



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:31 am BST

PDB ID : 4P1B
Title : CRYSTAL STRUCTURE OF THE TOLUENE 4-MONOOXYGENASE HYDROXYLASE-FERREDOXIN C7S E16C C84A C85A VARIANT ELECTRON-TRANSFER COMPLEX
Authors : Acheson, J.F.; Fox, B.G.
Deposited on : 2014-02-25
Resolution : 2.05 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 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 : 2.11
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) : 2.11

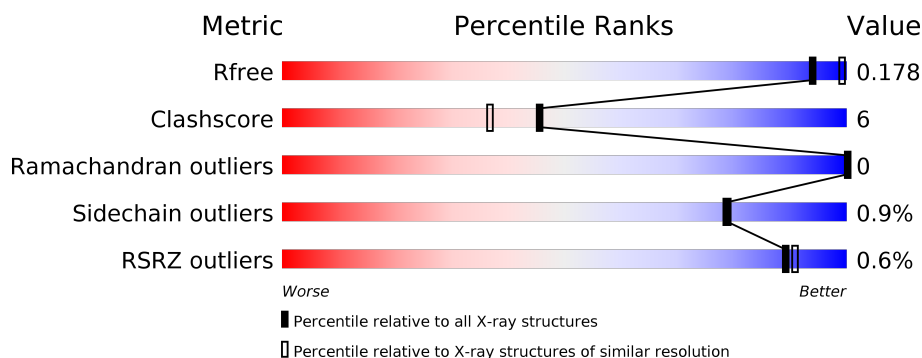
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 on 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	<div> <div style="width: 88%; background-color: green;"></div> <div style="width: 12%; background-color: yellow;"></div> </div> <div>88% 12%</div>
1	D	490	<div> <div style="width: 90%; background-color: green;"></div> <div style="width: 10%; background-color: yellow;"></div> </div> <div>90% 10%</div>
2	B	305	<div> <div style="width: 90%; background-color: green;"></div> <div style="width: 10%; background-color: yellow;"></div> </div> <div>90% 10%</div>
2	E	305	<div> <div style="width: 85%; background-color: green;"></div> <div style="width: 15%; background-color: yellow;"></div> </div> <div>85% 15%</div>
3	C	82	<div> <div style="width: 11%; background-color: red;"></div> <div style="width: 72%; background-color: green;"></div> <div style="width: 28%; background-color: yellow;"></div> </div> <div>11% 72% 28%</div>
3	F	82	<div> <div style="width: 88%; background-color: green;"></div> <div style="width: 11%; background-color: yellow;"></div> </div> <div>88% 11%</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	H	111	 87% 11% •
4	I	111	 93% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ACT	B	401	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18244 atoms, of which 18 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	3	0
			4050	2596	683	748	23			
1	D	490	Total	C	N	O	S	0	4	0
			4060	2602	684	751	23			

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	5	0
			2566	1622	448	481	15			
2	E	305	Total	C	N	O	S	0	3	0
			2557	1618	446	478	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	0	0	0
			654	412	117	121	4			
3	F	82	Total	C	N	O	S	0	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	3	0
			872	546	142	179	5			
4	I	111	Total	C	N	O	S	0	0	0
			848	531	137	175	5			

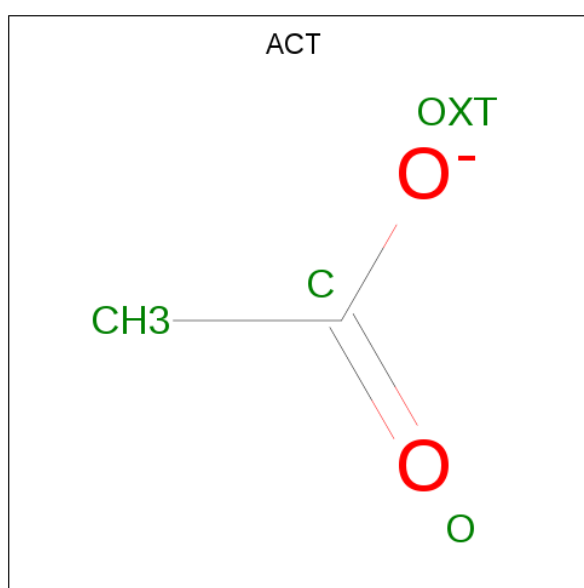
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	7	SER	CYS	engineered mutation	UNP Q00458
H	16	CYS	GLU	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	16	CYS	GLU	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 (three-letter code: 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 ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).

