



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:02 AM UTC

PDB ID : 1NDO / pdb_00001ndo
Title : NAPHTHALENE 1,2-DIOXYGENASE
Authors : Ramaswamy, S.; Kauppi, B.; Carredano, E.
Deposited on : 1998-01-11
Resolution : 2.25 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

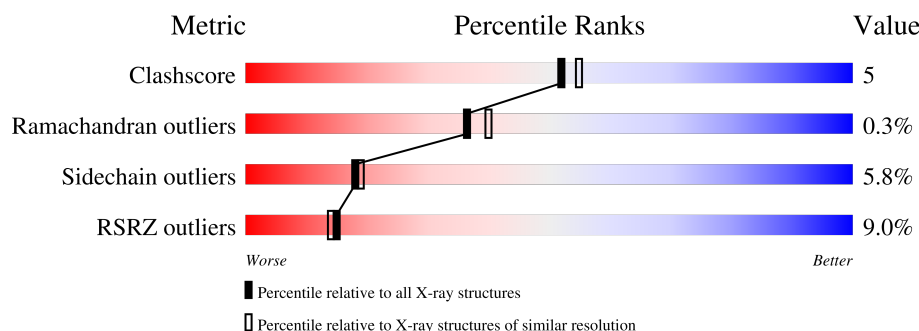
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	10% 78% 18% .
1	C	449	7% 78% 19% .
1	E	449	6% 76% 20% ..
2	B	194	12% 76% 19% ..
2	D	194	12% 74% 21% 5% .
2	F	194	13% 74% 21% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16326 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 NAPHTHALENE 1,2-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3480	2202	597	665	16			
1	C	447	Total	C	N	O	S	0	0	0
			3480	2202	597	665	16			
1	E	445	Total	C	N	O	S	0	0	0
			3466	2194	595	661	16			

- Molecule 2 is a protein called NAPHTHALENE 1,2-DIOXYGENASE.

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

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	E	1	Total	Fe	0	0
			1	1		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

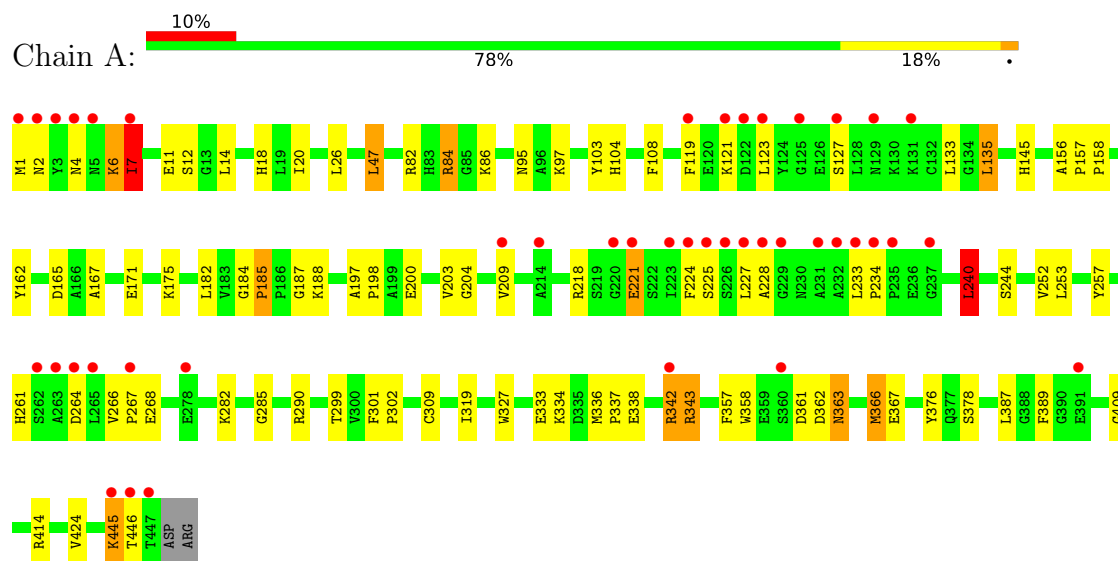
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	274	Total	O	0	0
			274	274		
5	B	97	Total	O	0	0
			97	97		
5	C	265	Total	O	0	0
			265	265		
5	D	112	Total	O	0	0
			112	112		
5	E	203	Total	O	0	0
			203	203		
5	F	110	Total	O	0	0
			110	110		

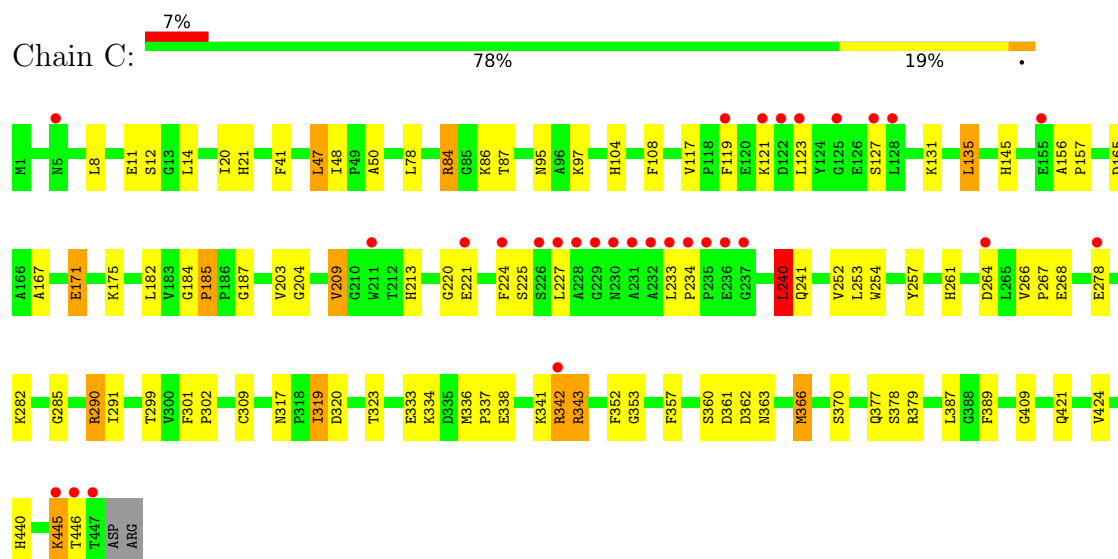
3 Residue-property plots [i](#)

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.

