYS:HE2	1.60	0.83
1:D:299:GLU:HA	1:D:302:LYS:HE3	1.62	0.81
1:D:215:PHE:CD1	1:D:216:PRO:HA	2.16	0.81
1:B:130:SER:HB2	1:B:134:ILE:CG1	2.13	0.78
1:D:235:LEU:HD11	1:D:245:LEU:HB2	1.65	0.78
1:D:227:THR:OG1	1:D:230:GLU:HG3	1.84	0.77
1:A:229:ALA:O	1:A:233:GLN:HG3	1.85	0.76
1:B:97:LEU:HD21	1:B:102:ASN:HA	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:THR:O	1:A:57:GLN:HG3	1.85	0.76
1:B:37:THR:HA	1:D:306:GLN:OE1	1.86	0.76
1:D:234:TRP:HB3	1:D:238:LEU:HD12	1.66	0.76
1:D:260:PRO:CG	1:D:301:MET:HE3	2.16	0.75
1:B:334:LEU:HD12	1:B:334:LEU:O	1.87	0.75
1:B:53:THR:O	1:B:57:GLN:HG3	1.87	0.74
1:B:178:LEU:HD22	1:C:318:LEU:HD22	1.69	0.74
1:C:178:LEU:HD11	1:C:287:TYR:OH	1.86	0.74
1:D:260:PRO:HB2	1:D:264:MET:HE2	1.70	0.74
1:B:215:PHE:CD1	1:B:216:PRO:HA	2.23	0.73
1:B:45:ILE:O	1:B:45:ILE:HG22	1.86	0.73
1:C:145:ILE:O	1:C:148:SER:HB3	1.87	0.73
1:A:110:SER:C	1:A:112:PRO:HD3	2.14	0.73
1:D:158:ALA:O	1:D:161:THR:HG22	1.88	0.72
1:B:134:ILE:O	1:B:137:MET:HB2	1.88	0.72
1:B:235:LEU:HD11	1:B:245:LEU:HB2	1.69	0.72
1:B:335:GLU:OE2	1:B:336:THR:HG23	1.89	0.72
1:B:177:TRP:HB3	1:B:190:ASP:HB3	1.73	0.71
1:D:260:PRO:O	1:D:264:MET:HG2	1.91	0.71
1:D:165:GLN:C	1:D:167:PHE:H	1.96	0.71
1:A:227:THR:HG23	1:A:230:GLU:OE2	1.91	0.71
1:D:227:THR:O	1:D:229:ALA:N	2.25	0.69
1:D:253:VAL:HG23	1:D:254:VAL:N	2.06	0.69
1:B:80:ARG:HG2	1:B:319:TYR:OH	1.93	0.69
1:B:87:LEU:HD22	1:B:138:VAL:HG11	1.74	0.69
1:B:63:GLN:HG3	1:B:63:GLN:O	1.93	0.69
1:A:171:LEU:HD11	1:D:325:VAL:HG11	1.74	0.69
1:A:188:LYS:HD3	3:A:1342:GOL:O2	1.93	0.68
1:A:55:ILE:HD12	1:A:330:ILE:HD12	1.76	0.68
1:D:165:GLN:HG3	1:D:166:ALA:N	2.07	0.68
1:A:187:VAL:HG21	1:A:287:TYR:CD1	2.28	0.68
1:B:131:ASP:C	1:B:133:GLU:H	2.01	0.68
1:B:87:LEU:HD13	1:B:138:VAL:CG1	2.21	0.68
1:C:187:VAL:O	1:C:281:GLU:HA	1.94	0.67
1:A:114:SER:OG	1:A:119:ALA:HB3	1.94	0.67
1:B:55:ILE:HG12	1:B:83:LEU:HD11	1.76	0.67
1:A:34:VAL:HG23	1:C:295:LYS:HE3	1.77	0.67
1:A:234:TRP:O	1:A:238:LEU:HG	1.95	0.66
1:C:183:ASP:C	1:C:185:ASN:H	2.03	0.66
1:B:97:LEU:HD12	1:B:101:GLN:OE1	1.95	0.65
1:D:212:THR:O	1:D:212:THR:HG22	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:THR:HG22	1:B:37:THR:O	1.96	0.65
1:D:215:PHE:CG	1:D:216:PRO:HA	2.32	0.65
1:A:181:GLY:HA3	1:A:186:THR:OG1	1.96	0.64
1:A:32:ALA:HA	1:C:295:LYS:HZ2	1.62	0.64
1:C:278:SER:OG	1:C:279:LYS:N	2.18	0.64
1:A:309:THR:HG21	1:D:336:THR:HB	1.79	0.64
1:A:55:ILE:CD1	1:A:330:ILE:HD12	2.28	0.64
1:A:37:THR:HG22	1:C:306:GLN:HE22	1.61	0.64