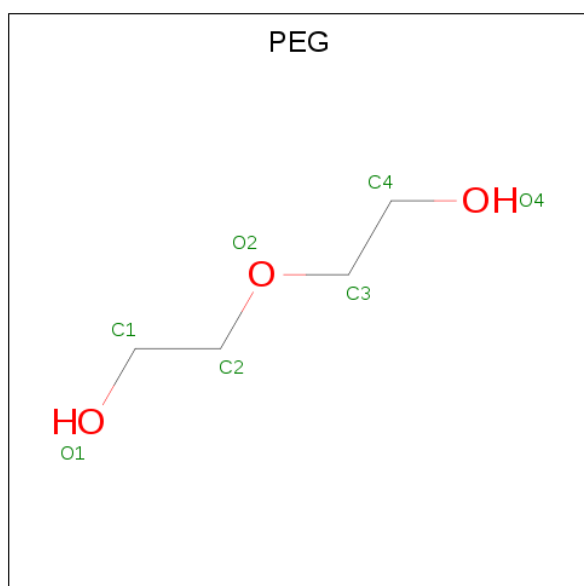


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 7 2 3 2	0	0
6	A	1	Total C H O 7 2 3 2	0	0
6	A	1	Total C H O 7 2 3 2	0	0
6	B	1	Total C H O 7 2 3 2	0	0
6	D	1	Total C H O 7 2 3 2	0	0
6	D	1	Total C H O 7 2 3 2	0	0
6	D	1	Total C O 4 2 2	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

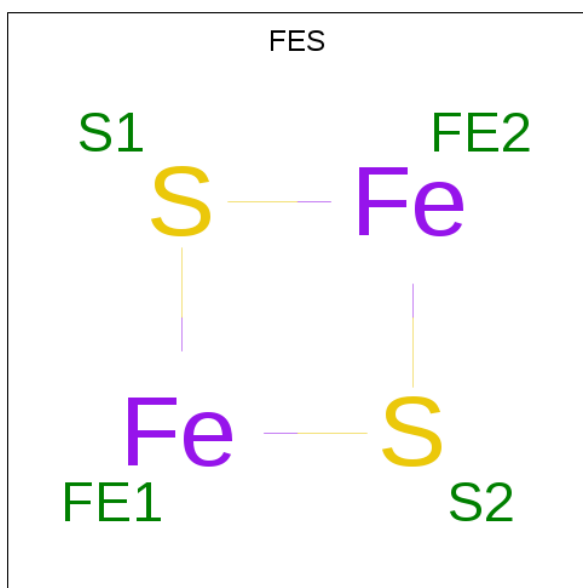
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total C O 7 4 3	0	0

