Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 04:58 AM EDT

PDB ID	:	3N5E
Title	:	Crystal Structure of human thymidylate synthase bound to a peptide inhibitor
Authors	:	Pozzi, C.; Cardinale, D.; Guaitoli, G.; Tondi, D.; Luciani, R.; Myllykallio, H.; Ferrari, S.; Costi, M.P.; Mangani, S.
Deposited on	:	2010-05-25
Resolution	:	2.26 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

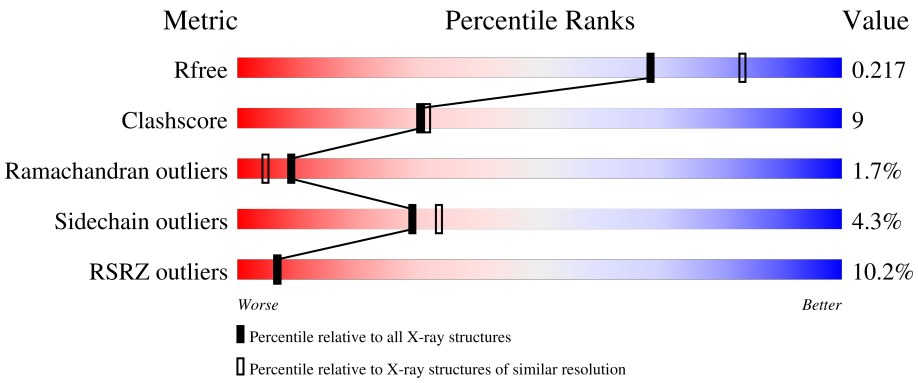
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 of 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	325	7%; 71%; 9%; •; 19%
2	B	325	8%; 66%; 11%; •; 19%
3	D	8	75%; 25%; 38%; 38%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4614 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 Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	2136	1369	372	380	15	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P04818
A	2	ARG	-	expression tag	UNP P04818
A	3	GLY	-	expression tag	UNP P04818
A	4	SER	-	expression tag	UNP P04818
A	5	HIS	-	expression tag	UNP P04818
A	6	HIS	-	expression tag	UNP P04818
A	7	HIS	-	expression tag	UNP P04818
A	8	HIS	-	expression tag	UNP P04818
A	9	HIS	-	expression tag	UNP P04818
A	10	HIS	-	expression tag	UNP P04818
A	11	GLY	-	expression tag	UNP P04818
A	12	SER	-	expression tag	UNP P04818

- Molecule 2 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	263	2134	1368	372	380	14	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP P04818
B	2	ARG	-	expression tag	UNP P04818
B	3	GLY	-	expression tag	UNP P04818
B	4	SER	-	expression tag	UNP P04818

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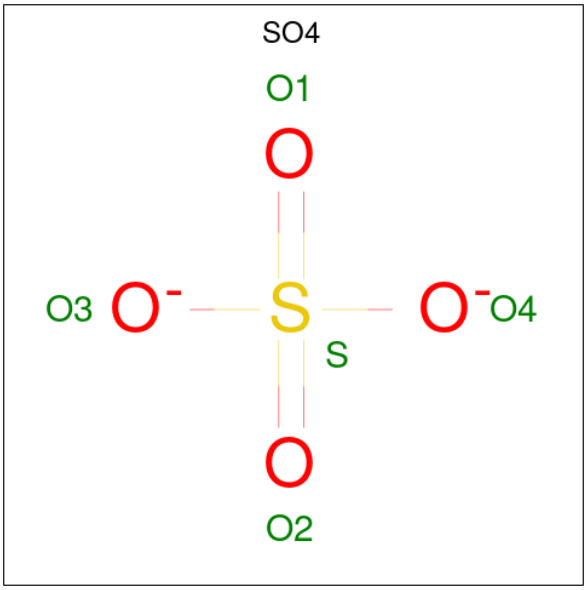
Chain	Residue	Modelled	Actual	Comment	Reference
B	5	HIS	-	expression tag	UNP P04818
B	6	HIS	-	expression tag	UNP P04818
B	7	HIS	-	expression tag	UNP P04818
B	8	HIS	-	expression tag	UNP P04818
B	9	HIS	-	expression tag	UNP P04818
B	10	HIS	-	expression tag	UNP P04818
B	11	GLY	-	expression tag	UNP P04818
B	12	SER	-	expression tag	UNP P04818

