



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:03 PM GMT

PDB ID : 1RV8  
Title : Class II fructose-1,6-bisphosphate aldolase from *Thermus aquaticus* in complex with cobalt  
Authors : Izard, T.; Sygusch, J.  
Deposited on : 2003-12-12  
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](mailto: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

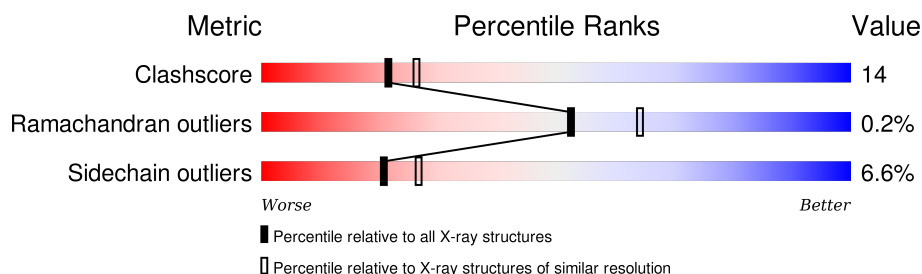
# 1 Overall quality at a glance

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  $\geq 3$ , 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	305	 72% 22% . .
1	B	305	 76% 20% .
1	C	305	 70% 28% .
1	D	305	 70% 25% .

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10343 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 fructose-1,6-bisphosphate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	10	0
			2338	1468	427	436	7			
1	B	305	Total	C	N	O	S	0	0	0
			2329	1464	421	437	7			
1	C	305	Total	C	N	O	S	0	2	0
			2346	1476	423	440	7			
1	D	305	Total	C	N	O	S	0	0	0
			2329	1464	421	437	7			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Co 1 1	0	0
3	A	2	Total Co 2 2	0	0
3	D	1	Total Co 1 1	0	0
3	C	1	Total Co 1 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

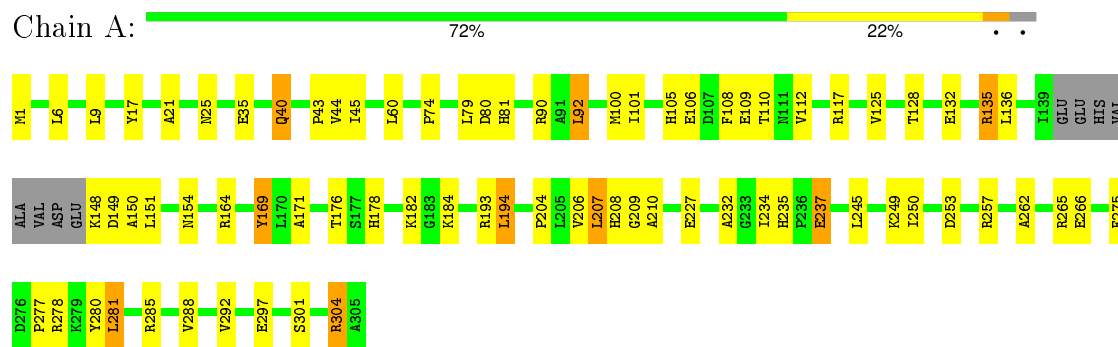
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	248	Total	O	0	0
			248	248		
5	B	234	Total	O	0	0
			234	234		
5	C	195	Total	O	0	0
			195	195		
5	D	255	Total	O	0	0
			255	255		

### 3 Residue-property plots

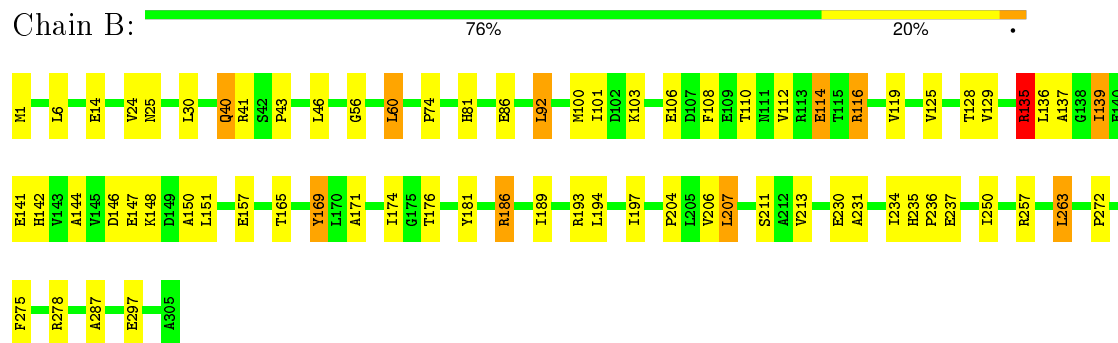
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