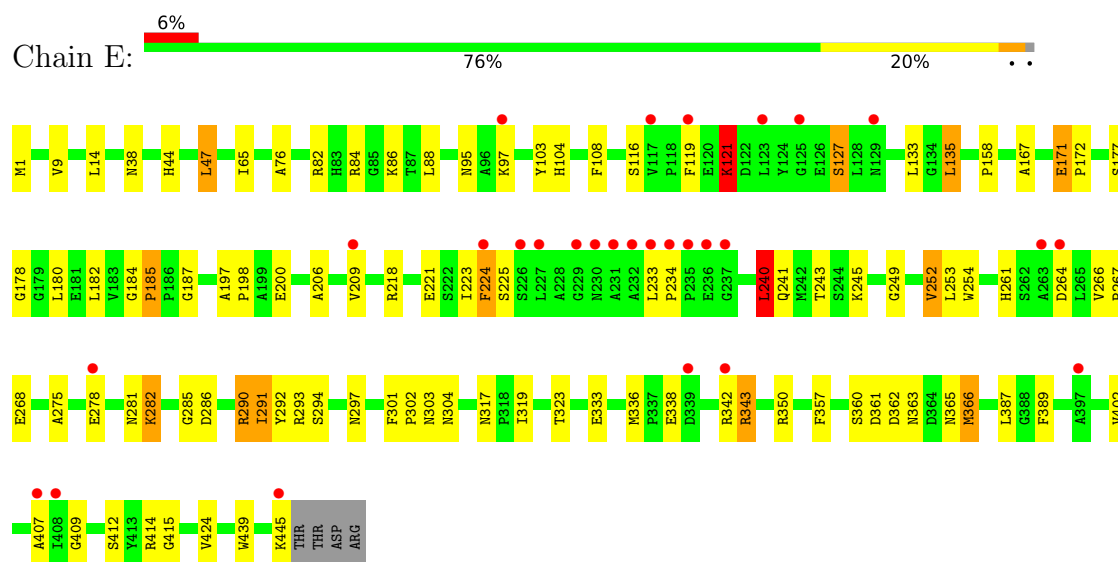
• Molecule 1: NAPHTHALENE 1,2-DIOXYGENASE



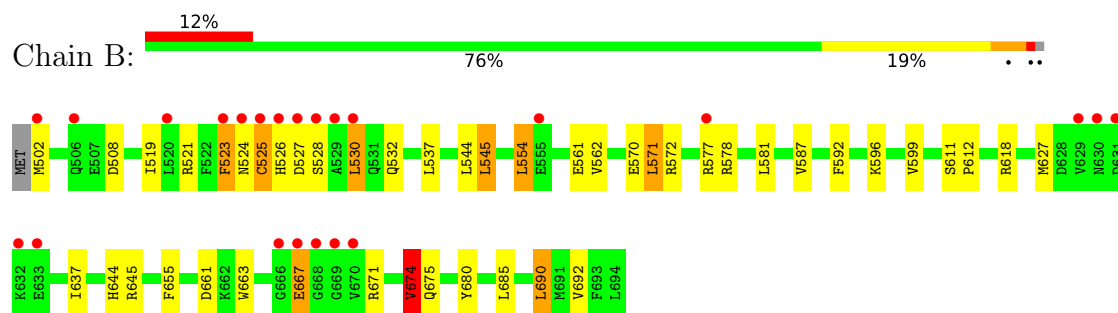
• Molecule 1: NAPHTHALENE 1,2-DIOXYGENASE



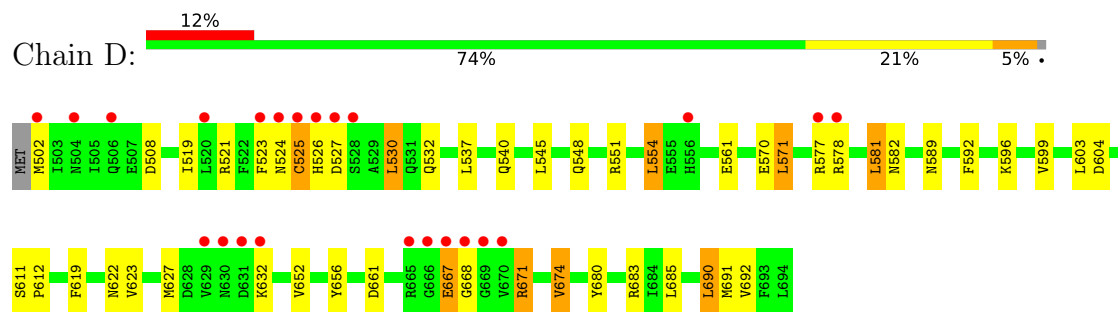
• Molecule 1: NAPHTHALENE 1,2-DIOXYGENASE



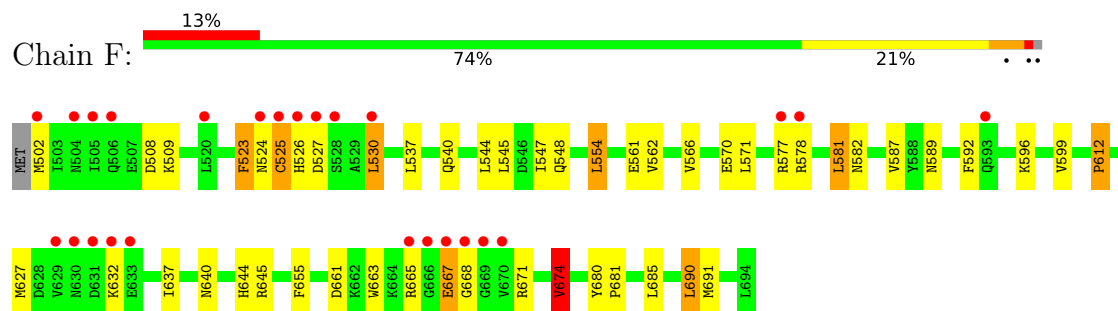
• Molecule 2: NAPHTHALENE 1,2-DIOXYGENASE



• Molecule 2: NAPHTHALENE 1,2-DIOXYGENASE



• Molecule 2: NAPHTHALENE 1,2-DIOXYGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	105.00Å 174.00Å 282.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.25 30.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	79.0 (30.00-2.25) 95.4 (30.00-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.24Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.240 0.184 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16326	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, 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	0.84	0/3572	1.73	49/4839 (1.0%)
1	C	0.83	0/3572	1.70	60/4839 (1.2%)
1	E	0.91	2/3558 (0.1%)	1.91	70/4819 (1.5%)
2	B	0.75	0/1638	1.63	19/2209 (0.9%)
2	D	0.71	0/1638	1.59	22/2209 (1.0%)
2	F	0.72	0/1638	1.62	16/2209 (0.7%)
All	All	0.82	2/15616 (0.0%)	1.73	236/21124 (1.1%)

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	E	0	4
2	D	0	2
2	F	0	1
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	414	ARG	NE-CZ	-5.62	1.26	1.33
1	E	121	LYS	CE-NZ	5.58	1.66	1.49

