



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:07 AM GMT

PDB ID : 1D6I
Title : CHALCONE SYNTHASE (H303Q MUTANT)
Authors : Jez, J.M.; Ferrer, J.L.; Bowman, M.E.; Dixon, R.A.; Noel, J.P.
Deposited on : 1999-10-13
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

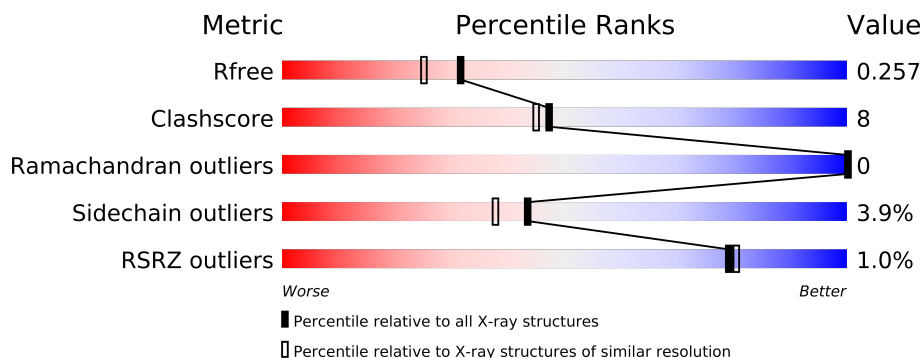
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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))
R_{free}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	388	
1	B	388	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6328 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

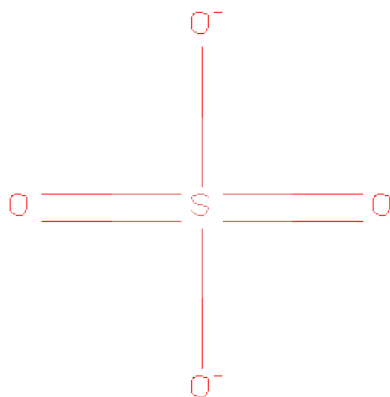
- Molecule 1 is a protein called CHALCONE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	1	0
			2996	1903	505	569	19			
1	B	388	Total	C	N	O	S	0	1	0
			2996	1903	505	569	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	303	GLN	HIS	ENGINEERED	UNP P30074
B	303	GLN	HIS	ENGINEERED	UNP P30074

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

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

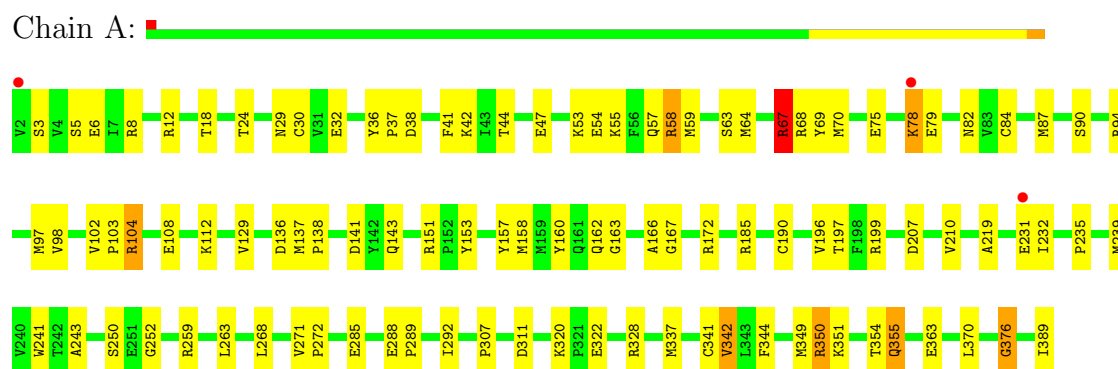
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	163	Total	O	0	0
			163	163		
3	B	163	Total	O	0	0
			163	163		