1:A:307:THR:HG22	1:A:311:LYS:HD2	1.81	0.63
1:B:109:PHE:N	1:B:109:PHE:HD1	1.96	0.63
1:B:234:TRP:HA	1:B:237:GLU:HB3	1.81	0.63
1:A:112:PRO:HB3	1:A:120:SER:O	2.00	0.62
1:C:139:SER:C	1:C:141:ASN:H	2.08	0.62
1:C:334:LEU:HD22	1:D:334:LEU:HD22	1.82	0.62
1:C:259:THR:CG2	1:C:260:PRO:HD3	2.30	0.62
1:D:229:ALA:O	1:D:233:GLN:N	2.31	0.62
1:B:45:ILE:O	1:B:45:ILE:CG2	2.47	0.62
1:C:321:ASN:O	1:C:325:VAL:HG23	2.00	0.61
1:B:109:PHE:N	1:B:109:PHE:CD1	2.66	0.61
1:B:40:HIS:HB3	1:B:45:ILE:CG1	2.25	0.61
1:C:129:ILE:HD11	1:D:140:GLN:O	2.01	0.61
1:D:164:TYR:OH	1:D:302:LYS:HG3	2.00	0.61
1:D:156:VAL:O	1:D:158:ALA:N	2.33	0.61
1:C:141:ASN:C	1:C:143:SER:H	2.10	0.60
1:B:42:GLY:HA3	1:D:164:TYR:OH	2.02	0.60
1:C:182:LYS:C	1:C:184:GLY:H	2.10	0.60
1:D:153:TYR:OH	1:D:311:LYS:HG2	2.02	0.60
1:B:97:LEU:CD2	1:B:102:ASN:HA	2.31	0.60
1:A:80:ARG:NH1	1:A:154:GLU:OE2	2.34	0.60
1:A:49:SER:HA	1:C:309:THR:HG21	1.82	0.59
1:B:76:ARG:NE	1:B:154:GLU:OE2	2.29	0.59
1:D:149:TYR:CD1	1:D:149:TYR:C	2.79	0.59
1:B:227:THR:HG23	1:B:230:GLU:OE2	2.02	0.59
1:D:232:ARG:HA	1:D:235:LEU:HD12	1.83	0.59
1:A:105:LEU:HB3	1:A:134:ILE:CD1	2.27	0.59
1:B:44:ASP:OD2	1:B:95:VAL:HA	2.03	0.59
1:D:326:LEU:O	1:D:330:ILE:HG13	2.03	0.59
1:A:34:VAL:HG11	1:C:296:ALA:HA	1.84	0.59
1:B:35:PRO:HG2	1:D:310:GLN:OE1	2.02	0.59
1:C:235:LEU:HD11	1:C:245:LEU:HB2	1.85	0.58
1:C:282:MET:HE2	1:C:287:TYR:CA	2.27	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:ILE:O	1:C:145:ILE:HG23	2.03	0.58
1:A:262:GLN:O	1:A:266:GLN:HG3	2.03	0.58
1:B:129:ILE:O	1:B:130:SER:HB3	2.02	0.58
1:C:283:ASP:O	1:C:284:ASN:C	2.46	0.58
1:B:40:HIS:NE2	1:B:96:SER:OG	2.33	0.58
1:B:157:VAL:O	1:B:161:THR:HG23	2.03	0.58
1:B:137:MET:HE2	1:B:137:MET:HA	1.86	0.58
1:B:42:GLY:CA	1:D:164:TYR:OH	2.52	0.57
1:C:227:THR:OG1	1:C:230:GLU:HG3	2.04	0.57
1:B:43:THR:O	1:B:46:ILE:HG22	2.05	0.57
1:A:38:THR:HG21	1:A:45:ILE:HD11	1.86	0.57
1:A:100:GLU:OE1	1:A:100:GLU:N	2.35	0.57
1:C:141:ASN:C	1:C:143:SER:N	2.60	0.57
1:C:259:THR:HG22	1:C:260:PRO:HD3	1.87	0.57
1:B:47:SER:HB3	1:B:90:LEU:HD23	1.87	0.57
1:A:112:PRO:HB3	1:A:120:SER:C	2.30	0.57
1:B:91:ALA:HB2	1:B:135:TRP:CB	2.33	0.57
1:A:259:THR:HB	1:A:260:PRO:HD3	1.87	0.56
1:B:51:ALA:O	1:B:55:ILE:HG13	2.04	0.56
1:B:68:ILE:HG13	1:B:68:ILE:O	2.05	0.56
1:C:334:LEU:HD22	1:D:334:LEU:CD2	2.36	0.56
1:D:227:THR:O	1:D:228:GLU:C	2.48	0.56
1:D:229:ALA:C	1:D:231:ALA:H	2.12	0.56
1:D:320:ASP:OD1	1:D:324:LYS:HE3	2.04	0.56
1:B:80:ARG:NH1	1:B:150:LEU:HD23	2.21	0.56
1:C:134:ILE:CD1	1:D:333:SER:HB3	2.36	0.56
