



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:14 AM UTC

PDB ID : 4P1C / pdb_00004p1c
Title : CRYSTAL STRUCTURE OF THE TOLUENE 4-MONOOXYGENASE HYDROXYLASE-FERREDOXIN C7S, C84A, C85A VARIANT ELECTRON-TRANSFER COMPLEX
Authors : Acheson, J.F.; Fox, B.G.
Deposited on : 2014-02-25
Resolution : 2.40 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

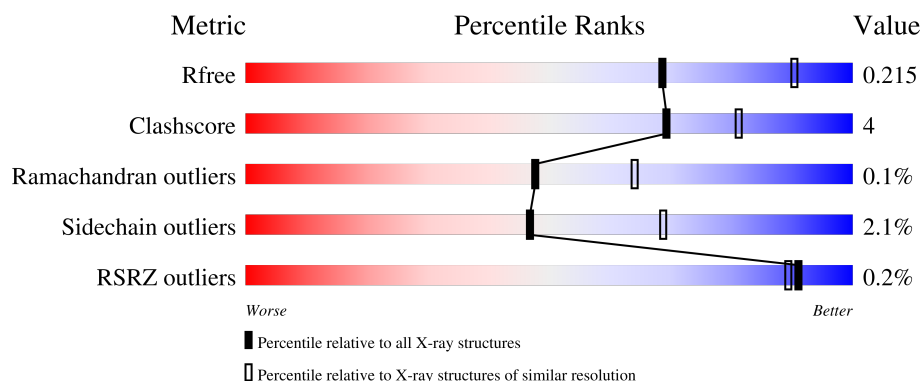
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	490	90% 9% .
1	D	490	86% 13% .
2	B	305	83% 16% .
2	E	305	89% 11%
3	C	82	87% 11% .

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Mol	Chain	Length	Quality of chain
3	F	82	85% 13%
4	H	111	95% 5%
4	I	111	89% 7%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16762 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 Toluene-4-monooxygenase system protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			4030	2584	681	743	22			
1	D	490	Total	C	N	O	S	0	0	0
			4030	2584	681	743	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	336	TRP	LEU	see remark 999	UNP Q00456
A	337	TYR	ASP	see remark 999	UNP Q00456
D	336	TRP	LEU	see remark 999	UNP Q00456
D	337	TYR	ASP	see remark 999	UNP Q00456

- Molecule 2 is a protein called Toluene-4-monooxygenase system protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	305	Total	C	N	O	S	0	0	0
			2528	1601	438	474	15			
2	E	305	Total	C	N	O	S	0	0	0
			2528	1601	438	474	15			

- Molecule 3 is a protein called Toluene-4-monooxygenase system protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	82	Total	C	N	O	S	1	0	0
			654	412	117	121	4			
3	F	82	Total	C	N	O	S	2	0	0
			654	412	117	121	4			

- Molecule 4 is a protein called Toluene-4-monooxygenase system ferredoxin subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	111	Total	C	N	O	S	0	0	0
			851	533	137	177	4			
4	I	111	Total	C	N	O	S	3	1	0
			854	535	138	177	4			

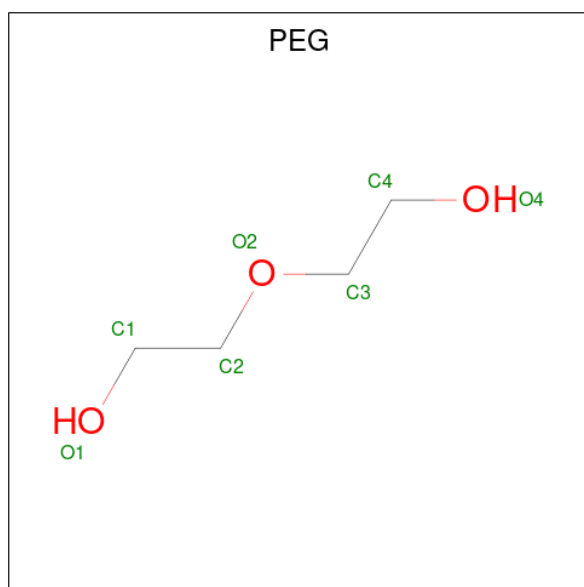
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	7	SER	CYS	engineered mutation	UNP Q00458
H	84	ALA	CYS	engineered mutation	UNP Q00458
H	85	ALA	CYS	engineered mutation	UNP Q00458
I	7	SER	CYS	engineered mutation	UNP Q00458
I	84	ALA	CYS	engineered mutation	UNP Q00458
I	85	ALA	CYS	engineered mutation	UNP Q00458

