



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:51 AM GMT

PDB ID : 2YM9
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

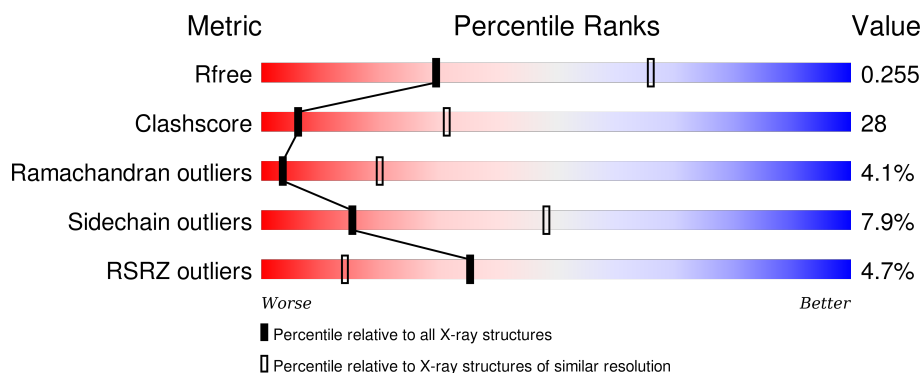
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	346	<div> <div>5%</div> <div>47%</div> <div>36%</div> <div>•</div> <div>13%</div> </div>
1	B	346	<div> <div>3%</div> <div>45%</div> <div>32%</div> <div>5%</div> <div>18%</div> </div>
1	C	346	<div> <div>3%</div> <div>36%</div> <div>23%</div> <div>• •</div> <div>38%</div> </div>
1	D	346	<div> <div>3%</div> <div>13%</div> <div>18%</div> <div>5%</div> <div>64%</div> </div>

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 (three-letter code: 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 (three-letter code: GOL) (formula: C₃H₈O₃).



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		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

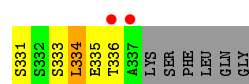
Chain A:

Sequence logo for Chain A. The y-axis represents information content in bits (0.00 to 0.25). The x-axis shows positions 1 to 100. A color key identifies amino acids: Gly (green), Leu (grey), Phe (dark grey), Ser (orange), Thr (red), Val (yellow), and others (grey). A bar chart at the top shows the percentage of each amino acid: Gly 47%, Val 36%, Ser 5%, and others 13%.

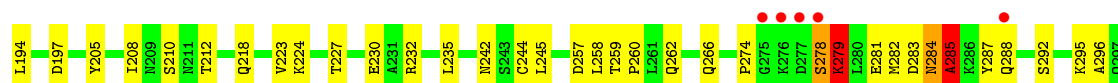
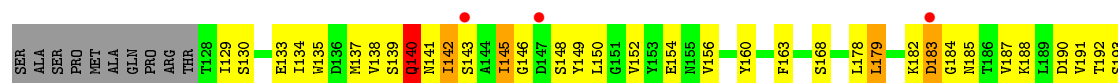
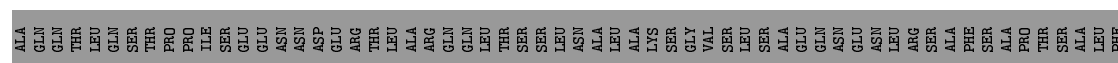
Chain B:

