



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2024 – 09:07 PM EST

PDB ID : 1NDO
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

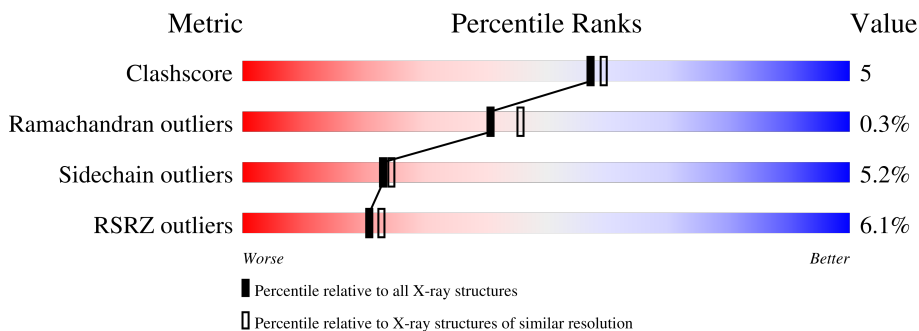
1 Overall quality at a glance

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	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (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	
1	C	449	
1	E	449	
2	B	194	
2	D	194	
2	F	194	

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
			Total	C	N	O	S			
1	A	447	3480	2202	597	665	16	0	0	0
1	C	447	3480	2202	597	665	16	0	0	0
1	E	445	3466	2194	595	661	16	0	0	0

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

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

- Molecule 3 is FE (III) ION (three-letter code: 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 (three-letter code: 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		

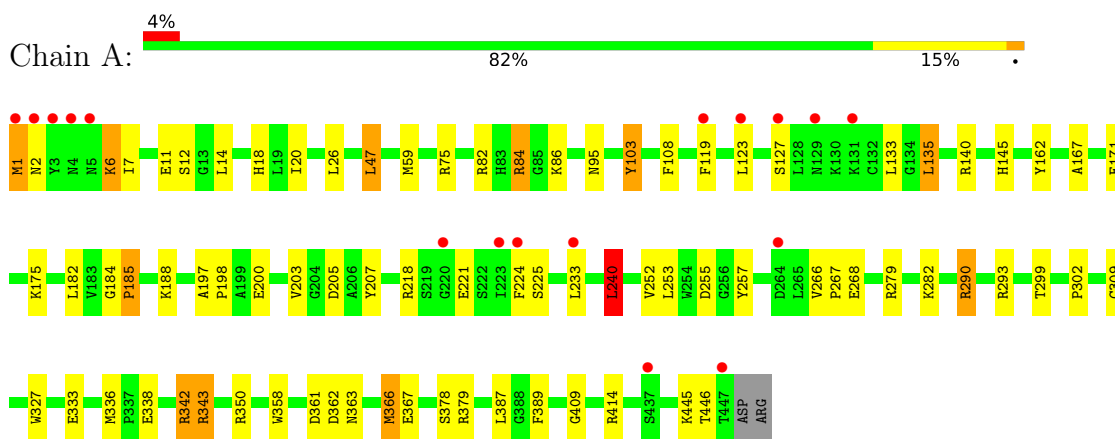
- Molecule 5 is water.

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		

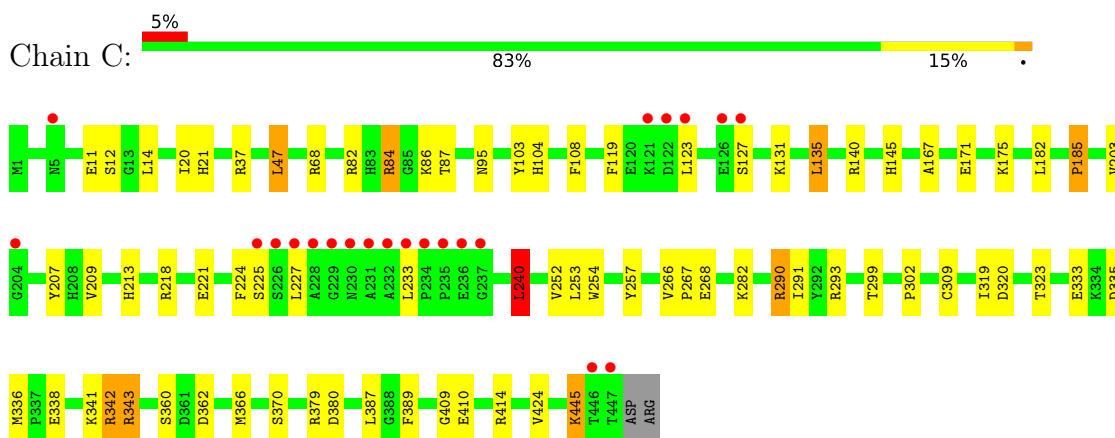
3 Residue-property plots [i](#)

