Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:42 PM GMT

PDB ID	:	3RUB
Title	:	CRYSTAL STRUCTURE OF THE UNACTIVATED FORM OF RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE FROM TOBACCO REFINED AT 2.0-ANGSTROMS RESOLUTION
Authors	:	Schreuder, H.; Cascio, D.; Curmi, P.M.G.; Chapman, M.S.; Suh, S.W.; Eisenberg, D.S.
Deposited on	:	1990-05-25
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

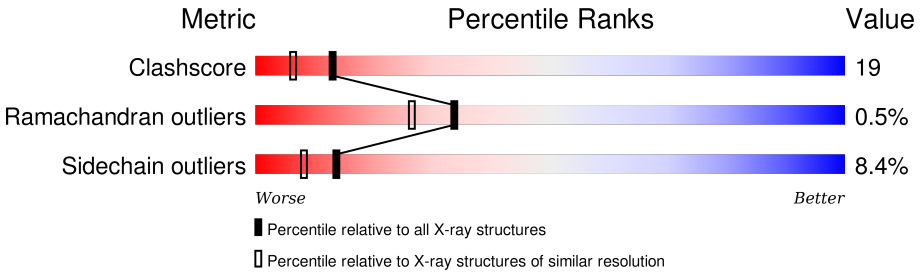
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.00 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	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	L	477	52% 32% 8% • 8%
2	S	123	59% 33% 8% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4716 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 RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE, FORM III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	441	3455	2194	612	633	16	0	0	0

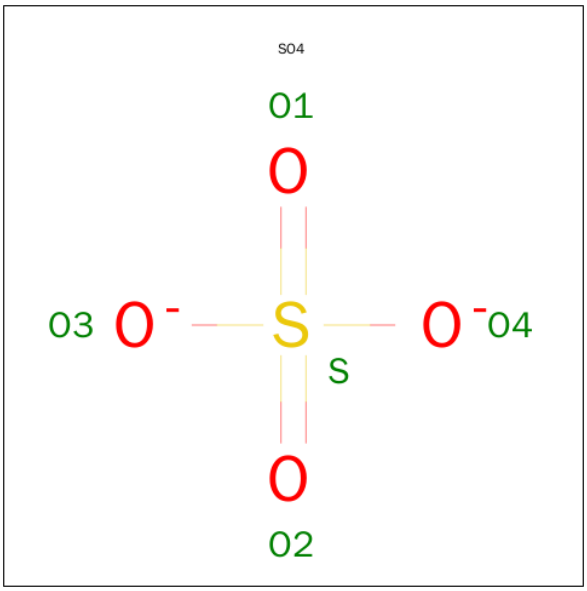
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	377	VAL	GLU	CONFLICT	UNP P00876
L	405	MET	GLY	CONFLICT	UNP P00876

- Molecule 2 is a protein called RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE, FORM III.

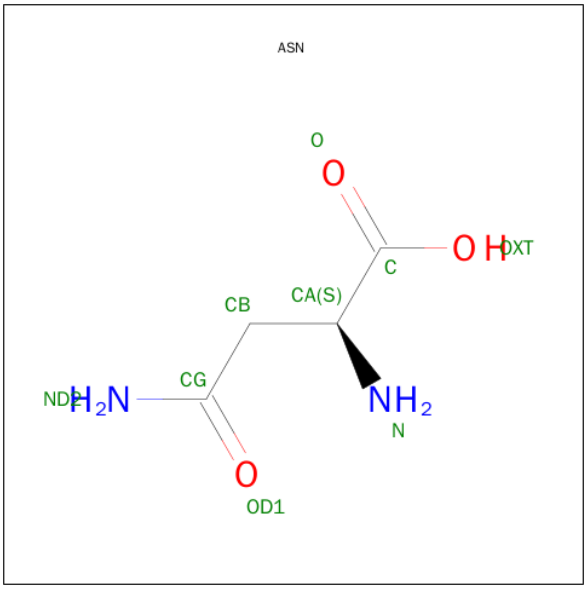
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	S	123	1029	672	163	188	6	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is ASPARAGINE (three-letter code: ASN) (formula: $C_4H_8N_2O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total N 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	179	Total O 179 179	0	0
5	S	37	Total O 37 37	0	0