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

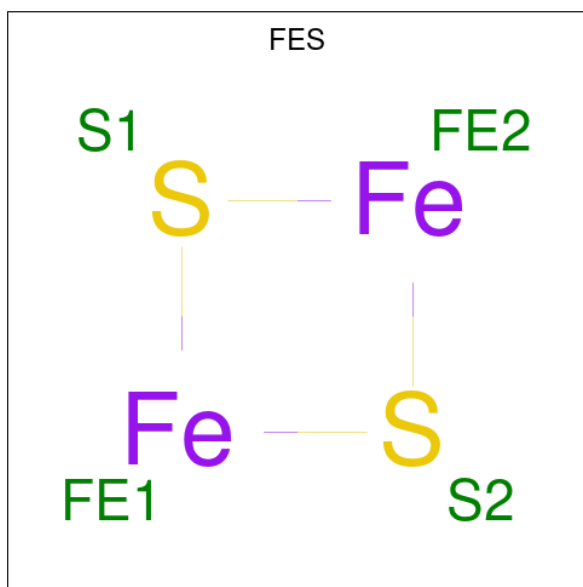
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Fe	0	0
			2	2		
5	D	2	Total	Fe	0	0
			2	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			5	3	2		
6	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	Fe	S	0	0
			4	2	2		
7	I	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	172	Total	O	0	0
			172	172		
8	B	78	Total	O	0	0
			78	78		
8	C	23	Total	O	0	0
			23	23		
8	D	154	Total	O	0	0
			154	154		
8	E	99	Total	O	0	0
			99	99		
8	F	6	Total	O	0	0
			6	6		

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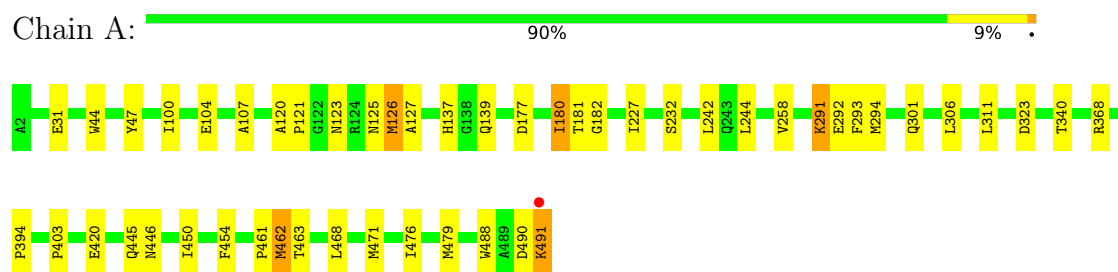
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	38	Total 38	O 38	0	0
8	I	39	Total 39	O 39	0	0

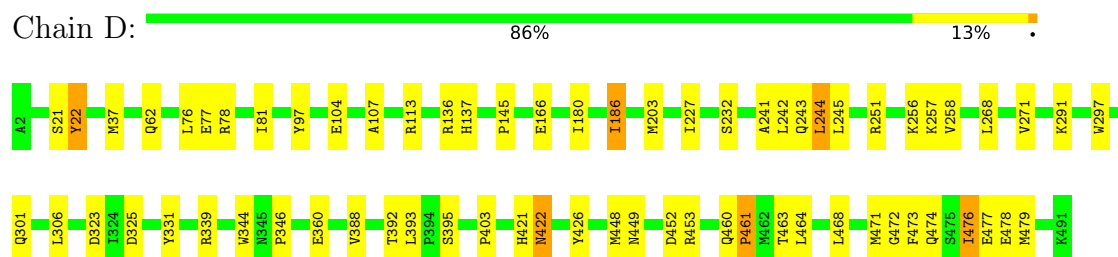
3 Residue-property plots

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.