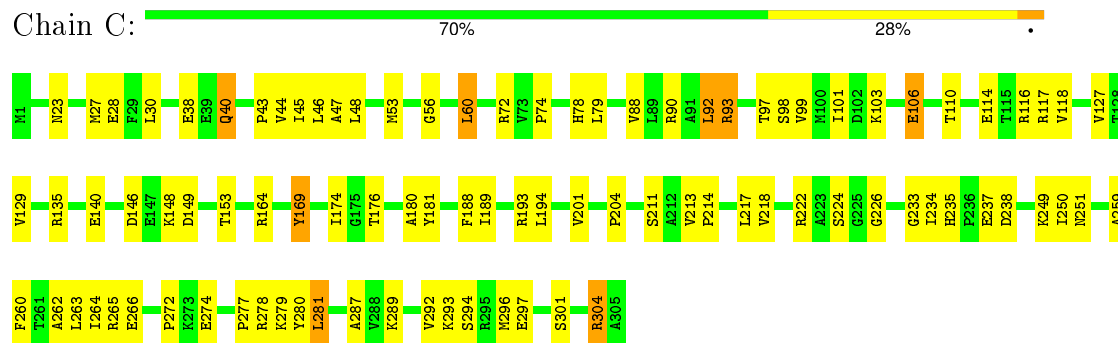
- Molecule 1: fructose-1,6-bisphosphate aldolase



- Molecule 1: fructose-1,6-bisphosphate aldolase

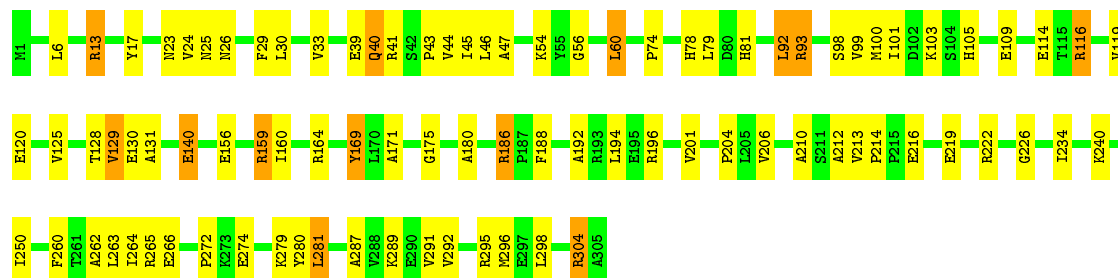


- Molecule 1: fructose-1,6-bisphosphate aldolase



● Molecule 1: fructose-1,6-bisphosphate aldolase

Chain D:  70% 25% .



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.35 Å   57.63 Å   138.58 Å 90.00°   90.23°   90.00°	Depositor
Resolution (Å)	40.43 – 2.30	Depositor
% Data completeness (in resolution range)	97.4 (40.43-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.211 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10343	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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: NA, CO, 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	0.36	0/2375	0.64	0/3200
1	B	0.33	0/2365	0.58	0/3190
1	C	0.32	0/2383	0.56	0/3215
1	D	0.35	0/2365	0.62	0/3190
All	All	0.34	0/9488	0.60	0/12795