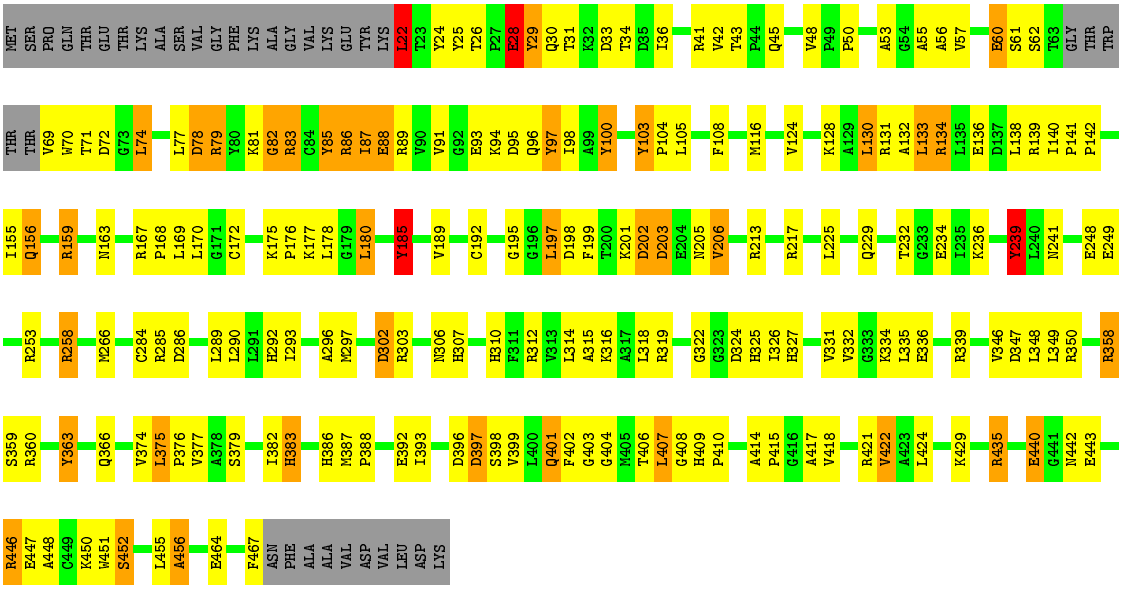
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

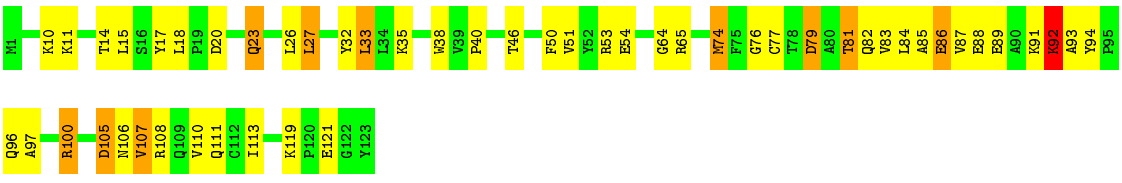
• Molecule 1: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE, FORM III

Chain L:



• Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE, FORM III

Chain S:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	148.70Å 148.70Å 137.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4716	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

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	L	1.09	4/3537 (0.1%)	1.97	89/4793 (1.9%)
2	S	1.03	1/1062 (0.1%)	1.98	25/1442 (1.7%)
All	All	1.08	5/4599 (0.1%)	1.97	114/6235 (1.8%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	322	GLY	N-CA	-6.08	1.36	1.46
1	L	248	GLU	CD-OE1	-5.67	1.19	1.25
1	L	234	GLU	CD-OE1	-5.15	1.20	1.25
2	S	100	ARG	CD-NE	-5.01	1.38	1.46
1	L	398	SER	CA-CB	5.00	1.60	1.52