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.

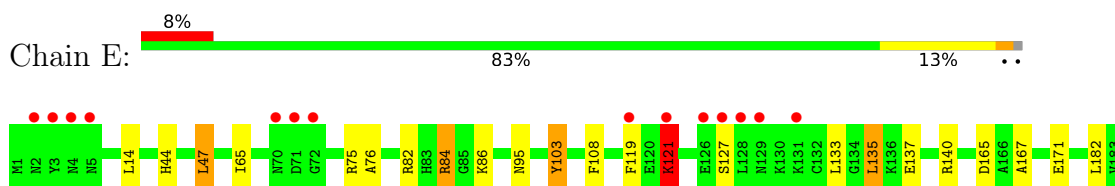
- Molecule 1: NAPHTHALENE 1,2-DIOXYGENASE

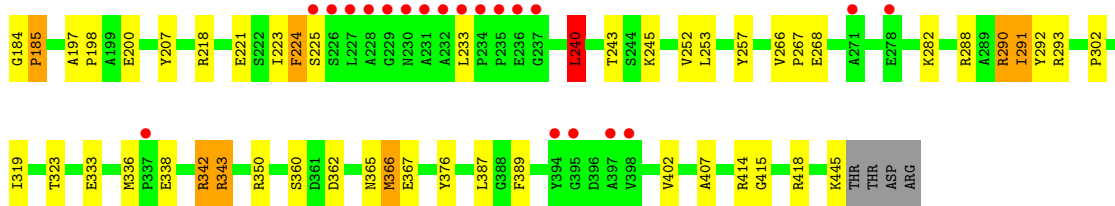


- Molecule 1: NAPHTHALENE 1,2-DIOXYGENASE

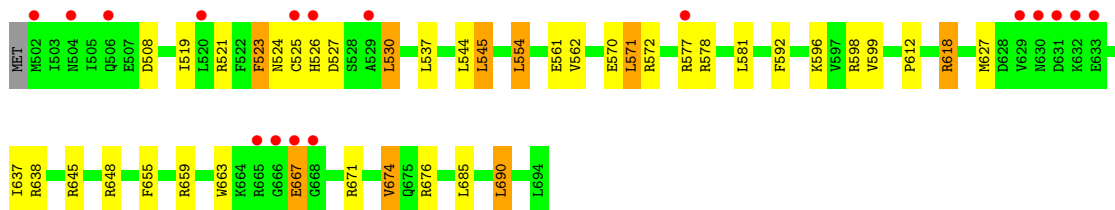
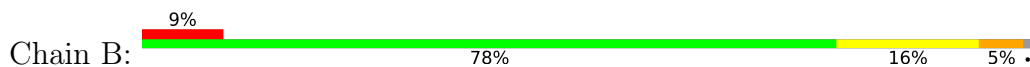