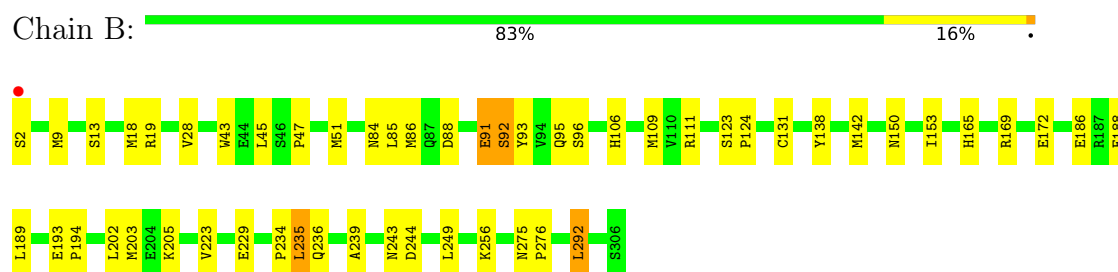
- Molecule 1: Toluene-4-monooxygenase system protein A



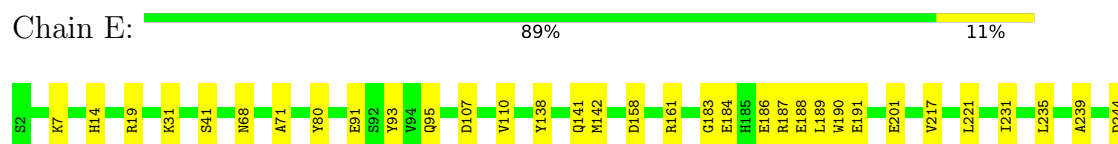
- Molecule 1: Toluene-4-monooxygenase system protein A



- Molecule 2: Toluene-4-monooxygenase system protein E



- Molecule 2: Toluene-4-monooxygenase system protein E





- Molecule 3: Toluene-4-monooxygenase system protein B

Chain C: 87% 11% .



- Molecule 3: Toluene-4-monooxygenase system protein B

Chain F: 85% 13% .



- Molecule 4: Toluene-4-monooxygenase system ferredoxin subunit

Chain H: 95% 5% .



- Molecule 4: Toluene-4-monooxygenase system ferredoxin subunit

Chain I: 89% 7% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.23Å 106.35Å 213.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.69 – 2.40 47.69 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.1 (47.69-2.40) 90.7 (47.69-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.37Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1184)	Depositor
R, R_{free}	0.153 , 0.215 0.157 , 0.215	Depositor DCC
R_{free} test set	4187 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16762	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 3.38% 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: PEG, 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	0.66	10/4159 (0.2%)	0.83	4/5648 (0.1%)
1	D	0.78	17/4159 (0.4%)	0.83	2/5648 (0.0%)
2	B	0.86	15/2603 (0.6%)	0.87	4/3537 (0.1%)
2	E	0.66	7/2603 (0.3%)	0.81	0/3537
3	C	0.76	4/666 (0.6%)	0.83	0/902
3	F	0.79	2/666 (0.3%)	0.92	2/902 (0.2%)
4	H	0.60	0/870	0.76	1/1182 (0.1%)
4	I	0.79	3/879 (0.3%)	0.79	0/1193
All	All	0.74	58/16605 (0.3%)	0.83	13/22549 (0.1%)