3% 45% 32% 5% 18%

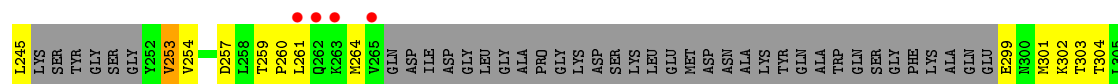
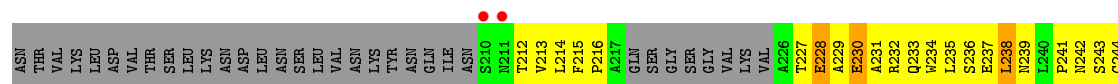
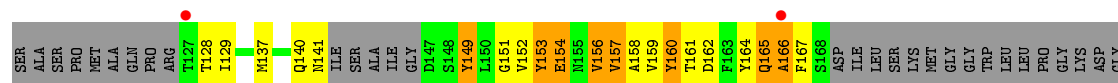
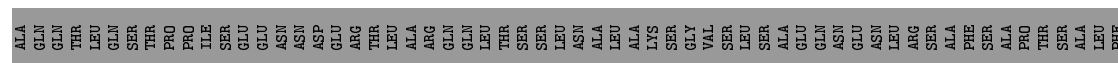
GLY SER HIS MET LEU ASN ILE GLN ASN TYR SER ALA SER PRO HIS PRO GLY ILE VAL ALA ALA GLU ARG PRO GLN THR PRO SER SER ALA SER GLU HIS VAL THR ALA VAL VAL P35 S36 T37 T38 E39 H40 R41 G42 LEU T43 D44 I45 I46 S47 Q50 A51 A52 T53 K54 I55 H56 Q57 A58



- 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) 97.2 (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 (5.04%)	DCC
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 , 66.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 34081 reflections (0.006%)	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.43	0/2321	0.64	1/3153 (0.0%)
1	B	0.39	0/2206	0.65	0/2993
1	C	0.40	0/1686	0.66	2/2286 (0.1%)
1	D	0.47	0/984	0.69	0/1335
All	All	0.42	0/7197	0.65	3/9767 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	ALA	N-CA-C	-5.52	96.09	111.00
1	C	279	LYS	N-CA-C	5.35	125.45	111.00
1	A	117	PHE	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2288	0	2253	113	0
1	B	2175	0	2135	123	0
1	C	1659	0	1633	99	0
1	D	972	0	943	99	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	395	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 28.