1:B:38:THR:OG1	1:B:39:GLU:N	2.31	0.56
1:C:154:GLU:HA	1:C:312:TYR:CE1	2.41	0.56
1:C:185:ASN:HB3	1:C:284:ASN:HD22	1.71	0.56
1:A:187:VAL:HG21	1:A:287:TYR:CG	2.41	0.56
1:B:35:PRO:HB2	1:D:306:GLN:NE2	2.21	0.56
1:C:242:ASN:C	1:C:244:CYS:H	2.13	0.55
1:A:42:GLY:O	1:A:46:ILE:HG13	2.05	0.55
1:D:212:THR:O	1:D:213:VAL:HG23	2.07	0.55
1:A:280:LEU:HD23	1:A:282:MET:HE2	1.88	0.55
1:C:140:GLN:HE21	1:D:129:ILE:HB	1.71	0.55
1:C:188:LYS:HE3	1:C:279:LYS:HA	1.87	0.55
1:B:264:MET:O	1:B:268:ILE:HG13	2.06	0.55
1:A:181:GLY:N	1:A:186:THR:O	2.39	0.54
1:B:50:GLN:HA	1:B:50:GLN:OE1	2.07	0.54
1:C:145:ILE:HB	1:C:319:TYR:CE1	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:LYS:O	1:C:184:GLY:N	2.40	0.54
1:D:314:ASN:C	1:D:316:ASN:H	2.14	0.54
1:B:335:GLU:CD	1:B:336:THR:HG23	2.33	0.54
1:B:46:ILE:O	1:B:50:GLN:HG2	2.07	0.54
1:D:165:GLN:O	1:D:167:PHE:N	2.40	0.54
1:B:259:THR:N	1:B:260:PRO:HD2	2.23	0.54
1:C:182:LYS:C	1:C:184:GLY:N	2.62	0.54
1:D:314:ASN:C	1:D:316:ASN:N	2.64	0.54
1:C:205:TYR:CD1	1:C:212:THR:HG22	2.43	0.54
1:D:244:CYS:SG	1:D:257:ASP:HA	2.48	0.54
1:B:131:ASP:C	1:B:133:GLU:N	2.66	0.53
1:A:34:VAL:HG13	1:A:35:PRO:HD2	1.90	0.53
1:A:109:PHE:O	1:A:141:ASN:ND2	2.40	0.53
1:A:178:LEU:O	1:A:179:LEU:HD23	2.08	0.53
1:C:185:ASN:C	1:C:284:ASN:ND2	2.67	0.53
1:B:97:LEU:HD23	1:B:102:ASN:OD1	2.09	0.52
1:B:227:THR:OG1	1:B:230:GLU:HG3	2.09	0.52
1:B:91:ALA:CB	1:B:135:TRP:HB2	2.37	0.52
1:A:234:TRP:CZ3	1:A:238:LEU:HD21	2.44	0.52
1:A:46:ILE:O	1:A:50:GLN:HG3	2.09	0.52
1:A:131:ASP:O	1:A:134:ILE:HG22	2.09	0.52
1:B:330:ILE:O	1:B:334:LEU:HB3	2.09	0.52
1:A:205:TYR:HA	1:A:212:THR:CG2	2.40	0.52
1:A:37:THR:HG23	1:A:336:THR:CG2	2.34	0.52
1:B:203:ASN:O	1:B:207:GLN:HG2	2.10	0.52
1:B:302:LYS:HG3	1:C:332:SER:HB2	1.91	0.52
1:A:260:PRO:HA	1:A:297:GLN:OE1	2.10	0.52
1:B:61:THR:C	1:B:63:GLN:H	2.18	0.52
1:D:159:VAL:HG21	1:D:213:VAL:O	2.09	0.51
1:B:178:LEU:CD2	1:C:318:LEU:HD22	2.39	0.51
1:C:137:MET:HE1	1:D:137:MET:CB	2.40	0.51
1:D:152:VAL:C	1:D:154:GLU:H	2.17	0.51
1:C:130:SER:OG	1:C:133:GLU:HG3	2.10	0.51
1:A:278:SER:OG	3:A:1342:GOL:H2	2.10	0.51
1:A:117:PHE:CD1	1:A:118:SER:N	2.67	0.51
1:C:142:ILE:C	1:C:145:ILE:HG23	2.36	0.51
1:B:98:SER:O	1:B:100:GLU:N	2.44	0.51
1:C:183:ASP:C	1:C:185:ASN:N	2.69	0.51
1:B:258:LEU:O	1:B:262:GLN:HG3	2.11	0.51
1:C:326:LEU:O	1:C:329:THR:HB	2.11	0.51
1:D:159:VAL:HB	1:D:214:LEU:HD23	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:VAL:CG1	1:D:308:LEU:HD13	2.41	0.50
1:A:111:ALA:O	1:A:120:SER:CB	2.59	0.50
