



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:44 PM GMT

PDB ID : 1GZS
Title : CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN THE GEF DOMAIN OF THE SALMONELLA TYPHIMURIUM SOPE TOXIN AND HUMAN CDC42
Authors : Buchwald, G.; Friebe, A.; Galan, J.E.; Hardt, W.D.; Wittinghofer, A.; Scheffzek, K.
Deposited on : 2002-06-05
Resolution : 2.30 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

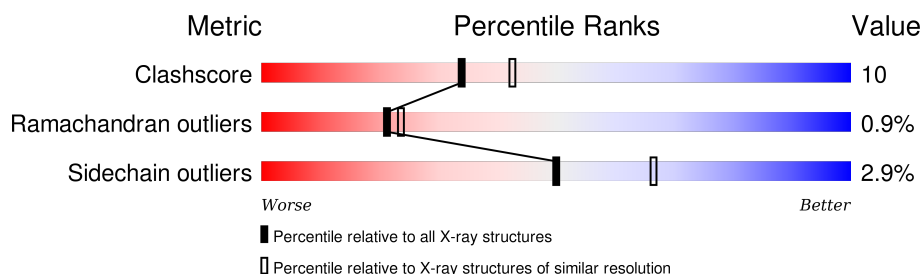
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	180	 79% 19% ..
1	C	180	 72% 24% ..
2	B	165	 82% 16% .
2	D	165	 70% 27% ...

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	SO4	C	406	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5498 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.

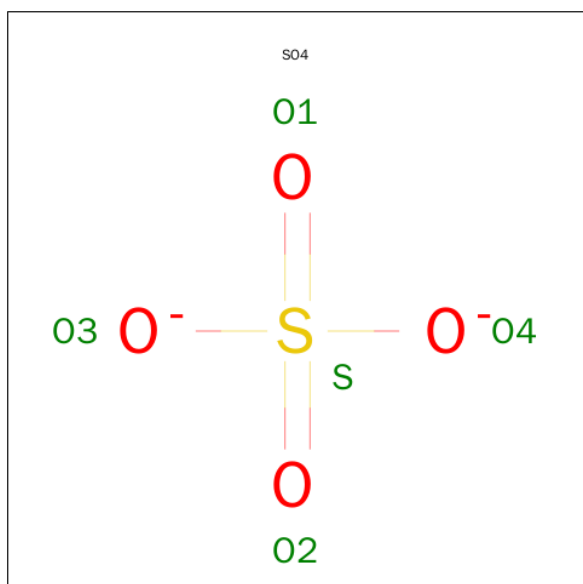
- Molecule 1 is a protein called GTP-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1389	893	221	268	7			
1	C	178	Total	C	N	O	S	0	0	0
			1389	893	221	268	7			

- Molecule 2 is a protein called SOPE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	165	Total	C	N	O	S	0	0	0
			1267	803	213	244	7			
2	D	164	Total	C	N	O	S	0	0	0
			1263	801	212	243	7			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

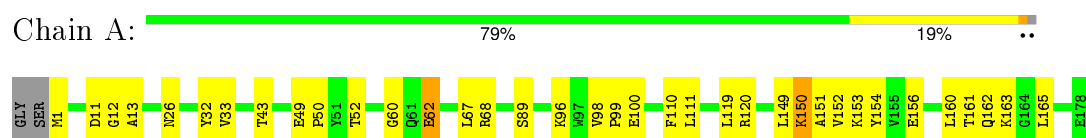
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	38	Total O 38 38	0	0
4	B	45	Total O 45 45	0	0
4	C	36	Total O 36 36	0	0
4	D	41	Total O 41 41	0	0

3 Residue-property plots

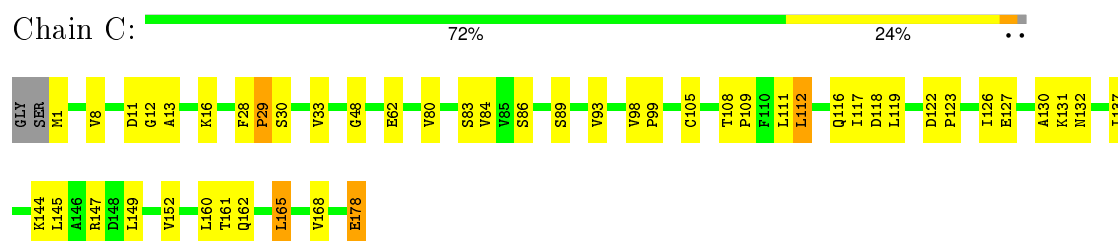
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

