Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 12:38 am BST

PDB ID	:	1I5N
Title	:	Crystal structure of the P1 domain of CheA from Salmonella typhimurium
Authors	:	Mourey, L.; Da Re, S.; Pedelacq, J.-D.; Tolstyk, T.; Faurie, C.; Guillet, V.; Stock, J.B.; Samama, J.-P.
Deposited on	:	2001-02-28
Resolution	:	2.14 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

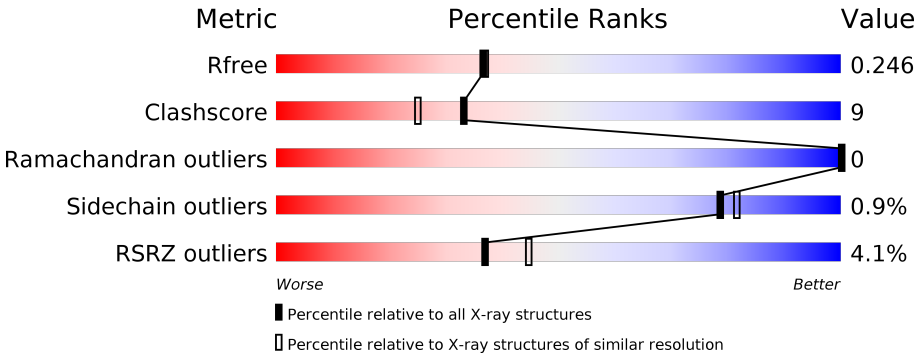
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.14 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 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 <=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	146	2% 71% 16% • 12%
1	B	146	3% 74% 12% 14%
1	C	146	3% 66% 19% 14%
1	D	146	5% 73% 15% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4244 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 CHEMOTAXIS PROTEIN CHEA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	128	Total	C	N	O	S	Se	0	3	0
			1019	639	164	211	1	4			
1	B	125	Total	C	N	O	S	Se	0	1	0
			990	622	160	203	1	4			
1	C	125	Total	C	N	O	S	Se	0	1	0
			998	627	160	206	1	4			
1	D	129	Total	C	N	O	S	Se	0	0	0
			1017	639	165	208	1	4			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P09384
A	3	MSE	MET	MODIFIED RESIDUE	UNP P09384
A	23	MSE	MET	MODIFIED RESIDUE	UNP P09384
A	69	MSE	MET	MODIFIED RESIDUE	UNP P09384
A	81	MSE	MET	MODIFIED RESIDUE	UNP P09384
A	98	MSE	MET	MODIFIED RESIDUE	UNP P09384
A	139	ARG	-	EXPRESSION TAG	UNP P09384
A	140	SER	-	EXPRESSION TAG	UNP P09384
A	141	HIS	-	EXPRESSION TAG	UNP P09384
A	142	HIS	-	EXPRESSION TAG	UNP P09384
A	143	HIS	-	EXPRESSION TAG	UNP P09384
A	144	HIS	-	EXPRESSION TAG	UNP P09384
A	145	HIS	-	EXPRESSION TAG	UNP P09384
A	146	HIS	-	EXPRESSION TAG	UNP P09384
B	1	MSE	MET	MODIFIED RESIDUE	UNP P09384
B	3	MSE	MET	MODIFIED RESIDUE	UNP P09384
B	23	MSE	MET	MODIFIED RESIDUE	UNP P09384
B	69	MSE	MET	MODIFIED RESIDUE	UNP P09384
B	81	MSE	MET	MODIFIED RESIDUE	UNP P09384
B	98	MSE	MET	MODIFIED RESIDUE	UNP P09384
B	139	ARG	-	EXPRESSION TAG	UNP P09384