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	290	ARG	CD-NE-CZ	36.68	175.75	124.40
1	A	290	ARG	CD-NE-CZ	35.89	174.64	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	290	ARG	CD-NE-CZ	32.60	170.04	124.40
1	E	414	ARG	CD-NE-CZ	31.89	169.05	124.40
2	B	577	ARG	CD-NE-CZ	16.03	146.84	124.40
2	D	577	ARG	CD-NE-CZ	14.23	144.32	124.40
1	E	224	PHE	CD1-CG-CD2	-14.17	97.35	118.60
1	E	224	PHE	CE1-CZ-CE2	-11.89	98.59	120.00
1	A	264	ASP	CA-CB-CG	11.15	123.75	112.60
1	A	343	ARG	CD-NE-CZ	10.77	139.47	124.40
2	F	577	ARG	CD-NE-CZ	10.05	138.46	124.40
2	B	527	ASP	CA-CB-CG	9.79	122.39	112.60
1	C	301	PHE	CA-C-O	-9.49	110.82	120.02
1	C	361	ASP	CA-CB-CG	9.48	122.08	112.60
1	C	157	PRO	N-CA-CB	9.30	108.40	103.19
2	B	612	PRO	N-CA-CB	9.26	112.79	102.60
1	E	301	PHE	CA-C-O	-9.08	111.21	120.02
2	F	612	PRO	N-CA-CB	8.87	112.36	102.60
1	C	264	ASP	CA-CB-CG	8.82	121.42	112.60
1	E	361	ASP	CA-CB-CG	8.76	121.36	112.60
1	C	421	GLN	OE1-CD-NE2	-8.55	114.05	122.60
2	D	527	ASP	CA-CB-CG	8.47	121.07	112.60
2	D	612	PRO	N-CA-CB	8.40	111.85	102.60
1	A	290	ARG	CA-CB-CG	8.32	130.73	114.10
1	E	184	GLY	O-C-N	8.31	130.08	121.77
2	F	527	ASP	CA-CB-CG	8.31	120.91	112.60
1	A	285	GLY	CA-C-N	8.22	131.30	120.28
1	A	285	GLY	C-N-CA	8.22	131.30	120.28
1	A	7	ILE	N-CA-CB	-8.17	101.80	111.60
1	E	261	HIS	CA-CB-CG	-8.16	105.64	113.80
1	C	302	PRO	N-CA-CB	8.15	111.56	102.60
1	C	343	ARG	CD-NE-CZ	7.96	135.55	124.40
1	E	363	ASN	CA-CB-CG	7.95	120.55	112.60
1	E	343	ARG	NE-CZ-NH2	-7.95	112.05	119.20
2	B	674	VAL	CB-CA-C	7.93	118.43	110.65
1	A	185	PRO	N-CA-CB	7.79	111.17	102.60
1	C	184	GLY	O-C-N	7.79	129.56	121.77
1	A	6	LYS	CA-C-O	7.77	129.59	120.58
1	E	185	PRO	N-CA-CB	7.71	111.08	102.60
1	E	178	GLY	N-CA-C	-7.68	104.69	114.37
1	C	377	GLN	OE1-CD-NE2	-7.67	114.93	122.60
1	C	285	GLY	CA-C-N	7.64	130.85	120.54
1	C	285	GLY	C-N-CA	7.64	130.85	120.54
2	B	645	ARG	CD-NE-CZ	7.61	135.06	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	ASP	CA-CB-CG	7.60	120.20	112.60
1	C	290	ARG	CA-CB-CG	7.60	129.30	114.10
1	A	157	PRO	N-CA-CB	7.59	107.44	103.19
1	C	209	VAL	N-CA-C	7.51	118.25	110.36
1	E	224	PHE	CB-CG-CD2	7.43	133.33	120.70
1	A	319	ILE	N-CA-C	-7.42	105.76	111.62
2	B	644	HIS	CA-CB-CG	7.41	121.21	113.80
1	E	290	ARG	CA-CB-CG	7.40	128.91	114.10
1	C	156	ALA	CA-C-N	7.38	125.05	119.66
1	C	156	ALA	C-N-CA	7.38	125.05	119.66
1	A	184	GLY	CA-C-O	-7.35	111.00	121.52
1	E	317	ASN	CA-C-O	7.34	125.11	119.46
1	E	343	ARG	CD-NE-CZ	7.30	134.63	124.40
1	C	261	HIS	CA-CB-CG	-7.30	106.50	113.80
1	C	440	HIS	CA-C-N	7.19	130.22	120.44
1	C	440	HIS	C-N-CA	7.19	130.22	120.44
2	F	674	VAL	CB-CA-C	7.16	117.66	110.65
1	C	185	PRO	N-CA-CB	7.13	110.45	102.60
1	E	218	ARG	CD-NE-CZ	7.09	134.33	124.40
2	B	661	ASP	CA-CB-CG	7.07	119.67	112.60
1	C	301	PHE	O-C-N	7.05	128.11	121.27
1	E	224	PHE	CG-CD2-CE2	7.03	132.65	120.70
1	E	184	GLY	CA-C-O	-7.02	111.48	121.52
1	A	358	TRP	O-C-N	-6.86	114.68	122.09
1	A	104	HIS	CA-CB-CG	-6.84	106.96	113.80
1	E	171	GLU	O-C-N	-6.83	114.22	120.92
1	E	116	SER	CA-C-O	6.83	128.63	120.99
1	A	302	PRO	N-CA-CB	6.76	110.03	102.60
2	F	645	ARG	CD-NE-CZ	6.73	133.82	124.40
1	E	302	PRO	N-CA-CB	6.64	109.90	102.60
1	A	6	LYS	N-CA-CB	6.63	119.92	109.71
1	A	218	ARG	CD-NE-CZ	6.62	133.66	124.40
1	E	409	GLY	O-C-N	-6.59	116.04	123.62
1	A	414	ARG	CD-NE-CZ	6.59	133.63	124.40
1	A	184	GLY	O-C-N	6.58	128.35	121.77
1	C	343	ARG	NE-CZ-NH2	-6.57	113.28	119.20
2	D	692	VAL	CA-C-O	-6.56	114.78	121.67
1	E	224	PHE	CD1-CE1-CZ	6.53	131.75	120.00
1	A	343	ARG	NE-CZ-NH2	-6.42	113.42	119.20
2	B	611	SER	CA-C-O	-6.39	113.17	119.69
1	E	278	GLU	CA-C-O	-6.33	113.84	120.55
1	C	84	ARG	CG-CD-NE	6.27	125.79	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	254	TRP	CA-C-O	-6.25	114.28	121.15
2	D	611	SER	CA-C-O	-6.25	113.55	119.55
1	A	337	PRO	N-CA-CB	6.24	108.89	103.27
2	F	644	HIS	CA-CB-CG	6.20	120.00	113.80
1	A	4	ASN	N-CA-C	-6.18	103.14	112.04
2	B	674	VAL	N-CA-CB	-6.14	103.83	112.12
2	F	674	VAL	N-CA-CB	-6.13	103.84	112.12
1	C	184	GLY	CA-C-O	-6.06	112.85	121.52
2	D	668	GLY	N-CA-C	-6.05	107.49	114.69
2	F	680	TYR	CA-CB-CG	-6.05	103.01	113.90
1	E	187	GLY	N-CA-C	-6.03	103.93	112.37
2	F	587	VAL	N-CA-C	-6.02	104.44	111.00
1	E	104	HIS	CA-CB-CG	-6.01	107.79	113.80
2	B	680	TYR	CA-C-N	6.00	125.55	119.19
2	B	680	TYR	C-N-CA	6.00	125.55	119.19
2	D	674	VAL	N-CA-CB	-5.99	104.03	112.12
1	C	41	PHE	CA-CB-CG	-5.99	107.81	113.80
1	C	157	PRO	O-C-N	5.96	124.05	121.31
1	E	9	VAL	CA-C-O	-5.95	114.14	120.39
1	A	302	PRO	N-CD-CG	5.95	110.94	103.80
1	C	320	ASP	CA-C-O	-5.94	114.95	121.31
1	E	439	TRP	CA-C-O	-5.94	114.25	120.55
1	C	8	LEU	CA-C-O	5.93	126.78	119.79
1	E	209	VAL	N-CA-C	5.89	116.35	110.23
1	E	240	LEU	N-CA-CB	-5.87	102.42	111.46
1	E	275	ALA	CA-C-O	-5.87	114.66	120.82
1	E	357	PHE	CA-CB-CG	5.87	119.67	113.80
1	C	224	PHE	CE1-CZ-CE2	-5.86	109.45	120.00
1	E	297	ASN	CA-C-O	-5.85	114.03	120.70
1	E	241	GLN	CA-C-O	-5.85	113.58	120.60
1	E	127	SER	N-CA-C	5.85	118.60	111.82