- Molecule 1: NAPHTHALENE 1,2-DIOXYGENASE

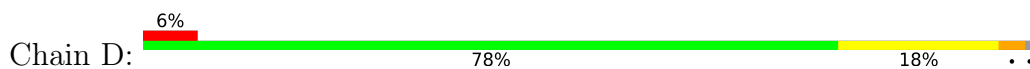




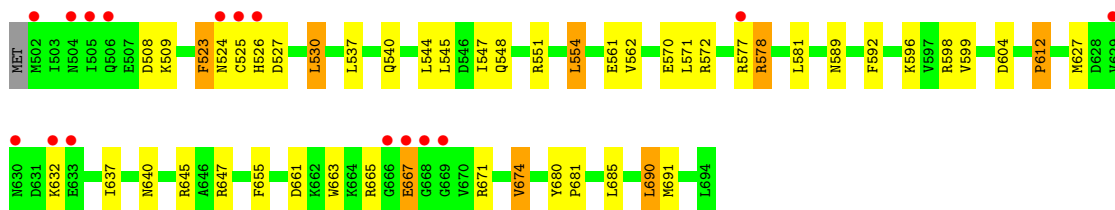
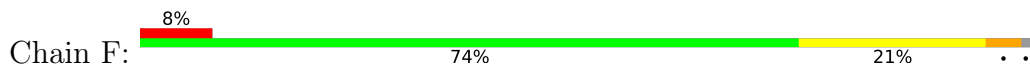
• Molecule 2: NAPHTHALENE 1,2-DIOXYGENASE



• 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 29.97 – 2.25	Depositor EDS
% Data completeness (in resolution range)	79.0 (30.00-2.25) 95.5 (29.97-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.24Å)	Xtrriage
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	Xtrriage
Anisotropy	0.365	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16326	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage'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	0.68	0/3572	1.45	32/4839 (0.7%)
1	C	0.67	0/3572	1.40	26/4839 (0.5%)
1	E	0.73	1/3558 (0.0%)	1.67	36/4819 (0.7%)
2	B	0.58	0/1638	1.33	11/2209 (0.5%)
2	D	0.55	0/1638	1.33	11/2209 (0.5%)
2	F	0.57	0/1638	1.27	14/2209 (0.6%)
All	All	0.66	1/15616 (0.0%)	1.45	130/21124 (0.6%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	121	LYS	CE-NZ	6.82	1.66	1.49