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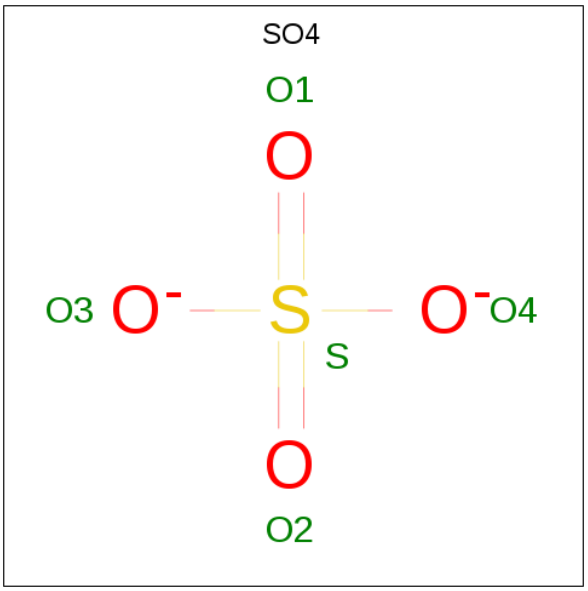
Chain	Residue	Modelled	Actual	Comment	Reference
B	140	SER	-	EXPRESSION TAG	UNP P09384
B	141	HIS	-	EXPRESSION TAG	UNP P09384
B	142	HIS	-	EXPRESSION TAG	UNP P09384
B	143	HIS	-	EXPRESSION TAG	UNP P09384
B	144	HIS	-	EXPRESSION TAG	UNP P09384
B	145	HIS	-	EXPRESSION TAG	UNP P09384
B	146	HIS	-	EXPRESSION TAG	UNP P09384
C	1	MSE	MET	MODIFIED RESIDUE	UNP P09384
C	3	MSE	MET	MODIFIED RESIDUE	UNP P09384
C	23	MSE	MET	MODIFIED RESIDUE	UNP P09384
C	69	MSE	MET	MODIFIED RESIDUE	UNP P09384
C	81	MSE	MET	MODIFIED RESIDUE	UNP P09384
C	98	MSE	MET	MODIFIED RESIDUE	UNP P09384
C	139	ARG	-	EXPRESSION TAG	UNP P09384
C	140	SER	-	EXPRESSION TAG	UNP P09384
C	141	HIS	-	EXPRESSION TAG	UNP P09384
C	142	HIS	-	EXPRESSION TAG	UNP P09384
C	143	HIS	-	EXPRESSION TAG	UNP P09384
C	144	HIS	-	EXPRESSION TAG	UNP P09384
C	145	HIS	-	EXPRESSION TAG	UNP P09384
C	146	HIS	-	EXPRESSION TAG	UNP P09384
D	1	MSE	MET	MODIFIED RESIDUE	UNP P09384
D	3	MSE	MET	MODIFIED RESIDUE	UNP P09384
D	23	MSE	MET	MODIFIED RESIDUE	UNP P09384
D	69	MSE	MET	MODIFIED RESIDUE	UNP P09384
D	81	MSE	MET	MODIFIED RESIDUE	UNP P09384
D	98	MSE	MET	MODIFIED RESIDUE	UNP P09384
D	139	ARG	-	EXPRESSION TAG	UNP P09384
D	140	SER	-	EXPRESSION TAG	UNP P09384
D	141	HIS	-	EXPRESSION TAG	UNP P09384
D	142	HIS	-	EXPRESSION TAG	UNP P09384
D	143	HIS	-	EXPRESSION TAG	UNP P09384
D	144	HIS	-	EXPRESSION TAG	UNP P09384
D	145	HIS	-	EXPRESSION TAG	UNP P09384
D	146	HIS	-	EXPRESSION TAG	UNP P09384

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

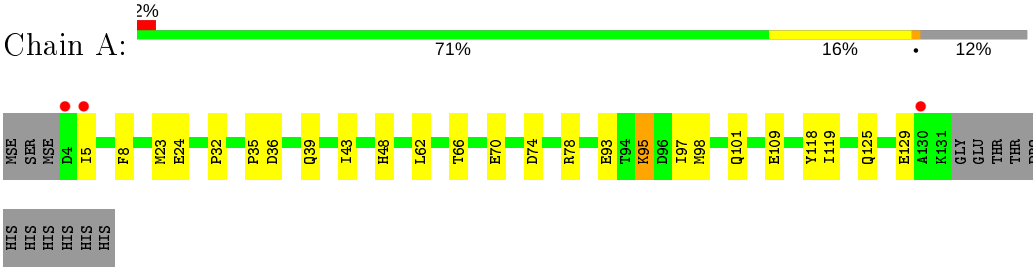
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	73	Total O 73 73	0	0
3	B	40	Total O 40 40	0	0
3	C	44	Total O 44 44	0	0
3	D	58	Total O 58 58	0	0

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.