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	100	ARG	NE-CZ-NH1	23.30	131.95	120.30
1	L	421	ARG	NE-CZ-NH2	-15.88	112.36	120.30
2	S	100	ARG	NE-CZ-NH2	-15.63	112.48	120.30
1	L	421	ARG	NE-CZ-NH1	13.32	126.96	120.30
1	L	360	ARG	NE-CZ-NH1	-13.16	113.72	120.30
1	L	312	ARG	NE-CZ-NH1	13.07	126.83	120.30
1	L	350	ARG	NE-CZ-NH1	12.92	126.76	120.30
1	L	213	ARG	NE-CZ-NH1	11.83	126.22	120.30
1	L	97	TYR	CB-CG-CD1	-11.53	114.08	121.00
2	S	100	ARG	CG-CD-NE	11.47	135.89	111.80
1	L	285	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	L	203	ASP	CB-CG-OD2	-10.47	108.88	118.30
2	S	65	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	L	253	ARG	NE-CZ-NH1	-10.22	115.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	134	ARG	NE-CZ-NH1	-10.01	115.29	120.30
1	L	22	LEU	CA-CB-CG	9.86	137.98	115.30
1	L	464	GLU	CA-CB-CG	9.70	134.74	113.40
1	L	435	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	L	396	ASP	CB-CG-OD2	-9.36	109.88	118.30
1	L	86	ARG	NE-CZ-NH1	9.31	124.95	120.30
1	L	302	ASP	CB-CG-OD2	9.16	126.55	118.30
1	L	339	ARG	CD-NE-CZ	9.07	136.30	123.60
1	L	401	GLN	CA-CB-CG	8.99	133.18	113.40
2	S	100	ARG	CB-CG-CD	8.95	134.88	111.60
1	L	258	ARG	CA-CB-CG	8.90	132.97	113.40
2	S	108	ARG	NE-CZ-NH1	8.87	124.74	120.30
1	L	134	ARG	CD-NE-CZ	-8.85	111.21	123.60
1	L	217	ARG	NE-CZ-NH2	8.41	124.51	120.30
1	L	83	ARG	NE-CZ-NH1	-8.08	116.26	120.30
1	L	22	LEU	CB-CA-C	7.97	125.35	110.20
1	L	185	TYR	CB-CG-CD2	7.92	125.75	121.00
2	S	100	ARG	CD-NE-CZ	7.86	134.60	123.60
2	S	105	ASP	CB-CG-OD2	7.63	125.17	118.30
2	S	65	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	L	206	VAL	CA-CB-CG2	7.49	122.13	110.90
2	S	108	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	L	185	TYR	CB-CG-CD1	-7.35	116.59	121.00
2	S	20	ASP	CB-CG-OD1	7.26	124.83	118.30
1	L	86	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	L	79	ARG	CA-CB-CG	7.07	128.95	113.40
1	L	440	GLU	OE1-CD-OE2	7.06	131.77	123.30
1	L	383	HIS	CA-CB-CG	-6.94	101.81	113.60
1	L	41	ARG	NE-CZ-NH2	6.83	123.72	120.30
1	L	116	MET	CG-SD-CE	6.67	110.88	100.20
1	L	217	ARG	NH1-CZ-NH2	-6.62	112.12	119.40
1	L	41	ARG	NE-CZ-NH1	-6.61	116.99	120.30
1	L	198	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	L	180	LEU	N-CA-CB	-6.60	97.21	110.40
1	L	452	SER	N-CA-CB	6.56	120.33	110.50
1	L	133	LEU	O-C-N	6.51	133.12	122.70
1	L	347	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	L	401	GLN	N-CA-CB	-6.50	98.90	110.60
1	L	139	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	L	286	ASP	CB-CG-OD2	-6.31	112.62	118.30
2	S	38	TRP	CA-CB-CG	-6.29	101.74	113.70