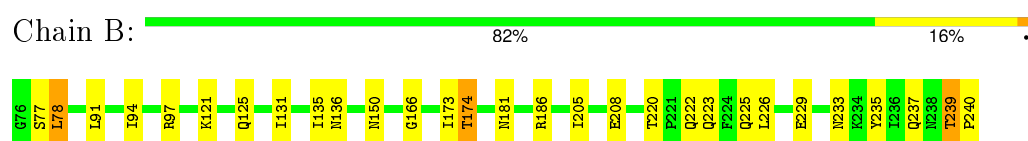
• Molecule 1: GTP-BINDING PROTEIN



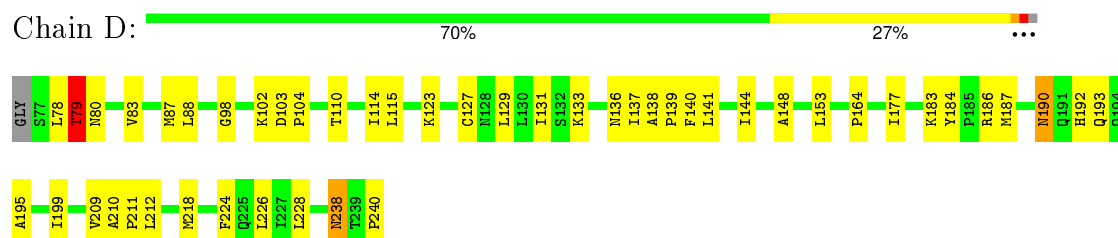
• Molecule 1: GTP-BINDING PROTEIN



• Molecule 2: SOPE



• Molecule 2: SOPE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.55Å 87.55Å 200.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.86 – 2.30	Depositor
% Data completeness (in resolution range)	99.8 (19.86-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.226 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5498	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	0/1419	0.64	0/1930
1	C	0.33	0/1419	0.61	0/1930
2	B	0.37	0/1291	0.55	0/1749
2	D	0.36	0/1287	0.53	0/1744
All	All	0.35	0/5416	0.59	0/7353

There are no bond length outliers.

There are no bond angle outliers.

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	1389	0	1405	23	0
1	C	1389	0	1405	36	0
2	B	1267	0	1276	22	0
2	D	1263	0	1273	36	0
3	A	20	0	0	0	0
3	C	10	0	0	2	0
4	A	38	0	0	1	0
4	B	45	0	0	0	0
4	C	36	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	41	0	0	0	0
All	All	5498	0	5359	108	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 10.

