



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:17 pm BST

PDB ID : 3LUQ  
Title : The Crystal Structure of a PAS Domain from a Sensory Box Histidine Kinase Regulator from *Geobacter sulfurreducens* to 2.5Å  
Authors : Stein, A.J.; Weger, A.; Duggan, E.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2010-02-18  
Resolution : 2.49 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

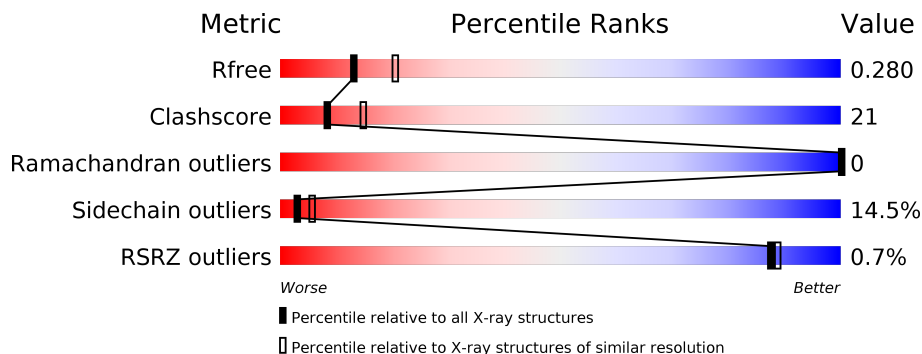
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	114	 64% 25% 9% ..
1	B	114	 58% 38% .
1	C	114	 % 60% 32% 9%
1	D	114	 2% 62% 30% . .

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3658 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 Sensor protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	112	Total 891	C 569	N 155	O 163	S 1	Se 3	0	0	0
1	B	114	Total 913	C 579	N 160	O 170	S 1	Se 3	0	0	0
1	C	114	Total 895	C 569	N 157	O 165	S 1	Se 3	0	0	0
1	D	110	Total 876	C 560	N 158	O 154	S 1	Se 3	0	0	0

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



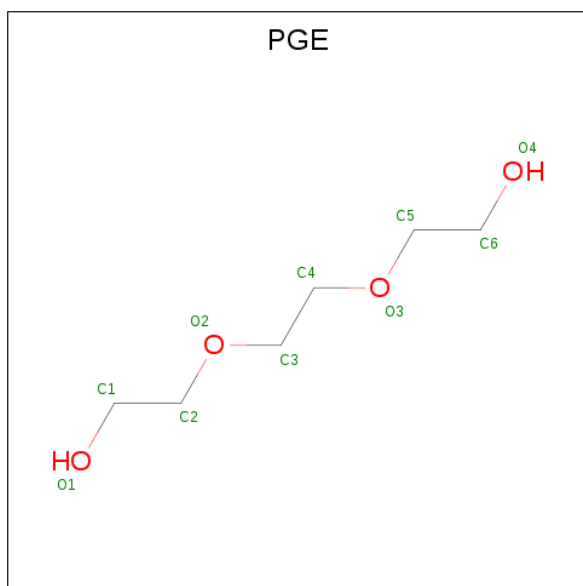
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0

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

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	8	Total	O	0	0
			8	8		
4	C	3	Total	O	0	0
			3	3		

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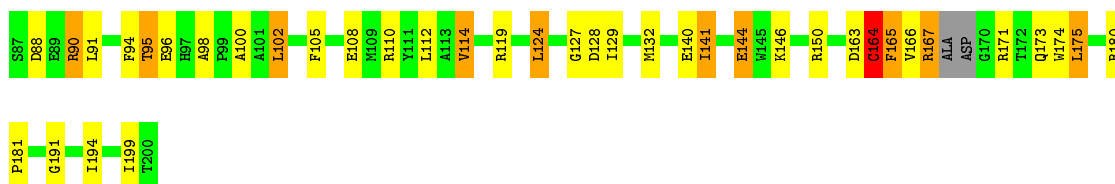
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	D	5	Total	O	0	0
			5	5		

