



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:43 AM UTC

PDB ID : 1EG9 / pdb_00001eg9
Title : NAPHTHALENE 1,2-DIOXYGENASE WITH INDOLE BOUND IN THE ACTIVE SITE.
Authors : Carredano, E.; Karlsson, A.; Kauppi, B.; Choudhury, D.; Parales, R.E.; Parales, J.V.; Lee, K.; Gibson, D.T.; Eklund, H.; Ramaswamy, S.
Deposited on : 2000-02-15
Resolution : 1.60 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

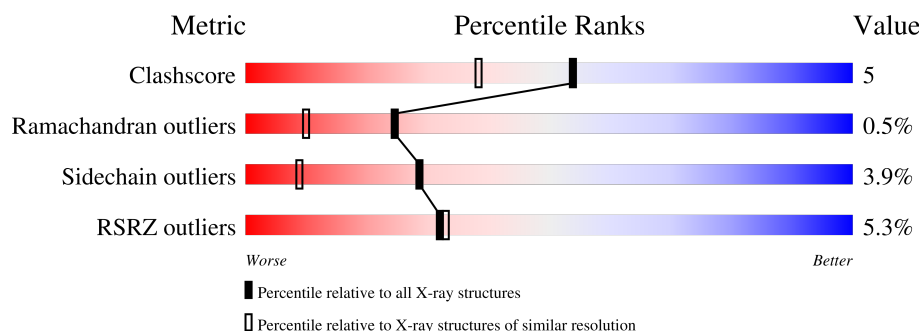
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	449	4% 82% 16% .
2	B	194	9% 71% 23% 5% ..

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5729 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.

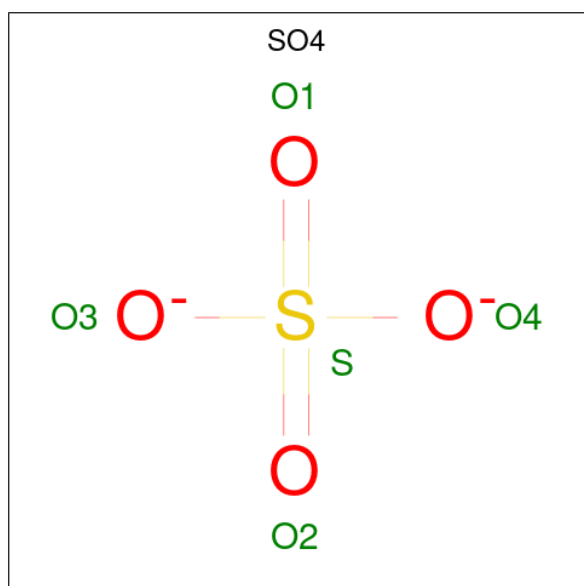
- Molecule 1 is a protein called PROTEIN (NAPHTHALENE 1,2-DIOXYGENASE ALPHA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3480	2202	597	665	16			

- Molecule 2 is a protein called PROTEIN (NAPHTHALENE 1,2-DIOXYGENASE BETA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	193	Total	C	N	O	S	0	0	0
			1608	1007	302	293	6			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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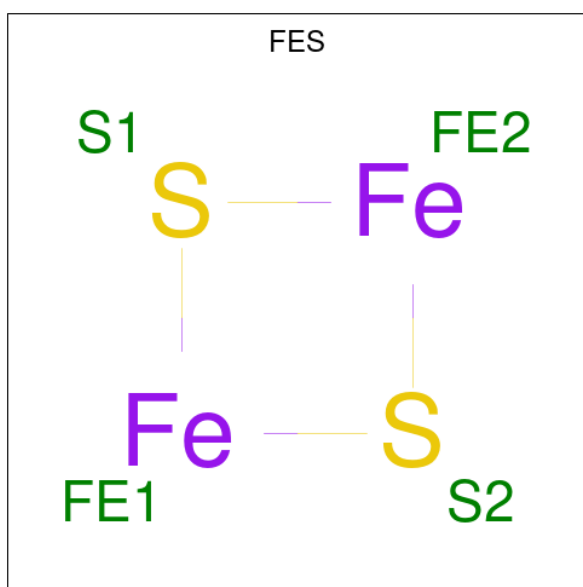
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