1:B:47:SER:HB3	1:B:90:LEU:CD2	2.40	0.50
1:C:179:LEU:O	1:C:179:LEU:HD12	2.11	0.50
1:C:208:ILE:HG12	1:C:208:ILE:O	2.12	0.50
1:D:227:THR:O	1:D:230:GLU:N	2.44	0.50
1:D:241:PRO:HG2	1:D:244:CYS:HB2	1.93	0.50
1:B:100:GLU:HG3	1:B:101:GLN:H	1.76	0.50
1:D:245:LEU:C	1:D:245:LEU:HD23	2.36	0.50
1:A:274:PRO:HA	1:A:280:LEU:HB2	1.94	0.50
1:D:213:VAL:HG13	1:D:215:PHE:O	2.11	0.50
1:B:38:THR:HG23	1:B:39:GLU:OE1	2.12	0.50
1:B:324:LYS:C	1:B:326:LEU:N	2.67	0.49
1:D:160:TYR:CD2	1:D:160:TYR:O	2.65	0.49
1:D:241:PRO:C	1:D:243:SER:N	2.68	0.49
1:A:37:THR:HG22	1:C:306:GLN:NE2	2.27	0.49
1:A:174:MET:HB3	1:D:322:LEU:HD21	1.93	0.49
1:D:215:PHE:CE1	1:D:216:PRO:HA	2.47	0.49
1:A:256:VAL:HG23	1:A:258:LEU:HD13	1.94	0.49
1:D:160:TYR:OH	1:D:301:MET:HG2	2.13	0.49
1:D:242:ASN:C	1:D:244:CYS:H	2.20	0.49
1:B:40:HIS:CB	1:B:45:ILE:HG13	2.27	0.49
1:C:178:LEU:HD11	1:C:287:TYR:CZ	2.48	0.49
1:B:179:LEU:HD12	1:B:279:LYS:NZ	2.27	0.49
1:C:274:PRO:HB2	1:C:278:SER:O	2.11	0.49
1:C:313:SER:O	1:C:314:ASN:C	2.54	0.49
1:A:205:TYR:HA	1:A:212:THR:HG21	1.94	0.49
1:B:36:SER:O	1:B:37:THR:C	2.54	0.49
1:D:229:ALA:O	1:D:231:ALA:N	2.45	0.49
1:A:101:GLN:HE22	1:A:333:SER:CA	2.26	0.49
1:D:310:GLN:O	1:D:314:ASN:HB2	2.13	0.49
1:D:259:THR:HB	1:D:260:PRO:HD3	1.94	0.48
1:A:105:LEU:HG	1:A:138:VAL:HG21	1.93	0.48
1:A:259:THR:HG22	1:A:263:LYS:NZ	2.28	0.48
1:C:208:ILE:HD11	1:C:223:VAL:HG11	1.94	0.48
1:A:77:THR:O	1:A:81:GLN:HG3	2.14	0.48
1:A:260:PRO:O	1:A:264:MET:HG3	2.13	0.48
1:D:259:THR:HB	1:D:260:PRO:CD	2.43	0.48
1:A:155:ASN:O	1:A:159:VAL:HG23	2.13	0.48
1:B:191:VAL:HG13	1:B:192:THR:N	2.28	0.48
1:C:257:ASP:OD1	1:C:259:THR:HG22	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:TRP:CE3	1:A:238:LEU:HD21	2.48	0.48
1:B:55:ILE:HA	1:B:83:LEU:CD1	2.42	0.48
1:B:80:ARG:NH1	1:B:146:GLY:O	2.46	0.48
1:D:156:VAL:O	1:D:157:VAL:C	2.56	0.48
1:D:236:SER:C	1:D:238:LEU:H	2.22	0.48
1:C:242:ASN:C	1:C:244:CYS:N	2.70	0.48
1:D:326:LEU:O	1:D:329:THR:HG22	2.13	0.48
1:C:295:LYS:O	1:C:299:GLU:HG2	2.14	0.48
1:A:63:GLN:NE2	1:D:343:GLY:HA2	2.28	0.48
1:B:208:ILE:O	1:B:208:ILE:HG22	2.14	0.48
1:A:282:MET:HB2	1:A:286:LYS:HD3	1.96	0.47
1:B:36:SER:OG	1:B:336:THR:HG22	2.13	0.47
1:B:181:GLY:HA3	1:B:186:THR:OG1	2.14	0.47
1:B:323:VAL:O	1:B:326:LEU:HB3	2.13	0.47
1:A:215:PHE:CD1	1:A:216:PRO:HA	2.49	0.47
1:A:225:VAL:HG11	1:A:248:TYR:O	2.14	0.47
1:C:285:ALA:H	1:C:287:TYR:H	1.62	0.47
1:D:141:ASN:OD1	1:D:141:ASN:C	2.57	0.47
1:A:134:ILE:O	1:A:138:VAL:HG23	2.14	0.47