### 3 Residue-property plots [i](#)

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

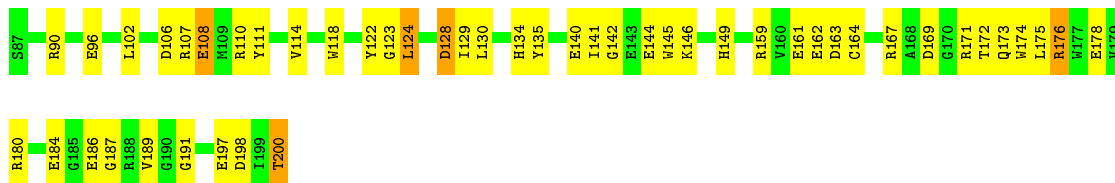
- Molecule 1: Sensor protein

Chain A: 



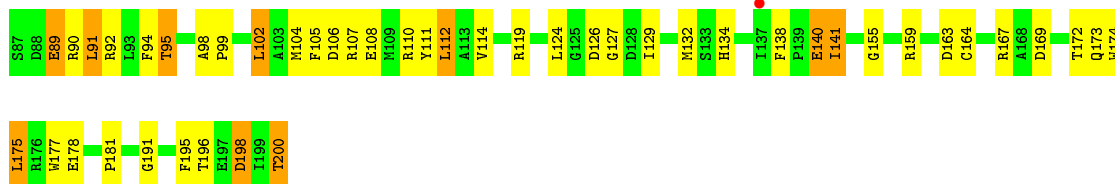
- Molecule 1: Sensor protein

Chain B: 



- Molecule 1: Sensor protein

Chain C: 



- Molecule 1: Sensor protein

Chain D: 



GLY	GLU	G187	R188	V189	I194	E197	D198	I199	THR
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.55Å 71.97Å 67.37Å 90.00° 113.05° 90.00°	Depositor
Resolution (Å)	35.99 – 2.49 35.99 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.6 (35.99-2.49) 97.6 (35.99-2.49)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.48Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.228 , 0.279 0.236 , 0.280	Depositor DCC
$R_{free}$ test set	970 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.3	Xtrriage
Anisotropy	0.129	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3658	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6198e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, 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	1.58	0/911	0.80	1/1229 (0.1%)
1	B	1.52	0/934	0.78	0/1261
1	C	1.51	1/915 (0.1%)	0.79	0/1238
1	D	1.45	0/896	0.76	1/1209 (0.1%)
All	All	1.52	1/3656 (0.0%)	0.78	2/4937 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	111	TYR	CD1-CE1	-5.59	1.30	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	CYS	CA-CB-SG	5.68	124.22	114.00
1	D	164	CYS	CA-CB-SG	5.43	123.78	114.00

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	891	0	819	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	913	0	834	54	0
1	C	895	0	814	40	0
1	D	876	0	802	31	0
2	A	10	0	0	1	0
2	B	5	0	0	0	0
3	A	10	0	14	0	0
3	B	20	0	28	2	0
3	C	20	0	28	2	0
4	A	2	0	0	0	0
4	B	8	0	0	1	0
4	C	3	0	0	0	0
4	D	5	0	0	0	0
All	All	3658	0	3339	146	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 21.