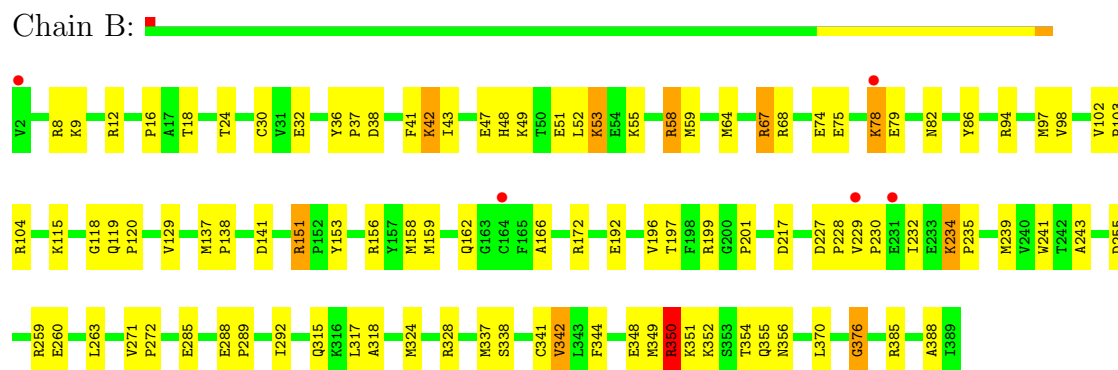
3 Residue-property plots

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

• Molecule 1: CHALCONE SYNTHASE



• Molecule 1: CHALCONE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	97.86Å 97.86Å 129.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	71.00 – 2.00 20.65 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.0 (71.00-2.00) 93.2 (20.65-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.196 , 0.269 0.200 , 0.257	Depositor DCC
R_{free} test set	2309 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 41.8	EDS
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 45648 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6328	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 80.67 % 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 4.2394e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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: CSD, 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	0.91	1/3027 (0.0%)	1.41	38/4095 (0.9%)
1	B	0.89	0/3027	1.41	40/4095 (1.0%)
All	All	0.90	1/6054 (0.0%)	1.41	78/8190 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	SER	CB-OG	5.29	1.49	1.42