1:C:208:ILE:HD11	1:C:223:VAL:CG1	2.44	0.47
1:D:159:VAL:C	1:D:161:THR:H	2.23	0.47
1:B:39:GLU:O	1:B:40:HIS:CG	2.68	0.47
1:A:111:ALA:O	1:A:120:SER:HB3	2.15	0.47
1:A:278:SER:OG	1:A:279:LYS:N	2.48	0.47
1:C:137:MET:HE1	1:D:137:MET:HB3	1.96	0.47
1:A:87:LEU:HD11	1:A:326:LEU:HD11	1.96	0.47
1:B:177:TRP:HB3	1:B:190:ASP:CB	2.43	0.47
1:C:284:ASN:HA	1:C:287:TYR:HB3	1.96	0.47
1:A:228:GLU:HB2	1:A:252:TYR:CE2	2.50	0.47
1:C:295:LYS:HA	1:C:298:GLU:HB3	1.96	0.47
1:D:233:GLN:O	1:D:236:SER:HB3	2.15	0.47
1:A:34:VAL:HG23	1:C:295:LYS:CE	2.43	0.46
1:C:135:TRP:CZ3	1:D:340:PHE:HB2	2.49	0.46
1:B:35:PRO:CG	1:D:310:GLN:OE1	2.64	0.46
1:B:328:SER:O	1:B:331:SER:N	2.48	0.46
1:D:215:PHE:HA	1:D:216:PRO:O	2.16	0.46
1:A:111:ALA:N	1:A:112:PRO:HD3	2.30	0.46
1:B:198:LEU:HD22	1:B:261:LEU:HD22	1.98	0.46
1:B:145:ILE:HG22	1:B:319:TYR:HD1	1.81	0.46
1:A:73:ASN:HD21	1:A:158:ALA:HB2	1.81	0.46
1:A:191:VAL:HG23	1:A:192:THR:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:SER:HB3	1:A:252:TYR:CE1	2.51	0.46
1:B:191:VAL:HG23	1:B:268:ILE:HG23	1.97	0.46
1:C:262:GLN:O	1:C:266:GLN:HG3	2.15	0.46
1:D:156:VAL:HG11	1:D:308:LEU:HD13	1.98	0.46
1:A:37:THR:HA	1:A:338:LYS:HB3	1.97	0.46
1:A:277:ASP:OD1	1:A:277:ASP:C	2.58	0.46
1:A:56:HIS:HB3	1:C:316:ASN:ND2	2.31	0.45
1:B:38:THR:OG1	1:B:39:GLU:HG3	2.16	0.45
1:D:257:ASP:C	1:D:259:THR:H	2.24	0.45
1:A:83:LEU:HD12	1:A:83:LEU:O	2.16	0.45
1:A:189:LEU:HD12	1:A:190:ASP:N	2.31	0.45
1:C:139:SER:C	1:C:141:ASN:N	2.72	0.45
1:A:130:SER:OG	1:A:133:GLU:HB2	2.16	0.45
1:D:151:GLY:O	1:D:154:GLU:N	2.44	0.45
1:A:98:SER:OG	1:A:101:GLN:HG3	2.17	0.45
1:B:189:LEU:O	1:B:191:VAL:N	2.46	0.45
1:B:293:GLY:O	1:B:296:ALA:HB3	2.16	0.45
1:C:140:GLN:NE2	1:D:129:ILE:HB	2.31	0.45
1:C:145:ILE:HG22	1:C:319:TYR:HE1	1.82	0.45
1:C:150:LEU:HD11	1:C:316:ASN:CG	2.41	0.45
1:D:164:TYR:OH	1:D:302:LYS:CG	2.64	0.45
1:D:314:ASN:O	1:D:316:ASN:N	2.50	0.45
1:A:58:ALA:HA	1:A:79:ALA:HB1	1.99	0.45
1:A:106:ARG:HG2	1:A:106:ARG:HH11	1.81	0.45
1:B:238:LEU:O	1:B:239:ASN:CB	2.64	0.45
1:C:139:SER:O	1:C:142:ILE:HG13	2.17	0.45
1:C:193:SER:O	1:C:194:LEU:C	2.59	0.45
1:C:332:SER:O	1:C:336:THR:HG23	2.17	0.45
1:D:160:TYR:OH	1:D:301:MET:CG	2.65	0.45
1:A:161:THR:HG22	1:A:162:ASP:N	2.32	0.45
1:C:150:LEU:HD11	1:C:316:ASN:OD1	2.17	0.45
1:A:91:ALA:HB2	1:A:135:TRP:CB	2.47	0.45
1:A:91:ALA:HB2	1:A:135:TRP:HB3	1.98	0.45
1:B:37:THR:OG1	1:D:303:THR:HG23	2.16	0.45
1:B:238:LEU:O	1:B:239:ASN:HB2	2.17	0.45
1:B:258:LEU:O	1:B:259:THR:C	2.60	0.45