All (395) 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: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: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:C:278:SER:OG	1:C:279:LYS:N	2.18	0.76
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
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:B:334:LEU:HD12	1:B:334:LEU:O	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:215:PHE:CD1	1:B:216:PRO:HA	2.23	0.73
1:B:45:ILE:HG22	1:B:45:ILE:O	1.86	0.73
1:C:145:ILE:O	1:C:148:SER:HB3	1.87	0.73
1:D:260:PRO:HB2	1:D:264:MET:HE2	1.71	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: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:87:LEU:HD22	1:B:138:VAL:HG11	1.74	0.69
1:B:80:ARG:HG2	1:B:319:TYR:OH	1.93	0.69
1:B:63:GLN:O	1:B:63:GLN:HG3	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:110:SER:C	1:A:112:PRO:HD3	2.14	0.68
1:D:165:GLN:HG3	1:D:166:ALA:N	2.07	0.68
1:A:55:ILE:HD12	1:A:330:ILE:HD12	1.76	0.68
1:A:187:VAL:HG21	1:A:287:TYR:CD1	2.28	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:D:165:GLN:C	1:D:167:PHE:H	1.96	0.66
1:B:97:LEU:HD12	1:B:101:GLN:OE1	1.95	0.65
1:D:212:THR:HG22	1:D:212:THR:O	1.96	0.65
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:PHE:N	1:B:109:PHE:HD1	1.96	0.63
1:B:131:ASP:C	1:B:133:GLU:H	2.01	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:334:LEU:HD22	1:D:334:LEU:HD22	1.82	0.62
1:D:229:ALA:O	1:D:233:GLN:N	2.31	0.62
1:C:259:THR:CG2	1:C:260:PRO:HD3	2.30	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:B:42:GLY:HA3	1:D:164:TYR:OH	2.02	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:B:129:ILE:O	1:B:130:SER:HB3	2.02	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:232:ARG:HA	1:D:235:LEU:HD12	1.83	0.59
1:B:227:THR:HG23	1:B:230:GLU:OE2	2.02	0.59
1:C:183:ASP:C	1:C:185:ASN:H	2.03	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: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: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: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:100:GLU:N	1:A:100:GLU:OE1	2.35	0.57
1:A:38:THR:HG21	1:A:45:ILE:HD11	1.86	0.57
1:C:139:SER:C	1:C:141:ASN:H	2.08	0.57
1:C:259:THR:HG22	1:C:260:PRO:HD3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:MET:CE	1:C:287:TYR:HA	2.35	0.57
1:B:47:SER:HB3	1:B:90:LEU:HD23	1.87	0.57
1:C:137:MET:HE1	1:D:137:MET:CB	2.35	0.57
1:B:91:ALA:HB2	1:B:135:TRP:CB	2.33	0.57
1:B:51:ALA:O	1:B:55:ILE:HG13	2.04	0.56
1:C:334:LEU:HD22	1:D:334:LEU:CD2	2.36	0.56
1:B:68:ILE:HG13	1:B:68:ILE:O	2.05	0.56