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ARG	NE-CZ-NH1	14.00	127.30	120.30
1	A	376	GLY	O-C-N	-12.99	101.92	122.70
1	B	376	GLY	O-C-N	-12.96	101.96	122.70
1	B	12	ARG	NE-CZ-NH2	-12.35	114.13	120.30
1	B	67	ARG	NE-CZ-NH1	11.31	125.95	120.30
1	A	67	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	B	328	ARG	CD-NE-CZ	10.77	138.68	123.60
1	B	376	GLY	CA-C-N	10.22	139.69	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	PRO	N-CA-CB	10.09	115.41	103.30
1	B	388	ALA	C-N-CA	10.03	146.78	121.70
1	A	157	TYR	CB-CG-CD2	9.77	126.86	121.00
1	A	136	ASP	CB-CG-OD2	9.41	126.77	118.30
1	A	328	ARG	CD-NE-CZ	9.33	136.66	123.60
1	A	259	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	A	376	GLY	CA-C-N	8.29	135.43	117.20
1	A	172	ARG	NE-CZ-NH2	7.99	124.29	120.30
1	A	12	ARG	CD-NE-CZ	7.74	134.44	123.60
1	A	185	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	B	58	ARG	NE-CZ-NH2	7.67	124.14	120.30
1	B	12	ARG	CD-NE-CZ	7.47	134.06	123.60
1	A	58	ARG	NE-CZ-NH2	7.45	124.02	120.30
1	A	311	ASP	CB-CG-OD1	7.45	125.00	118.30
1	B	156	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	A	8	ARG	NE-CZ-NH2	7.31	123.96	120.30
1	B	137	MET	CG-SD-CE	-7.30	88.52	100.20
1	A	199	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	A	185	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	B	86	TYR	CB-CG-CD2	-7.11	116.73	121.00
1	B	172	ARG	NE-CZ-NH2	7.11	123.85	120.30
1	B	199	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	B	259	ARG	NH1-CZ-NH2	-6.95	111.75	119.40
1	B	104	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	B	385	ARG	NE-CZ-NH2	6.89	123.74	120.30
1	B	151	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	B	8	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	A	68	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	B	68	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	A	322	GLU	OE1-CD-OE2	6.61	131.24	123.30
1	A	137	MET	CG-SD-CE	-6.61	89.62	100.20
1	A	104	ARG	NE-CZ-NH2	6.51	123.55	120.30
1	B	138	PRO	CA-N-CD	-6.44	102.49	111.50
1	A	138	PRO	N-CA-CB	6.40	110.98	103.30
1	A	94	ARG	NE-CZ-NH2	6.35	123.47	120.30
1	A	143	GLN	CA-CB-CG	6.29	127.23	113.40
1	B	217	ASP	CB-CG-OD1	6.24	123.91	118.30
1	A	59	MET	CG-SD-CE	6.21	110.14	100.20
1	B	337	MET	CG-SD-CE	6.14	110.03	100.20
1	B	94	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	A	70	MET	CG-SD-CE	6.11	109.98	100.20
1	A	87	MET	CG-SD-CE	6.05	109.87	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	TYR	CB-CG-CD1	-6.04	117.37	121.00
1	B	97	MET	CG-SD-CE	6.04	109.86	100.20
1	A	239	MET	CG-SD-CE	6.01	109.82	100.20
1	B	64	MET	CG-SD-CE	5.96	109.73	100.20
1	A	12	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	349	MET	CG-SD-CE	5.92	109.68	100.20
1	B	255	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	239	MET	CG-SD-CE	5.89	109.62	100.20
1	A	337	MET	CG-SD-CE	5.87	109.59	100.20
1	B	328	ARG	CG-CD-NE	5.86	124.10	111.80
1	A	97	MET	CG-SD-CE	5.77	109.43	100.20
1	B	349	MET	CG-SD-CE	5.69	109.30	100.20
1	B	159	MET	CG-SD-CE	5.66	109.26	100.20
1	B	324	MET	CG-SD-CE	5.65	109.24	100.20
1	B	138	PRO	N-CD-CG	5.56	111.54	103.20
1	B	350	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	A	350	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	B	158	MET	CG-SD-CE	5.40	108.83	100.20
1	A	311	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	B	59	MET	CG-SD-CE	5.36	108.78	100.20
1	A	136	ASP	OD1-CG-OD2	-5.29	113.24	123.30
1	A	160	TYR	CD1-CE1-CZ	5.27	124.55	119.80
1	A	160	TYR	CG-CD1-CE1	-5.19	117.14	121.30
1	A	158	MET	CG-SD-CE	5.15	108.44	100.20
1	B	255	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	B	260	GLU	OE1-CD-OE2	5.10	129.42	123.30
1	A	363	GLU	CG-CD-OE1	5.07	128.44	118.30
1	B	388	ALA	O-C-N	-5.00	114.70	122.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	GLY	Peptide
1	A	167	GLY	Mainchain
1	A	376	GLY	Mainchain
1	B	118	GLY	Mainchain
1	B	376	GLY	Mainchain
1	B	82[2]	ASN	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2996	0	3037	44	0
1	B	2996	0	3036	52	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	163	0	0	3	0
3	B	163	0	0	3	0
All	All	6328	0	6073	96	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (96) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:229:VAL:HG12	1:B:232:ILE:HG13	1.39	0.99
1:B:342:VAL:HG13	1:B:370:LEU:HD11	1.58	0.84