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	245	LEU	C-O	-7.60	1.15	1.24
2	E	189	LEU	C-O	-7.27	1.15	1.24
1	D	21	SER	C-O	-7.00	1.15	1.24
4	I	110	ALA	C-O	-6.93	1.15	1.24
1	A	125	ASN	C-O	-6.92	1.16	1.24
1	D	251	ARG	C-O	-6.80	1.16	1.24
2	B	235	LEU	C-O	-6.75	1.16	1.24
4	I	109	LYS	C-O	-6.75	1.16	1.24
1	A	294	MET	C-O	-6.73	1.16	1.24
2	B	84	ASN	C-O	-6.63	1.15	1.24
2	E	187	ARG	C-O	-6.55	1.16	1.24
1	A	127	ALA	C-O	-6.55	1.15	1.24
3	C	60	LEU	C-O	-6.54	1.16	1.23
2	E	191	GLU	C-O	-6.49	1.16	1.24
1	A	291	LYS	C-O	-6.40	1.16	1.24
2	B	43	TRP	C-O	-6.32	1.16	1.23
1	A	292	GLU	C-O	-6.29	1.16	1.24
2	E	190	TRP	C-O	-6.25	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	474	GLN	C-O	-6.25	1.16	1.24
2	B	106	HIS	C-O	-6.24	1.16	1.24
1	D	244	LEU	C-O	-6.24	1.16	1.24
1	D	243	GLN	C-O	-6.23	1.16	1.24
1	D	242	LEU	C-O	-6.08	1.17	1.24
2	B	188	GLU	C-O	-6.05	1.17	1.24
2	B	91	GLU	C-O	-5.99	1.16	1.24
1	D	241	ALA	C-O	-5.86	1.17	1.24
2	B	123	SER	C-N	5.83	1.40	1.34
1	D	472	GLY	C-O	-5.83	1.16	1.24
2	E	186	GLU	C-O	-5.81	1.17	1.24
2	B	236	GLN	C-O	-5.79	1.17	1.24
2	B	45	LEU	C-O	-5.77	1.17	1.24
1	D	477	GLU	C-O	-5.77	1.16	1.24
2	E	184	GLU	C-O	-5.67	1.15	1.23
3	F	61	PHE	C-N	5.65	1.41	1.33
1	D	477	GLU	N-CA	-5.61	1.39	1.46
1	A	368	ARG	CA-C	5.59	1.55	1.52
2	B	93	TYR	C-O	-5.58	1.17	1.24
3	C	58	THR	C-O	-5.56	1.16	1.24
3	C	60	LEU	CA-C	-5.46	1.46	1.52
3	F	62	PRO	C-O	-5.38	1.17	1.23
2	B	86	MET	C-O	-5.31	1.18	1.24
1	A	293	PHE	C-O	-5.22	1.17	1.24
2	B	91	GLU	CA-C	-5.21	1.45	1.52
3	C	59	GLU	C-O	-5.19	1.17	1.24
1	D	22	TYR	C-O	-5.19	1.17	1.24
2	B	124	PRO	C-O	-5.17	1.17	1.24
2	B	186	GLU	C-O	-5.17	1.18	1.24
2	E	183	GLY	C-O	-5.14	1.17	1.23
2	B	234	PRO	C-O	-5.13	1.18	1.24
1	D	478	GLU	C-O	-5.13	1.17	1.24
1	D	62	GLN	C-O	-5.12	1.17	1.24
1	A	126	MET	C-O	-5.11	1.18	1.24
4	I	108	ASN	C-O	-5.10	1.17	1.23
1	D	461	PRO	N-CD	5.09	1.54	1.47
1	A	294	MET	CA-C	-5.04	1.46	1.52
1	A	291	LYS	N-CA	-5.04	1.40	1.46
1	D	473	PHE	C-O	-5.03	1.17	1.23
1	D	460	GLN	C-O	-5.00	1.17	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	460	GLN	C-N-CD	8.46	139.21	120.60
1	A	100	ILE	N-CA-C	6.28	116.99	111.90
1	A	180	ILE	CB-CA-C	-6.06	106.56	111.71
2	B	186	GLU	N-CA-C	5.97	117.78	111.28
1	A	445	GLN	N-CA-C	5.83	117.63	111.28
2	B	123	SER	CA-C-N	-5.76	113.88	119.87
2	B	123	SER	C-N-CA	-5.76	113.88	119.87
4	H	79	ILE	N-CA-C	-5.58	107.38	111.90
1	A	125	ASN	N-CA-C	5.58	117.16	111.14
1	D	478	GLU	N-CA-C	5.40	118.08	111.82
2	B	124	PRO	CA-N-CD	-5.38	104.47	112.00
3	F	61	PHE	CA-C-N	-5.30	114.30	119.76
3	F	61	PHE	C-N-CA	-5.30	114.30	119.76

There are no chirality outliers.

