



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:46 AM UTC

PDB ID : 1D6I / pdb_00001d6i
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 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

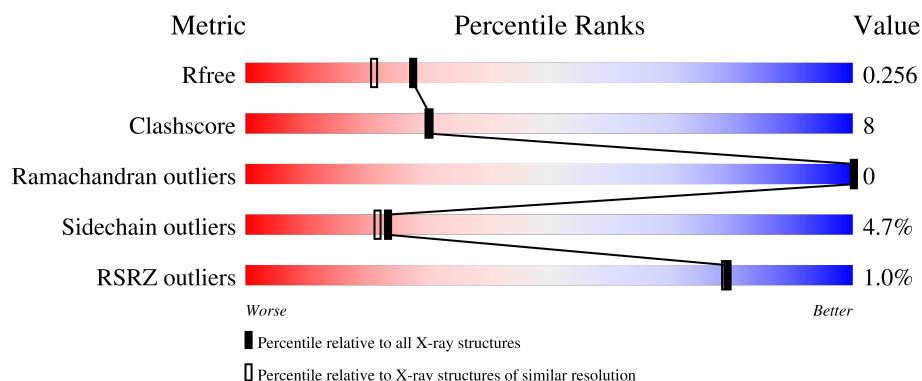
1 Overall quality at a glance

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))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	388	% 73% 24% .
1	B	388	% 73% 23% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6328 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 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 mutation	UNP P30074
B	303	GLN	HIS	engineered mutation	UNP P30074

- Molecule 2 is SULFATE ION (CCD ID: 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		

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 71.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.0 (71.00-2.00) 93.1 (71.00-2.00)	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 0.199 , 0.256	Depositor DCC
R_{free} test set	2309 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.07	3/3027 (0.1%)	1.64	35/4095 (0.9%)
1	B	1.02	4/3027 (0.1%)	1.64	49/4095 (1.2%)
All	All	1.05	7/6054 (0.1%)	1.64	84/8190 (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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	241	TRP	NE1-CE2	-5.41	1.31	1.37
1	A	241	TRP	NE1-CE2	-5.33	1.31	1.37
1	B	367	TRP	NE1-CE2	-5.31	1.31	1.37
1	A	117	TRP	NE1-CE2	-5.25	1.31	1.37
1	B	164	CSD	C-N	5.18	1.40	1.33
1	B	300	TRP	NE1-CE2	-5.17	1.31	1.37
1	A	300	TRP	NE1-CE2	-5.13	1.31	1.37