All (146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ASP:OD2	1:A:91:LEU:HD12	1.36	1.26
1:B:198:ASP:OD1	1:B:200:THR:HG23	1.30	1.25
1:B:164:CYS:SG	1:B:172:THR:CG2	2.31	1.18
1:D:176:ARG:NH2	1:D:197:GLU:OE2	1.82	1.11
1:B:198:ASP:OD1	1:B:200:THR:CG2	2.08	1.01
1:D:91:LEU:HB3	1:D:104:MSE:HE1	1.40	1.00
1:B:167:ARG:HE	1:B:173:GLN:HB2	1.28	0.99
1:B:164:CYS:SG	1:B:172:THR:HG21	2.01	0.97
1:B:167:ARG:NE	1:B:173:GLN:HB2	1.79	0.97
1:B:124:LEU:N	1:B:124:LEU:HD13	1.75	0.96
1:B:124:LEU:CD1	1:B:124:LEU:N	2.30	0.94
1:A:108:GLU:OE1	1:A:110:ARG:NH2	2.02	0.92
1:D:89:GLU:OE1	1:D:92:ARG:NH1	2.01	0.92
1:A:94:PHE:O	1:B:90:ARG:NH1	2.04	0.91
1:D:106:ASP:OD2	1:D:110:ARG:HD2	1.72	0.88
1:A:96:GLU:OE1	1:C:90:ARG:NH2	2.08	0.87
1:B:174:TRP:H	1:B:200:THR:CG2	1.87	0.86
1:B:164:CYS:SG	1:B:172:THR:HG23	2.14	0.86
1:D:178:GLU:OE1	1:D:180:ARG:NH1	2.15	0.79
1:D:99:PRO:O	1:D:117:ARG:NH2	2.18	0.76
1:D:167:ARG:O	1:D:170:GLY:N	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:SER:O	1:D:137:ILE:HG12	1.86	0.74
1:C:119:ARG:NH2	1:C:127:GLY:O	2.20	0.74
1:B:189:VAL:HG12	1:B:191:GLY:H	1.53	0.73
1:A:114:VAL:HG21	1:A:129:ILE:HD11	1.71	0.72
1:C:106:ASP:OD1	1:C:108:GLU:N	2.23	0.70
1:B:128:ASP:OD1	1:C:126:ASP:HB2	1.91	0.69
1:B:176:ARG:NH1	1:B:197:GLU:OE2	2.25	0.69
1:D:108:GLU:HG3	1:D:110:ARG:NH1	2.08	0.69
1:B:135:TYR:OH	1:B:149:HIS:HD2	1.77	0.67
1:B:108:GLU:HB2	1:B:110:ARG:HD2	1.77	0.67
1:C:106:ASP:OD1	1:C:106:ASP:C	2.33	0.67
1:B:174:TRP:HE3	1:B:200:THR:HB	1.60	0.67
1:B:174:TRP:H	1:B:200:THR:HG21	1.59	0.66
1:B:174:TRP:H	1:B:200:THR:HG22	1.58	0.65
1:C:91:LEU:O	1:C:95:THR:HG22	1.97	0.65
1:C:163:ASP:OD1	1:C:164:CYS:N	2.29	0.64
1:A:128:ASP:OD2	1:D:116:ARG:NH1	2.29	0.64
1:C:94:PHE:HB3	3:C:1:PGE:H62	1.81	0.63
1:B:167:ARG:HB2	1:B:171:ARG:O	1.98	0.63
1:B:142:GLY:HA3	1:B:144:GLU:OE2	1.99	0.63
1:D:110:ARG:HG3	1:D:131:GLY:HA2	1.80	0.62
1:C:177:TRP:HB3	1:C:196:THR:HG22	1.81	0.62
1:B:174:TRP:O	1:B:200:THR:HG22	1.99	0.61
1:A:91:LEU:O	1:A:95:THR:CG2	2.48	0.61
1:A:91:LEU:O	1:A:95:THR:HG23	2.01	0.61
1:C:155:GLY:HA2	1:C:181:PRO:HG3	1.83	0.61
1:B:184:GLU:O	1:B:187:GLY:CA	2.49	0.61
1:C:134:HIS:NE2	3:C:4:PGE:H4	2.16	0.60
1:C:89:GLU:HG3	1:C:92:ARG:HH22	1.67	0.59
1:B:184:GLU:O	1:B:187:GLY:HA3	2.02	0.59
1:C:174:TRP:H	1:C:200:THR:CG2	2.16	0.59
1:B:186:GLU:N	1:B:187:GLY:HA2	2.17	0.59
1:B:106:ASP:OD2	1:B:110:ARG:HD3	2.01	0.59
1:A:129:ILE:O	1:A:132:MSE:HG3	2.03	0.58
1:C:89:GLU:CG	1:C:92:ARG:NH2	2.66	0.58
1:A:167:ARG:HD3	1:A:171:ARG:O	2.04	0.58
1:B:140:GLU:N	1:B:140:GLU:OE1	2.30	0.58
1:A:165:PHE:CE1	1:A:167:ARG:HG3	2.39	0.57
1:A:90:ARG:HG2	1:A:91:LEU:N	2.19	0.56
1:C:89:GLU:HA	1:C:92:ARG:NH2	2.21	0.56
1:C:91:LEU:O	1:C:95:THR:CG2	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ALA:HB2	1:B:90:ARG:HH12	1.71	0.55
1:C:178:GLU:OE2	1:D:180:ARG:NH2	2.37	0.55
1:C:89:GLU:CG	1:C:92:ARG:HH22	2.18	0.55
1:D:167:ARG:O	1:D:170:GLY:CA	2.55	0.55
1:C:102:LEU:CD2	1:C:195:PHE:HB2	2.37	0.54
1:C:173:GLN:HG3	1:C:200:THR:HG21	1.90	0.54
1:B:123:GLY:C	1:B:124:LEU:HD13	2.28	0.54
1:D:167:ARG:O	1:D:170:GLY:HA2	2.07	0.54
1:D:160:VAL:HG11	1:D:163:ASP:HB2	1.89	0.53
1:B:111:TYR:OH	1:B:134:HIS:HD2	1.92	0.53
1:B:144:GLU:H	1:B:144:GLU:CD	2.11	0.53
1:C:198:ASP:OD1	1:C:200:THR:HG23	2.09	0.52
1:C:89:GLU:HG2	1:C:92:ARG:NH2	2.24	0.52
1:B:96:GLU:OE1	4:B:3:HOH:O	2.19	0.52
1:A:98:ALA:HB2	1:B:90:ARG:NH1	2.24	0.52
1:A:146:LYS:O	1:A:150:ARG:HB2	2.10	0.52
1:B:164:CYS:SG	1:B:172:THR:HG22	2.43	0.52