There are no planarity outliers.

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	4030	0	3786	23	0
1	D	4030	0	3786	34	0
2	B	2528	0	2408	24	0
2	E	2528	0	2408	18	0
3	C	654	0	649	4	0
3	F	654	0	649	10	0
4	H	851	0	792	3	0
4	I	854	0	797	5	0
5	A	2	0	0	0	0
5	D	2	0	0	0	0
6	A	5	0	4	1	0
6	D	7	0	9	1	0
7	H	4	0	0	0	0
7	I	4	0	0	0	0
8	A	172	0	0	0	0
8	B	78	0	0	1	0
8	C	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	154	0	0	0	0
8	E	99	0	0	0	0
8	F	6	0	0	1	0
8	H	38	0	0	0	0
8	I	39	0	0	0	0
All	All	16762	0	15288	111	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 4.

All (111) 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)
3:F:62:PRO:HD2	3:F:65:MET:HE2	1.13	1.12
3:F:62:PRO:HD2	3:F:65:MET:CE	1.78	1.12
2:E:19:ARG:NH2	4:I:10:ASP:OD1	2.15	0.78
1:A:491:LYS:HD3	1:A:491:LYS:H	1.51	0.76
3:F:62:PRO:CD	3:F:65:MET:CE	2.61	0.75
1:A:491:LYS:HD3	1:A:491:LYS:N	2.02	0.74
2:E:19:ARG:NH2	4:I:96:ASP:OD2	2.18	0.70
3:F:65:MET:HG3	3:F:69:GLU:HG3	1.72	0.69
3:F:53:ARG:HB3	3:F:60:LEU:HD23	1.74	0.68
1:D:448:MET:HE2	1:D:452:ASP:HB3	1.74	0.67
1:D:291:LYS:HD2	1:D:325:ASP:HB3	1.77	0.66
1:D:476:ILE:HD13	1:D:479:MET:CE	2.26	0.65
3:F:11:GLU:OE2	8:F:106:HOH:O	2.13	0.64
3:F:28:ASP:OD1	3:F:63:ARG:HB3	1.99	0.63
1:D:37:MET:HE2	1:D:257:LYS:HE2	1.82	0.61
2:B:91:GLU:OE1	2:B:165:HIS:NE2	2.29	0.61
2:B:19:ARG:NH2	4:H:96:ASP:OD2	2.32	0.61
1:D:258:VAL:HG11	1:D:306:LEU:HD21	1.83	0.61
1:D:203:MET:HE2	1:D:297:TRP:HB3	1.82	0.61
2:B:111:ARG:HH11	2:B:243:ASN:HB2	1.64	0.60
2:B:91:GLU:O	2:B:95:GLN:HG2	2.02	0.59
3:C:30:VAL:HG21	3:C:67:ILE:HD11	1.86	0.58
3:C:2:SER:HA	3:C:23:LEU:HD12	1.87	0.56
1:D:104:GLU:CD	6:D:503:PEG:H32	2.31	0.56
2:B:9:MET:HE1	2:B:13:SER:HB3	1.87	0.56
4:I:111:HIS:O	4:I:112:SER:HB2	2.07	0.55
1:A:394:PRO:HB2	1:A:403:PRO:HB3	1.91	0.53
1:D:422:ASN:N	1:D:422:ASN:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:VAL:HG23	1:D:331:TYR:HB3	1.93	0.51
1:D:461:PRO:C	1:D:463:THR:H	2.18	0.51
2:B:131:CYS:HB3	2:B:203:MET:HE2	1.93	0.51