1	C	171	GLU	CA-C-N	5.85	125.32	119.24
1	C	171	GLU	C-N-CA	5.85	125.32	119.24
1	C	334	LYS	CA-C-O	-5.81	113.69	120.20
1	C	187	GLY	N-CA-C	-5.80	104.65	112.14
1	E	240	LEU	CA-C-O	-5.77	115.26	121.38
1	C	204	GLY	CA-C-N	-5.77	114.28	122.41
1	C	204	GLY	C-N-CA	-5.77	114.28	122.41
1	C	224	PHE	CD1-CG-CD2	-5.74	109.99	118.60
1	C	353	GLY	CA-C-N	5.74	125.59	119.28
1	C	353	GLY	C-N-CA	5.74	125.59	119.28
1	E	285	GLY	CA-C-N	5.73	127.96	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	285	GLY	C-N-CA	5.73	127.96	120.28
2	D	680	TYR	CA-C-N	5.72	125.25	119.19
2	D	680	TYR	C-N-CA	5.72	125.25	119.19
1	C	157	PRO	CB-CA-C	-5.71	106.02	111.39
1	A	264	ASP	O-C-N	-5.69	115.56	122.11
1	E	286	ASP	N-CA-C	5.67	117.46	111.28
1	A	209	VAL	N-CA-C	5.64	116.10	110.23
2	B	572	ARG	CG-CD-NE	5.64	124.41	112.00
1	E	224	PHE	CG-CD1-CE1	5.63	130.28	120.70
1	A	158	PRO	N-CA-CB	5.63	108.05	103.32
1	A	334	LYS	CA-C-O	-5.61	113.76	120.10
1	A	162	TYR	CA-CB-CG	5.61	124.00	113.90
1	C	241	GLN	CB-CG-CD	-5.61	103.06	112.60
1	A	224	PHE	CE1-CZ-CE2	-5.60	109.92	120.00
1	E	264	ASP	CA-CB-CG	5.59	118.19	112.60
2	F	681	PRO	N-CA-CB	5.58	109.44	103.52
1	E	412	SER	CA-CB-OG	-5.58	99.95	111.10
1	A	240	LEU	CA-CB-CG	5.57	135.78	116.30
1	A	84	ARG	CB-CG-CD	5.56	124.09	111.30
2	B	528	SER	N-CA-C	5.52	117.30	111.28
1	C	366	MET	O-C-N	5.52	128.06	122.09
2	D	671	ARG	CD-NE-CZ	-5.51	116.68	124.40
2	D	692	VAL	CA-C-N	-5.51	115.09	122.42
2	D	692	VAL	C-N-CA	-5.51	115.09	122.42
1	C	234	PRO	N-CA-CB	5.50	108.42	103.08
1	E	206	ALA	N-CA-C	-5.50	106.74	113.50
1	E	350	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	C	352	PHE	CA-CB-CG	-5.48	108.32	113.80
1	E	88	LEU	N-CA-C	5.47	116.93	111.07
2	D	680	TYR	CA-CB-CG	-5.47	104.05	113.90
1	E	252	VAL	CA-C-O	-5.47	114.64	120.39
2	F	612	PRO	N-CD-CG	5.43	110.32	103.80
2	D	674	VAL	CB-CA-C	5.41	115.95	110.65
2	F	668	GLY	N-CA-C	-5.40	107.90	114.92
1	A	187	GLY	N-CA-C	-5.40	104.81	112.37
1	E	301	PHE	O-C-N	5.39	126.50	121.27
1	C	278	GLU	CA-C-O	-5.37	114.86	120.55
1	A	376	TYR	CA-C-O	-5.37	115.15	120.90
2	F	661	ASP	CA-CB-CG	5.37	117.97	112.60
1	E	38	ASN	CA-CB-CG	-5.36	107.24	112.60
1	A	261	HIS	CA-CB-CG	-5.36	108.44	113.80
2	D	623	VAL	O-C-N	-5.35	116.84	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	290	ARG	O-C-N	-5.34	115.17	122.33
1	C	165	ASP	CA-CB-CG	-5.34	107.26	112.60
2	D	656	TYR	CA-C-O	-5.33	114.53	120.66
2	D	661	ASP	CA-CB-CG	5.33	117.93	112.60
2	B	675	GLN	OE1-CD-NE2	-5.33	117.27	122.60
1	C	240	LEU	CA-CB-CG	5.31	134.89	116.30
2	D	604	ASP	CA-C-N	5.31	125.39	119.87
2	D	604	ASP	C-N-CA	5.31	125.39	119.87
1	A	204	GLY	CA-C-N	-5.31	114.90	123.23
1	A	204	GLY	C-N-CA	-5.31	114.90	123.23
2	B	525	CYS	N-CA-C	5.31	116.79	109.15
1	A	357	PHE	CA-CB-CG	5.30	119.10	113.80
1	C	302	PRO	N-CD-CG	5.30	110.16	103.80
1	C	363	ASN	CA-CB-CG	5.30	117.90	112.60
2	B	692	VAL	CA-C-O	-5.28	116.13	121.67
1	E	241	GLN	CB-CG-CD	-5.27	103.64	112.60
2	F	566	VAL	CA-C-N	-5.27	114.86	122.45
2	F	566	VAL	C-N-CA	-5.27	114.86	122.45
2	F	525	CYS	N-CA-C	5.27	116.74	109.15
1	A	156	ALA	CA-C-N	5.25	123.50	119.66
1	A	156	ALA	C-N-CA	5.25	123.50	119.66
1	E	185	PRO	N-CD-CG	5.25	110.09	103.80
1	C	185	PRO	N-CD-CG	5.24	110.09	103.80
1	A	221	GLU	O-C-N	-5.23	116.68	122.91
1	E	234	PRO	N-CA-CB	5.23	108.15	103.08
1	C	319	ILE	N-CA-C	-5.22	107.07	111.56
1	E	177	SER	CA-C-N	-5.21	116.04	123.08
1	E	177	SER	C-N-CA	-5.21	116.04	123.08
1	C	220	GLY	N-CA-C	5.21	121.11	114.66
1	A	301	PHE	O-C-N	5.19	127.29	121.32
1	E	281	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	E	224	PHE	CZ-CE2-CD2	5.19	129.34	120.00
1	E	407	ALA	N-CA-CB	-5.18	102.50	110.16
2	D	652	VAL	CA-C-O	-5.16	115.14	120.25
1	C	337	PRO	N-CA-CB	5.16	107.90	103.31
2	D	525	CYS	N-CA-C	5.14	116.55	109.15
1	E	282	LYS	CA-C-O	-5.14	114.98	120.42
1	E	294	SER	O-C-N	-5.14	117.19	123.10
1	E	240	LEU	CA-CB-CG	5.13	134.26	116.30
1	E	180	LEU	CA-C-N	-5.13	114.76	122.81
1	E	180	LEU	C-N-CA	-5.13	114.76	122.81
1	C	357	PHE	CA-CB-CG	5.12	118.92	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ASP	CA-CB-CG	-5.11	107.49	112.60
1	E	249	GLY	CA-C-O	-5.10	116.11	121.56
1	C	50	ALA	CA-C-N	5.09	126.21	119.84
1	C	50	ALA	C-N-CA	5.09	126.21	119.84
1	A	363	ASN	CA-CB-CG	5.08	117.68	112.60
1	C	317	ASN	CA-C-N	5.07	125.22	119.90
1	C	317	ASN	C-N-CA	5.07	125.22	119.90
1	E	285	GLY	O-C-N	-5.07	116.85	122.68
1	E	224	PHE	CB-CG-CD1	5.07	129.31	120.70
2	B	587	VAL	N-CA-C	-5.06	105.61	110.72
1	A	301	PHE	CA-C-O	-5.06	113.22	120.16
1	E	158	PRO	O-C-N	-5.05	116.58	122.99
1	C	48	ILE	CA-C-N	5.04	124.34	118.85
1	C	48	ILE	C-N-CA	5.04	124.34	118.85
2	D	622	ASN	OD1-CG-ND2	-5.04	117.56	122.60
2	B	674	VAL	CA-C-O	5.04	124.17	118.98
2	B	680	TYR	CA-CB-CG	-5.04	104.84	113.90
1	E	303	ASN	N-CA-C	5.04	116.91	110.61
1	E	304	ASN	CA-C-O	-5.03	114.93	120.36
1	A	234	PRO	CA-C-N	5.02	125.29	119.92
1	A	234	PRO	C-N-CA	5.02	125.29	119.92
1	C	302	PRO	CA-N-CD	-5.02	104.47	111.50
1	A	244	SER	CA-C-N	5.01	127.31	120.54
1	A	244	SER	C-N-CA	5.01	127.31	120.54