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	2338	0	2371	77	0
1	B	2329	0	2372	62	0
1	C	2346	0	2385	71	0
1	D	2329	0	2372	74	0
2	A	15	0	0	1	0
2	B	15	0	0	0	0
2	C	10	0	0	1	0
2	D	20	0	0	0	0
3	A	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	248	0	0	7	0
5	B	234	0	0	3	0
5	C	195	0	0	5	0
5	D	255	0	0	8	0
All	All	10343	0	9500	267	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 (267) 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:D:186:ARG:H	1:D:186:ARG:HD3	1.09	1.10
1:A:148:LYS:HD3	1:A:154:ASN:HD22	1.19	1.07
1:A:207[B]:LEU:HD22	1:A:210:ALA:HB2	1.38	1.04
1:A:148:LYS:HG3	1:A:193:ARG:HH12	1.25	1.02
1:C:189:ILE:HD12	1:C:238:ASP:HB3	1.52	0.92
1:B:40:GLN:HE21	1:B:40:GLN:HA	1.34	0.90
1:A:176:THR:HG21	1:A:207[B]:LEU:HD21	1.54	0.88
1:A:40:GLN:HE21	1:A:40:GLN:HA	1.39	0.87
1:C:103:LYS:HG3	1:C:114:GLU:HG2	1.56	0.87
1:B:186:ARG:HD3	1:B:186:ARG:H	1.38	0.87
1:D:159:ARG:HB3	1:D:159:ARG:HH11	1.39	0.86
1:D:186:ARG:H	1:D:186:ARG:CD	1.84	0.86
1:D:186:ARG:HD3	1:D:186:ARG:N	1.89	0.86
1:B:169:TYR:HB3	1:B:204:PRO:HG2	1.58	0.85
1:C:40:GLN:HE21	1:C:40:GLN:HA	1.42	0.85
1:D:263:LEU:HD22	1:D:287:ALA:HB2	1.59	0.84
1:D:103:LYS:HG3	1:D:114:GLU:HG2	1.59	0.84
1:A:148:LYS:HG3	1:A:193:ARG:NH1	1.97	0.80
1:D:40:GLN:HE21	1:D:40:GLN:HA	1.46	0.79
1:A:148:LYS:HD3	1:A:154:ASN:ND2	1.98	0.79
1:C:27:MET:HE1	1:D:60:LEU:HG	1.67	0.76
1:C:106:GLU:HG2	1:C:110:THR:HG21	1.68	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ALA:HA	1:D:234:ILE:HD13	1.70	0.73
1:A:148:LYS:HG2	1:A:149:ASP:N	2.03	0.72
1:A:253:ASP:OD1	1:A:257:ARG:HD2	1.89	0.72
1:A:43:PRO:HB3	1:A:74:PRO:HG2	1.69	0.72
1:B:135:ARG:HG3	1:B:135:ARG:HH11	1.54	0.72
1:A:265:ARG:NH2	1:B:272:PRO:HA	2.05	0.71
1:B:30:LEU:HD11	1:B:46:LEU:HD13	1.71	0.71
1:D:30:LEU:HD11	1:D:46:LEU:HD13	1.71	0.71
1:D:212:ALA:HB3	1:D:295:ARG:NH1	2.08	0.68
1:B:176:THR:HG21	1:B:207:LEU:HD21	1.75	0.67
1:A:182:LYS:HE3	1:A:209[B]:GLY:O	1.95	0.67
1:B:108:PHE:O	1:B:112:VAL:HG23	1.95	0.66
1:D:43:PRO:HB3	1:D:74:PRO:HG2	1.77	0.66
1:A:227:GLU:HG3	1:B:272:PRO:HB2	1.77	0.66
1:C:189:ILE:HD11	1:C:234:ILE:HG21	1.78	0.65
1:D:24:VAL:HG21	1:D:30:LEU:HD13	1.78	0.65
1:C:43:PRO:HB3	1:C:74:PRO:HG2	1.78	0.65
1:A:105:HIS:HA	1:A:135:ARG:NH1	2.11	0.65
1:B:136:LEU:HD11	1:B:142:HIS:HD2	1.62	0.64
1:C:30:LEU:HD11	1:C:46:LEU:HD13	1.78	0.64
1:B:40:GLN:NE2	1:B:40:GLN:HA	2.09	0.64
1:D:93:ARG:HD3	5:D:1852:HOH:O	1.97	0.64
1:A:17:TYR:CZ	1:A:304:ARG:HG2	2.33	0.63
1:D:140:GLU:HG2	1:D:140:GLU:O	1.97	0.62
1:C:146:ASP:OD2	1:C:148:LYS:HG2	1.99	0.61