1:A:259:THR:HB	1:A:260:PRO:HD3	1.87	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:B:35:PRO:HB2	1:D:306:GLN:NE2	2.21	0.56
1:A:187:VAL:HG21	1:A:287:TYR:CG	2.41	0.56
1:C:182:LYS:C	1:C:184:GLY:H	2.10	0.55
1:D:212:THR:O	1:D:213:VAL:HG23	2.07	0.55
1:A:42:GLY:O	1:A:46:ILE:HG13	2.05	0.55
1:C:140:GLN:HE21	1:D:129:ILE:HB	1.71	0.55
1:C:141:ASN:C	1:C:143:SER:H	2.10	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:C:282:MET:HE1	1:C:287:TYR:HA	1.88	0.55
1:D:149:TYR:C	1:D:149:TYR:CD1	2.79	0.55
1:C:145:ILE:HB	1:C:319:TYR:CE1	2.42	0.54
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:182:LYS:O	1:C:184:GLY:N	2.40	0.54
1:D:165:GLN:O	1:D:167:PHE:N	2.40	0.54
1:B:46:ILE:O	1:B:50:GLN:HG2	2.07	0.54
1:B:259:THR:N	1:B:260:PRO:HD2	2.23	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:C:283:ASP:O	1:C:284:ASN:C	2.46	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:D:229:ALA:C	1:D:231:ALA:H	2.12	0.53
1:C:141:ASN:C	1:C:143:SER:N	2.60	0.53
1:B:97:LEU:HD23	1:B:102:ASN:OD1	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:182:LYS:C	1:C:184:GLY:N	2.62	0.52
1:A:234:TRP:CZ3	1:A:238:LEU:HD21	2.44	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:46:ILE:O	1:A:50:GLN:HG3	2.09	0.52
1:A:205:TYR:HA	1:A:212:THR:CG2	2.40	0.52
1:D:227:THR:O	1:D:228:GLU:C	2.48	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:A:112:PRO:HB3	1:A:120:SER:C	2.30	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:HB3	1.92	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:33:VAL:H	1:C:295:LYS:HZ1	1.57	0.51
1:A:117:PHE:CD1	1:A:118:SER:N	2.67	0.51
1:B:98:SER:O	1:B:100:GLU:N	2.44	0.51
1:D:314:ASN:C	1:D:316:ASN:N	2.64	0.51
1:C:242:ASN:C	1:C:244:CYS:H	2.13	0.51
1:D:159:VAL:HB	1:D:214:LEU:HD23	1.92	0.51
1:C:326:LEU:O	1:C:329:THR:HB	2.11	0.51
1:B:258:LEU:O	1:B:262:GLN:HG3	2.11	0.51
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:HD12	1:C:179:LEU:O	2.11	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:C:208:ILE:O	1:C:208:ILE:HG12	2.12	0.50
1:B:100:GLU:HG3	1:B:101:GLN:H	1.76	0.50
1:D:314:ASN:C	1:D:316:ASN:H	2.14	0.50
1:D:213:VAL:HG13	1:D:215:PHE:O	2.11	0.50
1:A:274:PRO:HA	1:A:280:LEU:HB2	1.94	0.50
1:B:38:THR:HG23	1:B:39:GLU:OE1	2.12	0.50
1:D:160:TYR:CD2	1:D:160:TYR:O	2.65	0.49
1:D:215:PHE:CE1	1:D:216:PRO:HA	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:160:TYR:OH	1:D:301:MET:HG2	2.13	0.49
1:A:256:VAL:HG23	1:A:258:LEU:HD13	1.94	0.49
1:B:40:HIS:CB	1:B:45:ILE:HG13	2.27	0.49
1:B:335:GLU:CD	1:B:336:THR:HG23	2.33	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:D:229:ALA:O	1:D:231:ALA:N	2.45	0.49
1:A:205:TYR:HA	1:A:212:THR:HG21	1.94	0.49