All (108) 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)
2:D:190:ASN:HD21	2:D:192:HIS:HB3	1.37	0.90
4:A:2008:HOH:O	2:B:174:THR:HG21	1.73	0.87
2:B:222:GLN:O	2:B:226:LEU:HD23	1.82	0.80
1:C:165:LEU:O	1:C:168:VAL:HG12	1.85	0.76
1:C:112:LEU:HD11	1:C:145:LEU:HD12	1.71	0.73
1:C:29:PRO:HB2	1:C:33:VAL:HG22	1.70	0.73
1:C:8:VAL:HG12	1:C:16:LYS:HG2	1.73	0.70
1:A:62:GLU:CD	1:A:62:GLU:H	1.98	0.65
1:A:1:MET:HE3	2:B:186:ARG:HH22	1.61	0.65
1:A:1:MET:CE	2:B:186:ARG:HH22	2.11	0.64
1:C:11:ASP:OD2	1:C:89:SER:HA	1.97	0.64
1:A:153:LYS:HG2	1:A:154:TYR:N	2.14	0.63
1:C:116:GLN:HB3	1:C:119:LEU:HD23	1.79	0.63
1:A:150:LYS:HD3	1:A:150:LYS:N	2.12	0.63
1:A:98:VAL:HG21	1:A:149:LEU:HD13	1.81	0.62
2:D:209:VAL:HG13	2:D:212:LEU:HD22	1.82	0.62
1:C:80:VAL:O	1:C:80:VAL:HG23	1.99	0.61
1:C:162:GLN:HG2	1:C:165:LEU:HD12	1.83	0.60
2:D:190:ASN:ND2	2:D:192:HIS:HB3	2.13	0.59
2:B:91:LEU:HD12	2:B:94:ILE:HD11	1.85	0.59
1:A:163:LYS:HB2	1:A:163:LYS:NZ	2.18	0.58
1:A:153:LYS:HG2	1:A:154:TYR:H	1.67	0.58
2:D:115:LEU:HD11	2:D:218:MET:HG2	1.85	0.57
2:B:173:ILE:HD13	2:B:205:ILE:HD12	1.85	0.57
2:B:239:THR:H	2:B:240:PRO:HD2	1.70	0.57
2:D:195:ALA:O	2:D:199:ILE:HG12	2.06	0.56
1:C:80:VAL:HG23	1:C:112:LEU:HD23	1.88	0.55
1:C:108:THR:HG23	3:C:406:SO4:O3	2.07	0.55
2:D:210:ALA:HB3	2:D:211:PRO:HD3	1.89	0.55
1:C:137:ILE:HD12	1:C:137:ILE:N	2.22	0.55
1:C:1:MET:HB2	4:C:2001:HOH:O	2.07	0.55
2:D:87:MET:CE	2:D:177:ILE:HD13	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLU:HG3	1:A:50:PRO:HD2	1.88	0.54
1:C:83:SER:HB3	1:C:86:SER:HB3	1.89	0.54
1:C:80:VAL:HG22	1:C:111:LEU:O	2.07	0.54
1:C:137:ILE:HD12	1:C:137:ILE:H	1.72	0.54
2:D:190:ASN:ND2	2:D:193:GLN:H	2.07	0.53
2:D:238:ASN:ND2	2:D:240:PRO:HD3	2.24	0.52
1:C:84:VAL:HG21	1:C:117:ILE:HA	1.91	0.51
2:D:136:ASN:ND2	2:D:139:PRO:HD3	2.26	0.51
2:D:78:LEU:O	2:D:79:THR:HG23	2.10	0.51
2:B:91:LEU:O	2:B:94:ILE:HG12	2.12	0.50
2:B:220:THR:OG1	2:B:223:GLN:HG3	2.11	0.50
2:D:148:ALA:HB1	2:D:164:PRO:HG3	1.93	0.50
2:B:135:ILE:HG22	2:B:136:ASN:N	2.27	0.49
1:A:163:LYS:HB2	1:A:163:LYS:HZ2	1.77	0.49
2:B:235:TYR:O	2:B:239:THR:HG23	2.12	0.49
2:B:225:GLN:O	2:B:229:GLU:HG3	2.13	0.49
2:D:87:MET:HE1	2:D:177:ILE:HD13	1.95	0.49
1:C:62:GLU:H	1:C:62:GLU:CD	2.16	0.49
1:C:93:VAL:HG11	1:C:112:LEU:HD21	1.95	0.48
2:B:150:ASN:O	1:C:48:GLY:HA3	2.13	0.47
1:A:110:PHE:CE1	1:A:151:ALA:HB2	2.49	0.47
1:A:96:LYS:C	1:A:99:PRO:HD2	2.35	0.47
1:C:98:VAL:HB	1:C:99:PRO:HD3	1.97	0.47
2:D:209:VAL:O	2:D:209:VAL:HG12	2.13	0.47
2:D:78:LEU:C	2:D:80:ASN:H	2.18	0.47
2:D:140:PHE:CZ	2:D:144:ILE:HD13	2.50	0.47
1:C:12:GLY:O	1:C:13:ALA:HB3	2.15	0.47
1:A:111:LEU:HD23	1:A:152:VAL:HB	1.97	0.46
1:A:120:ARG:NH2	1:A:156:GLU:OE2	2.46	0.46
1:C:98:VAL:HG21	1:C:149:LEU:HD13	1.98	0.46
1:A:11:ASP:OD2	1:A:89:SER:HA	2.15	0.46
2:D:78:LEU:O	2:D:80:ASN:N	2.48	0.46
2:D:83:VAL:HG21	2:D:187:MET:HG2	1.98	0.46
2:D:127:CYS:O	2:D:131:ILE:HG12	2.16	0.46
1:C:127:GLU:O	1:C:131:LYS:HG3	2.16	0.45
2:B:239:THR:N	2:B:240:PRO:HD2	2.31	0.45
1:C:130:ALA:C	1:C:132:ASN:H	2.19	0.45
1:C:105:CYS:HA	3:C:406:SO4:O2	2.18	0.44
1:C:1:MET:CE	2:D:186:ARG:HD2	2.47	0.44
1:A:32:TYR:HB2	2:B:131:ILE:CD1	2.48	0.44
1:C:118:ASP:OD2	1:C:160:LEU:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:VAL:O	1:A:33:VAL:HG13	2.18	0.44
1:C:122:ASP:O	1:C:126:ILE:HG13	2.18	0.44
2:D:138:ALA:HB3	2:D:139:PRO:HD3	1.99	0.43
1:A:60:GLY:O	2:B:166:GLY:HA2	2.18	0.43
1:C:161:THR:O	1:C:162:GLN:HB2	2.19	0.43
2:B:226:LEU:HD12	1:C:178:GLU:HA	2.00	0.43
2:D:103:ASP:HA	2:D:104:PRO:HD2	1.89	0.43
2:B:97:ARG:HG3	2:B:208:GLU:OE1	2.19	0.43
1:A:68:ARG:HD2	1:A:100:GLU:OE2	2.18	0.43
2:B:121:LYS:O	2:B:125:GLN:HG3	2.18	0.43
2:D:129:LEU:O	2:D:133:LYS:HG3	2.18	0.43
1:C:109:PRO:HB2	1:C:152:VAL:HG21	2.01	0.43
1:A:160:LEU:C	1:A:160:LEU:HD23	2.39	0.42
2:D:88:LEU:HD12	2:D:88:LEU:HA	1.90	0.42
2:B:226:LEU:CD1	1:C:178:GLU:HA	2.49	0.42
1:A:12:GLY:O	1:A:13:ALA:HB3	2.20	0.42
2:D:224:PHE:O	2:D:228:LEU:HG	2.19	0.42
2:D:87:MET:HE3	2:D:177:ILE:HD13	2.02	0.42
2:D:137:ILE:HD12	2:D:141:LEU:HD11	2.02	0.42
2:D:127:CYS:SG	2:D:141:LEU:HD21	2.60	0.42
1:C:80:VAL:HG23	1:C:112:LEU:HA	2.02	0.42
2:D:110:THR:O	2:D:114:ILE:HG12	2.19	0.42
2:D:78:LEU:C	2:D:79:THR:CG2	2.87	0.42
2:D:183:LYS:HB3	2:D:184:TYR:CD1	2.55	0.42
1:C:144:LYS:O	1:C:147:ARG:HB2	2.20	0.41
1:C:122:ASP:HA	1:C:123:PRO:HD3	1.94	0.41
2:B:233:ASN:O	2:B:237:GLN:HG2	2.21	0.41
2:D:212:LEU:HD12	2:D:212:LEU:N	2.36	0.41
2:D:123:LYS:HE3	2:D:141:LEU:HD22	2.03	0.40
2:D:98:GLY:O	2:D:102:LYS:HG3	2.21	0.40
1:C:145:LEU:CD1	1:C:149:LEU:HD12	2.52	0.40
2:D:115:LEU:HB2	2:D:153:LEU:HD21	2.03	0.40
1:A:161:THR:O	1:A:162:GLN:HB2	2.21	0.40
2:D:78:LEU:O	2:D:79:THR:CG2	2.70	0.40
1:A:52:THR:CG2	2:B:181:ASN:HD21	2.35	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	176/180 (98%)	169 (96%)	7 (4%)	0	100	100
1	C	176/180 (98%)	165 (94%)	9 (5%)	2 (1%)	17	18
2	B	163/165 (99%)	157 (96%)	3 (2%)	3 (2%)	11	9
2	D	162/165 (98%)	159 (98%)	2 (1%)	1 (1%)	30	36
All	All	677/690 (98%)	650 (96%)	21 (3%)	6 (1%)	21	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	30	SER
2	B	77	SER
2	D	79	THR
2	B	78	LEU
2	B	239	THR
1	C	29	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	158/159 (99%)	151 (96%)	7 (4%)	35	46
1	C	158/159 (99%)	154 (98%)	4 (2%)	55	73
2	B	140/140 (100%)	138 (99%)	2 (1%)	74	86
2	D	140/140 (100%)	136 (97%)	4 (3%)	50	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	596/598 (100%)	579 (97%)	17 (3%)	50 66