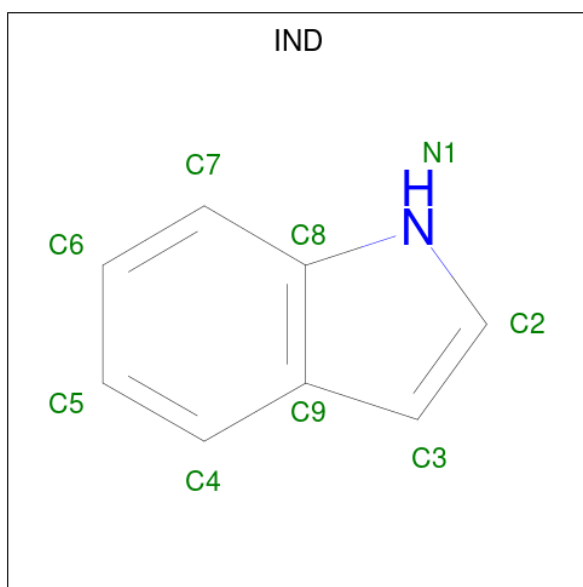
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Fe	0	0
			1	1		

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 6 is INDOLE (CCD ID: IND) (formula: C₈H₇N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			9	8	1		

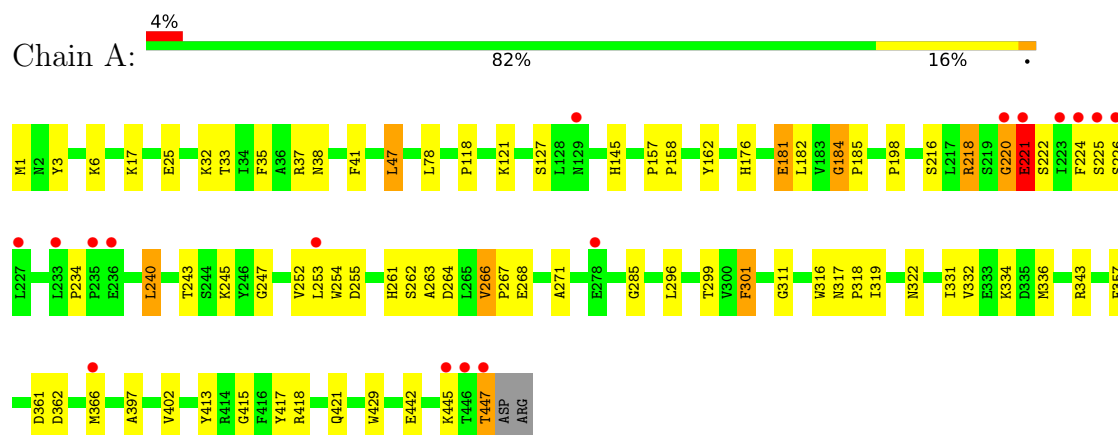
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	430	Total	O	0	0
			430	430		
7	B	182	Total	O	0	0
			182	182		

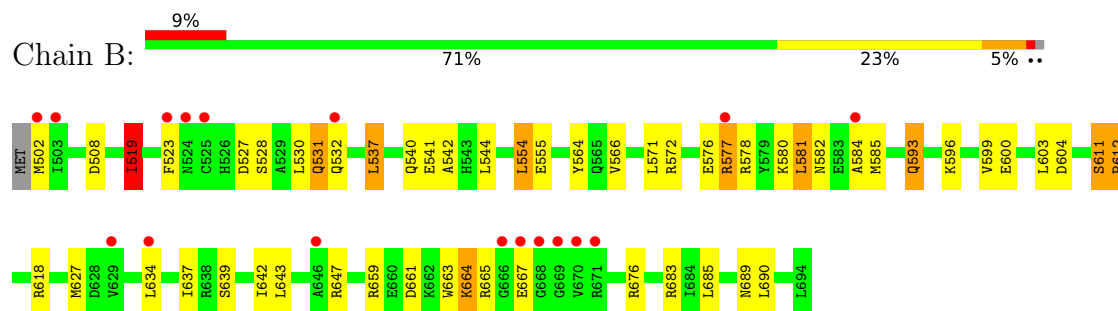
3 Residue-property plots [i](#)