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	290	ARG	CD-NE-CZ	37.25	175.75	123.60
1	A	290	ARG	CD-NE-CZ	36.46	174.64	123.60
1	C	290	ARG	CD-NE-CZ	33.17	170.04	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	414	ARG	CD-NE-CZ	32.46	169.05	123.60
1	E	224	PHE	CB-CG-CD2	17.90	133.33	120.80
2	B	577	ARG	CD-NE-CZ	16.60	146.84	123.60
1	E	343	ARG	NE-CZ-NH2	-16.51	112.05	120.30
1	E	224	PHE	CD1-CG-CD2	-16.11	97.35	118.30
2	D	577	ARG	CD-NE-CZ	14.80	144.32	123.60
1	C	343	ARG	NE-CZ-NH2	-14.03	113.28	120.30
1	A	343	ARG	NE-CZ-NH2	-13.76	113.42	120.30
1	E	290	ARG	NE-CZ-NH1	12.36	126.48	120.30
1	E	224	PHE	CB-CG-CD1	12.16	129.31	120.80
1	E	224	PHE	CE1-CZ-CE2	-11.89	98.59	120.00
1	A	218	ARG	NE-CZ-NH1	11.64	126.12	120.30
2	D	618	ARG	NE-CZ-NH1	11.59	126.10	120.30
1	A	343	ARG	NE-CZ-NH1	11.57	126.09	120.30
1	C	343	ARG	NE-CZ-NH1	11.57	126.09	120.30
1	A	343	ARG	CD-NE-CZ	11.34	139.47	123.60
1	E	224	PHE	CG-CD2-CE2	10.77	132.65	120.80
2	F	577	ARG	CD-NE-CZ	10.62	138.46	123.60
1	E	343	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	E	288	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	E	218	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	E	224	PHE	CD1-CE1-CZ	9.71	131.75	120.10
1	E	418	ARG	NE-CZ-NH1	9.16	124.88	120.30
2	B	618	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	A	240	LEU	CA-CB-CG	8.90	135.78	115.30
2	D	577	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	E	224	PHE	CG-CD1-CE1	8.61	130.28	120.80
1	C	343	ARG	CD-NE-CZ	8.53	135.55	123.60
1	C	240	LEU	CA-CB-CG	8.52	134.89	115.30
1	E	240	LEU	CA-CB-CG	8.24	134.26	115.30
2	B	645	ARG	CD-NE-CZ	8.18	135.06	123.60
1	C	224	PHE	CB-CG-CD2	8.00	126.40	120.80
2	B	612	PRO	N-CA-CB	7.91	112.79	103.30
1	A	290	ARG	CA-CB-CG	7.88	130.73	113.40
1	E	343	ARG	CD-NE-CZ	7.88	134.63	123.60
1	A	279	ARG	NE-CZ-NH2	-7.77	116.42	120.30
2	B	638	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	E	224	PHE	CZ-CE2-CD2	7.70	129.34	120.10
1	E	350	ARG	NE-CZ-NH2	7.69	124.15	120.30
1	E	218	ARG	CD-NE-CZ	7.66	134.33	123.60
2	F	612	PRO	N-CA-CB	7.55	112.36	103.30
1	E	165	ASP	CB-CG-OD2	7.50	125.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	645	ARG	CD-NE-CZ	7.30	133.82	123.60
1	C	290	ARG	CA-CB-CG	7.23	129.30	113.40
1	A	218	ARG	CD-NE-CZ	7.19	133.66	123.60
1	C	68	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	A	414	ARG	CD-NE-CZ	7.16	133.63	123.60
1	C	82	ARG	NE-CZ-NH1	7.12	123.86	120.30
2	D	612	PRO	N-CA-CB	7.12	111.85	103.30
2	D	527	ASP	CB-CG-OD1	7.08	124.68	118.30
2	B	676	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	140	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	E	290	ARG	CA-CB-CG	7.05	128.91	113.40
1	C	302	PRO	N-CA-CB	6.89	111.56	103.30
1	E	257	TYR	CB-CG-CD2	-6.88	116.87	121.00
2	F	647	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	E	140	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	C	84	ARG	CG-CD-NE	6.66	125.79	111.80
1	E	75	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	255	ASP	CB-CG-OD2	6.60	124.24	118.30
1	C	290	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	A	185	PRO	N-CA-CB	6.55	111.17	103.30
1	E	376	TYR	CB-CG-CD2	-6.53	117.08	121.00
1	C	414	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	E	185	PRO	N-CA-CB	6.48	111.08	103.30
2	D	604	ASP	CB-CG-OD1	6.47	124.12	118.30
1	C	380	ASP	CB-CG-OD1	6.43	124.09	118.30
1	C	37	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	C	379	ARG	NE-CZ-NH1	-6.39	117.10	120.30
1	C	224	PHE	CD1-CG-CD2	-6.39	109.99	118.30
1	E	84	ARG	NE-CZ-NH2	6.39	123.49	120.30
1	A	379	ARG	NE-CZ-NH2	6.35	123.47	120.30
1	C	140	ARG	NE-CZ-NH2	6.26	123.43	120.30
2	D	683	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	75	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	F	598	ARG	NE-CZ-NH2	6.17	123.39	120.30
2	B	598	ARG	NE-CZ-NH2	-6.14	117.23	120.30
2	B	659	ARG	NE-CZ-NH2	-6.04	117.28	120.30
2	B	572	ARG	CG-CD-NE	6.00	124.41	111.80
1	C	335	ASP	CB-CG-OD1	6.00	123.70	118.30
2	B	648	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	C	185	PRO	N-CA-CB	5.96	110.45	103.30
2	D	598	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	E	257	TYR	CB-CG-CD1	5.89	124.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	224	PHE	CE1-CZ-CE2	-5.86	109.45	120.00
2	D	618	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	B	527	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	205	ASP	CB-CG-OD1	5.79	123.51	118.30
2	F	578	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	218	ARG	NH1-CZ-NH2	-5.65	113.18	119.40
1	A	302	PRO	N-CA-CB	5.61	110.03	103.30
1	A	224	PHE	CE1-CZ-CE2	-5.60	109.92	120.00
2	F	527	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	162	TYR	CA-CB-CG	5.58	124.00	113.40
1	C	320	ASP	CB-CG-OD1	5.57	123.31	118.30
1	E	367	GLU	OE1-CD-OE2	-5.55	116.64	123.30
1	A	59	MET	CG-SD-CE	5.54	109.06	100.20
1	E	302	PRO	N-CA-CB	5.50	109.90	103.30
2	F	680	TYR	CA-CB-CG	-5.47	103.01	113.40
1	C	410	GLU	OE1-CD-OE2	-5.45	116.76	123.30
2	F	572	ARG	CD-NE-CZ	5.45	131.23	123.60
1	E	137	GLU	OE1-CD-OE2	-5.43	116.78	123.30
2	F	661	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	E	407	ALA	N-CA-CB	-5.43	102.50	110.10
1	A	184	GLY	CA-C-O	-5.33	111.00	120.60
1	A	84	ARG	CG-CD-NE	5.32	122.97	111.80
2	D	676	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	366	MET	CA-CB-CG	5.22	122.17	113.30
1	A	6	LYS	N-CA-CB	5.18	119.92	110.60
1	E	414	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	E	290	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	302	PRO	N-CD-CG	5.16	110.94	103.20
1	A	350	ARG	CD-NE-CZ	5.14	130.79	123.60
1	A	361	ASP	CB-CG-OD1	5.12	122.91	118.30
2	F	681	PRO	N-CA-CB	5.12	109.44	103.30
2	F	551	ARG	CD-NE-CZ	5.11	130.75	123.60
1	C	218	ARG	CD-NE-CZ	5.11	130.75	123.60
2	D	659	ARG	NE-CZ-NH1	-5.11	117.75	120.30
2	F	604	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	1	MET	CA-CB-CG	5.09	121.96	113.30
1	C	379	ARG	NE-CZ-NH2	5.09	122.85	120.30
2	F	578	ARG	CD-NE-CZ	5.09	130.72	123.60
1	E	184	GLY	CA-C-O	-5.07	111.48	120.60
1	C	302	PRO	CA-N-CD	-5.02	104.47	111.50
1	A	224	PHE	CB-CG-CD2	5.02	124.31	120.80
1	A	358	TRP	O-C-N	-5.01	114.68	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	ARG	NE-CZ-NH2	5.01	122.81	120.30