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	548	GLN	Mainchain
2	D	589	ASN	Mainchain
1	E	245	LYS	Mainchain
1	E	291	ILE	Mainchain
1	E	402	VAL	Mainchain
1	E	44	HIS	Mainchain
2	F	589	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	3480	0	3316	43	0
1	C	3480	0	3316	36	0
1	E	3466	0	3302	38	0
2	B	1608	0	1583	18	0
2	D	1608	0	1583	18	0
2	F	1608	0	1583	24	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	4	0	0	0	0
4	C	4	0	0	1	0
4	E	4	0	0	0	0
5	A	274	0	0	1	0
5	B	97	0	0	0	0
5	C	265	0	0	2	0
5	D	112	0	0	1	0
5	E	203	0	0	1	0
5	F	110	0	0	0	0
All	All	16326	0	14683	154	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 (154) 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:333:GLU:H	1:A:336:MET:HE3	1.34	0.92
1:E:333:GLU:H	1:E:336:MET:HE3	1.44	0.81
1:C:333:GLU:H	1:C:336:MET:HE3	1.45	0.81
1:E:171:GLU:OE2	5:E:554:HOH:O	2.07	0.72
1:C:171:GLU:OE2	5:C:570:HOH:O	2.08	0.71
1:C:167:ALA:O	1:C:171:GLU:HG3	1.93	0.69
1:A:119:PHE:CG	1:E:233:LEU:HD13	2.29	0.67
1:E:167:ALA:O	1:E:171:GLU:HG3	1.95	0.67
1:C:47:LEU:HD22	1:C:182:LEU:HD23	1.77	0.66
2:B:530:LEU:HD21	2:B:627:MET:HG2	1.79	0.65
1:A:47:LEU:HD22	1:A:182:LEU:HD23	1.79	0.64
1:A:47:LEU:CD2	1:A:182:LEU:HD23	2.30	0.61
1:A:119:PHE:CD2	1:E:233:LEU:HD13	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PHE:CD1	1:A:135:LEU:HD13	2.35	0.61
2:D:530:LEU:HD21	2:D:627:MET:HG2	1.81	0.61
1:C:145:HIS:CE1	1:C:175:LYS:HB2	2.36	0.60
1:C:266:VAL:HB	1:C:267:PRO:HD3	1.84	0.60
2:D:554:LEU:HD22	2:D:599:VAL:HG21	1.84	0.60
1:E:108:PHE:CD1	1:E:135:LEU:HD13	2.37	0.60
1:E:266:VAL:HB	1:E:267:PRO:HD3	1.85	0.59
1:A:167:ALA:O	1:A:171:GLU:HG3	2.03	0.58
1:C:366:MET:HA	1:C:366:MET:HE2	1.86	0.58
2:F:530:LEU:HD21	2:F:627:MET:HG2	1.85	0.58
1:A:366:MET:HA	1:A:366:MET:HE2	1.87	0.57
2:B:537:LEU:HD11	2:B:671:ARG:HG2	1.87	0.56
1:A:342:ARG:NH1	5:A:718:HOH:O	2.39	0.56
1:E:366:MET:HA	1:E:366:MET:HE2	1.88	0.56
1:E:291:ILE:O	1:E:292:TYR:C	2.49	0.55
2:D:592:PHE:CE2	2:D:596:LYS:HD2	2.42	0.55
2:B:667:GLU:HA	2:B:667:GLU:OE1	2.05	0.55
1:A:268:GLU:CD	1:A:343:ARG:HH22	2.15	0.54
1:E:47:LEU:HD22	1:E:182:LEU:HD23	1.88	0.54
2:F:685:LEU:CD1	2:F:690:LEU:HB2	2.37	0.54
2:B:685:LEU:HD11	2:B:690:LEU:HB2	1.89	0.54
2:F:685:LEU:HD11	2:F:690:LEU:HB2	1.90	0.54
1:C:203:VAL:HG23	1:C:299:THR:HB	1.90	0.54
1:C:268:GLU:CD	1:C:343:ARG:HH22	2.16	0.54
2:B:554:LEU:HD22	2:B:599:VAL:HG21	1.90	0.53
2:D:685:LEU:CD1	2:D:690:LEU:HB2	2.37	0.53
1:E:362:ASP:O	1:E:366:MET:HG2	2.09	0.53
2:B:685:LEU:CD1	2:B:690:LEU:HB2	2.38	0.53
2:D:667:GLU:HA	2:D:667:GLU:OE1	2.08	0.53
2:F:554:LEU:HD22	2:F:599:VAL:HG21	1.91	0.53
1:C:108:PHE:CD1	1:C:135:LEU:HD13	2.44	0.52
1:A:203:VAL:HG23	1:A:299:THR:HB	1.91	0.52
1:E:86:LYS:HD2	1:E:103:TYR:HB2	1.92	0.52
1:E:268:GLU:CD	1:E:343:ARG:HH22	2.18	0.52
2:D:571:LEU:HD22	2:D:683:ARG:HG2	1.92	0.51
1:E:333:GLU:N	1:E:336:MET:HE3	2.19	0.51
1:E:338:GLU:O	1:E:342:ARG:HG2	2.11	0.51
1:E:95:ASN:OD1	2:F:578:ARG:NH1	2.44	0.51
1:E:240:LEU:HD22	1:E:252:VAL:CG2	2.41	0.51
1:C:14:LEU:HD21	1:C:389:PHE:CG	2.46	0.51
2:D:551:ARG:HD3	5:D:803:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:592:PHE:CE2	2:B:596:LYS:HD2	2.45	0.51
1:A:145:HIS:CE1	1:A:175:LYS:HB2	2.45	0.50
2:D:685:LEU:HD11	2:D:690:LEU:HB2	1.93	0.50
1:E:360:SER:OG	2:F:691:MET:HG3	2.11	0.50
2:F:592:PHE:CE2	2:F:596:LYS:HD2	2.46	0.50
1:A:233:LEU:HD13	1:C:119:PHE:CG	2.46	0.49
1:A:333:GLU:N	1:A:336:MET:HE3	2.15	0.49
1:A:14:LEU:HD21	1:A:389:PHE:CG	2.46	0.49
1:E:197:ALA:O	1:E:200:GLU:HG2	2.12	0.49
1:E:14:LEU:HD21	1:E:389:PHE:CG	2.48	0.49
1:A:1:MET:SD	1:A:6:LYS:HG2	2.53	0.49
2:F:685:LEU:HD21	2:F:690:LEU:HD22	1.95	0.48
1:A:266:VAL:HB	1:A:267:PRO:HD3	1.95	0.48
1:E:223:ILE:HG13	1:E:224:PHE:CD1	2.47	0.48
1:A:7:ILE:HG22	1:A:7:ILE:O	2.13	0.48
1:A:86:LYS:HD2	1:A:103:TYR:HB2	1.96	0.48
1:C:221:GLU:HA	1:C:225:SER:OG	2.14	0.48
2:D:603:LEU:HB3	2:F:509:LYS:HE3	1.95	0.48
1:A:197:ALA:O	1:A:200:GLU:HG2	2.14	0.47
2:B:544:LEU:HD23	2:D:519:ILE:HD13	1.96	0.47