1:C:188:LYS:CE	1:C:279:LYS:HA	2.46	0.45
1:C:257:ASP:CG	1:C:259:THR:HG22	2.42	0.45
1:D:160:TYR:OH	1:D:304:THR:OG1	2.34	0.45
1:B:324:LYS:C	1:B:326:LEU:H	2.24	0.44
1:C:292:SER:CA	1:C:295:LYS:HE2	2.39	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:MET:O	1:B:141:ASN:HB2	2.17	0.44
1:C:138:VAL:HG12	1:C:138:VAL:O	2.17	0.44
1:B:188:LYS:HE2	1:B:281:GLU:OE2	2.17	0.44
1:A:278:SER:CB	3:A:1342:GOL:HO3	2.30	0.44
1:D:229:ALA:HA	1:D:232:ARG:HB3	2.00	0.44
1:A:56:HIS:ND1	1:C:316:ASN:HB3	2.33	0.44
1:B:63:GLN:O	1:B:63:GLN:CG	2.64	0.44
1:C:210:SER:HG	1:C:218:GLN:HB2	1.82	0.44
1:A:326:LEU:HD23	1:A:326:LEU:HA	1.80	0.44
1:B:35:PRO:HB3	1:B:335:GLU:HA	2.00	0.44
1:B:316:ASN:HD22	1:C:343:GLY:C	2.25	0.44
1:C:187:VAL:HG13	1:C:284:ASN:OD1	2.17	0.44
1:B:40:HIS:O	1:B:41:ARG:C	2.59	0.43
1:C:175:GLY:C	1:C:177:TRP:H	2.26	0.43
1:C:299:GLU:O	1:C:300:ASN:C	2.61	0.43
1:D:153:TYR:CE1	1:D:311:LYS:HB3	2.52	0.43
1:B:151:GLY:HA2	1:B:154:GLU:OE1	2.18	0.43
1:B:177:TRP:O	1:B:189:LEU:HD12	2.18	0.43
1:B:188:LYS:HG2	1:B:281:GLU:CG	2.39	0.43
1:B:192:THR:HG22	1:B:193:SER:N	2.32	0.43
1:D:164:TYR:CD1	1:D:164:TYR:C	2.95	0.43
1:B:288:GLN:HA	1:B:288:GLN:NE2	2.32	0.43
1:C:210:SER:OG	1:C:218:GLN:HB2	2.18	0.43
1:B:259:THR:HB	1:B:260:PRO:CD	2.48	0.43
1:C:139:SER:O	1:C:141:ASN:N	2.51	0.43
1:B:65:THR:O	1:B:76:ARG:HD2	2.17	0.43
1:D:156:VAL:HG12	1:D:157:VAL:N	2.33	0.43
1:A:150:LEU:HG	1:A:154:GLU:OE2	2.19	0.43
1:A:208:ILE:O	1:A:208:ILE:HG22	2.18	0.43
1:D:210:SER:C	1:D:212:THR:H	2.27	0.43
1:D:226:ALA:O	1:D:227:THR:C	2.61	0.43
1:B:130:SER:HB2	1:B:134:ILE:CD1	2.48	0.43
1:C:138:VAL:CG1	1:D:341:LEU:HD21	2.49	0.43
1:A:264:MET:O	1:A:268:ILE:HG13	2.19	0.43
1:A:41:ARG:H	1:A:44:ASP:HB2	1.84	0.43
1:B:37:THR:O	1:B:37:THR:CG2	2.66	0.43
1:B:42:GLY:HA2	1:D:164:TYR:OH	2.17	0.43
1:A:101:GLN:HE22	1:A:333:SER:HA	1.83	0.43
1:B:69:SER:HB3	1:B:72:ASN:HB2	2.01	0.43
1:A:41:ARG:HB3	1:A:43:THR:HG22	2.02	0.42
1:A:150:LEU:O	1:A:154:GLU:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HD21	1:D:325:VAL:CG1	2.49	0.42
1:B:67:PRO:O	1:B:157:VAL:HG12	2.18	0.42
1:B:256:VAL:HG23	1:B:258:LEU:HD13	2.00	0.42
1:D:263:LYS:C	1:D:265:VAL:H	2.27	0.42
1:B:179:LEU:HD12	1:B:279:LYS:HZ2	1.83	0.42
1:B:264:MET:HE2	1:B:297:GLN:HB2	2.01	0.42
1:B:284:ASN:O	1:B:285:ALA:C	2.62	0.42
1:D:156:VAL:O	1:D:159:VAL:N	2.51	0.42
1:D:253:VAL:C	1:D:254:VAL:HG23	2.44	0.42
1:A:112:PRO:O	1:A:113:THR:HG22	2.20	0.42
1:A:189:LEU:C	1:A:191:VAL:H	2.26	0.42
1:B:230:GLU:HG3	1:B:230:GLU:H	1.67	0.42