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 [i](#)

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	41	0
1	C	3480	0	3316	36	0
1	E	3466	0	3302	35	0
2	B	1608	0	1583	18	0
2	D	1608	0	1583	17	0
2	F	1608	0	1583	23	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	147	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 (147) 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	1.49	0.77
1:E:333:GLU:H	1:E:336:MET:HE3	1.54	0.73
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
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
2:F:530:LEU:HD21	2:F:627:MET:HG2	1.85	0.58
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
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: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
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:D:667:GLU:HA	2:D:667:GLU:OE1	2.08	0.53
2:B:685:LEU:CD1	2:B:690:LEU:HB2	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:571:LEU:HD22	2:D:683:ARG:HG2	1.92	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:E:333:GLU:H	1:E:336:MET:CE	2.22	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
1:E:291:ILE:O	1:E:292:TYR:C	2.49	0.51
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
1:A:268:GLU:CD	1:A:343:ARG:HH22	2.15	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:C:333:GLU:H	1:C:336:MET:HE3	1.77	0.49
1:A:14:LEU:HD21	1:A:389:PHE:CG	2.46	0.49
1:C:268:GLU:CD	1:C:343:ARG:HH22	2.16	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
1:C:333:GLU:H	1:C:336:MET:CE	2.26	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:A:333:GLU:H	1:A:336:MET:CE	2.22	0.47
1:E:268:GLU:CD	1:E:343:ARG:HH22	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:547:ILE:O	2:F:548:GLN:HB2	2.15	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
1:C:333:GLU:HB2	1:C:336:MET:HE2	1.99	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
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
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: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
1:E:333:GLU:HB2	1:E:336:MET:HE2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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 [\(i\)](#)