2:F:667:GLU:HA	2:F:667:GLU:OE1	2.15	0.47
1:C:257:TYR:O	1:C:309:CYS:HB3	2.15	0.47
1:E:185:PRO:HB3	2:F:570:GLU:HB2	1.97	0.47
1:C:95:ASN:OD1	2:D:578:ARG:NH1	2.48	0.46
1:A:240:LEU:HD22	1:A:252:VAL:CG2	2.46	0.46
2:B:655:PHE:CE2	2:B:690:LEU:HD13	2.50	0.46
1:A:108:PHE:CE1	1:A:135:LEU:HD13	2.51	0.46
1:C:338:GLU:O	1:C:342:ARG:HG2	2.16	0.46
2:B:571:LEU:HG	2:F:612:PRO:CG	2.46	0.46
2:D:537:LEU:HD11	2:D:671:ARG:HG2	1.98	0.46
1:A:363:ASN:O	1:A:367:GLU:HG3	2.16	0.46
2:B:637:ILE:HD12	2:B:663:TRP:CD1	2.51	0.46
1:A:95:ASN:OD1	2:B:578:ARG:NH1	2.48	0.46
2:F:547:ILE:O	2:F:548:GLN:HB2	2.15	0.45
1:A:387:LEU:HG	1:A:409:GLY:HA2	1.97	0.45
1:A:197:ALA:HB3	1:A:198:PRO:HD3	1.97	0.45
1:C:21:HIS:HB3	1:C:370:SER:HA	1.99	0.45
1:C:387:LEU:HG	1:C:409:GLY:HA2	1.98	0.45
2:D:540:GLN:HB3	2:F:523:PHE:CE1	2.51	0.45
2:D:685:LEU:HD21	2:D:690:LEU:HD22	1.99	0.45
1:E:221:GLU:HA	1:E:225:SER:OG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:THR:HG22	1:A:446:THR:O	2.16	0.45
2:B:685:LEU:HD21	2:B:690:LEU:HD22	1.98	0.45
1:C:233:LEU:HD13	1:E:119:PHE:CG	2.52	0.45
2:D:581:LEU:O	2:D:582:ASN:C	2.60	0.45
1:C:104:HIS:HB2	4:C:451:FES:S1	2.57	0.44
1:A:257:TYR:O	1:A:309:CYS:HB3	2.17	0.44
1:E:333:GLU:H	1:E:336:MET:CE	2.22	0.44
1:E:319:ILE:HB	1:E:323:THR:HB	1.99	0.44
1:A:18:HIS:HB3	1:A:378:SER:O	2.18	0.44
1:A:123:LEU:HB3	1:E:387:LEU:HD11	1.99	0.44
2:B:519:ILE:HD13	2:F:544:LEU:HD23	2.00	0.44
2:F:537:LEU:HD11	2:F:671:ARG:HG2	1.99	0.44
1:A:362:ASP:O	1:A:366:MET:HG2	2.17	0.44
2:B:523:PHE:CE1	2:F:540:GLN:HB3	2.53	0.44
1:A:11:GLU:O	1:A:12:SER:HB2	2.18	0.44
2:B:545:LEU:HB3	2:B:618:ARG:CZ	2.48	0.44
1:C:254:TRP:CZ3	1:C:291:ILE:HD13	2.52	0.44
1:C:360:SER:OG	2:D:691:MET:HG3	2.18	0.43
1:A:2:ASN:O	1:A:6:LYS:N	2.45	0.43
1:A:338:GLU:O	1:A:342:ARG:HG2	2.18	0.43
1:A:387:LEU:HD11	1:C:123:LEU:HB3	2.00	0.43
2:B:562:VAL:HA	2:B:674:VAL:O	2.19	0.43
1:C:227:LEU:HB3	5:C:710:HOH:O	2.19	0.43
1:E:243:THR:OG1	1:E:415:GLY:HA3	2.18	0.43
1:A:119:PHE:CE1	1:E:233:LEU:HB2	2.53	0.42
1:E:47:LEU:CD2	1:E:182:LEU:HD23	2.49	0.42
1:A:227:LEU:O	1:A:228:ALA:C	2.62	0.42
1:C:319:ILE:HB	1:C:323:THR:HB	2.01	0.42
1:A:86:LYS:HE3	1:E:365:ASN:OD1	2.19	0.42
1:E:82:ARG:HG3	1:E:133:LEU:O	2.19	0.42
2:D:619:PHE:CE2	2:F:640:ASN:HB3	2.55	0.42
1:E:1:MET:HE3	1:E:1:MET:HB2	1.91	0.42
1:E:240:LEU:HD22	1:E:252:VAL:HG21	2.01	0.42
1:A:188:LYS:HE2	1:A:327:TRP:CE2	2.55	0.42
1:C:240:LEU:HD22	1:C:252:VAL:CG2	2.50	0.42
1:C:342:ARG:HH11	1:C:342:ARG:HD3	1.71	0.41
1:C:378:SER:O	1:C:379:ARG:C	2.63	0.41
1:A:20:ILE:HA	1:A:26:LEU:HD23	2.03	0.41
1:A:185:PRO:HB3	2:B:570:GLU:HB2	2.03	0.41
1:C:362:ASP:O	1:C:366:MET:HG2	2.20	0.41
1:E:197:ALA:N	1:E:198:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:PRO:HB3	2:D:570:GLU:HB2	2.02	0.41
2:F:562:VAL:HA	2:F:674:VAL:O	2.21	0.41
2:F:665:ARG:HG2	2:F:671:ARG:HD3	2.02	0.41
1:C:209:VAL:O	1:C:213:HIS:HB2	2.21	0.41
2:F:637:ILE:HD12	2:F:663:TRP:CD1	2.55	0.41
1:E:121:LYS:HE2	1:E:121:LYS:HB3	1.89	0.41
1:A:82:ARG:HG3	1:A:133:LEU:O	2.21	0.41
1:A:221:GLU:HA	1:A:225:SER:OG	2.21	0.41
2:F:592:PHE:CD2	2:F:596:LYS:HD2	2.56	0.41
1:C:11:GLU:O	1:C:12:SER:HB2	2.21	0.41
1:C:47:LEU:CD2	1:C:182:LEU:HD23	2.46	0.41
1:C:336:MET:O	1:C:341:LYS:HE3	2.21	0.41
1:C:20:ILE:HD13	1:C:20:ILE:HG21	1.90	0.40
1:E:171:GLU:O	1:E:172:PRO:C	2.64	0.40
2:F:581:LEU:O	2:F:582:ASN:C	2.64	0.40
1:C:86:LYS:HG2	1:C:87:THR:N	2.37	0.40
1:E:65:ILE:O	1:E:76:ALA:HA	2.21	0.40
2:F:655:PHE:CE2	2:F:690:LEU:HD13	2.57	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%)	432 (97%)	12 (3%)	1 (0%)	43	50
1	C	445/449 (99%)	432 (97%)	12 (3%)	1 (0%)	43	50
1	E	443/449 (99%)	431 (97%)	12 (3%)	0	100	100
2	B	191/194 (98%)	184 (96%)	6 (3%)	1 (0%)	24	24
2	D	191/194 (98%)	184 (96%)	6 (3%)	1 (0%)	24	24
2	F	191/194 (98%)	185 (97%)	5 (3%)	1 (0%)	24	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1906/1929 (99%)	1848 (97%)	53 (3%)	5 (0%)	36	40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	524	ASN
2	D	524	ASN
2	F	524	ASN
1	A	445	LYS
1	C	445	LYS