1:A:82[1]:ASN:CG	3:A:551:HOH:O	2.17	0.83
1:A:18:THR:HG21	1:A:235:PRO:HB3	1.61	0.83
1:A:342:VAL:HG13	1:A:370:LEU:HD11	1.62	0.80
1:A:42:LYS:HG2	1:A:47:GLU:CD	2.03	0.79
1:B:18:THR:HG21	1:B:235:PRO:HB3	1.73	0.70
1:B:229:VAL:CG1	1:B:232:ILE:HG13	2.20	0.69
1:B:234:LYS:HE2	3:B:533:HOH:O	1.92	0.68
1:B:42:LYS:NZ	1:B:47:GLU:OE2	2.28	0.66
1:A:231:GLU:O	1:A:232:ILE:HD13	1.97	0.65
1:B:98:VAL:HG11	1:B:196:VAL:HG23	1.78	0.65
1:B:75:GLU:O	1:B:78:LYS:HD2	1.97	0.64
1:A:102:VAL:HB	1:A:103:PRO:HD3	1.80	0.64
1:A:54:GLU:O	1:A:58:ARG:HG3	1.98	0.63
1:B:55:LYS:HA	1:B:58:ARG:HE	1.62	0.63
1:B:42:LYS:HG3	1:B:47:GLU:OE2	1.99	0.62
1:A:342:VAL:HB	3:A:489:HOH:O	1.97	0.62
1:A:78:LYS:O	1:A:78:LYS:HG2	1.99	0.60
1:B:348:GLU:OE2	1:B:352:LYS:HE2	2.02	0.60
1:A:63:SER:O	1:A:307:PRO:HG3	2.01	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:75:GLU:O	1:A:79:GLU:HG3	2.03	0.58
1:A:3:SER:OG	1:A:6:GLU:HG3	2.04	0.58
1:B:55:LYS:HA	1:B:58:ARG:NE	2.19	0.57
1:A:82[1]:ASN:HB2	1:A:90:SER:HB3	1.85	0.56
1:B:102:VAL:HB	1:B:103:PRO:HD3	1.85	0.56
1:A:288:GLU:N	1:A:289:PRO:HD2	2.21	0.56
1:B:38:ASP:O	1:B:42:LYS:HD3	2.07	0.55
1:A:98:VAL:HG11	1:A:196:VAL:HG23	1.89	0.55
1:A:32:GLU:OE2	1:A:67:ARG:HD3	2.07	0.54
1:A:197:THR:CG2	1:A:263:LEU:HD23	2.38	0.53
1:B:42:LYS:CE	1:B:47:GLU:OE2	2.56	0.53
1:A:82[1]:ASN:ND2	3:A:551:HOH:O	2.40	0.52
1:A:162:GLN:HB3	1:A:166:ALA:HB2	1.91	0.51
1:B:192:GLU:HG3	1:B:338:SER:HB3	1.92	0.51
1:B:355:GLN:HG2	1:B:356:ASN:ND2	2.26	0.51
1:B:129:VAL:HG21	1:B:141:ASP:HA	1.91	0.51
1:A:351:LYS:O	1:A:355:GLN:HB3	2.10	0.51
1:B:42:LYS:CD	1:B:47:GLU:OE2	2.58	0.51
1:B:115:LYS:NZ	3:B:540:HOH:O	2.44	0.51
1:A:129:VAL:HG21	1:A:141:ASP:HA	1.93	0.50
1:A:288:GLU:N	1:A:289:PRO:CD	2.74	0.50
1:A:18:THR:CG2	1:A:235:PRO:HB3	2.37	0.49
1:B:271:VAL:N	1:B:272:PRO:HD2	2.27	0.49
1:B:197:THR:HG23	1:B:263:LEU:HD23	1.95	0.49
1:B:78:LYS:HD2	1:B:79:GLU:HG3	1.95	0.48
1:B:24:THR:HB	1:B:344:PHE:CZ	2.48	0.48
1:A:41:PHE:CG	1:A:53:LYS:HG3	2.49	0.48
1:A:64:MET:HE2	1:A:64:MET:HA	1.96	0.47
1:B:74:GLU:O	1:B:78:LYS:HG3	2.14	0.47
1:B:52:LEU:HD21	1:B:201:PRO:HB2	1.97	0.46
1:B:162:GLN:HB3	1:B:166:ALA:HB2	1.98	0.46
1:B:288:GLU:N	1:B:289:PRO:HD2	2.30	0.46
1:A:252:GLY:O	1:A:268:LEU:HB2	2.16	0.46
1:B:317:LEU:O	1:B:318:ALA:HB3	2.15	0.45
1:B:32:GLU:OE2	1:B:67:ARG:HD3	2.17	0.45
1:B:228:PRO:O	1:B:230:PRO:HD3	2.16	0.45
1:A:241:TRP:CH2	1:A:243:ALA:HB2	2.51	0.45
1:B:18:THR:CG2	1:B:235:PRO:HB3	2.43	0.45
1:B:42:LYS:CG	1:B:47:GLU:OE2	2.64	0.45
1:A:37:PRO:HG2	1:A:57:GLN:OE1	2.17	0.45
1:B:48:HIS:CD2	1:B:49:LYS:HG2	2.52	0.44
1:B:43:ILE:HD13	1:B:74:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:197:THR:CG2	1:B:263:LEU:HD23	2.46	0.44
1:A:271:VAL:HB	1:A:272:PRO:HD3	1.98	0.44
1:A:38:ASP:O	1:A:42:LYS:HG3	2.17	0.44
1:A:24:THR:HB	1:A:344:PHE:CZ	2.52	0.44
1:B:241:TRP:CH2	1:B:243:ALA:HB2	2.53	0.44
1:B:151:ARG:HD3	1:B:153:TYR:CZ	2.53	0.44
1:B:119:GLN:HB3	1:B:120:PRO:HD2	1.99	0.44
1:A:104:ARG:NH1	1:A:108:GLU:OE2	2.49	0.43
1:B:288:GLU:N	1:B:289:PRO:CD	2.82	0.43
1:B:41:PHE:CG	1:B:53:LYS:HG2	2.53	0.43
1:A:29:ASN:O	1:A:69:TYR:HA	2.18	0.43
1:A:108:GLU:O	1:A:112:LYS:HG3	2.18	0.43
1:B:272:PRO:HG2	3:B:447:HOH:O	2.19	0.43
1:A:151:ARG:HD2	1:A:153:TYR:OH	2.19	0.43
1:A:207:ASP:O	1:A:210:VAL:HB	2.19	0.42
1:B:241:TRP:HH2	1:B:285:GLU:HG2	1.84	0.42
1:B:288:GLU:HB3	1:B:289:PRO:HD3	2.00	0.42
1:B:30:CYS:SG	1:B:67:ARG:HD2	2.59	0.42
1:B:227:ASP:N	1:B:228:PRO:HD3	2.34	0.42
1:A:102:VAL:HB	1:A:103:PRO:CD	2.48	0.42
1:B:271:VAL:N	1:B:272:PRO:CD	2.82	0.41
1:A:36:TYR:N	1:A:37:PRO:HD2	2.35	0.41
1:A:64:MET:HA	1:A:64:MET:CE	2.49	0.41
1:B:36:TYR:N	1:B:37:PRO:CD	2.83	0.41
1:A:30:CYS:SG	1:A:67:ARG:HD2	2.60	0.41
1:A:41:PHE:CZ	1:A:53:LYS:HA	2.55	0.41
1:A:42:LYS:HG2	1:A:47:GLU:OE2	2.20	0.41
1:B:351:LYS:O	1:B:355:GLN:HB3	2.20	0.41
1:A:44:THR:HA	1:A:84:CYS:HB3	2.03	0.41
1:B:271:VAL:HB	1:B:272:PRO:HD3	2.03	0.41
1:B:342:VAL:HG11	1:B:370:LEU:HD21	2.02	0.40
1:A:190:CYS:O	1:A:219:ALA:HA	2.22	0.40
1:B:350:ARG:O	1:B:354:THR:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/388 (100%)	375 (97%)	11 (3%)	0	100	100
1	B	386/388 (100%)	370 (96%)	16 (4%)	0	100	100
All	All	772/776 (100%)	745 (96%)	27 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	322/323 (100%)	309 (96%)	13 (4%)	42	36
1	B	322/323 (100%)	310 (96%)	12 (4%)	45	40
All	All	644/646 (100%)	619 (96%)	25 (4%)	43	38