1	L	29	TYR	C-N-CA	6.13	137.02	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	312	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	L	79	ARG	N-CA-CB	6.08	121.54	110.60
1	L	339	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	L	363	TYR	CB-CG-CD2	-6.06	117.36	121.00
1	L	85	TYR	CB-CG-CD1	6.05	124.63	121.00
2	S	32	TYR	CB-CG-CD2	-6.02	117.39	121.00
1	L	159	ARG	NE-CZ-NH2	-6.02	117.29	120.30
2	S	33	LEU	O-C-N	6.00	132.29	122.70
1	L	82	GLY	N-CA-C	-5.92	98.29	113.10
1	L	83	ARG	NH1-CZ-NH2	5.91	125.90	119.40
1	L	346	VAL	CA-CB-CG2	-5.87	102.09	110.90
1	L	241	ASN	CB-CG-OD1	5.85	133.31	121.60
1	L	93	GLU	CA-C-O	5.81	132.31	120.10
2	S	38	TRP	O-C-N	5.81	131.99	122.70
1	L	180	LEU	CB-CA-C	5.78	121.18	110.20
2	S	79	ASP	CB-CG-OD2	5.69	123.42	118.30
1	L	97	TYR	CB-CG-CD2	5.68	124.41	121.00
2	S	53	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	L	285	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	L	285	ARG	CD-NE-CZ	5.63	131.49	123.60
1	L	360	ARG	CD-NE-CZ	-5.62	115.74	123.60
1	L	253	ARG	CD-NE-CZ	5.58	131.41	123.60
1	L	33	ASP	CB-CG-OD1	-5.55	113.30	118.30
1	L	450	LYS	N-CA-CB	5.55	120.59	110.60
1	L	232	THR	CA-CB-CG2	5.54	120.15	112.40
1	L	88	GLU	CB-CA-C	5.53	121.46	110.40
1	L	60	GLU	N-CA-CB	5.50	120.49	110.60
1	L	397	ASP	CB-CG-OD1	5.47	123.23	118.30
1	L	392	GLU	CG-CD-OE2	-5.47	107.36	118.30
1	L	103	TYR	CG-CD2-CE2	-5.43	116.96	121.30
1	L	234	GLU	OE1-CD-OE2	5.42	129.81	123.30
1	L	156	GLN	O-C-N	5.39	131.32	122.70
1	L	249	GLU	CA-CB-CG	5.38	125.24	113.40
1	L	100	TYR	O-C-N	5.36	131.28	122.70
1	L	202	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	L	360	ARG	NH1-CZ-NH2	5.32	125.25	119.40
2	S	54	GLU	CG-CD-OE2	-5.32	107.66	118.30
1	L	130	LEU	O-C-N	5.29	131.16	122.70
1	L	139	ARG	NE-CZ-NH1	-5.26	117.67	120.30
2	S	94	TYR	CB-CG-CD1	-5.26	117.85	121.00
1	L	310	HIS	CA-CB-CG	-5.20	104.77	113.60
2	S	86	GLU	CG-CD-OE2	-5.17	107.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	28	GLU	CG-CD-OE2	5.16	128.63	118.30
1	L	456	ALA	CB-CA-C	5.16	117.85	110.10
1	L	213	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
1	L	88	GLU	CA-CB-CG	5.11	124.64	113.40
1	L	56	ALA	CB-CA-C	5.10	117.75	110.10
1	L	29	TYR	CA-C-O	5.09	130.80	120.10
2	S	64	GLY	CA-C-O	-5.08	111.45	120.60
2	S	86	GLU	OE1-CD-OE2	5.05	129.36	123.30
1	L	258	ARG	CB-CG-CD	5.05	124.73	111.60
2	S	107	VAL	CB-CA-C	5.05	120.99	111.40
1	L	350	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	S	92	LYS	N-CA-CB	5.02	119.64	110.60
1	L	392	GLU	CG-CD-OE1	5.02	128.33	118.30
1	L	325	HIS	CA-CB-CG	5.01	122.12	113.60
2	S	74	MET	CA-CB-CG	-5.01	104.79	113.30
1	L	239	TYR	CG-CD1-CE1	5.00	125.30	121.30