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	367/369 (100%)	353 (96%)	14 (4%)	29	36
1	C	367/369 (100%)	350 (95%)	17 (5%)	24	28
1	E	365/369 (99%)	351 (96%)	14 (4%)	29	36
2	B	172/173 (99%)	156 (91%)	16 (9%)	8	6
2	D	172/173 (99%)	155 (90%)	17 (10%)	7	5
2	F	172/173 (99%)	157 (91%)	15 (9%)	9	8
All	All	1615/1626 (99%)	1522 (94%)	93 (6%)	18	19

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	47	LEU
1	A	84	ARG
1	A	97	LYS
1	A	121	LYS
1	A	127	SER
1	A	135	LEU

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Mol	Chain	Res	Type
1	A	240	LEU
1	A	253	LEU
1	A	282	LYS
1	A	342	ARG
1	A	366	MET
1	A	424	VAL
1	A	445	LYS
2	B	502	MET
2	B	508	ASP
2	B	521	ARG
2	B	523	PHE
2	B	525	CYS
2	B	526	HIS
2	B	530	LEU
2	B	532	GLN
2	B	545	LEU
2	B	554	LEU
2	B	561	GLU
2	B	571	LEU
2	B	581	LEU
2	B	667	GLU
2	B	674	VAL
2	B	690	LEU
1	C	47	LEU
1	C	78	LEU
1	C	84	ARG
1	C	97	LYS
1	C	117	VAL
1	C	121	LYS
1	C	127	SER
1	C	131	LYS
1	C	135	LEU
1	C	240	LEU
1	C	253	LEU
1	C	282	LYS
1	C	290	ARG
1	C	342	ARG
1	C	424	VAL
1	C	445	LYS
1	C	446	THR
2	D	502	MET
2	D	508	ASP

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Mol	Chain	Res	Type
2	D	521	ARG
2	D	523	PHE
2	D	525	CYS
2	D	526	HIS
2	D	530	LEU
2	D	532	GLN
2	D	545	LEU
2	D	554	LEU
2	D	561	GLU
2	D	571	LEU
2	D	581	LEU
2	D	632	LYS
2	D	667	GLU
2	D	674	VAL
2	D	690	LEU
1	E	47	LEU
1	E	84	ARG
1	E	97	LYS
1	E	121	LYS
1	E	127	SER
1	E	135	LEU
1	E	240	LEU
1	E	253	LEU
1	E	282	LYS
1	E	290	ARG
1	E	293	ARG
1	E	366	MET
1	E	424	VAL
1	E	445	LYS
2	F	502	MET
2	F	508	ASP
2	F	523	PHE
2	F	525	CYS
2	F	526	HIS
2	F	530	LEU
2	F	545	LEU
2	F	554	LEU
2	F	561	GLU
2	F	571	LEU
2	F	581	LEU
2	F	632	LYS
2	F	667	GLU

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Mol	Chain	Res	Type
2	F	674	VAL
2	F	690	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	5	ASN
1	A	21	HIS
1	A	115	GLN
1	A	154	GLN
2	B	514	HIS
2	B	548	GLN
2	B	593	GLN
1	C	4	ASN
1	C	21	HIS
1	C	115	GLN
2	D	514	HIS
2	D	543	HIS
2	D	593	GLN
1	E	4	ASN
1	E	21	HIS
1	E	115	GLN
1	E	201	ASN
2	F	514	HIS
2	F	593	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - 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	$\# Z > 2$
4	FES	E	451	1	0,4,4	-	-	-		
4	FES	A	451	1	0,4,4	-	-	-		
4	FES	C	451	1	0,4,4	-	-	-		

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
4	FES	E	451	1	-	-	0/1/1/1
4	FES	A	451	1	-	-	0/1/1/1
4	FES	C	451	1	-	-	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	451	FES	1	0