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	55	LYS
1	A	67	ARG
1	A	78	LYS
1	A	285	GLU
1	A	292	ILE
1	A	320	LYS
1	A	341	CYS
1	A	342	VAL
1	A	350	ARG
1	A	354	THR
1	A	355	GLN
1	A	389	ILE
1	B	9	LYS
1	B	16	PRO
1	B	42	LYS
1	B	51	GLU

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Mol	Chain	Res	Type
1	B	53	LYS
1	B	78	LYS
1	B	234	LYS
1	B	292	ILE
1	B	315	GLN
1	B	341	CYS
1	B	342	VAL
1	B	350	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	A	356	ASN
1	B	312	GLN
1	B	356	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 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	CSD	A	164	1	7,7,8	7.26	2 (28%)	6,8,10	1.74	1 (16%)
1	CSD	B	164	1	7,7,8	7.24	2 (28%)	6,8,10	1.74	1 (16%)

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	CSD	A	164	1	-	0/3/6/8	0/0/0/0
1	CSD	B	164	1	-	0/3/6/8	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	CSD	O-C	19.01	1.24	1.11
1	B	164	CSD	O-C	18.94	1.24	1.11
1	B	164	CSD	CA-C	2.17	1.52	1.48
1	A	164	CSD	CA-C	2.13	1.52	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	CSD	OD2-SG-OD1	3.30	114.87	109.39
1	A	164	CSD	OD2-SG-OD1	3.30	114.86	109.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	$\# Z > 2$
2	SO4	A	390	-	4,4,4	1.12	0	6,6,6	0.25	0
2	SO4	B	391	-	4,4,4	1.04	0	6,6,6	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	390	-	-	0/0/0/0	0/0/0/0
2	SO4	B	391	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	388/388 (100%)	-0.21	3 (0%) 83 84	15, 26, 39, 54	0
1	B	388/388 (100%)	-0.22	5 (1%) 74 74	13, 26, 40, 52	0
All	All	776/776 (100%)	-0.21	8 (1%) 79 80	13, 26, 40, 54	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	GLU	3.1
1	A	78	LYS	2.8
1	A	2	VAL	2.7
1	B	231	GLU	2.4
1	B	164	CSD	2.3
1	B	78	LYS	2.2
1	B	2	VAL	2.2
1	B	229	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CSD	B	164	8/9	0.20	2.76	2,12,17,22	0
1	CSD	A	164	8/9	0.15	1.83	11,12,17,22	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	390	5/5	0.12	-0.67	36,38,38,39	0
2	SO4	B	391	5/5	0.11	-1.02	39,40,40,41	0

6.5 Other polymers

There are no such residues in this entry.