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	L	3455	0	3389	137	1
2	S	1029	0	994	38	0
3	L	15	0	0	1	0
4	L	1	0	0	0	0
5	L	179	0	0	2	0
5	S	37	0	0	0	0
All	All	4716	0	4383	169	1

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 19.

All (169) 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:L:172:CYS:HB2	1:L:197:LEU:HD23	1.34	1.07
1:L:140:ILE:H	1:L:366:GLN:HE22	1.21	0.89
2:S:27:LEU:HD12	2:S:84:LEU:HD22	1.54	0.88
1:L:443:GLU:O	1:L:447:GLU:HG3	1.73	0.88
1:L:69:VAL:O	1:L:72:ASP:HB2	1.75	0.86
1:L:170:LEU:HD21	1:L:424:LEU:HD22	1.59	0.83
2:S:86:GLU:HA	2:S:86:GLU:OE1	1.81	0.80
2:S:11:LYS:HG3	2:S:17:TYR:CE1	2.16	0.80
1:L:172:CYS:HB2	1:L:197:LEU:CD2	2.12	0.79
1:L:156:GLN:HG2	2:S:110:VAL:HG12	1.65	0.78
1:L:156:GLN:HG2	2:S:110:VAL:CG1	2.14	0.78
1:L:30:GLN:HG2	1:L:30:GLN:O	1.86	0.76
1:L:132:ALA:CB	1:L:306:ASN:HD22	1.99	0.76
2:S:105:ASP:OD1	2:S:107:VAL:HG22	1.86	0.75
1:L:57:VAL:O	1:L:61:SER:CB	2.35	0.74
2:S:88:GLU:OE2	2:S:91:LYS:HE3	1.89	0.73
1:L:57:VAL:O	1:L:61:SER:HB3	1.90	0.72
2:S:33:LEU:CD1	2:S:113:ILE:HD13	2.18	0.72
1:L:406:THR:OG1	1:L:407:LEU:HD23	1.90	0.72
2:S:82:GLN:O	2:S:85:ALA:HB3	1.90	0.72
1:L:70:TRP:CZ3	1:L:74:LEU:HD21	2.24	0.71
2:S:40:PRO:HG2	2:S:74:MET:HE3	1.71	0.71
1:L:98:ILE:HD13	1:L:363:TYR:CE2	2.26	0.70
1:L:70:TRP:HZ3	1:L:74:LEU:HD21	1.56	0.70
1:L:50:PRO:O	1:L:53:ALA:HB3	1.92	0.69
1:L:69:VAL:HG23	1:L:72:ASP:OD1	1.93	0.69
1:L:156:GLN:CG	2:S:110:VAL:HG12	2.23	0.68
1:L:446:ARG:HG3	1:L:467:PHE:CE2	2.29	0.68
1:L:22:LEU:HD23	1:L:25:TYR:HB3	1.76	0.67
2:S:33:LEU:HD12	2:S:113:ILE:HD13	1.77	0.67
1:L:36:ILE:HD13	1:L:108:PHE:CE2	2.30	0.66
2:S:27:LEU:HD12	2:S:84:LEU:CD2	2.27	0.65
1:L:71:THR:HA	1:L:74:LEU:HD22	1.80	0.64
1:L:69:VAL:CG2	1:L:72:ASP:OD1	2.46	0.63
1:L:156:GLN:CG	2:S:110:VAL:CG1	2.75	0.63
1:L:43:THR:HA	1:L:95:ASP:O	1.98	0.63
2:S:40:PRO:HG2	2:S:74:MET:CE	2.28	0.63
1:L:172:CYS:CB	1:L:197:LEU:HD23	2.22	0.63
1:L:316:LYS:NZ	1:L:366:GLN:HE21	1.98	0.62
1:L:43:THR:HG22	1:L:131:ARG:HB3	1.80	0.62
1:L:29:TYR:CE2	1:L:31:THR:HA	2.35	0.62
1:L:403:GLY:HA3	3:L:490:SO4:O2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:98:ILE:HD13	1:L:363:TYR:HE2	1.63	0.61
2:S:92:LYS:HD2	2:S:93:ALA:N	2.14	0.61
1:L:138:LEU:O	1:L:316:LYS:NZ	2.33	0.61
1:L:57:VAL:O	1:L:61:SER:HB2	1.99	0.61
1:L:442:ASN:O	1:L:446:ARG:HB2	2.00	0.61
1:L:132:ALA:HB1	1:L:306:ASN:HD22	1.65	0.60
1:L:414:ALA:HB3	1:L:415:PRO:HD3	1.82	0.60
1:L:88:GLU:OE2	1:L:358:ARG:NH1	2.32	0.60
1:L:422:VAL:CG2	1:L:455:LEU:HD22	2.32	0.60
1:L:61:SER:HB2	1:L:124:VAL:HG11	1.83	0.60