1:B:122:TYR:O	1:B:124:LEU:CD1	2.58	0.52
1:D:129:ILE:O	1:D:132:MSE:HB2	2.10	0.52
1:D:88:ASP:N	1:D:91:LEU:HD22	2.24	0.51
1:B:163:ASP:O	1:B:174:TRP:HA	2.09	0.51
1:C:140:GLU:CD	1:C:140:GLU:H	2.14	0.51
1:B:159:ARG:HB2	1:B:178:GLU:HG3	1.93	0.51
1:A:167:ARG:CD	1:A:171:ARG:O	2.58	0.51
1:C:178:GLU:CD	1:D:180:ARG:HH22	2.14	0.51
1:B:123:GLY:C	1:B:124:LEU:CD1	2.79	0.50
1:B:114:VAL:HG21	1:B:129:ILE:HD11	1.94	0.49
1:A:119:ARG:NH2	1:A:127:GLY:O	2.44	0.49
1:C:159:ARG:NH1	1:C:178:GLU:OE2	2.42	0.49
1:B:164:CYS:HG	1:B:172:THR:HG21	1.78	0.48
1:A:100:ALA:HB3	2:A:3:SO4:O2	2.13	0.48
1:B:161:GLU:O	1:B:176:ARG:HG3	2.14	0.48
1:B:174:TRP:CE3	1:B:200:THR:HB	2.45	0.48
1:A:163:ASP:OD1	1:A:164:CYS:N	2.47	0.47
1:C:177:TRP:CB	1:C:196:THR:HG22	2.44	0.47
1:B:184:GLU:O	1:B:187:GLY:HA2	2.14	0.47
1:D:106:ASP:OD2	1:D:110:ARG:CD	2.54	0.47
1:C:173:GLN:NE2	1:C:198:ASP:OD2	2.48	0.47
1:B:135:TYR:OH	1:B:149:HIS:CD2	2.63	0.46
1:D:137:ILE:HG12	1:D:137:ILE:H	1.57	0.46
1:D:175:LEU:HD12	1:D:175:LEU:HA	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:HD23	1:A:194:ILE:O	2.16	0.46
1:C:167:ARG:C	1:C:169:ASP:N	2.66	0.46
1:B:145:TRP:CE3	3:B:5:PGE:H62	2.51	0.46
1:B:124:LEU:HA	1:B:124:LEU:HD12	1.70	0.45
1:B:107:ARG:NH1	1:B:189:VAL:O	2.49	0.45
1:D:132:MSE:HE2	1:D:137:ILE:CD1	2.46	0.45
1:B:174:TRP:N	1:B:200:THR:HG22	2.30	0.45
1:C:106:ASP:OD1	1:C:107:ARG:N	2.49	0.45
1:C:129:ILE:O	1:C:132:MSE:HB2	2.16	0.45
1:C:98:ALA:HA	1:C:99:PRO:HD2	1.70	0.45
1:A:132:MSE:HE2	1:A:132:MSE:HB3	1.92	0.45
1:B:124:LEU:HD12	1:B:124:LEU:N	2.22	0.45
1:D:102:LEU:HD23	1:D:102:LEU:HA	1.72	0.45
1:D:133:SER:O	1:D:137:ILE:CG1	2.63	0.45
1:B:142:GLY:O	1:B:146:LYS:HG3	2.17	0.45
1:C:141:ILE:HG21	1:C:141:ILE:HD12	1.72	0.44
1:D:116:ARG:O	1:D:119:ARG:HB2	2.16	0.44
1:B:141:ILE:HD11	3:B:5:PGE:H1	1.99	0.44
1:D:94:PHE:CD2	1:D:94:PHE:N	2.85	0.44
1:D:98:ALA:HA	1:D:99:PRO:HD3	1.57	0.44
1:B:189:VAL:HG12	1:B:191:GLY:N	2.27	0.44
1:A:175:LEU:HD22	1:A:175:LEU:HA	1.75	0.43
1:B:169:ASP:HB3	1:B:171:ARG:HG3	2.00	0.43
1:C:138:PHE:HA	1:C:140:GLU:OE2	2.18	0.43
1:D:179:VAL:HG22	1:D:194:ILE:HG12	2.00	0.42
1:A:124:LEU:HD12	1:A:124:LEU:HA	1.77	0.42
1:A:180:ARG:HB2	1:A:181:PRO:HD2	2.01	0.42
1:C:174:TRP:O	1:C:200:THR:HG22	2.19	0.42
1:A:144:GLU:H	1:A:144:GLU:HG3	1.37	0.42
1:D:91:LEU:HD12	1:D:91:LEU:HA	1.78	0.42
1:D:183:TYR:CE1	1:D:189:VAL:HG22	2.55	0.41
1:C:105:PHE:O	1:C:191:GLY:HA3	2.19	0.41
1:D:132:MSE:CE	1:D:137:ILE:CD1	2.98	0.41
1:C:138:PHE:CA	1:C:140:GLU:OE2	2.69	0.41
1:C:102:LEU:HD21	1:C:195:PHE:HB2	2.03	0.41
1:B:118:TRP:O	1:B:122:TYR:HB2	2.21	0.41
1:C:104:MSE:CE	1:C:112:LEU:HD23	2.51	0.41
1:A:129:ILE:H	1:A:129:ILE:HG13	1.71	0.41
1:C:141:ILE:HD13	1:C:141:ILE:HG23	1.69	0.41
1:A:105:PHE:O	1:A:191:GLY:HA3	2.21	0.40
1:C:175:LEU:HD22	1:C:175:LEU:HA	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:HD13	1:A:141:ILE:HA	1.87	0.40
1:A:174:TRP:HB3	1:A:199:ILE:HD11	2.03	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	108/114 (95%)	108 (100%)	0	0	100	100
1	B	112/114 (98%)	112 (100%)	0	0	100	100
1	C	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
1	D	106/114 (93%)	106 (100%)	0	0	100	100
All	All	438/456 (96%)	435 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	86/92 (94%)	71 (83%)	15 (17%)	2	3
1	B	88/92 (96%)	78 (89%)	10 (11%)	5	11
1	C	84/92 (91%)	70 (83%)	14 (17%)	2	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	81/92 (88%)	71 (88%)	10 (12%)	4	9
All	All	339/368 (92%)	290 (86%)	49 (14%)	3	6