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: PROTEIN (NAPHTHALENE 1,2-DIOXYGENASE ALPHA SUBUNIT)



- Molecule 2: PROTEIN (NAPHTHALENE 1,2-DIOXYGENASE BETA SUBUNIT)



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	140.17Å 140.17Å 209.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.60 20.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.60) 99.3 (20.00-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.220 0.177 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.1	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5729	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SO4, FE, IND, FES

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	0.81	1/3572 (0.0%)	1.65	56/4839 (1.2%)
2	B	0.91	0/1638	1.81	47/2209 (2.1%)
All	All	0.84	1/5210 (0.0%)	1.70	103/7048 (1.5%)

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	8
2	B	0	4
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	318	PRO	CA-CB	5.38	1.60	1.53

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	611	SER	CA-C-O	-11.78	105.91	120.04
1	A	225	SER	N-CA-C	11.00	124.44	111.02
2	B	527	ASP	CA-CB-CG	10.25	122.85	112.60
1	A	184	GLY	CA-C-O	-9.99	107.23	121.52
1	A	264	ASP	CA-CB-CG	9.38	121.98	112.60
1	A	271	ALA	CA-C-O	-9.08	110.79	120.42
2	B	665	ARG	CA-C-O	-8.82	111.20	120.55
1	A	184	GLY	CA-C-N	8.51	129.14	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	GLY	C-N-CA	8.51	129.14	120.38
1	A	221	GLU	CA-C-O	8.42	132.54	120.51
2	B	661	ASP	CA-CB-CG	8.28	120.88	112.60
2	B	618	ARG	NE-CZ-NH1	-8.25	113.25	121.50
2	B	647	ARG	O-C-N	8.14	131.51	123.46
2	B	612	PRO	N-CA-CB	8.01	111.41	102.60
2	B	639	SER	O-C-N	7.96	131.93	123.42
1	A	218	ARG	CD-NE-CZ	7.68	135.15	124.40
1	A	429	TRP	CB-CG-CD1	7.65	138.37	126.90
1	A	185	PRO	N-CA-CB	7.60	110.45	103.08
1	A	218	ARG	NE-CZ-NH2	-7.53	112.42	119.20
2	B	540	GLN	O-C-N	7.50	130.70	122.15
1	A	185	PRO	CA-N-CD	-7.30	101.78	112.00
2	B	611	SER	O-C-N	7.29	128.52	121.66
1	A	262	SER	CA-C-N	7.24	130.96	120.38
1	A	262	SER	C-N-CA	7.24	130.96	120.38
2	B	618	ARG	NE-CZ-NH2	7.20	125.68	119.20
2	B	637	ILE	O-C-N	7.12	130.88	123.20
1	A	262	SER	CA-C-O	7.11	130.06	122.03
2	B	647	ARG	NE-CZ-NH2	7.04	125.53	119.20
2	B	659	ARG	CD-NE-CZ	-6.84	114.83	124.40
1	A	317	ASN	CA-C-O	6.83	124.72	119.46
1	A	421	GLN	N-CA-CB	6.80	119.86	110.01
2	B	537	LEU	O-C-N	6.68	128.95	122.07
1	A	224	PHE	CA-C-N	6.64	130.02	120.79
1	A	224	PHE	C-N-CA	6.64	130.02	120.79
1	A	318	PRO	CA-C-N	-6.61	116.15	123.16
1	A	318	PRO	C-N-CA	-6.61	116.15	123.16
2	B	604	ASP	CA-C-N	6.59	126.28	119.56
2	B	604	ASP	C-N-CA	6.59	126.28	119.56
2	B	612	PRO	CA-N-CD	-6.51	102.38	111.50
1	A	157	PRO	N-CA-CB	6.48	109.37	103.08
1	A	225	SER	CB-CA-C	-6.39	100.77	110.92
2	B	544	LEU	O-C-N	6.38	128.64	122.07
1	A	397	ALA	CA-C-N	-6.35	116.50	122.66
1	A	397	ALA	C-N-CA	-6.35	116.50	122.66
2	B	572	ARG	CD-NE-CZ	6.29	133.20	124.40
1	A	221	GLU	CB-CG-CD	6.25	123.22	112.60
2	B	540	GLN	CA-C-O	-6.22	113.83	120.42