2:S:46:THR:HG22	2:S:97:ALA:HB2	1.84	0.59
2:S:79:ASP:OD1	2:S:81:THR:OG1	2.12	0.59
1:L:316:LYS:HZ3	1:L:366:GLN:HE21	1.49	0.59
1:L:167:ARG:HG3	1:L:168:PRO:O	2.02	0.59
1:L:203:ASP:HB3	1:L:206:VAL:HG13	1.84	0.59
1:L:155:ILE:HG12	1:L:375:LEU:HD13	1.84	0.59
2:S:106:ASN:OD1	2:S:106:ASN:C	2.40	0.58
2:S:33:LEU:HD11	2:S:113:ILE:HD13	1.85	0.57
1:L:86:ARG:HG2	1:L:100:TYR:CD1	2.39	0.57
1:L:201:LYS:HG2	1:L:202:ASP:O	2.05	0.56
1:L:435:ARG:HH22	1:L:447:GLU:CD	2.09	0.56
1:L:85:TYR:O	1:L:86:ARG:HB2	2.04	0.56
1:L:42:VAL:HG23	1:L:130:LEU:HD22	1.88	0.56
1:L:379:SER:HB3	1:L:401:GLN:HB3	1.88	0.56
1:L:70:TRP:CZ3	1:L:74:LEU:CD2	2.90	0.55
2:S:14:THR:HG22	2:S:15:LEU:HG	1.89	0.54
1:L:382:ILE:HG21	1:L:402:PHE:HE1	1.71	0.54
1:L:42:VAL:HG23	1:L:130:LEU:CD2	2.37	0.54
1:L:78:ASP:HA	1:L:81:LYS:HE3	1.91	0.53
1:L:414:ALA:N	1:L:415:PRO:CD	2.71	0.53
1:L:404:GLY:O	1:L:408:GLY:HA3	2.09	0.53
1:L:382:ILE:HG21	1:L:402:PHE:CE1	2.44	0.52
1:L:358:ARG:HD2	5:L:669:HOH:O	2.09	0.52
1:L:452:SER:O	1:L:456:ALA:N	2.35	0.52
1:L:178:LEU:HD21	1:L:205:ASN:HB2	1.91	0.51
2:S:35:LYS:HG3	2:S:35:LYS:O	2.11	0.51
1:L:318:LEU:C	1:L:318:LEU:HD13	2.30	0.51
1:L:442:ASN:ND2	5:L:552:HOH:O	2.29	0.51
1:L:451:TRP:CE3	1:L:451:TRP:O	2.64	0.51
1:L:22:LEU:O	1:L:22:LEU:HD22	2.11	0.50
2:S:87:VAL:O	2:S:91:LYS:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:45:GLN:O	1:L:48:VAL:HG22	2.12	0.50
2:S:11:LYS:HG3	2:S:17:TYR:CZ	2.47	0.50
1:L:451:TRP:HE3	1:L:451:TRP:O	1.95	0.50
2:S:33:LEU:HG	2:S:113:ILE:HG21	1.94	0.50
1:L:382:ILE:CG2	1:L:402:PHE:HE1	2.25	0.49
1:L:176:PRO:HD2	1:L:180:LEU:HD22	1.94	0.49
2:S:79:ASP:C	2:S:81:THR:N	2.65	0.49
1:L:88:GLU:O	1:L:97:TYR:HA	2.12	0.49
1:L:387:MET:N	1:L:388:PRO:CD	2.75	0.49
1:L:169:LEU:HB2	1:L:399:VAL:HG22	1.95	0.49
1:L:409:HIS:CG	1:L:410:PRO:HD2	2.48	0.49
1:L:418:VAL:O	1:L:422:VAL:HG13	2.13	0.49
1:L:29:TYR:CD1	1:L:83:ARG:HD2	2.47	0.48
1:L:134:ARG:HD3	1:L:136:GLU:OE2	2.12	0.48
1:L:331:VAL:HG21	1:L:393:ILE:HG21	1.95	0.48
1:L:42:VAL:O	1:L:96:GLN:HA	2.13	0.48
2:S:23:GLN:HG3	2:S:84:LEU:HD21	1.95	0.48
2:S:35:LYS:O	2:S:35:LYS:CG	2.55	0.48
1:L:318:LEU:HG	1:L:326:ILE:HD12	1.94	0.48
1:L:26:THR:HB	1:L:28:GLU:OE1	2.14	0.48
1:L:315:ALA:HB1	1:L:349:LEU:HD21	1.96	0.48
1:L:62:SER:OG	1:L:82:GLY:N	2.35	0.48
1:L:414:ALA:O	1:L:418:VAL:HG23	2.15	0.47
1:L:422:VAL:HG23	1:L:455:LEU:HD22	1.96	0.47
1:L:175:LYS:HA	1:L:176:PRO:C	2.34	0.47
1:L:382:ILE:CG2	1:L:402:PHE:CE1	2.98	0.47
1:L:159:ARG:O	1:L:163:ASN:N	2.48	0.47
1:L:383:HIS:N	1:L:386:HIS:ND1	2.63	0.46
1:L:376:PRO:HD2	1:L:397:ASP:O	2.14	0.46