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	43	THR
1	A	62	GLU
1	A	67	LEU
1	A	119	LEU
1	A	150	LYS
1	A	165	LEU
2	B	78	LEU
2	B	174	THR
1	C	28	PHE
1	C	112	LEU
1	C	165	LEU
1	C	178	GLU
2	D	79	THR
2	D	190	ASN
2	D	226	LEU
2	D	238	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	162	GLN
2	B	128	ASN
2	B	159	ASN
2	B	230	ASN
2	B	233	ASN
2	B	237	GLN
2	D	136	ASN
2	D	150	ASN
2	D	159	ASN
2	D	190	ASN
2	D	193	GLN
2	D	237	GLN
2	D	238	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 ⓘ

6 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	SO4	A	401	-	4,4,4	0.32	0	6,6,6	0.08	0
3	SO4	A	402	-	4,4,4	0.22	0	6,6,6	0.08	0
3	SO4	A	403	-	4,4,4	0.27	0	6,6,6	0.13	0
3	SO4	A	405	-	4,4,4	0.28	0	6,6,6	0.10	0
3	SO4	C	404	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	C	406	-	4,4,4	0.21	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	SO4	A	401	-	-	0/0/0/0	0/0/0/0
3	SO4	A	402	-	-	0/0/0/0	0/0/0/0
3	SO4	A	403	-	-	0/0/0/0	0/0/0/0
3	SO4	A	405	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	C	404	-	-	0/0/0/0	0/0/0/0
3	SO4	C	406	-	-	0/0/0/0	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	406	SO4	2	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.