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	445/449 (99%)	432 (97%)	12 (3%)	1 (0%)	47	55
1	C	445/449 (99%)	432 (97%)	12 (3%)	1 (0%)	47	55
1	E	443/449 (99%)	431 (97%)	12 (3%)	0	100	100
2	B	191/194 (98%)	184 (96%)	6 (3%)	1 (0%)	29	29
2	D	191/194 (98%)	184 (96%)	6 (3%)	1 (0%)	29	29
2	F	191/194 (98%)	185 (97%)	5 (3%)	1 (0%)	29	29
All	All	1906/1929 (99%)	1848 (97%)	53 (3%)	5 (0%)	41	46

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 [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%)	355 (97%)	12 (3%)	38	46
1	C	367/369 (100%)	352 (96%)	15 (4%)	30	36
1	E	365/369 (99%)	350 (96%)	15 (4%)	30	36
2	B	172/173 (99%)	158 (92%)	14 (8%)	11	10
2	D	172/173 (99%)	158 (92%)	14 (8%)	11	10
2	F	172/173 (99%)	158 (92%)	14 (8%)	11	10
All	All	1615/1626 (99%)	1531 (95%)	84 (5%)	23	24

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	84	ARG
1	A	103	TYR
1	A	127	SER
1	A	135	LEU
1	A	207	TYR
1	A	240	LEU
1	A	253	LEU
1	A	282	LYS
1	A	290	ARG
1	A	293	ARG
1	A	342	ARG
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	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	84	ARG
1	C	103	TYR
1	C	127	SER
1	C	131	LYS
1	C	135	LEU
1	C	207	TYR
1	C	240	LEU
1	C	253	LEU
1	C	282	LYS
1	C	290	ARG
1	C	293	ARG
1	C	342	ARG
1	C	424	VAL
1	C	445	LYS
2	D	508	ASP
2	D	523	PHE