1:A:182:LYS:HE3	1:A:209[A]:GLY:O	2.00	0.61
1:D:101:ILE:HG22	5:D:1823:HOH:O	1.99	0.61
1:D:212:ALA:O	1:D:214:PRO:HD3	2.00	0.61
1:A:194:LEU:HD13	1:A:245:LEU:HB2	1.81	0.61
1:B:263:LEU:HD13	1:B:287:ALA:HB2	1.83	0.60
1:A:235:HIS:CD2	1:A:237:GLU:H	2.20	0.60
1:A:250:ILE:N	1:A:250:ILE:HD12	2.17	0.60
1:A:148:LYS:HG2	1:A:149:ASP:H	1.66	0.60
1:C:249:LYS:NZ	1:C:251:ASN:HD21	1.99	0.60
1:B:43:PRO:HB3	1:B:74:PRO:HG2	1.83	0.59
1:A:182:LYS:HB2	1:A:232:ALA:O	2.02	0.59
1:C:181[B]:TYR:HH	1:C:188:PHE:HE2	1.50	0.59
1:C:289:LYS:O	1:C:293:LYS:HG3	2.03	0.58
1:D:222:ARG:HA	1:D:226:GLY:O	2.03	0.58
1:A:171:ALA:HA	1:A:206:VAL:HB	1.85	0.58
1:C:222:ARG:HA	1:C:226:GLY:O	2.04	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:LEU:CD2	1:D:287:ALA:HB2	2.32	0.58
1:C:93:ARG:HD3	5:C:1812:HOH:O	2.04	0.58
1:B:263:LEU:HD13	1:B:287:ALA:CB	2.34	0.57
1:C:249:LYS:HZ2	1:C:251:ASN:HD21	1.50	0.57
1:D:116:ARG:HD3	1:D:116:ARG:O	2.04	0.57
1:C:272:PRO:O	1:D:226:GLY:HA2	2.04	0.57
1:B:103:LYS:HG3	1:B:114:GLU:HG2	1.87	0.57
1:A:285:ARG:HD2	5:A:1874:HOH:O	2.03	0.57
1:C:277:PRO:O	1:C:281:LEU:HB2	2.03	0.57
1:D:180:ALA:HB3	5:D:1794:HOH:O	2.05	0.57
1:B:92:LEU:HG	1:B:125:VAL:HG21	1.85	0.57
1:A:234:ILE:N	1:A:234:ILE:HD12	2.19	0.57
1:D:105:HIS:H	1:D:105:HIS:CD2	2.23	0.57
1:A:265:ARG:HH21	1:B:272:PRO:HA	1.69	0.57
1:A:301:SER:O	1:A:304:ARG:HB2	2.05	0.56
1:B:135:ARG:NH1	1:B:135:ARG:HG3	2.18	0.56
1:A:277:PRO:O	1:A:281:LEU:HB2	2.05	0.56
1:A:148:LYS:CD	1:A:154:ASN:HB2	2.36	0.56
1:C:117:ARG:HD3	5:C:1782:HOH:O	2.06	0.56
1:B:213:VAL:HG11	1:B:231:ALA:HB1	1.87	0.56
1:B:135:ARG:HD3	1:B:150:ALA:O	2.06	0.56
1:C:235:HIS:CE1	1:C:237:GLU:H	2.24	0.55
1:C:103:LYS:CG	1:C:114:GLU:HG2	2.34	0.55
1:C:90:ARG:HD2	5:C:1784:HOH:O	2.06	0.55
1:A:40:GLN:HE21	1:A:40:GLN:CA	2.16	0.55
1:D:156:GLU:OE1	1:D:159:ARG:NH1	2.39	0.55
1:A:182:LYS:HG2	1:A:234:ILE:HD12	1.88	0.55
1:D:13:ARG:HD3	5:D:1798:HOH:O	2.07	0.55
1:B:116:ARG:HD2	1:B:165:THR:HA	1.89	0.55
1:D:40:GLN:HA	1:D:40:GLN:NE2	2.21	0.55
1:A:21:ALA:HA	1:A:45:ILE:HB	1.89	0.55
1:A:178[A]:HIS:HE1	1:A:208[A]:HIS:HB3	1.72	0.55
1:A:101:ILE:HG23	1:A:101:ILE:O	2.08	0.54
1:C:174:ILE:HD12	1:C:189:ILE:HG23	1.90	0.54
1:C:56:GLY:HA3	1:C:60:LEU:HD12	1.90	0.54
1:C:38:GLU:OE1	1:C:72:ARG:HB2	2.08	0.54
1:C:164:ARG:HD2	5:C:1830:HOH:O	2.07	0.53
1:D:262:ALA:O	1:D:266:GLU:HG3	2.08	0.53
1:D:116:ARG:HG3	5:D:1936:HOH:O	2.08	0.53
1:A:149:ASP:H	1:A:193:ARG:HH22	1.55	0.53
1:C:222:ARG:HH11	1:C:222:ARG:HG3	1.73	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:O	1:A:292:VAL:HG23	2.08	0.53