- Molecule 3 is a protein called Synthetic peptide LR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	8	69	43	13	12	1	0	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

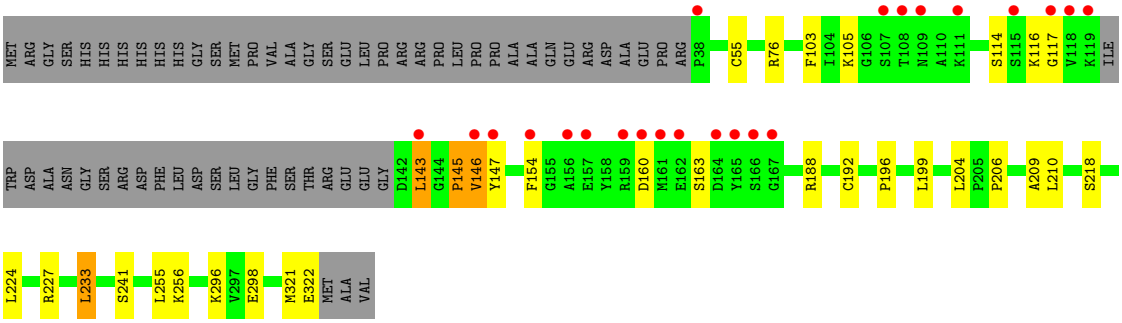
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	125	125	125	0	0
			Total	O		
5	B	130	130	130	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

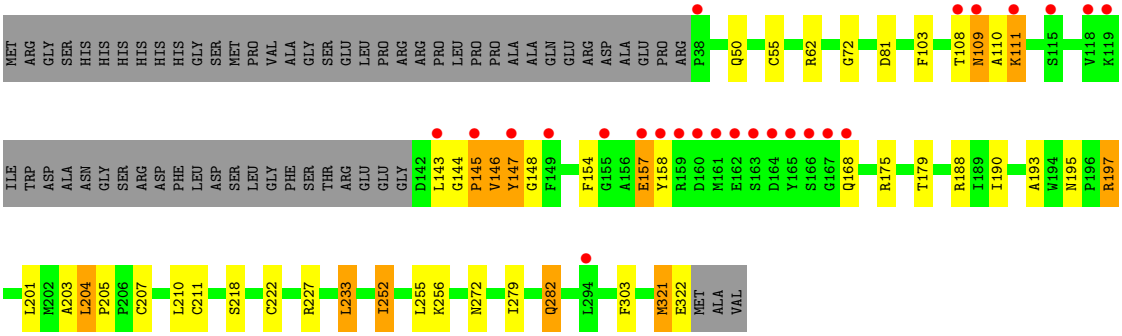
- Molecule 1: Thymidylate synthase

Chain A:



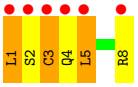
- Molecule 2: Thymidylate synthase

Chain B:



- Molecule 3: Synthetic peptide LR

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	96.11Å 96.11Å 82.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	83.23 – 2.26 83.23 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.7 (83.23-2.26) 99.7 (83.23-2.26)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.87 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.188 , 0.221 0.183 , 0.217	Depositor DCC
R_{free} test set	1990 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l 0.487 for h,-h-k,-l 0.024 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4614	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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 (i)

5.1 Standard geometry (i)

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

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	0.64	0/2164	0.65	0/2921
2	B	0.66	1/2171 (0.0%)	0.68	0/2932
3	D	0.61	0/69	1.38	0/91
All	All	0.65	1/4404 (0.0%)	0.68	0/5944

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	203	ALA	C-N	-5.57	1.21	1.34