1:D:162:ASP:O	1:D:163:PHE:C	2.63	0.42
1:D:229:ALA:C	1:D:231:ALA:N	2.75	0.42
1:C:341:LEU:O	1:C:342:GLN:C	2.63	0.42
1:C:163:PHE:CE2	1:C:301:MET:HE3	2.54	0.42
1:D:263:LYS:C	1:D:265:VAL:N	2.77	0.42
1:A:210:SER:HA	1:A:218:GLN:HG3	2.02	0.42
1:D:238:LEU:HD23	1:D:308:LEU:HD21	2.01	0.42
1:B:102:ASN:OD1	1:B:134:ILE:HG13	2.20	0.42
1:C:142:ILE:O	1:C:145:ILE:HG12	2.20	0.42
1:A:181:GLY:O	1:A:182:LYS:C	2.62	0.42
1:A:274:PRO:O	1:A:275:GLY:O	2.37	0.42
1:A:54:LYS:HD2	1:A:82:GLN:HB3	2.01	0.42
1:A:112:PRO:HA	1:A:120:SER:HB2	2.02	0.42
1:A:190:ASP:O	1:A:191:VAL:C	2.62	0.42
1:A:214:LEU:HD21	1:A:256:VAL:HG12	2.00	0.42
1:B:40:HIS:HB2	1:B:45:ILE:HD11	2.02	0.42
1:B:36:SER:HB2	1:B:336:THR:HA	2.02	0.41
1:C:282:MET:HE3	1:C:286:LYS:HG3	2.02	0.41
1:D:303:THR:C	1:D:305:LEU:H	2.28	0.41
1:B:37:THR:CG2	1:D:303:THR:OG1	2.68	0.41
1:B:100:GLU:O	1:B:103:GLU:HB3	2.20	0.41
1:B:163:PHE:CZ	1:B:301:MET:HE3	2.55	0.41
1:C:138:VAL:HG11	1:D:341:LEU:HD21	2.01	0.41
1:D:261:LEU:HA	1:D:264:MET:HG2	2.02	0.41
1:A:41:ARG:O	1:A:44:ASP:HB2	2.20	0.41
1:A:156:VAL:HG22	1:A:214:LEU:HB3	2.03	0.41
1:A:36:SER:O	1:A:338:LYS:HB2	2.20	0.41
1:A:170:ILE:HD13	1:A:197:ASP:HB3	2.02	0.41
1:A:111:ALA:N	1:A:112:PRO:CD	2.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:SER:HA	1:C:295:LYS:HG2	2.02	0.41
1:A:291:GLN:O	1:A:292:SER:C	2.63	0.41
1:A:322:LEU:HD23	1:A:322:LEU:HA	1.82	0.41
1:C:145:ILE:HG21	1:C:319:TYR:OH	2.20	0.41
1:C:234:TRP:O	1:C:235:LEU:C	2.63	0.41
1:A:185:ASN:HB3	1:A:284:ASN:OD1	2.20	0.41
1:B:58:ALA:HA	1:B:79:ALA:HB1	2.02	0.41
1:B:231:ALA:HB1	1:B:245:LEU:CD1	2.51	0.41
1:C:149:TYR:CD1	1:C:149:TYR:N	2.89	0.41
1:C:319:TYR:O	1:C:323:VAL:HG13	2.21	0.41
1:A:278:SER:OG	3:A:1342:GOL:O3	2.25	0.41
1:C:190:ASP:O	1:C:192:THR:N	2.54	0.41
1:A:306:GLN:OE1	1:D:335:GLU:HG2	2.21	0.40
1:B:145:ILE:CG2	1:B:319:TYR:HD1	2.35	0.40
1:C:232:ARG:HG2	1:C:232:ARG:HH11	1.85	0.40
1:A:115:ALA:O	1:A:116:LEU:C	2.64	0.40
1:B:54:LYS:HA	1:B:54:LYS:HD3	1.92	0.40
1:B:134:ILE:C	1:B:136:ASP:N	2.79	0.40
1:C:145:ILE:HA	1:C:148:SER:HB3	2.03	0.40
1:C:152:VAL:O	1:C:156:VAL:HG23	2.22	0.40
1:C:329:THR:HG22	1:C:330:ILE:N	2.35	0.40
1:D:238:LEU:O	1:D:239:ASN:HB3	2.21	0.40
1:D:321:ASN:O	1:D:325:VAL:HG23	2.21	0.40
1:A:284:ASN:O	1:A:288:GLN:HG2	2.20	0.40
1:B:295:LYS:HG2	1:B:299:GLU:OE2	2.21	0.40
1:C:235:LEU:HD23	1:C:235:LEU:HA	1.91	0.40
1:D:257:ASP:OD2	1:D:259:THR:HB	2.21	0.40
1:A:237:GLU:O	1:A:311:LYS:NZ	2.49	0.40
1:B:169:ASP:OD1	1:B:169:ASP:N	2.55	0.40