1:D:310:GLN:O	1:D:314:ASN:HB2	2.13	0.49
1:A:101:GLN:HE22	1:A:333:SER:CA	2.26	0.49
1:D:165:GLN:C	1:D:167:PHE:N	2.64	0.49
1:B:137:MET:HA	1:B:137:MET:HE2	1.95	0.48
1:D:259:THR:HB	1:D:260:PRO:HD3	1.94	0.48
1:B:131:ASP:C	1:B:133:GLU:N	2.66	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:260:PRO:O	1:A:264:MET:HG3	2.13	0.48
1:A:77:THR:O	1:A:81:GLN:HG3	2.14	0.48
1:D:259:THR:HB	1:D:260:PRO:CD	2.43	0.48
1:C:185:ASN:C	1:C:284:ASN:ND2	2.67	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
1:A:155:ASN:O	1:A:159:VAL:HG23	2.13	0.48
1:B:80:ARG:NH1	1:B:146:GLY:O	2.46	0.48
1:B:55:ILE:HA	1:B:83:LEU:CD1	2.42	0.48
1:A:234:TRP:CE3	1:A:238:LEU:HD21	2.48	0.48
1:B:324:LYS:C	1:B:326:LEU:N	2.67	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:D:260:PRO:HG3	1:D:301:MET:CE	2.44	0.48
1:A:32:ALA:HA	1:C:295:LYS:HZ2	1.78	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:B:36:SER:OG	1:B:336:THR:HG22	2.13	0.47
1:B:323:VAL:O	1:B:326:LEU:HB3	2.13	0.47
1:A:282:MET:HB2	1:A:286:LYS:HD3	1.96	0.47
1:B:181:GLY:HA3	1:B:186:THR:OG1	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PHE:CD1	1:A:216:PRO:HA	2.49	0.47
1:C:285:ALA:H	1:C:287:TYR:H	1.62	0.47
1:A:225:VAL:HG11	1:A:248:TYR:O	2.14	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:B:39:GLU:O	1:B:40:HIS:CG	2.68	0.47
1:B:61:THR:C	1:B:63:GLN:H	2.18	0.47
1:A:278:SER:OG	1:A:279:LYS:N	2.48	0.47
1:A:111:ALA:O	1:A:120:SER:HB3	2.15	0.47
1:A:111:ALA:N	1:A:112:PRO:HD3	2.30	0.47
1:A:87:LEU:HD11	1:A:326:LEU:HD11	1.96	0.47
1:C:284:ASN:HA	1:C:287:TYR:HB3	1.96	0.47
1:B:177:TRP:HB3	1:B:190:ASP:CB	2.43	0.47
1:D:152:VAL:C	1:D:154:GLU:H	2.17	0.47
1:D:233:GLN:O	1:D:236:SER:HB3	2.15	0.47
1:C:295:LYS:HA	1:C:298:GLU:HB3	1.96	0.47
1:A:228:GLU:HB2	1:A:252:TYR:CE2	2.50	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:C:142:ILE:C	1:C:145:ILE:HG23	2.36	0.46
1:D:215:PHE:HA	1:D:216:PRO:O	2.16	0.46
1:B:198:LEU:HD22	1:B:261:LEU:HD22	1.98	0.46
1:C:183:ASP:C	1:C:185:ASN:N	2.69	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
1:D:156:VAL:HG11	1:D:308:LEU:HD13	1.98	0.46
1:B:191:VAL:HG23	1:B:268:ILE:HG23	1.97	0.46
1:A:247:SER:HB3	1:A:252:TYR:CE1	2.51	0.46
1:C:262:GLN:O	1:C:266:GLN:HG3	2.15	0.46
1:A:37:THR:HA	1:A:338:LYS:HB3	1.97	0.46
1:B:38:THR:OG1	1:B:39:GLU:HG3	2.16	0.45
1:A:56:HIS:HB3	1:C:316:ASN:ND2	2.31	0.45
1:A:83:LEU:O	1:A:83:LEU:HD12	2.16	0.45
1:A:189:LEU:HD12	1:A:190:ASP:N	2.31	0.45
1:D:151:GLY:O	1:D:154:GLU:N	2.44	0.45
1:A:130:SER:OG	1:A:133:GLU:HB2	2.16	0.45
1:B:189:LEU:O	1:B:191:VAL:N	2.46	0.45
1:C:140:GLN:NE2	1:D:129:ILE:HB	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:SER:OG	1:A:101:GLN:HG3	2.17	0.45