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ARG
1	A	95	THR
1	A	102	LEU
1	A	112	LEU
1	A	114	VAL
1	A	124	LEU
1	A	140	GLU
1	A	141	ILE
1	A	144	GLU
1	A	164	CYS
1	A	165	PHE
1	A	166	VAL
1	A	167	ARG
1	A	173	GLN
1	A	175	LEU
1	B	102	LEU
1	B	108	GLU
1	B	124	LEU
1	B	128	ASP
1	B	130	LEU
1	B	162	GLU
1	B	175	LEU
1	B	176	ARG
1	B	180	ARG
1	B	200	THR
1	C	89	GLU
1	C	91	LEU
1	C	95	THR
1	C	102	LEU
1	C	110	ARG
1	C	112	LEU
1	C	114	VAL
1	C	124	LEU
1	C	140	GLU
1	C	141	ILE
1	C	172	THR

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Mol	Chain	Res	Type
1	C	175	LEU
1	C	198	ASP
1	C	200	THR
1	D	89	GLU
1	D	90	ARG
1	D	91	LEU
1	D	95	THR
1	D	110	ARG
1	D	112	LEU
1	D	116	ARG
1	D	124	LEU
1	D	137	ILE
1	D	159	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	HIS
1	B	149	HIS
1	D	173	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	PGE	A	201	-	9,9,9	0.36	0	8,8,8	0.34	0
3	PGE	B	201	-	9,9,9	0.74	0	8,8,8	0.48	0
3	PGE	B	5	-	9,9,9	0.49	0	8,8,8	0.36	0
2	SO4	A	1	-	4,4,4	0.35	0	6,6,6	0.23	0
3	PGE	C	1	-	9,9,9	0.46	0	8,8,8	0.29	0
3	PGE	C	4	-	9,9,9	0.45	0	8,8,8	0.42	0
2	SO4	B	2	-	4,4,4	0.24	0	6,6,6	0.23	0
2	SO4	A	3	-	4,4,4	0.07	0	6,6,6	0.29	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	PGE	B	5	-	-	5/7/7/7	-
3	PGE	A	201	-	-	6/7/7/7	-
3	PGE	B	201	-	-	1/7/7/7	-
3	PGE	C	1	-	-	5/7/7/7	-
3	PGE	C	4	-	-	5/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	4	PGE	O2-C3-C4-O3
3	A	201	PGE	O1-C1-C2-O2
3	C	1	PGE	O3-C5-C6-O4
3	B	5	PGE	O3-C5-C6-O4
3	C	4	PGE	O3-C5-C6-O4
3	C	1	PGE	O1-C1-C2-O2
3	A	201	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
3	C	4	PGE	O1-C1-C2-O2
3	B	5	PGE	O2-C3-C4-O3
3	A	201	PGE	O3-C5-C6-O4
3	C	4	PGE	C4-C3-O2-C2
3	A	201	PGE	C3-C4-O3-C5
3	C	1	PGE	C6-C5-O3-C4
3	B	5	PGE	C6-C5-O3-C4
3	A	201	PGE	C4-C3-O2-C2
3	B	201	PGE	C3-C4-O3-C5
3	B	5	PGE	O1-C1-C2-O2
3	B	5	PGE	C3-C4-O3-C5
3	A	201	PGE	C6-C5-O3-C4
3	C	1	PGE	C4-C3-O2-C2
3	C	1	PGE	O2-C3-C4-O3
3	C	4	PGE	C3-C4-O3-C5