4:I:8:SER:OG	4:I:11:ASP:OD1	2.27	0.51
1:D:421:HIS:HB3	1:D:426:TYR:HE1	1.77	0.50
1:D:301:GLN:N	1:D:301:GLN:OE1	2.44	0.50
1:D:476:ILE:HD13	1:D:479:MET:HE1	1.94	0.49
1:A:258:VAL:HG11	1:A:306:LEU:HD21	1.94	0.49
2:B:202:LEU:HD21	2:B:223:VAL:HG22	1.95	0.49
1:D:421:HIS:HB3	1:D:426:TYR:CE1	2.47	0.49
1:A:44:TRP:HA	1:A:244:LEU:HD11	1.94	0.49
3:F:66:THR:OG1	3:F:69:GLU:HG2	2.13	0.49
1:A:450:ILE:HD13	1:A:471:MET:HE2	1.95	0.48
3:C:49:VAL:HG13	3:C:83:GLU:HB2	1.94	0.48
3:F:25:ASP:O	3:F:66:THR:HA	2.13	0.48
4:H:5:LYS:HG3	4:H:99:TYR:CZ	2.50	0.47
1:A:182:GLY:HA2	2:B:51:MET:HG2	1.97	0.47
1:A:476:ILE:HA	1:A:479:MET:HE2	1.97	0.47
1:D:344:TRP:O	1:D:346:PRO:HD3	2.14	0.47
1:A:104:GLU:OE1	6:A:503:PEG:H42	2.15	0.46
2:E:68:ASN:ND2	2:E:71:ALA:HB2	2.29	0.46
4:I:20:PHE:CD2	4:I:30:ILE:HD12	2.50	0.46
3:F:28:ASP:OD2	3:F:63:ARG:NH2	2.37	0.46
1:A:491:LYS:N	1:A:491:LYS:CD	2.75	0.46
2:E:188:GLU:H	2:E:188:GLU:CD	2.24	0.46
1:A:139:GLN:HG2	2:B:28:VAL:HB	1.96	0.46
2:E:231:ILE:O	2:E:235:LEU:HB2	2.16	0.46
1:A:177:ASP:HA	1:A:181:THR:OG1	2.16	0.45
2:B:88:ASP:O	2:B:92:SER:HB3	2.17	0.45
3:C:65:MET:HG3	3:C:69:GLU:HG3	1.99	0.45
2:B:239:ALA:HB1	2:B:244:ASP:HB3	1.99	0.45
1:A:137:HIS:CE1	1:A:227:ILE:HG23	2.51	0.44
1:D:468:LEU:HD13	1:D:479:MET:SD	2.57	0.44
2:B:193:GLU:HA	2:B:194:PRO:HD3	1.87	0.44
1:A:488:TRP:HA	1:A:491:LYS:HE2	2.00	0.44
2:E:7:LYS:HD3	2:E:7:LYS:HA	1.79	0.44
1:D:137:HIS:CE1	1:D:227:ILE:HG23	2.52	0.44
1:D:476:ILE:HD13	1:D:476:ILE:HA	1.72	0.44
2:E:14:HIS:CD2	2:E:31:LYS:HD2	2.53	0.44
1:D:81:ILE:HD13	1:D:81:ILE:HA	1.84	0.44
2:B:18:MET:HE3	8:B:425:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:THR:OG1	1:D:393:LEU:N	2.51	0.44
2:E:91:GLU:O	2:E:95:GLN:HG2	2.18	0.44
2:B:275:ASN:HA	2:B:276:PRO:HD2	1.88	0.43
1:D:339:ARG:HH12	1:D:388:VAL:HG23	1.83	0.43
1:D:449:ASN:O	1:D:453:ARG:HG3	2.18	0.43
2:B:169:ARG:NH2	2:B:172:GLU:OE2	2.50	0.43
1:D:268:LEU:O	1:D:271:VAL:HG12	2.19	0.43
2:E:158:ASP:O	2:E:161:ARG:HB3	2.17	0.43
2:B:189:LEU:HD23	2:B:193:GLU:HB2	1.99	0.43