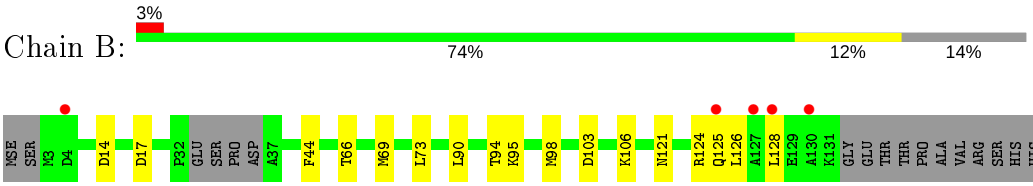
• Molecule 1: CHEMOTAXIS PROTEIN CHEA

Chain A:



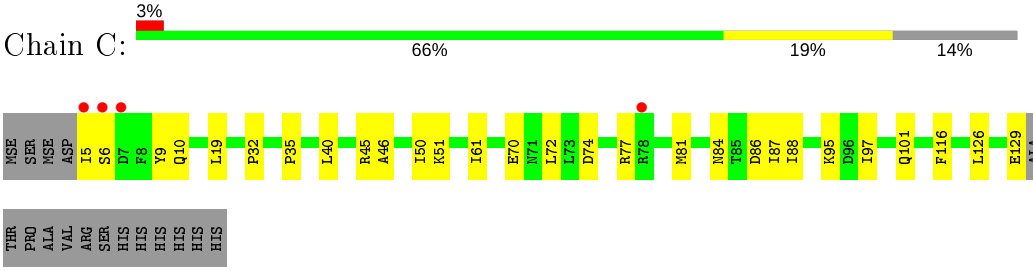
• Molecule 1: CHEMOTAXIS PROTEIN CHEA

Chain B:



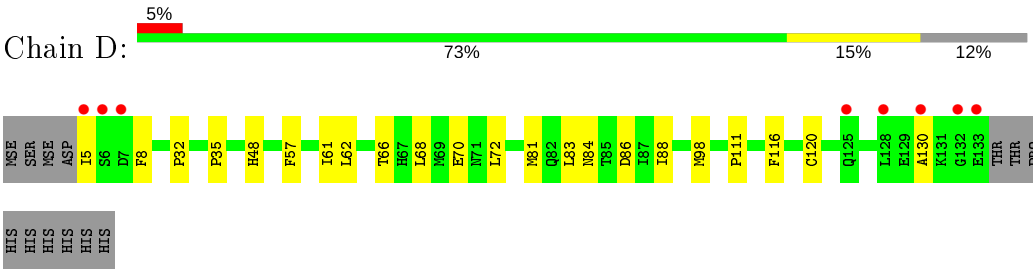
• Molecule 1: CHEMOTAXIS PROTEIN CHEA

Chain C:



• Molecule 1: CHEMOTAXIS PROTEIN CHEA

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.95Å 88.72Å 115.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.30 – 2.14 36.36 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.3 (35.30-2.14) 98.5 (36.36-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.22 (at 2.14Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.210 , 0.248 0.210 , 0.246	Depositor DCC
R_{free} test set	1548 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	17.1	Xtriage
Anisotropy	0.783	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4244	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.39	0/1047	0.56	0/1409
1	B	0.39	0/1013	0.53	0/1362
1	C	0.39	0/1015	0.52	0/1364
1	D	0.39	0/1029	0.53	0/1384
All	All	0.39	0/4104	0.54	0/5519

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

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	1019	0	957	16	0
1	B	990	0	930	15	0
1	C	998	0	933	24	0
1	D	1017	0	963	17	0
2	A	5	0	0	0	0
3	A	73	0	0	0	0
3	B	40	0	0	0	0
3	C	44	0	0	0	0
3	D	58	0	0	0	0
All	All	4244	0	3783	67	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 9.