2	B	611	SER	CB-CA-C	6.22	118.21	108.88
2	B	639	SER	CA-C-O	-6.11	114.70	121.23
1	A	218	ARG	NE-CZ-NH1	6.07	127.57	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	612	PRO	N-CD-CG	6.04	111.04	103.80
2	B	685	LEU	CA-C-O	-5.99	114.45	121.16
2	B	585	MET	O-C-N	-5.96	115.32	122.65
2	B	643	LEU	CA-C-O	-5.95	113.93	120.30
1	A	413	TYR	CA-CB-CG	5.92	124.56	113.90
1	A	261	HIS	CA-CB-CG	-5.91	107.89	113.80
1	A	33	THR	CA-C-O	5.88	126.15	119.27
1	A	266	VAL	O-C-N	-5.84	114.44	121.10
1	A	262	SER	O-C-N	-5.82	115.82	122.68
1	A	299	THR	O-C-N	5.78	130.17	123.30
2	B	584	ALA	CA-C-N	-5.74	109.18	121.45
2	B	584	ALA	C-N-CA	-5.74	109.18	121.45
1	A	362	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	145	HIS	CA-CB-CG	-5.67	108.13	113.80
1	A	429	TRP	CD2-CE3-CZ3	5.62	125.91	118.60
2	B	643	LEU	O-C-N	5.62	129.79	123.27
1	A	176	HIS	CA-CB-CG	-5.61	108.19	113.80
1	A	357	PHE	CA-CB-CG	5.61	119.41	113.80
2	B	593	GLN	CB-CG-CD	5.59	122.10	112.60
1	A	322	ASN	CA-CB-CG	5.58	118.18	112.60
1	A	285	GLY	CA-C-O	-5.56	118.40	122.23
2	B	566	VAL	CA-C-O	-5.55	114.67	120.27
2	B	676	ARG	NE-CZ-NH1	5.50	127.00	121.50
1	A	234	PRO	N-CA-CB	5.44	108.36	103.08
1	A	255	ASP	N-CA-C	5.43	119.73	113.38
2	B	544	LEU	CA-C-O	-5.33	115.22	120.82
1	A	301	PHE	CA-C-O	-5.33	112.86	120.16
1	A	41	PHE	CA-CB-CG	-5.31	108.49	113.80
1	A	162	TYR	CA-CB-CG	5.29	123.43	113.90
2	B	564	TYR	CA-C-O	-5.29	114.67	120.70
2	B	642	ILE	O-C-N	-5.29	117.63	123.18
1	A	247	GLY	O-C-N	5.28	128.26	122.56
1	A	158	PRO	N-CA-CB	5.27	107.93	103.35
1	A	118	PRO	N-CA-CB	5.26	107.85	103.17
1	A	417	TYR	CA-C-O	-5.21	113.64	119.79
2	B	585	MET	N-CA-C	5.21	117.25	110.53
1	A	35	PHE	N-CA-C	5.17	117.82	111.82
1	A	222	SER	N-CA-C	5.17	118.08	110.59
2	B	683	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	A	319	ILE	N-CA-CB	-5.12	107.44	111.64
2	B	663	TRP	CA-C-N	-5.11	114.78	122.81
2	B	663	TRP	C-N-CA	-5.11	114.78	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	LYS	N-CA-CB	-5.11	102.57	110.13
2	B	637	ILE	CA-C-O	-5.10	114.95	120.36
1	A	254	TRP	O-C-N	5.09	129.17	123.06
2	B	676	ARG	CA-C-O	-5.08	114.68	120.32
2	B	541	GLU	O-C-N	5.08	127.30	122.07
2	B	584	ALA	N-CA-C	5.08	117.43	108.75
2	B	647	ARG	NH1-CZ-NH2	-5.07	112.71	119.30
2	B	519	ILE	CB-CG1-CD1	5.04	124.39	113.80
2	B	689	ASN	O-C-N	5.03	128.32	123.29
1	A	38	ASN	N-CA-CB	-5.03	103.21	110.70
1	A	361	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	SER	Mainchain
1	A	184	GLY	Mainchain,Peptide
1	A	220	GLY	Mainchain
1	A	301	PHE	Mainchain,Peptide
1	A	336	MET	Mainchain
1	A	402	VAL	Mainchain
2	B	542	ALA	Mainchain
2	B	580	LYS	Mainchain
2	B	611	SER	Mainchain,Peptide

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	3480	0	3316	26	0
2	B	1608	0	1583	23	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
4	A	1	0	0	0	0
5	A	4	0	0	0	0
6	A	9	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	430	0	0	7	0
7	B	182	0	0	3	0
All	All	5729	0	4906	49	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 5.