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	2136	0	2124	29	0
2	B	2134	0	2122	55	0
3	D	69	0	71	30	0
4	A	15	0	0	0	0
4	B	5	0	0	0	0
5	A	125	0	0	0	0
5	B	130	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4614	0	4317	81	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 (81) 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:B:175:ARG:HH21	3:D:2:SER:HB3	1.22	1.02
1:A:192:SCH:CE	3:D:4:GLN:HG2	1.94	0.98
2:B:154:PHE:HZ	3:D:5:LEU:HA	1.29	0.97
2:B:175:ARG:HH21	3:D:2:SER:CB	1.78	0.95
2:B:175:ARG:NH2	3:D:2:SER:HB3	1.88	0.87
2:B:154:PHE:CZ	3:D:5:LEU:HA	2.09	0.87
2:B:195:ASN:OD1	2:B:197:ARG:HG3	1.76	0.86
1:A:145:PRO:HG2	1:A:196:PRO:HB3	1.59	0.82
1:A:192:SCH:HE1	3:D:4:GLN:HG2	1.60	0.81
2:B:175:ARG:HH21	3:D:2:SER:CA	1.97	0.77
2:B:50:GLN:HG3	5:B:595:HOH:O	1.86	0.75
2:B:175:ARG:HG2	3:D:1:LEU:HB3	1.68	0.74
2:B:205:PRO:HD2	3:D:5:LEU:HG	1.70	0.74
1:A:146:VAL:HG12	1:A:147:TYR:H	1.52	0.74
1:A:206:PRO:HB3	3:D:2:SER:O	1.90	0.72
2:B:147:TYR:CD2	2:B:193:ALA:HB1	2.26	0.70
2:B:146:VAL:O	2:B:148:GLY:N	2.27	0.68
1:A:204:LEU:HD23	3:D:2:SER:HB2	1.76	0.67
2:B:144:GLY:HA2	2:B:158:TYR:CE2	2.30	0.66
2:B:204:LEU:CD2	3:D:4:GLN:HG3	2.26	0.66
2:B:143:LEU:C	2:B:145:PRO:HD3	2.17	0.65
2:B:175:ARG:NH2	3:D:2:SER:CB	2.52	0.64
1:A:103:PHE:HE1	1:A:146:VAL:HG12	1.66	0.61
1:A:154:PHE:CE1	3:D:8:ARG:HD2	2.36	0.59
2:B:109:ASN:HD21	2:B:111:LYS:HG2	1.68	0.59
2:B:204:LEU:HD21	3:D:4:GLN:HG3	1.85	0.58
1:A:199:LEU:HD22	3:D:8:ARG:HD3	1.85	0.58
2:B:252:ILE:HD12	2:B:303:PHE:HE2	1.70	0.57
2:B:145:PRO:O	2:B:146:VAL:O	2.22	0.57
1:A:233:LEU:HD22	1:A:321:MET:HB2	1.88	0.56
1:A:204:LEU:HD13	2:B:154:PHE:CE1	2.40	0.56
2:B:272:ASN:ND2	2:B:322:GLU:O	2.39	0.56
2:B:321:MET:O	2:B:322:GLU:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:VAL:HG12	1:A:147:TYR:N	2.19	0.55
2:B:175:ARG:NH2	3:D:2:SER:HA	2.23	0.54
2:B:175:ARG:NH2	3:D:2:SER:CA	2.70	0.53
2:B:204:LEU:HD22	3:D:4:GLN:OE1	2.10	0.52
1:A:143:LEU:C	1:A:145:PRO:HD3	2.31	0.51
2:B:233:LEU:HD13	2:B:321:MET:HG3	1.92	0.51
2:B:204:LEU:HD22	3:D:4:GLN:HG3	1.92	0.50
1:A:321:MET:O	1:A:322:GLU:HB2	2.11	0.50