1:B:174:ILE:HD12	1:B:189:ILE:HG23	1.89	0.53
1:A:184:LYS:O	1:A:184:LYS:HG3	2.09	0.52
1:C:272:PRO:HA	1:D:265:ARG:NH2	2.24	0.52
1:B:235:HIS:CE1	1:B:237:GLU:HG2	2.44	0.52
1:D:212:ALA:HB3	1:D:295:ARG:HH12	1.73	0.52
1:D:169:TYR:HB3	1:D:204:PRO:HG2	1.91	0.51
1:C:294:SER:O	1:C:297:GLU:HB3	2.09	0.51
1:B:40:GLN:HE21	1:B:40:GLN:CA	2.15	0.51
1:C:103:LYS:HE3	1:C:114:GLU:HG2	1.92	0.51
1:D:159:ARG:NH1	1:D:159:ARG:HB3	2.18	0.51
1:A:235:HIS:CD2	1:A:237:GLU:HB2	2.45	0.51
1:B:171:ALA:HA	1:B:206:VAL:HB	1.91	0.51
1:B:147:GLU:O	1:B:151:LEU:HD13	2.11	0.51
1:C:260:PHE:CE2	1:C:264:ILE:HD11	2.46	0.50
1:D:92:LEU:HG	1:D:125:VAL:HG21	1.93	0.50
1:D:109:GLU:CD	1:D:164:ARG:HH22	2.13	0.50
1:D:171:ALA:HA	1:D:206:VAL:HB	1.91	0.50
1:C:40:GLN:HE21	1:C:40:GLN:CA	2.18	0.50
1:A:109:GLU:OE2	1:A:164:ARG:NH2	2.44	0.50
1:D:250:ILE:HD12	1:D:250:ILE:N	2.27	0.50
1:A:275:PHE:O	1:B:257:ARG:HB3	2.11	0.50
1:D:81:HIS:HA	1:D:100:MET:SD	2.52	0.50
1:B:186:ARG:HD3	1:B:186:ARG:N	2.19	0.49
1:C:201:VAL:HG13	5:C:1827:HOH:O	2.12	0.49
1:B:101:ILE:HG23	1:B:101:ILE:O	2.13	0.49
1:C:40:GLN:NE2	1:C:40:GLN:HA	2.21	0.48
1:A:148:LYS:HD2	1:A:154:ASN:HB2	1.96	0.48
1:D:212:ALA:O	1:D:214:PRO:CD	2.62	0.48
1:A:108:PHE:O	1:A:112:VAL:HG23	2.13	0.48
1:A:151:LEU:HD22	5:A:1925:HOH:O	2.12	0.48
1:D:159:ARG:HH12	1:D:160:ILE:HG13	1.79	0.48
1:A:44:VAL:HG22	1:A:45:ILE:N	2.29	0.48
1:B:106:GLU:HG2	1:B:110:THR:HG21	1.95	0.48
1:A:280:TYR:CD1	1:A:281:LEU:HD13	2.49	0.48
1:D:41:ARG:HD2	5:D:1843:HOH:O	2.12	0.48
1:B:106:GLU:HG3	5:B:1870:HOH:O	2.14	0.47
1:C:214:PRO:O	1:C:218:VAL:HG23	2.14	0.47
1:C:277:PRO:HA	1:C:280:TYR:CZ	2.49	0.47
1:B:81:HIS:HA	1:B:100:MET:SD	2.54	0.47
1:A:92:LEU:HG	1:A:125:VAL:HG21	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ASN:HA	1:C:47:ALA:O	2.14	0.47
1:B:6:LEU:CB	1:B:128:THR:HG21	2.44	0.47
1:C:265:ARG:NH2	1:D:272:PRO:HA	2.30	0.47
1:C:213:VAL:HG23	1:C:213:VAL:O	2.15	0.47
1:C:272:PRO:HA	1:D:265:ARG:HH21	1.79	0.47
1:A:235:HIS:HD2	1:A:237:GLU:HB2	1.78	0.47
1:B:6:LEU:HB3	1:B:128:THR:HG21	1.95	0.47
1:C:44:VAL:HG22	1:C:45:ILE:N	2.29	0.47
1:A:17:TYR:CE1	1:A:304:ARG:HG2	2.49	0.47
1:B:234:ILE:HD12	1:B:234:ILE:N	2.29	0.47
1:C:116:ARG:NH1	2:C:1609:SO4:O2	2.45	0.47
1:C:292:VAL:O	1:C:296:MET:HG3	2.15	0.47
1:C:78:HIS:HA	1:C:98:SER:O	2.14	0.47
1:A:184:LYS:HG2	5:A:1950:HOH:O	2.15	0.47
1:D:23:ASN:HA	1:D:47:ALA:O	2.15	0.47
1:B:136:LEU:HD23	1:B:157:GLU:OE1	2.15	0.46
1:A:204:PRO:HD3	5:A:1732:HOH:O	2.15	0.46
1:C:263:LEU:HD22	1:C:287:ALA:HB2	1.96	0.46
1:A:25:ASN:OD1	1:B:278:ARG:HD3	2.15	0.46