1:L:239:TYR:HB3	1:L:266:MET:HB2	1.97	0.46
2:S:79:ASP:C	2:S:81:THR:H	2.18	0.46
1:L:98:ILE:CD1	1:L:363:TYR:HE2	2.27	0.46
1:L:177:LYS:HE3	1:L:205:ASN:ND2	2.30	0.46
1:L:24:TYR:HB2	1:L:55:ALA:HB1	1.97	0.46
1:L:81:LYS:O	1:L:81:LYS:HG3	2.16	0.46
1:L:180:LEU:HA	1:L:180:LEU:HD12	1.56	0.46
1:L:42:VAL:CG1	1:L:97:TYR:HB2	2.46	0.46
1:L:296:ALA:O	1:L:297:MET:CB	2.64	0.45
2:S:79:ASP:O	2:S:81:THR:N	2.49	0.45
1:L:85:TYR:O	1:L:86:ARG:CB	2.63	0.45
1:L:169:LEU:O	1:L:399:VAL:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:43:THR:HG22	1:L:131:ARG:CB	2.45	0.45
1:L:172:CYS:SG	1:L:407:LEU:HD21	2.57	0.45
1:L:302:ASP:C	1:L:302:ASP:OD1	2.55	0.45
1:L:316:LYS:HE3	1:L:348:LEU:HD13	1.99	0.45
1:L:199:PHE:HB3	1:L:239:TYR:CE1	2.52	0.45
1:L:435:ARG:NH1	1:L:440:GLU:OE1	2.34	0.44
1:L:87:ILE:HG22	1:L:88:GLU:N	2.33	0.44
2:S:26:LEU:HD12	2:S:26:LEU:HA	1.81	0.44
1:L:318:LEU:HD13	1:L:318:LEU:O	2.18	0.44
2:S:106:ASN:OD1	2:S:107:VAL:N	2.51	0.44
1:L:34:THR:HB	1:L:105:LEU:HD22	1.99	0.44
1:L:448:ALA:HA	1:L:451:TRP:NE1	2.33	0.43
1:L:197:LEU:HD21	1:L:406:THR:HG21	2.00	0.43
1:L:293:ILE:HG13	1:L:318:LEU:HD21	2.00	0.43
1:L:133:LEU:O	1:L:307:HIS:HA	2.19	0.42
1:L:327:HIS:HA	1:L:377:VAL:HB	2.01	0.42
2:S:74:MET:HE3	2:S:83:VAL:HG22	2.00	0.42
1:L:141:PRO:HA	1:L:142:PRO:HD3	1.87	0.42
1:L:383:HIS:HB2	1:L:386:HIS:CE1	2.54	0.42
1:L:195:GLY:HA3	1:L:417:ALA:HB3	2.01	0.42
1:L:103:TYR:HA	1:L:104:PRO:HD3	1.79	0.42
2:S:79:ASP:O	2:S:82:GLN:N	2.48	0.42
1:L:319:ARG:HG3	1:L:374:VAL:HG23	2.02	0.42
1:L:36:ILE:HD13	1:L:108:PHE:CD2	2.54	0.42
2:S:10:LYS:HB3	2:S:50:PHE:CZ	2.55	0.42
1:L:89:ARG:HE	1:L:97:TYR:HE1	1.69	0.41
1:L:297:MET:HG2	1:L:297:MET:O	2.20	0.41
1:L:284:CYS:HB3	1:L:289:LEU:O	2.21	0.41
1:L:446:ARG:HD3	1:L:446:ARG:HH11	1.65	0.41
1:L:43:THR:CG2	1:L:131:ARG:HB3	2.48	0.41
1:L:387:MET:HG2	1:L:424:LEU:HA	2.01	0.41
1:L:156:GLN:HG3	2:S:110:VAL:CG1	2.50	0.41
1:L:178:LEU:HD21	1:L:205:ASN:CB	2.50	0.41
1:L:290:LEU:HA	1:L:324:ASP:OD2	2.20	0.41
1:L:50:PRO:HG3	1:L:97:TYR:CZ	2.55	0.41
1:L:429:LYS:HD3	2:S:18:LEU:HD13	2.03	0.41
1:L:229:GLN:HE21	1:L:236:LYS:H	1.68	0.41
1:L:306:ASN:ND2	1:L:307:HIS:HB2	2.36	0.41
2:S:40:PRO:CG	2:S:74:MET:HE3	2.45	0.40
1:L:239:TYR:CE2	1:L:292:HIS:CE1	3.09	0.40
1:L:98:ILE:HG22	1:L:100:TYR:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:89:ARG:HG3	1:L:97:TYR:CE1	2.55	0.40
1:L:178:LEU:HD23	1:L:206:VAL:HG12	2.04	0.40
1:L:185:TYR:O	1:L:189:VAL:HG23	2.22	0.40
1:L:358:ARG:HB3	1:L:358:ARG:HE	1.01	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:71:THR:OG1	1:L:175:LYS:O[7_556]	2.13	0.07