2:B:109:ASN:C	2:B:109:ASN:HD22	2.15	0.50
2:B:179:THR:HG21	3:D:1:LEU:HD13	1.94	0.49
1:A:233:LEU:CD2	1:A:321:MET:HB2	2.42	0.49
1:A:160:ASP:HB3	1:A:163:SER:OG	2.12	0.48
2:B:144:GLY:HA2	2:B:158:TYR:CZ	2.48	0.48
2:B:190:ILE:H	3:D:1:LEU:HA	1.79	0.48
2:B:157:GLU:H	2:B:157:GLU:HG2	1.46	0.47
2:B:175:ARG:HH21	3:D:2:SER:HA	1.73	0.47
2:B:154:PHE:CZ	3:D:5:LEU:HD22	2.49	0.47
3:D:2:SER:O	3:D:3:CYS:SG	2.72	0.47
1:A:227:ARG:CZ	2:B:188:ARG:HG2	2.44	0.47
2:B:154:PHE:CD1	2:B:154:PHE:C	2.88	0.46
2:B:256:LYS:HE3	2:B:256:LYS:HB2	1.76	0.46
1:A:145:PRO:HB3	1:A:199:LEU:HD12	1.99	0.45
2:B:81:ASP:HB3	5:B:557:HOH:O	2.16	0.45
2:B:204:LEU:HD23	2:B:204:LEU:HA	1.80	0.45
2:B:109:ASN:ND2	2:B:111:LYS:HG2	2.29	0.45
2:B:279:ILE:O	2:B:282:GLN:HG2	2.17	0.45
2:B:211:CYS:HG	2:B:222:CYS:HG	1.59	0.44
2:B:143:LEU:O	2:B:145:PRO:HD3	2.17	0.44
2:B:108:THR:HB	2:B:144:GLY:H	1.82	0.44
3:D:2:SER:O	3:D:3:CYS:CB	2.65	0.44
3:D:1:LEU:HG	3:D:1:LEU:O	2.18	0.44
2:B:103:PHE:CE1	2:B:147:TYR:HB2	2.53	0.44
1:A:204:LEU:CD2	3:D:2:SER:HB2	2.45	0.43
1:A:206:PRO:HG2	2:B:188:ARG:HB3	2.00	0.43
2:B:144:GLY:N	2:B:145:PRO:HD3	2.34	0.43
2:B:252:ILE:HD12	2:B:303:PHE:CE2	2.50	0.42
1:A:103:PHE:CD1	1:A:147:TYR:HB2	2.55	0.42
1:A:143:LEU:O	1:A:145:PRO:HD3	2.19	0.42
1:A:218:SER:HA	1:A:255:LEU:HD22	2.02	0.41
1:A:209:ALA:HB1	1:A:224:LEU:HD11	2.02	0.41
2:B:62:ARG:HB2	5:B:524:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ARG:HG2	2:B:227:ARG:CZ	2.50	0.41
2:B:218:SER:HA	2:B:255:LEU:HD22	2.01	0.41
2:B:109:ASN:HD22	2:B:110:ALA:N	2.19	0.41
1:A:204:LEU:HG	3:D:3:CYS:H	1.85	0.41
1:A:76:ARG:NH1	2:B:72:GLY:O	2.54	0.40
1:A:210:LEU:HD11	2:B:207:SCH:SD	2.61	0.40
1:A:256:LYS:HE2	1:A:256:LYS:HB2	1.60	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	256/325 (79%)	241 (94%)	11 (4%)	4 (2%)	9 5
2	B	257/325 (79%)	247 (96%)	7 (3%)	3 (1%)	13 9
3	D	6/8 (75%)	2 (33%)	2 (33%)	2 (33%)	0 0
All	All	519/658 (79%)	490 (94%)	20 (4%)	9 (2%)	9 4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	PRO
1	A	146	VAL
2	B	145	PRO
2	B	146	VAL
2	B	147	TYR
3	D	3	CYS
3	D	5	LEU
1	A	114	SER
1	A	117	GLY