1:C:153:THR:O	1:C:193:ARG:HD3	2.15	0.46
1:C:251:ASN:HD22	1:C:251:ASN:N	2.12	0.46
1:B:148:LYS:NZ	1:B:186:ARG:HH12	2.14	0.46
1:A:9:LEU:HD11	1:A:249:LYS:HD2	1.96	0.46
1:B:230:GLU:OE2	1:C:135:ARG:NH2	2.46	0.46
1:C:97:THR:C	1:C:127:VAL:HG13	2.36	0.46
1:A:176:THR:HG21	1:A:207[A]:LEU:HD22	1.97	0.46
1:B:151:LEU:HD23	1:B:181:TYR:HA	1.97	0.46
1:B:41:ARG:HD2	5:B:1817:HOH:O	2.16	0.46
1:D:240:LYS:HE2	1:D:298:LEU:HD12	1.98	0.46
1:B:147:GLU:N	1:B:147:GLU:OE2	2.49	0.46
1:B:86:GLU:CD	1:B:86:GLU:H	2.17	0.46
1:C:93:ARG:O	1:C:93:ARG:HG3	2.15	0.45
1:C:47:ALA:C	1:C:48:LEU:HD12	2.37	0.45
1:A:262:ALA:O	1:A:266:GLU:HG3	2.15	0.45
1:D:131:ALA:HA	5:D:1776:HOH:O	2.16	0.45
1:C:262:ALA:O	1:C:266:GLU:HG3	2.16	0.45
1:A:132[A]:GLU:OE1	1:A:136:LEU:HG	2.17	0.45
1:D:234:ILE:N	1:D:234:ILE:HD12	2.31	0.45
1:A:182:LYS:NZ	2:A:1604:SO4:O2	2.39	0.45
1:B:106:GLU:HG2	1:B:110:THR:CG2	2.46	0.45
1:B:135:ARG:HA	1:B:151:LEU:O	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ALA:CA	1:B:206:VAL:HB	2.47	0.45
1:C:169:TYR:HB3	1:C:204:PRO:HG2	1.99	0.45
1:C:27:MET:HE1	1:D:60:LEU:CG	2.43	0.45
1:C:274:GLU:OE2	1:C:279:LYS:HG3	2.16	0.45
1:D:119:VAL:HA	1:D:129:VAL:HG11	1.99	0.45
1:C:217:LEU:HD11	1:C:259:ALA:HA	1.98	0.45
1:A:80[A]:ASP:O	1:A:81[A]:HIS:HB2	2.17	0.45
1:C:280:TYR:CD1	1:C:281:LEU:HD13	2.52	0.44
1:D:292:VAL:O	1:D:296:MET:HG3	2.17	0.44
1:B:139:ILE:C	1:B:141:GLU:H	2.21	0.44
1:A:135:ARG:HE	1:A:151:LEU:HD13	1.83	0.44
1:A:106:GLU:HG2	1:A:110:THR:CG2	2.48	0.44
1:C:222:ARG:NH1	1:C:222:ARG:HG3	2.33	0.44
1:C:301:SER:O	1:C:304:ARG:HB2	2.17	0.44
1:D:6:LEU:CB	1:D:128:THR:HG21	2.47	0.44
1:A:182:LYS:HG2	1:A:234:ILE:CD1	2.48	0.44
1:D:6:LEU:HB3	1:D:128:THR:HG21	2.00	0.44
1:A:90:ARG:NH1	5:A:1833:HOH:O	2.50	0.44
1:D:263:LEU:HD22	1:D:287:ALA:CB	2.40	0.44
1:C:27:MET:CE	1:D:26:ASN:HA	2.48	0.43
1:A:277:PRO:HA	1:A:280:TYR:CZ	2.53	0.43
1:D:13:ARG:NH2	1:D:201:VAL:O	2.51	0.43
1:C:224:SER:HB2	1:C:265:ARG:HB3	2.01	0.43
1:D:29:PHE:O	1:D:33:VAL:HG23	2.19	0.43
1:D:39:GLU:OE2	1:D:289:LYS:NZ	2.42	0.43
1:D:44:VAL:HG22	1:D:45:ILE:N	2.34	0.43
1:B:137:ALA:HB3	1:B:139:ILE:HG12	2.01	0.43
1:B:56:GLY:HA3	1:B:60:LEU:HB2	2.00	0.43
1:A:106:GLU:HG3	5:A:1850:HOH:O	2.19	0.43
1:B:193:ARG:O	1:B:197:ILE:HG13	2.19	0.43
1:B:119:VAL:HA	1:B:129:VAL:HG11	2.01	0.43
1:D:78:HIS:HA	1:D:98:SER:O	2.19	0.43
1:A:40:GLN:NE2	1:A:40:GLN:HA	2.19	0.43
1:D:17:TYR:CE2	1:D:304:ARG:HG3	2.54	0.43
1:A:149:ASP:OD2	1:A:149:ASP:C	2.58	0.42
1:B:146:ASP:OD1	1:B:147:GLU:N	2.52	0.42
1:D:280:TYR:CD1	1:D:281:LEU:HD13	2.54	0.42
1:A:150:ALA:O	1:A:151:LEU:HD23	2.19	0.42