All (49) 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:A:37:ARG:NH2	7:A:1010:HOH:O	2.05	0.81
1:A:181:GLU:HG2	1:A:334:LYS:HG2	1.62	0.81
1:A:240:LEU:HD13	1:A:252:VAL:HB	1.68	0.74
2:B:576:GLU:HA	2:B:577:ARG:NH1	2.02	0.73
2:B:519:ILE:HD13	2:B:523:PHE:CZ	2.27	0.69
2:B:577:ARG:HH21	2:B:578:ARG:HE	1.40	0.68
1:A:266:VAL:HB	1:A:267:PRO:HD3	1.74	0.67
1:A:1:MET:HE2	1:A:6:LYS:HG2	1.81	0.62
1:A:220:GLY:HA3	7:A:894:HOH:O	1.98	0.62
2:B:577:ARG:NH2	2:B:578:ARG:HE	2.02	0.57
2:B:577:ARG:HH21	2:B:578:ARG:NE	2.01	0.56
2:B:634:LEU:HD23	2:B:664:LYS:HB2	1.88	0.56
1:A:366:MET:HE2	7:A:1180:HOH:O	2.04	0.56
1:A:245:LYS:O	1:A:418:ARG:NH2	2.40	0.55
1:A:47:LEU:HD22	1:A:182:LEU:HD23	1.88	0.55
2:B:531:GLN:NE2	2:B:532:GLN:OE1	2.41	0.53
1:A:181:GLU:HG3	1:A:332:VAL:HG23	1.89	0.53
2:B:577:ARG:HD2	2:B:578:ARG:HG3	1.90	0.53
2:B:576:GLU:HA	2:B:577:ARG:HH11	1.72	0.52
1:A:181:GLU:CG	1:A:334:LYS:HG2	2.37	0.51
2:B:555:GLU:HG3	7:B:843:HOH:O	2.11	0.49
1:A:447:THR:HB	7:A:1034:HOH:O	2.12	0.49
2:B:519:ILE:HG23	2:B:523:PHE:CE1	2.48	0.49
1:A:221:GLU:O	1:A:263:ALA:N	2.46	0.48
1:A:216:SER:O	1:A:220:GLY:HA3	2.13	0.48
2:B:530:LEU:HD21	2:B:627:MET:HG2	1.96	0.48
1:A:218:ARG:HD3	7:A:1149:HOH:O	2.15	0.47
2:B:577:ARG:HH21	2:B:578:ARG:HB2	1.80	0.47
2:B:581:LEU:O	2:B:582:ASN:C	2.59	0.46
2:B:554:LEU:HD22	2:B:599:VAL:HG21	1.99	0.45
2:B:519:ILE:HD13	2:B:523:PHE:CE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLY:HA2	1:A:331:ILE:HG13	1.96	0.45
1:A:25:GLU:HB3	7:A:1079:HOH:O	2.16	0.45
2:B:577:ARG:NH2	2:B:578:ARG:NE	2.62	0.45
1:A:252:VAL:HG22	1:A:296:LEU:HD22	1.99	0.45
2:B:577:ARG:CZ	2:B:577:ARG:H	2.30	0.45
1:A:268:GLU:CD	1:A:343:ARG:HH22	2.25	0.44
2:B:528:SER:O	2:B:532:GLN:NE2	2.51	0.44
1:A:216:SER:O	1:A:220:GLY:N	2.51	0.43
2:B:577:ARG:NE	2:B:577:ARG:N	2.67	0.42
1:A:198:PRO:HB2	1:A:316:TRP:CE2	2.55	0.42
1:A:442:GLU:O	1:A:445:LYS:HG2	2.20	0.42
2:B:537:LEU:HD12	7:B:750:HOH:O	2.18	0.42
1:A:243:THR:OG1	1:A:415:GLY:HA3	2.20	0.42
1:A:1:MET:HG2	1:A:3:TYR:CE2	2.55	0.41
2:B:596:LYS:NZ	2:B:600:GLU:OE1	2.52	0.41
1:A:37:ARG:HB2	7:A:1007:HOH:O	2.20	0.41
1:A:17:LYS:HD3	1:A:17:LYS:HA	1.87	0.41
2:B:664:LYS:HG2	7:B:880:HOH:O	2.21	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	445/449 (99%)	429 (96%)	14 (3%)	2 (0%)	30	14
2	B	191/194 (98%)	184 (96%)	6 (3%)	1 (0%)	24	10
All	All	636/643 (99%)	613 (96%)	20 (3%)	3 (0%)	24	10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	GLU
1	A	226	SER
2	B	612	PRO