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	228/278 (82%)	221 (97%)	7 (3%)	40	49
2	B	229/279 (82%)	217 (95%)	12 (5%)	23	24
3	D	8/8 (100%)	7 (88%)	1 (12%)	4	3
All	All	465/565 (82%)	445 (96%)	20 (4%)	29	33

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LYS
1	A	116	LYS
1	A	143	LEU
1	A	233	LEU
1	A	241	SER
1	A	296	LYS
1	A	298	GLU
2	B	109	ASN
2	B	111	LYS
2	B	157	GLU
2	B	168	GLN
2	B	197	ARG
2	B	201	LEU
2	B	204	LEU
2	B	210	LEU
2	B	233	LEU
2	B	252	ILE
2	B	282	GLN
2	B	321	MET
3	D	1	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	HIS

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Mol	Chain	Res	Type
2	B	109	ASN
2	B	282	GLN
2	B	309	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)

5 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	SCH	A	55	1	6,7,8	0.72	0	3,7,9	1.48	1 (33%)
1	SCH	A	207	1	6,7,8	0.74	0	3,7,9	1.07	0
1	SCH	A	192	1	6,7,8	0.69	0	3,7,9	1.13	0
2	SCH	B	207	2	6,7,8	0.77	0	3,7,9	0.48	0
2	SCH	B	55	2	6,7,8	0.78	0	3,7,9	1.87	1 (33%)

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
1	SCH	A	55	1	-	0/2/6/8	-
1	SCH	A	207	1	-	0/2/6/8	-
1	SCH	A	192	1	-	0/2/6/8	-
2	SCH	B	207	2	-	0/2/6/8	-
2	SCH	B	55	2	-	0/2/6/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	55	SCH	CB-SG-SD	2.71	110.83	103.82
1	A	55	SCH	CB-SG-SD	2.31	109.80	103.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	192	SCH	2	0
2	B	207	SCH	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
4	SO4	A	401	-	4,4,4	0.27	0	6,6,6	0.33	0
4	SO4	B	401	-	4,4,4	0.13	0	6,6,6	0.53	0
4	SO4	A	403	-	4,4,4	0.28	0	6,6,6	0.71	0
4	SO4	A	402	-	4,4,4	0.31	0	6,6,6	0.37	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 (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, 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	260/325 (80%)	-0.07	23 (8%)	10	11	15, 24, 65, 89	0
2	B	261/325 (80%)	-0.01	25 (9%)	8	8	14, 24, 67, 86	0
3	D	8/8 (100%)	3.11	6 (75%)	0	0	58, 66, 78, 80	8 (100%)
All	All	529/658 (80%)	0.01	54 (10%)	6	6	14, 24, 68, 89	8 (1%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	VAL	7.4
3	D	2	SER	6.6
2	B	111	LYS	5.6
2	B	145	PRO	4.8
1	A	117	GLY	4.6
1	A	108	THR	4.6
2	B	160	ASP	4.5
2	B	143	LEU	4.5
1	A	115	SER	4.4
1	A	162	GLU	4.4
1	A	166	SER	4.4
2	B	165	TYR	4.2
3	D	1	LEU	4.1
2	B	166	SER	4.1
2	B	164	ASP	4.1
2	B	108	THR	3.9
1	A	160	ASP	3.7
2	B	38	PRO	3.6
1	A	164	ASP	3.6
3	D	3	CYS	3.5
2	B	147	TYR	3.5
2	B	167	GLY	3.5
2	B	115	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	161	MET	3.2
2	B	161	MET	3.2
2	B	163	SER	3.1
3	D	5	LEU	3.1
1	A	147	TYR	3.1
2	B	155	GLY	3.1
2	B	118	VAL	3.0
1	A	165	TYR	2.9
1	A	38	PRO	2.9
1	A	167	GLY	2.8
1	A	107	SER	2.8
1	A	109	ASN	2.8
2	B	119	LYS	2.7
3	D	8	ARG	2.7
3	D	4	GLN	2.7
1	A	143	LEU	2.7
2	B	159	ARG	2.6
2	B	168	GLN	2.6
1	A	146	VAL	2.6
1	A	111	LYS	2.6
2	B	158	TYR	2.5
1	A	157	GLU	2.5
1	A	154	PHE	2.4
2	B	157	GLU	2.4
2	B	162	GLU	2.4
2	B	149	PHE	2.4
1	A	156	ALA	2.3
2	B	109	ASN	2.3
1	A	119	LYS	2.3
1	A	159	ARG	2.0
2	B	294	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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	B-factors(Å^2)	Q<0.9
1	SCH	A	55	8/9	0.93	0.10	28,29,39,41	0
2	SCH	B	55	8/9	0.94	0.08	29,30,38,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SCH	A	192	8/9	0.95	0.11	25,26,36,38	0
2	SCH	B	207	8/9	0.95	0.12	22,25,38,40	0
1	SCH	A	207	8/9	0.96	0.12	23,25,41,41	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
4	SO4	A	403	5/5	0.96	0.10	36,38,41,42	0
4	SO4	A	402	5/5	0.98	0.12	32,32,35,38	0
4	SO4	B	401	5/5	0.98	0.06	38,41,42,43	0
4	SO4	A	401	5/5	0.99	0.11	36,38,39,40	0

6.5 Other polymers (i)

There are no such residues in this entry.