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Mol	Chain	Res	Type
2	D	525	CYS
2	D	526	HIS
2	D	530	LEU
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	103	TYR
1	E	121	LYS
1	E	127	SER
1	E	135	LEU
1	E	207	TYR
1	E	240	LEU
1	E	253	LEU
1	E	282	LYS
1	E	290	ARG
1	E	293	ARG
1	E	342	ARG
1	E	366	MET
1	E	445	LYS
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
2	F	674	VAL
2	F	690	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	5	ASN
1	A	115	GLN
2	B	514	HIS
1	C	115	GLN
2	D	514	HIS
2	D	624	GLN
1	E	4	ASN
1	E	115	GLN
2	F	514	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	451	1	0,4,4	-	-	-		
4	FES	A	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	C	451	1	-	-	0/1/1/1
4	FES	A	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 [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%)	-0.10	17 (3%) 40 43	18, 27, 55, 86	0
1	C	447/449 (99%)	-0.11	22 (4%) 29 32	18, 27, 55, 86	0
1	E	445/449 (99%)	-0.01	34 (7%) 13 15	18, 28, 55, 86	0
2	B	193/194 (99%)	0.07	17 (8%) 10 11	21, 32, 78, 96	0
2	D	193/194 (99%)	-0.07	11 (5%) 23 25	21, 32, 78, 96	0
2	F	193/194 (99%)	0.01	16 (8%) 11 12	21, 32, 78, 96	0
All	All	1918/1929 (99%)	-0.05	117 (6%) 21 23	18, 29, 64, 96	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	447	THR	12.4
1	E	232	ALA	11.7
1	C	231	ALA	10.3
2	F	525	CYS	7.9
2	D	666	GLY	7.2
2	F	667	GLU	7.0
2	D	667	GLU	7.0
1	E	233	LEU	6.8
1	E	231	ALA	6.5
2	D	629	VAL	6.3
1	E	236	GLU	6.2
1	E	229	GLY	6.1
2	B	666	GLY	5.8
2	B	526	HIS	5.8
2	F	666	GLY	5.7
1	E	235	PRO	5.7
1	C	446	THR	5.5
2	D	525	CYS	5.4
1	E	234	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
1	E	226	SER	5.3
2	F	506	GLN	5.2
1	A	5	ASN	5.0
2	F	526	HIS	4.9
2	B	525	CYS	4.9
2	B	577	ARG	4.8
1	C	235	PRO	4.8
2	B	667	GLU	4.8
1	C	229	GLY	4.7
1	A	220	GLY	4.7
1	E	397	ALA	4.7
2	D	526	HIS	4.6
2	B	502	MET	4.6
1	C	236	GLU	4.5
2	D	668	GLY	4.4
1	E	237	GLY	4.4
2	D	632	LYS	4.3
1	A	119	PHE	4.2
1	E	228	ALA	4.1
1	A	1	MET	4.1
2	F	577	ARG	4.1
1	C	234	PRO	3.9
1	C	122	ASP	3.9
2	F	502	MET	3.8
2	D	669	GLY	3.7
1	C	127	SER	3.7
1	A	264	ASP	3.7
1	A	3	TYR	3.7
1	C	233	LEU	3.6
1	A	131	LYS	3.6
2	F	668	GLY	3.6
1	C	228	ALA	3.6
1	C	121	LYS	3.6
1	A	447	THR	3.5
1	E	119	PHE	3.5
1	C	232	ALA	3.5
2	F	524	ASN	3.5
2	B	632	LYS	3.5
2	B	529	ALA	3.4
1	A	2	ASN	3.4
2	F	632	LYS	3.4
1	A	4	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
2	F	629	VAL	3.4
1	E	121	LYS	3.4
1	C	126	GLU	3.3
1	E	230	ASN	3.3
1	C	226	SER	3.3
1	E	127	SER	3.3
1	E	398	VAL	3.2
1	E	5	ASN	3.0
2	B	520	LEU	3.0
1	E	225	SER	2.9
1	C	5	ASN	2.9
1	E	126	GLU	2.9
1	E	72	GLY	2.9
2	B	631	ASP	2.9
2	B	506	GLN	2.8
1	C	230	ASN	2.8
1	E	71	ASP	2.8
2	F	630	ASN	2.8
2	F	669	GLY	2.8
2	B	629	VAL	2.8
2	B	630	ASN	2.8
1	E	227	LEU	2.7
1	E	131	LYS	2.7
1	E	128	LEU	2.7
1	E	337	PRO	2.6
1	E	278	GLU	2.6
2	B	668	GLY	2.6
2	B	504	ASN	2.5
2	B	633	GLU	2.5
2	D	631	ASP	2.5
1	C	227	LEU	2.5
1	E	70	ASN	2.5
1	A	129	ASN	2.4
1	A	223	ILE	2.4
1	A	123	LEU	2.4
1	E	129	ASN	2.4
1	A	437	SER	2.3
1	E	394	TYR	2.3
1	E	2	ASN	2.3
1	C	237	GLY	2.2
1	A	233	LEU	2.2
1	C	204	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	3	TYR	2.2
2	D	630	ASN	2.2
1	C	225	SER	2.2
2	F	505	ILE	2.2
1	A	224	PHE	2.2
2	D	524	ASN	2.1
2	F	504	ASN	2.1
2	B	665	ARG	2.1
1	E	271	ALA	2.1
1	E	4	ASN	2.1
2	F	633	GLU	2.1
1	A	127	SER	2.1
1	C	123	LEU	2.1
1	E	395	GLY	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 monosaccharides 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	0.95	0.07	36,36,36,36	0
3	FE	C	452	1/1	0.96	0.08	35,35,35,35	0
3	FE	E	452	1/1	0.98	0.06	36,36,36,36	0
4	FES	A	451	4/4	0.99	0.04	25,26,28,28	0
4	FES	C	451	4/4	0.99	0.08	22,23,24,26	0
4	FES	E	451	4/4	1.00	0.04	25,26,27,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.