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	367/369 (100%)	359 (98%)	8 (2%)	45	22
2	B	172/173 (99%)	159 (92%)	13 (8%)	12	2
All	All	539/542 (99%)	518 (96%)	21 (4%)	28	9

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	78	LEU
1	A	121	LYS
1	A	181	GLU
1	A	221	GLU
1	A	240	LEU
1	A	253	LEU
1	A	447	THR
2	B	502	MET
2	B	508	ASP
2	B	519	ILE
2	B	531	GLN
2	B	554	LEU
2	B	571	LEU
2	B	577	ARG
2	B	581	LEU
2	B	593	GLN
2	B	603	LEU
2	B	664	LYS
2	B	667	GLU
2	B	690	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	115	GLN
1	A	201	ASN
2	B	514	HIS
2	B	531	GLN
2	B	532	GLN
2	B	556	HIS
2	B	675	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
6	IND	A	708	-	10,10,10	0.68	0	13,13,13	1.11	1 (7%)
3	SO4	B	702	-	4,4,4	0.68	0	6,6,6	0.11	0
5	FES	A	751	1	0,4,4	-	-	-		
3	SO4	B	707	-	4,4,4	0.59	0	6,6,6	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	717	-	4,4,4	1.91	2 (50%)	6,6,6	0.93	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
6	IND	A	708	-	-	-	0/2/2/2
5	FES	A	751	1	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	717	SO4	O1-S	3.07	1.63	1.44
3	A	717	SO4	O3-S	-2.21	1.30	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	708	IND	C5-C4-C9	-2.24	117.56	120.95

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

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	447/449 (99%)	-0.08	17 (3%) 44 46	11, 16, 35, 55	0
2	B	193/194 (99%)	0.17	17 (8%) 15 15	11, 16, 40, 56	0
All	All	640/643 (99%)	-0.01	34 (5%) 32 33	11, 16, 37, 56	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	THR	8.6
1	A	446	THR	7.2
2	B	523	PHE	6.2
1	A	224	PHE	5.6
2	B	525	CYS	5.2
1	A	225	SER	5.2
1	A	223	ILE	5.1
1	A	221	GLU	4.9
2	B	666	GLY	4.6
1	A	220	GLY	4.5
1	A	226	SER	4.3
1	A	236	GLU	4.1
2	B	669	GLY	4.1
2	B	502	MET	3.9
2	B	524	ASN	3.8
2	B	577	ARG	3.5
1	A	278	GLU	3.3
2	B	503	ILE	3.3
1	A	445	LYS	3.3
2	B	629	VAL	3.3
1	A	366	MET	3.1
2	B	584	ALA	3.0
1	A	233	LEU	2.9
1	A	227	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	235	PRO	2.6
2	B	667	GLU	2.5
1	A	129	ASN	2.4
2	B	634	LEU	2.4
2	B	532	GLN	2.4
2	B	646	ALA	2.4
2	B	670	VAL	2.4
2	B	668	GLY	2.3
2	B	671	ARG	2.2
1	A	253	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
3	SO4	B	702	5/5	0.75	0.15	70,70,71,71	0
6	IND	A	708	9/9	0.80	0.14	32,34,36,36	0
3	SO4	B	707	5/5	0.90	0.12	39,40,41,42	0
3	SO4	A	717	5/5	0.94	0.27	20,20,20,20	0
5	FES	A	751	4/4	0.99	0.06	8,10,16,17	0
4	FE	A	752	1/1	0.99	0.10	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.