1:B:293:GLY:O	1:B:296:ALA:HB3	2.16	0.45
1:C:145:ILE:HG22	1:C:319:TYR:HE1	1.82	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:C:139:SER:O	1:C:142:ILE:HG13	2.17	0.45
1:D:160:TYR:OH	1:D:301:MET:CG	2.65	0.45
1:C:332:SER:O	1:C:336:THR:HG23	2.17	0.45
1:A:106:ARG:HH11	1:A:106:ARG:HG2	1.81	0.45
1:A:58:ALA:HA	1:A:79:ALA:HB1	1.99	0.45
1:B:238:LEU:O	1:B:239:ASN:CB	2.64	0.45
1:C:150:LEU:HD11	1:C:316:ASN:OD1	2.17	0.45
1:A:161:THR:HG22	1:A:162:ASP:N	2.32	0.45
1:D:245:LEU:C	1:D:245:LEU:HD23	2.36	0.45
1:B:37:THR:OG1	1:D:303:THR:HG23	2.16	0.45
1:D:242:ASN:C	1:D:244:CYS:H	2.20	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:C:188:LYS:CE	1:C:279:LYS:HA	2.46	0.45
1:D:241:PRO:C	1:D:243:SER:N	2.68	0.45
1:D:160:TYR:OH	1:D:304:THR:OG1	2.34	0.45
1:B:238:LEU:O	1:B:239:ASN:HB2	2.17	0.45
1:C:292:SER:CA	1:C:295:LYS:HE2	2.39	0.44
1:C:138:VAL:O	1:C:138:VAL:HG12	2.17	0.44
1:B:137:MET:O	1:B:141:ASN:HB2	2.17	0.44
1:D:260:PRO:HG3	1:D:301:MET:HE3	1.99	0.44
1:C:313:SER:O	1:C:314:ASN:C	2.54	0.44
1:B:188:LYS:HE2	1:B:281:GLU:OE2	2.17	0.44
1:B:36:SER:O	1:B:37:THR:C	2.54	0.44
1:D:229:ALA:HA	1:D:232:ARG:HB3	2.00	0.44
1:A:278:SER:CB	3:A:1342:GOL:HO3	2.30	0.44
1:B:63:GLN:O	1:B:63:GLN:CG	2.64	0.44
1:A:56:HIS:ND1	1:C:316:ASN:HB3	2.33	0.44
1:B:35:PRO:HB3	1:B:335:GLU:HA	2.00	0.44
1:C:187:VAL:HG13	1:C:284:ASN:OD1	2.17	0.44
1:A:326:LEU:HD23	1:A:326:LEU:HA	1.80	0.44
1:D:153:TYR:CE1	1:D:311:LYS:HB3	2.52	0.43
1:C:242:ASN:C	1:C:244:CYS:N	2.70	0.43
1:B:288:GLN:HA	1:B:288:GLN:NE2	2.32	0.43
1:B:188:LYS:HG2	1:B:281:GLU:CG	2.39	0.43
1:B:177:TRP:O	1:B:189:LEU:HD12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:THR:HG22	1:B:193:SER:N	2.32	0.43
1:B:151:GLY:HA2	1:B:154:GLU:OE1	2.18	0.43
1:A:271:LEU:HD13	1:A:282:MET:HE1	1.99	0.43
1:D:156:VAL:O	1:D:157:VAL:C	2.56	0.43
1:D:236:SER:C	1:D:238:LEU:H	2.22	0.43
1:C:210:SER:OG	1:C:218:GLN:HB2	2.18	0.43
1:C:139:SER:O	1:C:141:ASN:N	2.51	0.43
1:B:259:THR:HB	1:B:260:PRO:CD	2.48	0.43
1:D:156:VAL:HG12	1:D:157:VAL:N	2.33	0.43
1:B:65:THR:O	1:B:76:ARG:HD2	2.17	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:C:138:VAL:CG1	1:D:341:LEU:HD21	2.49	0.43
1:B:130:SER:HB2	1:B:134:ILE:CD1	2.48	0.43
1:A:264:MET:O	1:A:268:ILE:HG13	2.19	0.43
1:B:42:GLY:HA2	1:D:164:TYR:OH	2.17	0.43
1:B:37:THR:CG2	1:B:37:THR:O	2.66	0.43
1:A:41:ARG:H	1:A:44:ASP:HB2	1.84	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:D:141:ASN:C	1:D:141:ASN:OD1	2.57	0.42
1:A:171:LEU:HD21	1:D:325:VAL:CG1	2.49	0.42