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	L	437/477 (92%)	413 (94%)	22 (5%)	2 (0%)	34	26
2	S	121/123 (98%)	112 (93%)	8 (7%)	1 (1%)	24	15
All	All	558/600 (93%)	525 (94%)	30 (5%)	3 (0%)	34	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	94	LYS
2	S	76	GLY
1	L	332	VAL

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	L	357/387 (92%)	330 (92%)	27 (8%)	16 10
2	S	110/110 (100%)	98 (89%)	12 (11%)	8 4
All	All	467/497 (94%)	428 (92%)	39 (8%)	14 8

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	22	LEU
1	L	28	GLU
1	L	60	GLU
1	L	74	LEU
1	L	77	LEU
1	L	78	ASP
1	L	79	ARG
1	L	87	ILE
1	L	91	VAL
1	L	128	LYS
1	L	185	TYR
1	L	192	CYS
1	L	197	LEU
1	L	225	LEU
1	L	239	TYR
1	L	258	ARG
1	L	303	ARG
1	L	314	LEU
1	L	334	LYS
1	L	335	LEU
1	L	336	GLU
1	L	358	ARG
1	L	359	SER
1	L	375	LEU
1	L	407	LEU
1	L	422	VAL
1	L	446	ARG
2	S	23	GLN
2	S	27	LEU
2	S	51	VAL
2	S	77	CYS
2	S	81	THR
2	S	89	GLU

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Mol	Chain	Res	Type
2	S	92	LYS
2	S	96	GLN
2	S	100	ARG
2	S	111	GLN
2	S	119	LYS
2	S	121	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	45	GLN
1	L	207	ASN
1	L	229	GLN
1	L	306	ASN
1	L	366	GLN
2	S	36	ASN
2	S	55	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is modelled with single atom - leaving 3 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	$\#\|Z\| > 2$
3	SO4	L	490	-	4,4,4	0.94	0	6,6,6	0.29	0
3	SO4	L	491	-	4,4,4	1.19	0	6,6,6	1.27	1 (16%)
3	SO4	L	492	-	4,4,4	1.10	0	6,6,6	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	L	490	-	-	0/0/0/0	0/0/0/0
3	SO4	L	491	-	-	0/0/0/0	0/0/0/0
3	SO4	L	492	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	491	SO4	O2-S-O1	-2.10	102.85	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	490	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.