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	GLY	O-C-N	-15.99	101.92	122.70
1	B	376	GLY	O-C-N	-15.96	101.96	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	388	ALA	CA-C-N	13.93	146.78	121.70
1	B	388	ALA	C-N-CA	13.93	146.78	121.70
1	B	265	PHE	CA-CB-CG	12.00	125.80	113.80
1	B	138	PRO	N-CA-CB	11.64	115.41	102.60
1	B	137	MET	CA-C-O	-10.53	109.75	119.86
1	B	328	ARG	CD-NE-CZ	10.20	138.68	124.40
1	A	137	MET	CA-C-O	-9.99	110.27	119.86
1	B	137	MET	O-C-N	8.92	129.94	121.38
1	A	328	ARG	CD-NE-CZ	8.76	136.66	124.40
1	A	137	MET	O-C-N	8.56	129.60	121.38
1	B	45	ASN	CB-CA-C	-7.69	100.57	111.80
1	A	138	PRO	N-CA-CB	7.62	110.98	102.60
1	A	249	ASP	CA-CB-CG	-7.24	105.36	112.60
1	A	12	ARG	CD-NE-CZ	7.17	134.44	124.40
1	B	12	ARG	CD-NE-CZ	6.90	134.06	124.40
1	A	167	GLY	N-CA-C	-6.88	103.96	112.77
1	A	338	SER	CB-CA-C	-6.77	108.77	116.63
1	B	119	GLN	OE1-CD-NE2	6.70	129.30	122.60
1	B	26	ASN	CB-CG-ND2	6.67	126.41	116.40
1	B	388	ALA	O-C-N	-6.66	114.70	122.95
1	B	26	ASN	O-C-N	6.59	125.93	121.71
1	A	143	GLN	CA-CB-CG	6.57	127.23	114.10
1	B	138	PRO	N-CD-CG	6.45	111.54	103.80
1	B	138	PRO	CA-N-CD	-6.44	102.49	111.50
1	B	338	SER	CB-CA-C	-6.25	109.36	116.54
1	B	236	ILE	O-C-N	-6.24	117.11	121.85
1	A	315	GLN	OE1-CD-NE2	-6.17	116.43	122.60
1	A	265	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	127	LEU	CA-C-N	-6.03	115.72	123.19
1	A	127	LEU	C-N-CA	-6.03	115.72	123.19
1	B	187	LEU	CA-C-O	-5.98	114.32	120.54
1	B	128	ILE	CA-C-N	-5.97	114.82	123.06
1	B	128	ILE	C-N-CA	-5.97	114.82	123.06
1	A	251	GLU	CA-CB-CG	-5.81	102.47	114.10
1	B	259	ARG	NH1-CZ-NH2	-5.81	111.75	119.30
1	B	259	ARG	NE-CZ-NH1	5.80	127.30	121.50
1	A	138	PRO	CA-C-N	-5.78	116.54	122.27
1	A	138	PRO	C-N-CA	-5.78	116.54	122.27
1	A	172	ARG	NE-CZ-NH2	5.66	124.29	119.20
1	A	135	VAL	O-C-N	-5.66	116.78	123.00
1	B	12	ARG	NE-CZ-NH2	-5.64	114.13	119.20
1	B	137	MET	CG-SD-CE	-5.63	88.52	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ALA	N-CA-C	5.60	117.38	111.28
1	B	31	VAL	N-CA-C	5.59	115.64	107.37
1	B	328	ARG	CG-CD-NE	5.50	124.10	112.00
1	B	58	ARG	NE-CZ-NH2	5.48	124.14	119.20
1	A	311	ASP	O-C-N	5.48	128.40	122.15
1	B	118	GLY	CA-C-O	-5.46	112.96	119.07
1	A	201	PRO	CB-CA-C	-5.42	102.88	110.63
1	B	217	ASP	CA-C-O	-5.37	114.91	121.36
1	A	104	ARG	CA-C-O	5.37	126.46	120.82
1	A	58	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	B	180	ASN	OD1-CG-ND2	5.34	127.94	122.60
1	B	156	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	A	327	THR	N-CA-C	-5.29	105.41	111.07
1	A	8	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	B	38	ASP	CA-CB-CG	-5.28	107.32	112.60
1	B	232	ILE	O-C-N	5.28	125.86	121.85
1	A	199	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	A	22	ILE	CA-C-O	-5.26	114.70	120.43
1	B	27	PRO	CB-CA-C	-5.24	104.52	111.23
1	B	71	TYR	O-C-N	5.24	127.47	122.07
1	B	167	GLY	N-CA-C	-5.21	106.47	112.73
1	B	26	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	A	130	CYS	CA-C-O	-5.18	114.57	120.32
1	B	172	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	B	199	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	A	315	GLN	CB-CG-CD	5.15	121.36	112.60
1	A	388	ALA	CA-C-N	5.13	130.94	121.70
1	A	388	ALA	C-N-CA	5.13	130.94	121.70
1	A	137	MET	CG-SD-CE	-5.12	89.62	100.90
1	B	162	GLN	N-CA-C	5.12	117.65	111.40
1	A	81	PRO	N-CA-C	-5.11	106.75	113.65
1	B	232	ILE	CB-CA-C	-5.10	107.38	111.71
1	B	25	ALA	O-C-N	-5.08	117.58	123.33
1	B	375	PRO	O-C-N	-5.08	116.44	122.89
1	B	104	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	B	385	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	B	216	GLY	O-C-N	-5.04	118.88	123.57
1	A	249	ASP	CB-CA-C	-5.03	104.45	111.80
1	B	201	PRO	CB-CA-C	-5.03	103.44	110.63
1	B	151	ARG	NE-CZ-NH2	5.01	123.71	119.20

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 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	2996	0	3037	46	0
1	B	2996	0	3037	55	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	6074	101	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 8.