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	447/449 (99%)	0.21	43 (9%) 13 12	18, 27, 55, 86	0
1	C	447/449 (99%)	0.12	30 (6%) 24 22	18, 27, 55, 86	0
1	E	445/449 (99%)	0.28	28 (6%) 26 24	18, 28, 55, 86	0
2	B	193/194 (99%)	0.47	23 (11%) 9 8	21, 32, 78, 96	0
2	D	193/194 (99%)	0.49	23 (11%) 9 8	21, 32, 78, 96	0
2	F	193/194 (99%)	0.46	25 (12%) 7 6	21, 32, 78, 96	0
All	All	1918/1929 (99%)	0.28	172 (8%) 15 14	18, 29, 64, 96	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	447	THR	11.7
2	F	525	CYS	6.2
1	E	235	PRO	6.0
1	A	264	ASP	6.0
1	C	235	PRO	5.9
2	F	629	VAL	5.9
2	B	526	HIS	5.7
2	D	666	GLY	5.7
1	C	231	ALA	5.6
1	A	220	GLY	5.6
2	B	525	CYS	5.5
2	D	525	CYS	5.5
2	D	669	GLY	5.5
1	A	235	PRO	5.3
1	E	232	ALA	5.2
2	B	502	MET	5.1
2	D	524	ASN	5.0
2	D	502	MET	4.8
1	E	231	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
2	F	666	GLY	4.7
2	D	526	HIS	4.7
1	E	227	LEU	4.6
1	A	263	ALA	4.6
1	A	224	PHE	4.5
1	A	119	PHE	4.5
1	E	229	GLY	4.5
2	F	630	ASN	4.5
1	C	127	SER	4.4
1	C	446	THR	4.3
1	C	229	GLY	4.3
1	A	226	SER	4.3
1	E	233	LEU	4.3
2	F	502	MET	4.3
1	A	5	ASN	4.1
1	A	1	MET	4.1
2	B	668	GLY	4.1
2	D	629	VAL	4.1
2	D	667	GLU	3.9
2	B	524	ASN	3.9
1	C	233	LEU	3.9
1	E	445	LYS	3.8
1	E	234	PRO	3.7
2	B	666	GLY	3.7
1	C	236	GLU	3.7
1	C	232	ALA	3.7
2	F	526	HIS	3.7
2	D	528	SER	3.7
1	E	237	GLY	3.7
2	B	577	ARG	3.7
1	A	127	SER	3.7
1	E	230	ASN	3.6
1	A	233	LEU	3.6
1	E	119	PHE	3.6
1	A	123	LEU	3.6
1	E	224	PHE	3.5
2	F	524	ASN	3.5
2	B	667	GLU	3.5
2	D	632	LYS	3.5
1	A	234	PRO	3.4
1	A	3	TYR	3.3
1	C	230	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	234	PRO	3.3
2	B	629	VAL	3.3
1	A	4	ASN	3.3
2	F	528	SER	3.3
1	A	231	ALA	3.2
1	E	209	VAL	3.3
1	C	122	ASP	3.2
1	C	121	LYS	3.2
1	A	232	ALA	3.2
2	B	632	LYS	3.2
1	C	224	PHE	3.2
2	D	506	GLN	3.2
1	E	226	SER	3.1
1	C	228	ALA	3.1
2	B	529	ALA	3.1
2	D	670	VAL	3.1
1	A	262	SER	3.1
2	B	523	PHE	3.1
2	F	668	GLY	3.1
1	A	7	ILE	3.1
1	C	226	SER	3.1
2	D	527	ASP	3.1
2	D	577	ARG	3.0
2	F	505	ILE	3.0
1	A	360	SER	3.0
1	A	125	GLY	3.0
1	C	227	LEU	3.0
1	A	447	THR	3.0
1	C	237	GLY	2.9
2	F	631	ASP	2.9
2	D	523	PHE	2.9
1	C	278	GLU	2.9
1	A	225	SER	2.9
1	C	123	LEU	2.9
2	B	520	LEU	2.9
1	E	236	GLU	2.9
1	C	119	PHE	2.8
1	A	446	THR	2.8
2	D	665	ARG	2.8
2	F	665	ARG	2.8
2	B	669	GLY	2.8
1	A	221	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	129	ASN	2.7
1	A	214	ALA	2.7
2	D	630	ASN	2.7
2	F	527	ASP	2.7
2	B	555	GLU	2.7
1	A	227	LEU	2.7
2	F	520	LEU	2.7
1	A	131	LYS	2.6
2	B	633	GLU	2.6
2	D	520	LEU	2.6
2	F	632	LYS	2.6
1	A	2	ASN	2.6
1	A	445	LYS	2.6
1	C	445	LYS	2.6
1	C	264	ASP	2.6
2	B	528	SER	2.6
2	F	577	ARG	2.6
2	D	556	HIS	2.6
2	F	578	ARG	2.5
2	D	504	ASN	2.5
1	E	263	ALA	2.5
1	A	223	ILE	2.5
1	A	278	GLU	2.4
2	F	667	GLU	2.4
1	A	342	ARG	2.4
1	E	397	ALA	2.4
2	B	527	ASP	2.4
1	C	125	GLY	2.4
1	E	129	ASN	2.4
2	B	630	ASN	2.4
1	A	228	ALA	2.4
1	E	125	GLY	2.4
1	E	97	LYS	2.3
2	B	631	ASP	2.3
1	A	267	PRO	2.3
1	A	209	VAL	2.3
1	E	278	GLU	2.3
2	B	530	LEU	2.3
1	C	342	ARG	2.3
2	D	578	ARG	2.3
1	E	407	ALA	2.2
2	F	633	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	408	ILE	2.2
1	C	128	LEU	2.2
1	E	264	ASP	2.2
1	A	229	GLY	2.2
2	F	506	GLN	2.2
2	F	530	LEU	2.1
1	A	122	ASP	2.1
2	B	670	VAL	2.1
2	F	504	ASN	2.1
1	A	237	GLY	2.1
1	A	265	LEU	2.1
1	C	5	ASN	2.1
2	D	631	ASP	2.1
2	B	506	GLN	2.1
1	A	121	LYS	2.1
1	E	117	VAL	2.1
1	C	155	GLU	2.1
1	E	123	LEU	2.1
1	E	339	ASP	2.1
2	F	669	GLY	2.1
1	C	211	TRP	2.1
1	A	391	GLU	2.0
1	C	221	GLU	2.0
2	F	670	VAL	2.0
2	D	668	GLY	2.0
2	F	593	GLN	2.0
1	E	342	ARG	2.0

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	FE	A	452	1/1	0.96	0.06	36,36,36,36	0
3	FE	E	452	1/1	0.96	0.04	36,36,36,36	0
3	FE	C	452	1/1	0.97	0.04	35,35,35,35	0
4	FES	A	451	4/4	0.99	0.05	25,26,28,28	0
4	FES	C	451	4/4	0.99	0.04	22,23,24,26	0
4	FES	E	451	4/4	0.99	0.04	25,26,27,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.