All (67) 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:5:ILE:CG2	1:C:5:ILE:CG1	2.50	0.89
1:C:5:ILE:CG2	1:C:5:ILE:CA	2.52	0.88
1:C:5:ILE:CG1	1:C:5:ILE:CA	2.53	0.87
1:B:69:MSE:HE3	1:B:94:THR:HB	1.65	0.77
1:A:66[A]:THR:HG22	1:A:98:MSE:HE3	1.68	0.75
1:D:66:THR:HG22	1:D:98:MSE:HE3	1.73	0.70
1:B:14[A]:ASP:OD2	1:C:45:ARG:HG2	1.91	0.69
1:C:126:LEU:HD23	1:C:126:LEU:O	1.96	0.64
1:A:62:LEU:O	1:A:66[A]:THR:HG23	1.99	0.62
1:D:62:LEU:O	1:D:66:THR:HG23	2.01	0.61
1:A:109:GLU:HG2	1:C:10:GLN:HB3	1.83	0.61
1:D:5:ILE:HG23	1:D:57:PHE:CE2	2.36	0.60
1:D:61:ILE:HD12	1:D:111:PRO:HG2	1.84	0.60
1:C:51:LYS:HD3	1:C:70:GLU:OE2	2.03	0.59
1:C:46:ALA:O	1:C:50[A]:ILE:HG12	2.04	0.58
1:B:69:MSE:HE3	1:B:94:THR:CB	2.34	0.57
1:C:6:SER:HA	1:C:9:TYR:CD2	2.39	0.57
1:C:61:ILE:HG23	1:C:116:PHE:CD1	2.39	0.57
1:C:46:ALA:O	1:C:50[B]:ILE:HG13	2.04	0.57
1:B:103:ASP:HA	1:B:106:LYS:HD3	1.87	0.56
1:A:97[B]:ILE:HD12	1:A:119:ILE:HB	1.87	0.56
1:C:19:LEU:HB2	1:C:50[A]:ILE:HD11	1.86	0.56
1:A:24:GLU:HB2	1:A:95:LYS:HE2	1.88	0.56
1:A:125:GLN:O	1:A:129:GLU:HG3	2.07	0.55
1:C:72:LEU:HD22	1:C:126:LEU:HD22	1.89	0.53
1:B:69:MSE:HE3	1:B:94:THR:CG2	2.40	0.52
1:A:36:ASP:OD2	1:A:39:GLN:HG3	2.08	0.52
1:C:126:LEU:HD23	1:C:126:LEU:C	2.30	0.52
1:B:66:THR:OG1	1:B:98:MSE:HE3	2.10	0.51
1:B:125:GLN:O	1:B:128:LEU:HB3	2.12	0.50
1:C:32:PRO:O	1:C:35:PRO:HD3	2.11	0.50
1:B:90:LEU:HD23	1:B:126:LEU:HD12	1.92	0.50
1:C:40:LEU:HD23	1:C:77:ARG:HA	1.94	0.49
1:C:32:PRO:HB2	1:C:84:ASN:HA	1.94	0.49
1:C:84:ASN:O	1:C:88:ILE:HG12	2.12	0.49
1:A:32:PRO:O	1:A:35:PRO:HD3	2.13	0.48
1:D:81:MSE:HB2	1:D:130:ALA:HB1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:CD2	1:B:126:LEU:HD12	2.44	0.47
1:D:66:THR:HG22	1:D:98:MSE:CE	2.43	0.47
1:D:72:LEU:HD11	1:D:81:MSE:SE	2.64	0.46
1:D:48:HIS:HA	1:D:70:GLU:OE1	2.15	0.46
1:A:74:ASP:O	1:A:78:ARG:HG2	2.16	0.45
1:D:32:PRO:HG3	1:D:88:ILE:HD12	1.98	0.45
1:A:93:GLU:O	1:A:97[B]:ILE:HG13	2.16	0.45
1:D:61:ILE:HG23	1:D:116:PHE:CD1	2.53	0.44
1:A:48:HIS:HA	1:A:70:GLU:OE1	2.17	0.44
1:D:66:THR:CG2	1:D:98:MSE:HE3	2.45	0.44
1:A:23:MSE:HG3	1:A:43:ILE:HG23	1.99	0.43
1:B:95:LYS:HD3	1:B:95:LYS:C	2.38	0.43
1:B:124:ARG:O	1:B:128:LEU:HB2	2.17	0.43
1:A:5:ILE:HG13	1:D:8:PHE:CE2	2.54	0.43
1:C:95:LYS:HD3	1:C:95:LYS:C	2.40	0.43
1:B:17:ASP:OD2	1:C:45:ARG:NH2	2.45	0.43
1:D:68:LEU:HD12	1:D:120:CYS:SG	2.59	0.42
1:B:44:PHE:CZ	1:B:73:LEU:HB3	2.54	0.42
1:D:61:ILE:CD1	1:D:111:PRO:HG2	2.48	0.42
1:C:97:ILE:O	1:C:101:GLN:HG3	2.18	0.42
1:C:87:ILE:HG23	1:C:126:LEU:HD11	2.01	0.42
1:D:35:PRO:HB3	1:D:83:LEU:HD12	2.01	0.42
1:A:93:GLU:O	1:A:97[A]:ILE:HG12	2.19	0.42
1:C:81:MSE:SE	1:C:126:LEU:HD21	2.69	0.42
1:C:84:ASN:OD1	1:C:86:ASP:N	2.52	0.42
1:B:121:ASN:O	1:B:125:GLN:HG2	2.20	0.42
1:D:84:ASN:OD1	1:D:86:ASP:HB2	2.20	0.41
1:A:8:PHE:HZ	1:D:5:ILE:HG12	1.85	0.41