All (101) 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:B:229:VAL:HG12	1:B:232:ILE:HG13	1.39	0.99
1:A:82[1]:ASN:CG	3:A:551:HOH:O	2.17	0.86
1:B:342:VAL:HG13	1:B:370:LEU:HD11	1.58	0.84
1:A:42:LYS:HG2	1:A:47:GLU:CD	2.03	0.84
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: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:A:64:MET:HA	1:A:64:MET:HE2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:129:VAL:HG21	1:B:141:ASP:HA	1.91	0.51
1:B:355:GLN:HG2	1:B:356:ASN:ND2	2.26	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:42:LYS:HZ2	1:B:47:GLU:CD	2.19	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:B:74:GLU:O	1:B:78:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:37:PRO:HG2	1:A:57:GLN:OE1	2.17	0.45
1:B:42:LYS:CG	1:B:47:GLU:OE2	2.64	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
1:B:197:THR:CG2	1:B:263:LEU:HD23	2.46	0.44
1:A:71:TYR:CD2	1:A:71:TYR:C	2.95	0.44
1:A:271:VAL:HB	1:A:272:PRO:HD3	1.98	0.44
1:A:24:THR:HB	1:A:344:PHE:CZ	2.52	0.44
1:A:38:ASP:O	1:A:42:LYS:HG3	2.17	0.44
1:B:241:TRP:CH2	1:B:243:ALA:HB2	2.53	0.44
1:B:119:GLN:HB3	1:B:120:PRO:HD2	1.99	0.44
1:B:151:ARG:HD3	1:B:153:TYR:CZ	2.53	0.44
1:A:104:ARG:NH1	1:A:108:GLU:OE2	2.49	0.43
1:B:41:PHE:CG	1:B:53:LYS:HG2	2.53	0.43
1:B:288:GLU:N	1:B:289:PRO:CD	2.82	0.43
1:A:63:SER:C	1:A:307:PRO:HG3	2.42	0.43
1:A:29:ASN:O	1:A:69:TYR:HA	2.18	0.43
1:B:377:LEU:HD23	1:B:377:LEU:C	2.44	0.43
1:A:108:GLU:O	1:A:112:LYS:HG3	2.18	0.43
1:A:151:ARG:HD2	1:A:153:TYR:OH	2.19	0.43
1:B:272:PRO:HG2	3:B:447:HOH:O	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:A:64:MET:HE2	1:A:64:MET:CA	2.48	0.42
1:A:36:TYR:N	1:A:37:PRO:HD2	2.35	0.41
1:B:271:VAL:N	1:B:272:PRO:CD	2.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:44:THR:HA	1:A:84:CYS:HB3	2.03	0.41
1:B:351:LYS:O	1:B:355:GLN:HB3	2.20	0.41
1:B:271:VAL:HB	1:B:272:PRO:HD3	2.03	0.41
1:B:230:PRO:C	1:B:232:ILE:H	2.28	0.40
1:A:190:CYS:O	1:A:219:ALA:HA	2.22	0.40
1:B:342:VAL:HG11	1:B:370:LEU:HD21	2.02	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 [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	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 [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	322/323 (100%)	306 (95%)	16 (5%)	22	20
1	B	322/323 (100%)	308 (96%)	14 (4%)	26	25
All	All	644/646 (100%)	614 (95%)	30 (5%)	23	22

All (30) 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	115	LYS
1	A	210	VAL
1	A	269	LYS
1	A	284	VAL
1	A	285	GLU
1	A	292	ILE
1	A	320	LYS
1	A	341	CYS
1	A	342	VAL
1	A	354	THR
1	A	355	GLN
1	A	389	ILE
1	B	9	LYS
1	B	42	LYS
1	B	51	GLU
1	B	53	LYS
1	B	78	LYS
1	B	115	LYS
1	B	151	ARG
1	B	232	ILE
1	B	234	LYS
1	B	284	VAL
1	B	292	ILE
1	B	315	GLN
1	B	341	CYS
1	B	342	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	356	ASN
1	B	181	ASN
1	B	312	GLN
1	B	356	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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	4,7,8	1.33	1 (25%)	1,8,10	1.60	0
1	CSD	B	164	1	4,7,8	1.36	1 (25%)	1,8,10	1.60	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
1	CSD	A	164	1	-	0/2/6/8	-
1	CSD	B	164	1	-	0/2/6/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	CSD	OD1-SG	-2.30	1.45	1.47
1	A	164	CSD	OD1-SG	-2.22	1.45	1.47

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.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	391	-	4,4,4	0.64	0	6,6,6	0.33	0
2	SO4	A	390	-	4,4,4	0.73	0	6,6,6	0.42	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 ⓘ

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	387/388 (99%)	-0.03	5 (1%) 75 74	14, 26, 39, 54	1 (0%)
1	B	387/388 (99%)	-0.04	3 (0%) 82 82	14, 26, 40, 52	1 (0%)
All	All	774/776 (99%)	-0.03	8 (1%) 79 79	14, 26, 40, 54	2 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	LEU	3.6
1	B	389	ILE	3.0
1	B	58	ARG	2.9
1	A	354	THR	2.9
1	B	82[1]	ASN	2.6
1	A	389	ILE	2.5
1	A	78	LYS	2.5
1	A	357	GLY	2.2

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	CSD	B	164	8/9	0.89	0.20	2,12,17,22	0
1	CSD	A	164	8/9	0.93	0.15	11,12,17,22	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	SO4	B	391	5/5	0.95	0.07	39,40,40,41	0
2	SO4	A	390	5/5	0.96	0.06	36,38,38,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.