1:D:22:TYR:CD2	2:E:201:GLU:HA	2.54	0.43
2:E:138:TYR:CZ	2:E:142:MET:HG3	2.53	0.43
1:A:446:ASN:HB2	2:B:47:PRO:HD2	2.01	0.43
1:A:242:LEU:HD22	1:A:311:LEU:HD11	2.01	0.43
2:B:96:SER:HB2	2:E:93:TYR:CD1	2.54	0.43
1:D:395:SER:O	1:D:403:PRO:HA	2.18	0.42
1:A:454:PHE:O	1:A:462:MET:HE3	2.19	0.42
1:D:76:LEU:C	1:D:78:ARG:H	2.27	0.42
4:H:111:HIS:CD2	4:H:111:HIS:H	2.38	0.42
1:A:468:LEU:HD13	1:A:479:MET:SD	2.59	0.42
1:A:107:ALA:HA	1:A:180:ILE:HG21	2.00	0.42
2:B:109:MET:O	2:B:243:ASN:ND2	2.52	0.42
1:A:461:PRO:C	1:A:463:THR:H	2.27	0.42
2:B:249:LEU:HD23	2:B:249:LEU:HA	1.92	0.42
2:B:205:LYS:HD2	2:B:292:LEU:HD21	2.01	0.41
1:D:136:ARG:HB2	2:E:80:TYR:CZ	2.55	0.41
2:E:239:ALA:HB1	2:E:244:ASP:HB3	2.01	0.41
2:B:150:ASN:HA	2:B:153:ILE:HD12	2.01	0.41
1:D:461:PRO:O	1:D:463:THR:N	2.47	0.41
2:B:138:TYR:CZ	2:B:142:MET:HG3	2.56	0.41
2:B:169:ARG:HA	2:B:169:ARG:HD2	1.88	0.41
1:A:47:TYR:CZ	1:A:123:ASN:HB2	2.56	0.41
1:A:120:ALA:HA	1:A:121:PRO:HD3	1.93	0.41
1:D:107:ALA:HA	1:D:180:ILE:HG21	2.02	0.41
2:E:217:VAL:HG13	2:E:221:LEU:HD12	2.00	0.41
1:D:97:TYR:CD2	1:D:145:PRO:HB3	2.56	0.41
1:D:268:LEU:HD12	1:D:268:LEU:HA	1.92	0.41
2:E:107:ASP:O	2:E:110:VAL:HG22	2.21	0.41
1:A:301:GLN:OE1	1:A:301:GLN:N	2.50	0.40
1:D:113:ARG:NH1	2:E:141:GLN:OE1	2.51	0.40
2:E:255:LEU:HD23	2:E:255:LEU:HA	1.88	0.40
1:D:186:ILE:HA	1:D:186:ILE:HD13	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:GLU:HA	1:D:471:MET:HG2	2.04	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	488/490 (100%)	470 (96%)	17 (4%)	1 (0%)	43	58
1	D	488/490 (100%)	468 (96%)	20 (4%)	0	100	100
2	B	303/305 (99%)	299 (99%)	4 (1%)	0	100	100
2	E	303/305 (99%)	297 (98%)	6 (2%)	0	100	100
3	C	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
3	F	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
4	H	109/111 (98%)	103 (94%)	6 (6%)	0	100	100
4	I	110/111 (99%)	104 (94%)	5 (4%)	1 (1%)	14	22
All	All	1961/1976 (99%)	1894 (97%)	65 (3%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	110	ALA
1	A	490	ASP