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	129/146 (88%)	128 (99%)	1 (1%)	0	100	100
1	B	123/146 (84%)	121 (98%)	2 (2%)	0	100	100
1	C	124/146 (85%)	121 (98%)	3 (2%)	0	100	100
1	D	127/146 (87%)	127 (100%)	0	0	100	100
All	All	503/584 (86%)	497 (99%)	6 (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	110/119 (92%)	108 (98%)	2 (2%)	59	60
1	B	105/119 (88%)	105 (100%)	0	100	100
1	C	107/119 (90%)	105 (98%)	2 (2%)	57	59
1	D	107/119 (90%)	107 (100%)	0	100	100
All	All	429/476 (90%)	425 (99%)	4 (1%)	78	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LYS
1	A	118	TYR
1	C	74	ASP
1	C	129	GLU

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	71	ASN
1	B	10	GLN
1	B	25	GLN

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Mol	Chain	Res	Type
1	B	39	GLN
1	B	63	GLN
1	B	71	ASN
1	B	82	GLN
1	B	99	GLN
1	C	39	GLN
1	C	82	GLN
1	C	99	GLN
1	D	10	GLN
1	D	71	ASN
1	D	82	GLN

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

1 ligand is 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	147	-	4,4,4	0.30	0	6,6,6	0.08	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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	124/146 (84%)	-0.03	3 (2%)	59	65	8, 18, 39, 46	0
1	B	120/146 (82%)	0.06	5 (4%)	36	44	10, 21, 45, 52	0
1	C	121/146 (82%)	0.05	4 (3%)	46	54	11, 20, 46, 55	0
1	D	125/146 (85%)	0.02	8 (6%)	19	24	11, 20, 45, 59	0
All	All	490/584 (83%)	0.03	20 (4%)	37	45	8, 20, 44, 59	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	ALA	7.1
1	B	128	LEU	5.5
1	D	132	GLY	4.8
1	D	5	ILE	4.1
1	C	6	SER	3.4
1	B	125	GLN	3.3
1	C	5	ILE	3.3
1	D	6	SER	3.0
1	D	133	GLU	2.9
1	D	130	ALA	2.9
1	C	7	ASP	2.9
1	D	128	LEU	2.7
1	D	7	ASP	2.5
1	A	130	ALA	2.5
1	B	127	ALA	2.5
1	C	78	ARG	2.4
1	D	125	GLN	2.3
1	A	4	ASP	2.3
1	B	4	ASP	2.1
1	A	5	ILE	2.1

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^{th} 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(Å^2)	Q<0.9
2	SO4	A	147	5/5	0.87	0.26	54,54,56,57	0

6.5 Other polymers (i)

There are no such residues in this entry.