1:B:235:HIS:ND1	1:B:236:PRO:HD2	2.34	0.42
1:D:92:LEU:HD13	1:D:99:VAL:HG11	2.01	0.42
1:D:260:PHE:O	1:D:264:ILE:HG13	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:TYR:HB3	1:A:204:PRO:HG2	2.00	0.42
1:C:250:ILE:N	1:C:250:ILE:HD12	2.34	0.42
1:A:278:ARG:HD3	1:B:25:ASN:OD1	2.20	0.42
1:A:235:HIS:HD2	1:A:237:GLU:H	1.64	0.42
1:B:230:GLU:CD	1:C:180[B]:ALA:HB1	2.39	0.42
1:D:17:TYR:CE2	1:D:304:ARG:CG	3.02	0.42
1:A:257:ARG:HB3	1:B:275:PHE:O	2.20	0.42
1:B:250:ILE:HD12	1:B:250:ILE:N	2.35	0.41
1:D:192:ALA:O	1:D:196:ARG:HG3	2.19	0.41
1:D:56:GLY:HA3	1:D:60:LEU:HB2	2.01	0.41
1:D:100:MET:HB2	1:D:130:GLU:HB3	2.01	0.41
1:C:56:GLY:HA3	1:C:60:LEU:HB2	2.03	0.41
1:A:106:GLU:CG	1:A:110:THR:HG21	2.50	0.41
1:C:213:VAL:HG22	1:C:233:GLY:HA3	2.02	0.41
1:C:92:LEU:HD13	1:C:99:VAL:HG11	2.02	0.41
1:A:6:LEU:HB3	1:A:128:THR:HG21	2.03	0.41
1:D:116:ARG:NE	1:D:120:GLU:OE1	2.53	0.41
1:D:274:GLU:OE2	1:D:279:LYS:HG3	2.21	0.41
1:A:148:LYS:NZ	1:A:150:ALA:O	2.54	0.41
1:B:144:ALA:CB	1:B:150:ALA:HB2	2.51	0.41
1:C:103:LYS:HG3	1:C:114:GLU:CG	2.37	0.41
1:A:171:ALA:HB1	1:A:208[B]:HIS:CD2	2.56	0.41
1:D:204:PRO:HD3	5:D:1724:HOH:O	2.20	0.41
1:C:149:ASP:HA	1:C:193:ARG:NH2	2.36	0.41
1:C:278:ARG:HD3	1:D:25:ASN:OD1	2.21	0.41
1:D:287:ALA:O	1:D:291:VAL:HG23	2.21	0.41
1:C:101:ILE:HB	1:C:118:VAL:HG21	2.02	0.41
1:B:24:VAL:HG21	1:B:30:LEU:HD13	2.03	0.40
1:A:109:GLU:CD	1:A:164:ARG:HH22	2.24	0.40
1:A:106:GLU:HG2	1:A:110:THR:HG21	2.02	0.40
1:D:291:VAL:O	1:D:295:ARG:HG2	2.21	0.40
1:A:194:LEU:HD13	1:A:245:LEU:CB	2.51	0.40
1:C:88:VAL:HG11	1:C:118:VAL:HG13	2.03	0.40
1:B:1:MET:HB2	5:B:1709:HOH:O	2.21	0.40
1:B:186:ARG:CD	1:B:186:ARG:H	2.11	0.40
1:C:235:HIS:ND1	1:C:237:GLU:N	2.64	0.40
1:B:14:GLU:HA	1:B:14:GLU:OE2	2.21	0.40
1:D:175:GLY:HA3	1:D:188:PHE:O	2.21	0.40
1:A:35:GLU:HG3	5:A:1842:HOH:O	2.20	0.40
1:D:281:LEU:HD12	1:D:281:LEU:HA	1.95	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	303/305 (99%)	295 (97%)	8 (3%)	0	100	100
1	B	303/305 (99%)	290 (96%)	11 (4%)	2 (1%)	26	31
1	C	305/305 (100%)	291 (95%)	14 (5%)	0	100	100
1	D	303/305 (99%)	293 (97%)	9 (3%)	1 (0%)	46	57
All	All	1214/1220 (100%)	1169 (96%)	42 (4%)	3 (0%)	52	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	139	ILE
1	B	135	ARG
1	D	213	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	237/237 (100%)	221 (93%)	16 (7%)	20	25
1	B	237/237 (100%)	224 (94%)	13 (6%)	27	36
1	C	238/237 (100%)	222 (93%)	16 (7%)	20	26
1	D	237/237 (100%)	219 (92%)	18 (8%)	16	20
All	All	949/948 (100%)	886 (93%)	63 (7%)	21	27