1:A:150:LEU:O	1:A:154:GLU:HG3	2.19	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:A:41:ARG:HB3	1:A:43:THR:HG22	2.02	0.42
1:D:156:VAL:O	1:D:159:VAL:N	2.51	0.42
1:D:159:VAL:C	1:D:161:THR:H	2.23	0.42
1:A:112:PRO:O	1:A:113:THR:HG22	2.20	0.42
1:B:230:GLU:H	1:B:230:GLU:HG3	1.67	0.42
1:D:238:LEU:HD23	1:D:308:LEU:HD21	2.01	0.42
1:A:210:SER:HA	1:A:218:GLN:HG3	2.02	0.42
1:C:142:ILE:O	1:C:145:ILE:HG12	2.20	0.42
1:B:102:ASN:OD1	1:B:134:ILE:HG13	2.20	0.42
1:A:274:PRO:O	1:A:275:GLY:O	2.37	0.42
1:B:40:HIS:HB2	1:B:45:ILE:HD11	2.02	0.42
1:A:112:PRO:HA	1:A:120:SER:HB2	2.02	0.42
1:A:214:LEU:HD21	1:A:256:VAL:HG12	2.00	0.42
1:A:54:LYS:HD2	1:A:82:GLN:HB3	2.01	0.42
1:B:36:SER:HB2	1:B:336:THR:HA	2.02	0.41
1:C:138:VAL:HG11	1:D:341:LEU:HD21	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:GLU:O	1:B:103:GLU:HB3	2.20	0.41
1:B:37:THR:CG2	1:D:303:THR:OG1	2.68	0.41
1:D:261:LEU:HA	1:D:264:MET:HG2	2.02	0.41
1:B:163:PHE:CZ	1:B:301:MET:HE3	2.55	0.41
1:A:156:VAL:HG22	1:A:214:LEU:HB3	2.03	0.41
1:A:41:ARG:O	1:A:44:ASP:HB2	2.20	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:277:ASP:OD1	1:A:277:ASP:C	2.58	0.41
1:C:163:PHE:CE2	1:C:301:MET:HE3	2.56	0.41
1:A:111:ALA:N	1:A:112:PRO:CD	2.84	0.41
1:C:150:LEU:HD11	1:C:316:ASN:CG	2.41	0.41
1:C:292:SER:HA	1:C:295:LYS:HG2	2.02	0.41
1:B:324:LYS:C	1:B:326:LEU:H	2.24	0.41
1:C:145:ILE:HG21	1:C:319:TYR:OH	2.20	0.41
1:A:322:LEU:HA	1:A:322:LEU:HD23	1.82	0.41
1:C:139:SER:C	1:C:141:ASN:N	2.72	0.41
1:C:319:TYR:O	1:C:323:VAL:HG13	2.21	0.41
1:D:257:ASP:C	1:D:259:THR:H	2.24	0.41
1:B:231:ALA:HB1	1:B:245:LEU:CD1	2.51	0.41
1:B:58:ALA:HA	1:B:79:ALA:HB1	2.02	0.41
1:C:149:TYR:CD1	1:C:149:TYR:N	2.89	0.41
1:A:185:ASN:HB3	1:A:284:ASN:OD1	2.20	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:C:145:ILE:HA	1:C:148:SER:HB3	2.03	0.40
1:D:238:LEU:O	1:D:239:ASN:HB3	2.21	0.40
1:C:329:THR:HG22	1:C:330:ILE:N	2.35	0.40
1:D:321:ASN:O	1:D:325:VAL:HG23	2.21	0.40
1:B:54:LYS:HD3	1:B:54:LYS:HA	1.92	0.40
1:C:152:VAL:O	1:C:156:VAL:HG23	2.22	0.40
1:D:257:ASP:OD2	1:D:259:THR:HB	2.21	0.40
1:C:235:LEU:HA	1:C:235:LEU:HD23	1.91	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:A:237:GLU:O	1:A:311:LYS:NZ	2.49	0.40
1:C:258:LEU:O	1:C:262:GLN:HG3	2.21	0.40
1:B:169:ASP:OD1	1:B:169:ASP:N	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:SER:O	1:C:194:LEU:C	2.59	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	298/346 (86%)	269 (90%)	20 (7%)	9 (3%)	5	29
1	B	281/346 (81%)	232 (83%)	38 (14%)	11 (4%)	4	21
1	C	214/346 (62%)	176 (82%)	32 (15%)	6 (3%)	6	30
1	D	112/346 (32%)	65 (58%)	36 (32%)	11 (10%)	1	3
All	All	905/1384 (65%)	742 (82%)	126 (14%)	37 (4%)	3	20