1:C:145:ILE:C	1:C:148:SER:HB3	2.47	0.40
1:C:258:LEU:O	1:C:262:GLN:HG3	2.21	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	298/346 (86%)	269 (90%)	20 (7%)	9 (3%)	3	19
1	B	281/346 (81%)	232 (83%)	38 (14%)	11 (4%)	2	14
1	C	214/346 (62%)	176 (82%)	32 (15%)	6 (3%)	4	21
1	D	112/346 (32%)	65 (58%)	36 (32%)	11 (10%)	0	2
All	All	905/1384 (65%)	742 (82%)	126 (14%)	37 (4%)	2	13

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	HIS
1	B	130	SER
1	C	285	ALA
1	D	156	VAL
1	D	157	VAL
1	D	166	ALA
1	D	228	GLU
1	D	342	GLN
1	A	96	SER
1	A	112	PRO
1	A	275	GLY
1	A	336	THR
1	B	36	SER
1	B	39	GLU
1	B	42	GLY
1	B	99	ALA
1	C	140	GLN
1	C	191	VAL
1	D	160	TYR
1	D	230	GLU
1	D	237	GLU
1	D	253	VAL
1	A	191	VAL
1	B	37	THR
1	B	69	SER
1	B	140	GLN
1	C	183	ASP
1	C	284	ASN
1	A	119	ALA
1	A	182	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	62	LEU
1	B	93	SER
1	C	279	LYS
1	D	165	GLN
1	D	306	GLN
1	A	223	VAL
1	A	274	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	A	1342	-	5,5,5	0.32	0	5,5,5	0.24	0
2	SO4	A	1341	-	4,4,4	0.39	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	1340	-	4,4,4	0.44	0	6,6,6	0.18	0
3	GOL	B	1339	-	5,5,5	0.35	0	5,5,5	0.32	0
2	SO4	B	1338	-	4,4,4	0.44	0	6,6,6	0.11	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	B	1339	-	-	0/4/4/4	-
3	GOL	A	1342	-	-	0/4/4/4	-

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.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1342	GOL	4	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	302/346 (87%)	-0.40	5 (1%) 69 45	35, 63, 128, 157	0
1	B	285/346 (82%)	-0.16	5 (1%) 67 44	43, 74, 143, 157	0
1	C	216/346 (62%)	-0.25	3 (1%) 73 51	45, 74, 134, 155	0
1	D	124/346 (35%)	0.38	6 (4%) 35 19	41, 109, 136, 157	0
All	All	927/1384 (66%)	-0.19	19 (2%) 65 41	35, 73, 140, 157	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	343	GLY	5.0
1	A	116	LEU	4.7
1	D	168	SER	3.6
1	B	132	ALA	3.3
1	B	337	ALA	3.1
1	C	144	ALA	3.1
1	A	117	PHE	3.0
1	A	337	ALA	2.9
1	D	252	TYR	2.9
1	A	33	VAL	2.9
1	D	261	LEU	2.9
1	B	129	ILE	2.8
1	B	134	ILE	2.8
1	B	35	PRO	2.3
1	A	118	SER	2.3
1	D	260	PRO	2.3
1	D	304	THR	2.2
1	D	163	PHE	2.1
1	C	274	PRO	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
2	SO4	B	1338	5/5	0.68	0.17	88,90,93,97	5
2	SO4	A	1341	5/5	0.80	0.11	88,91,96,96	5
3	GOL	A	1342	6/6	0.83	0.12	86,90,93,94	0
3	GOL	B	1339	6/6	0.84	0.13	76,87,90,91	0
2	SO4	A	1340	5/5	0.91	0.07	77,77,87,88	5

6.5 Other polymers [i](#)

There are no such residues in this entry.