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5	PGE	2	0
3	C	1	PGE	1	0
3	C	4	PGE	1	0
2	A	3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	109/114 (95%)	-0.03	0 <a href="#">100</a> <a href="#">100</a>	35, 51, 73, 81	0
1	B	111/114 (97%)	0.01	0 <a href="#">100</a> <a href="#">100</a>	37, 55, 74, 84	0
1	C	111/114 (97%)	-0.02	1 (0%) <a href="#">84</a> <a href="#">86</a>	37, 55, 69, 83	0
1	D	107/114 (93%)	0.06	2 (1%) <a href="#">66</a> <a href="#">69</a>	20, 60, 74, 93	0
All	All	438/456 (96%)	0.00	3 (0%) <a href="#">87</a> <a href="#">89</a>	20, 56, 74, 93	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	137	ILE	4.1
1	C	137	ILE	3.0
1	D	136	ASP	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PGE	C	4	10/10	0.81	0.18	64,69,71,71	0
3	PGE	B	201	10/10	0.82	0.23	46,50,52,53	0
3	PGE	B	5	10/10	0.85	0.19	71,71,72,72	0
3	PGE	A	201	10/10	0.86	0.19	80,83,86,86	0
3	PGE	C	1	10/10	0.91	0.19	65,66,66,66	0
2	SO4	B	2	5/5	0.94	0.18	56,57,57,60	0
2	SO4	A	3	5/5	0.94	0.16	65,66,67,69	0
2	SO4	A	1	5/5	0.98	0.12	45,46,47,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.