- Molecule 9 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

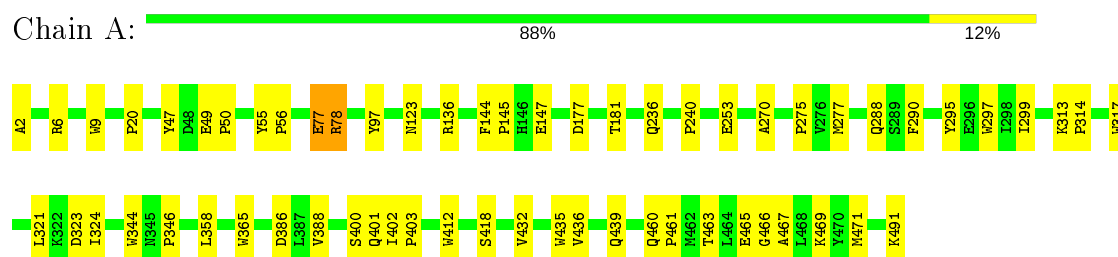
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	478	Total	O	0	0
			478	478		
10	B	326	Total	O	0	0
			326	326		
10	C	45	Total	O	0	0
			45	45		
10	D	432	Total	O	0	0
			432	432		
10	E	278	Total	O	0	0
			278	278		
10	F	86	Total	O	0	0
			86	86		
10	H	155	Total	O	0	0
			155	155		
10	I	117	Total	O	0	0
			117	117		

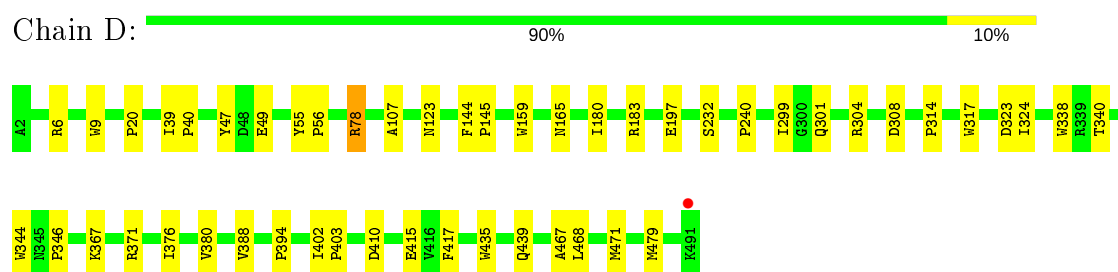
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

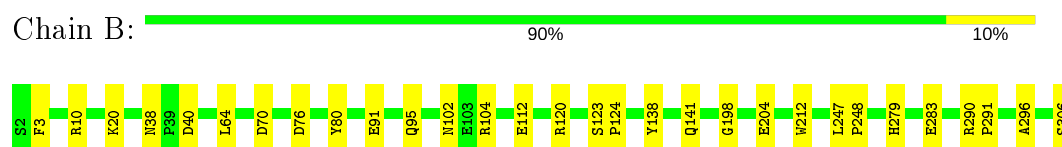
- Molecule 1: Toluene-4-monooxygenase system protein A



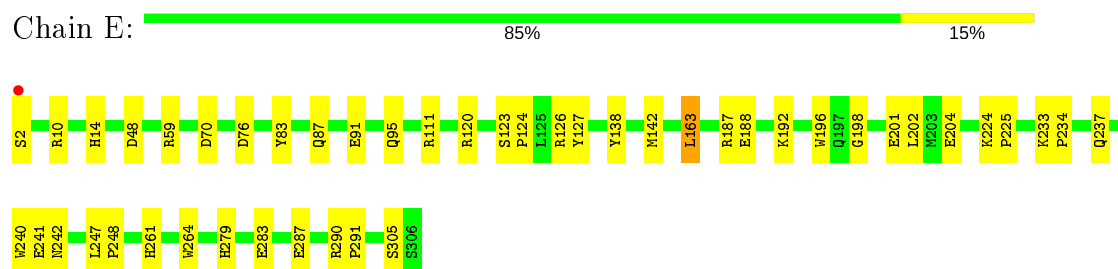
- Molecule 1: Toluene-4-monooxygenase system protein A



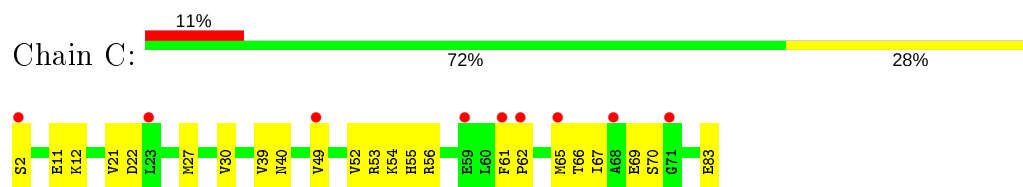
- Molecule 2: Toluene-4-monooxygenase system protein E