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	40	GLN
1	A	60	LEU
1	A	79	LEU
1	A	92	LEU
1	A	100	MET
1	A	117	ARG
1	A	135	ARG
1	A	169	TYR
1	A	194	LEU
1	A	207[A]	LEU
1	A	207[B]	LEU
1	A	237	GLU
1	A	281	LEU
1	A	297	GLU
1	A	304	ARG
1	B	40	GLN
1	B	60	LEU
1	B	92	LEU
1	B	114	GLU
1	B	116	ARG
1	B	135	ARG
1	B	169	TYR
1	B	186	ARG
1	B	194	LEU
1	B	207	LEU
1	B	211	SER
1	B	263	LEU
1	B	297	GLU
1	C	28	GLU
1	C	40	GLN
1	C	53	MET
1	C	60	LEU
1	C	79	LEU
1	C	92	LEU
1	C	93	ARG
1	C	106	GLU
1	C	129	VAL
1	C	140	GLU
1	C	169	TYR
1	C	176	THR
1	C	194	LEU
1	C	211	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	281	LEU
1	C	304	ARG
1	D	13	ARG
1	D	40	GLN
1	D	54	LYS
1	D	60	LEU
1	D	79	LEU
1	D	92	LEU
1	D	93	ARG
1	D	116	ARG
1	D	129	VAL
1	D	140	GLU
1	D	159	ARG
1	D	169	TYR
1	D	186	ARG
1	D	194	LEU
1	D	216	GLU
1	D	219	GLU
1	D	281	LEU
1	D	304	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	154	ASN
1	A	235	HIS
1	B	40	GLN
1	B	142	HIS
1	C	40	GLN
1	C	251	ASN
1	D	40	GLN
1	D	105	HIS

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 for Mogul analysis.

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	1603	-	4,4,4	0.11	0	6,6,6	0.08	0
2	SO4	A	1604	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	1612	-	4,4,4	0.17	0	6,6,6	0.07	0
2	SO4	B	1601	-	4,4,4	0.19	0	6,6,6	0.19	0
2	SO4	B	1602	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	B	1610	-	4,4,4	0.18	0	6,6,6	0.07	0
2	SO4	C	1608	-	4,4,4	0.20	0	6,6,6	0.11	0
2	SO4	C	1609	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	D	1605	-	4,4,4	0.20	0	6,6,6	0.11	0
2	SO4	D	1606	-	4,4,4	0.19	0	6,6,6	0.12	0
2	SO4	D	1607	-	4,4,4	0.17	0	6,6,6	0.16	0
2	SO4	D	1611	-	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
2	SO4	A	1603	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1604	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1612	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	B	1601	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1602	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1610	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1608	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1609	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1605	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1606	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1607	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1611	-	-	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1604	SO4	1	0
2	C	1609	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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.