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 ⓘ

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	259/297 (87%)	244 (94%)	15 (6%)	25	63
1	B	247/297 (83%)	224 (91%)	23 (9%)	11	39
1	C	187/297 (63%)	172 (92%)	15 (8%)	15	47
1	D	113/297 (38%)	102 (90%)	11 (10%)	10	37
All	All	806/1188 (68%)	742 (92%)	64 (8%)	15	48

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	63	GLN
1	A	160	TYR
1	A	178	LEU
1	A	183	ASP
1	A	197	ASP
1	A	224	LYS
1	A	258	LEU
1	A	276	LYS
1	A	277	ASP
1	A	280	LEU
1	A	313	SER
1	A	328	SER
1	A	333	SER
1	A	338	LYS
1	B	39	GLU
1	B	44	ASP
1	B	61	THR
1	B	81	GLN
1	B	98	SER
1	B	100	GLU
1	B	109	PHE
1	B	129	ILE
1	B	160	TYR
1	B	162	ASP
1	B	171	LEU
1	B	174	MET
1	B	178	LEU
1	B	183	ASP
1	B	187	VAL
1	B	224	LYS
1	B	258	LEU
1	B	292	SER
1	B	299	GLU
1	B	302	LYS
1	B	312	TYR
1	B	333	SER
1	B	334	LEU
1	C	140	GLN
1	C	142	ILE
1	C	145	ILE
1	C	160	TYR
1	C	168	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	179	LEU
1	C	197	ASP
1	C	224	LYS
1	C	278	SER
1	C	288	GLN
1	C	313	SER
1	C	320	ASP
1	C	329	THR
1	C	336	THR
1	C	342	GLN
1	D	128	THR
1	D	149	TYR
1	D	153	TYR
1	D	154	GLU
1	D	162	ASP
1	D	238	LEU
1	D	311	LYS
1	D	312	TYR
1	D	318	LEU
1	D	329	THR
1	D	336	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	C	300	ASN
1	C	306	GLN
1	D	140	GLN
1	D	155	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
2	SO4	A	1340	-	4,4,4	0.31	0	6,6,6	0.17	0
2	SO4	A	1341	-	4,4,4	0.29	0	6,6,6	0.12	0
3	GOL	A	1342	-	5,5,5	0.26	0	5,5,5	0.17	0
2	SO4	B	1338	-	4,4,4	0.35	0	6,6,6	0.11	0
3	GOL	B	1339	-	5,5,5	0.28	0	5,5,5	0.26	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
2	SO4	A	1340	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1341	-	-	0/0/0/0	0/0/0/0
3	GOL	A	1342	-	-	0/4/4/4	0/0/0/0
2	SO4	B	1338	-	-	0/0/0/0	0/0/0/0
3	GOL	B	1339	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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%)	-0.30	16 (5%)	30	12	35, 63, 128, 157	0
1	B	285/346 (82%)	-0.13	10 (3%)	48	21	43, 74, 143, 157	0
1	C	216/346 (62%)	-0.22	9 (4%)	40	16	45, 74, 134, 155	0
1	D	124/346 (35%)	0.23	9 (7%)	18	6	41, 109, 136, 157	0
All	All	927/1384 (66%)	-0.16	44 (4%)	35	14	35, 73, 140, 157	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	ALA	13.3
1	A	32	ALA	6.1
1	D	127	THR	5.8
1	B	336	THR	5.1
1	D	262	GLN	4.5
1	C	343	GLY	4.4
1	A	120	SER	4.4
1	B	35	PRO	4.1
1	D	343	GLY	4.0
1	B	277	ASP	4.0
1	C	275	GLY	3.9
1	C	277	ASP	3.9
1	A	127	THR	3.8
1	C	147	ASP	3.7
1	A	338	LYS	3.5
1	C	143	SER	3.4
1	D	263	LYS	3.3
1	D	261	LEU	3.3
1	C	276	LYS	3.3
1	C	278	SER	3.2
1	B	129	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	182	LYS	3.1
1	B	38	THR	2.9
1	A	113	THR	2.9
1	A	114	SER	2.9
1	D	211	ASN	2.8
1	A	339	SER	2.8
1	B	276	LYS	2.8
1	A	33	VAL	2.8
1	A	128	THR	2.7
1	A	337	ALA	2.6
1	D	265	VAL	2.6
1	A	34	VAL	2.5
1	B	131	ASP	2.5
1	C	288	GLN	2.4
1	A	117	PHE	2.3
1	B	43	THR	2.3
1	A	35	PRO	2.2
1	A	39	GLU	2.2
1	A	36	SER	2.2
1	D	166	ALA	2.1
1	D	210	SER	2.1
1	C	183	ASP	2.0
1	B	100	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	B	1338	5/5	0.89	0.17	-0.70	88,90,93,97	5
3	GOL	A	1342	6/6	0.89	0.19	-	86,90,93,94	0
2	SO4	A	1340	5/5	0.95	0.16	-	77,77,87,88	5
2	SO4	A	1341	5/5	0.93	0.27	-	88,91,96,96	5
3	GOL	B	1339	6/6	0.84	0.47	-	76,87,90,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.