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	415/415 (100%)	406 (98%)	9 (2%)	45	67
1	D	415/415 (100%)	405 (98%)	10 (2%)	43	65
2	B	276/276 (100%)	269 (98%)	7 (2%)	42	64
2	E	276/276 (100%)	275 (100%)	1 (0%)	84	92
3	C	73/73 (100%)	71 (97%)	2 (3%)	39	62
3	F	73/73 (100%)	72 (99%)	1 (1%)	59	79
4	H	93/93 (100%)	91 (98%)	2 (2%)	45	67
4	I	94/93 (101%)	90 (96%)	4 (4%)	26	44
All	All	1715/1714 (100%)	1679 (98%)	36 (2%)	47	69

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	126	MET
1	A	232	SER
1	A	291	LYS
1	A	323	ASP
1	A	340	THR
1	A	420	GLU
1	A	462	MET
1	A	491	LYS
2	B	2	SER
2	B	85	LEU
2	B	92	SER
2	B	229	GLU
2	B	235	LEU
2	B	256	LYS
2	B	292	LEU
3	C	58	THR
3	C	59	GLU
1	D	77	GLU
1	D	186	ILE
1	D	232	SER
1	D	244	LEU
1	D	256	LYS
1	D	323	ASP

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Mol	Chain	Res	Type
1	D	360	GLU
1	D	422	ASN
1	D	464	LEU
1	D	476	ILE
2	E	41	SER
3	F	23	LEU
4	H	5	LYS
4	H	10	ASP
4	I	10	ASP
4	I	49	GLU
4	I	109	LYS
4	I	112	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	438	GLN
2	B	38	ASN
2	B	68	ASN
2	B	155	GLN
2	B	220	ASN
1	D	222	ASN
2	E	68	ASN
2	E	155	GLN
2	E	220	ASN
2	E	237	GLN
4	I	36	HIS

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	PEG	A	503	5	4,4,6	0.75	0	3,3,5	0.44	0
7	FES	H	201	4	0,4,4	-	-	-		
6	PEG	D	503	5	6,6,6	0.44	0	5,5,5	0.31	0
7	FES	I	201	4	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
6	PEG	A	503	5	-	2/2/2/4	-
7	FES	H	201	4	-	-	0/1/1/1
6	PEG	D	503	5	-	3/4/4/4	-
7	FES	I	201	4	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	503	PEG	O1-C1-C2-O2
6	D	503	PEG	O2-C3-C4-O4
6	A	503	PEG	C4-C3-O2-C2
6	A	503	PEG	O2-C3-C4-O4
6	D	503	PEG	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	503	PEG	1	0
6	D	503	PEG	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	490/490 (100%)	-0.83	1 (0%) 91 89	8, 15, 28, 48	0
1	D	490/490 (100%)	-0.79	0 100 100	9, 17, 32, 49	0
2	B	305/305 (100%)	-0.60	1 (0%) 90 88	11, 22, 39, 53	0
2	E	305/305 (100%)	-0.78	1 (0%) 90 88	8, 18, 34, 60	0
3	C	82/82 (100%)	-0.79	0 100 100	10, 20, 30, 43	1 (1%)
3	F	82/82 (100%)	-0.14	0 100 100	17, 37, 51, 59	2 (2%)
4	H	111/111 (100%)	-0.73	0 100 100	10, 18, 35, 44	0
4	I	111/111 (100%)	-0.71	0 100 100	8, 19, 39, 42	1 (0%)
All	All	1976/1976 (100%)	-0.73	3 (0%) 91 89	8, 18, 37, 60	4 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	491	LYS	3.7
2	B	2	SER	2.3
2	E	306	SER	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($\text{\AA}^2$)	Q<0.9
6	PEG	A	503	5/7	0.90	0.12	26,29,35,40	0
6	PEG	D	503	7/7	0.90	0.13	18,21,28,38	7
5	FE	A	502	1/1	0.97	0.04	25,25,25,25	0
5	FE	D	502	1/1	0.99	0.03	24,24,24,24	0
5	FE	A	501	1/1	0.99	0.02	19,19,19,19	0
5	FE	D	501	1/1	0.99	0.03	18,18,18,18	0
7	FES	H	201	4/4	0.99	0.02	10,11,11,12	0
7	FES	I	201	4/4	0.99	0.02	9,11,11,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.