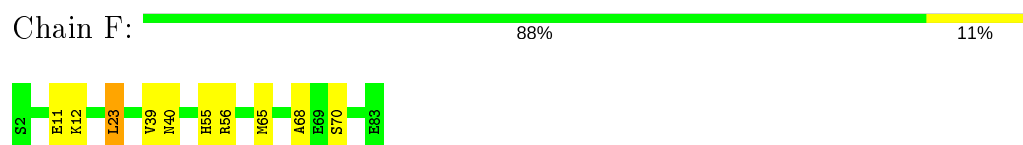
- Molecule 2: Toluene-4-monooxygenase system protein E



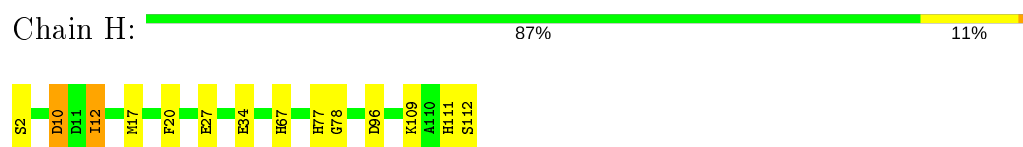
- Molecule 3: Toluene-4-monooxygenase system protein B



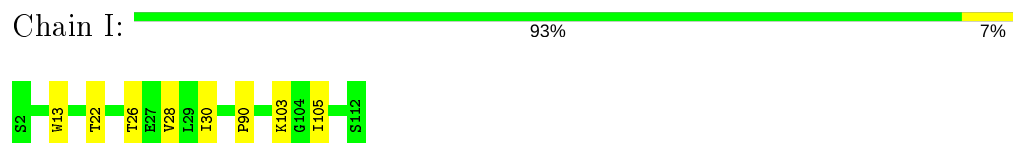
- Molecule 3: Toluene-4-monooxygenase system protein B



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.37Å 128.37Å 284.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.95 – 2.05 47.95 – 1.98	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.95-2.05) 94.5 (47.95-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.98Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1186)	Depositor
R, R_{free}	0.146 , 0.177 0.147 , 0.178	Depositor DCC
R_{free} test set	9442 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18244	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: NA, PEG, FE, FES, ACT

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	0.32	0/4182	0.43	0/5678
1	D	0.31	0/4192	0.43	0/5692
2	B	0.29	0/2645	0.43	0/3595
2	E	0.28	0/2634	0.42	0/3579
3	C	0.27	0/666	0.43	0/902
3	F	0.28	0/666	0.45	0/902
4	H	0.29	0/891	0.48	0/1209
4	I	0.28	0/867	0.45	0/1178
All	All	0.30	0/16743	0.43	0/22735

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4050	0	3804	49	0
1	D	4060	0	3811	37	0
2	B	2566	0	2441	36	0
2	E	2557	0	2427	41	0
3	C	654	0	649	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	654	0	649	6	0
4	H	872	0	812	21	0
4	I	848	0	791	9	0
5	A	2	0	0	0	0
5	D	2	0	0	0	0
6	A	12	9	9	0	0
6	B	4	3	3	3	0
6	D	12	6	9	0	0
7	A	1	0	0	0	0
8	D	7	0	10	0	0
9	H	4	0	0	1	0
9	I	4	0	0	0	0
10	A	478	0	0	7	0
10	B	326	0	0	10	2
10	C	45	0	0	1	0
10	D	432	0	0	11	0
10	E	278	0	0	11	1
10	F	86	0	0	0	1
10	H	155	0	0	6	0
10	I	117	0	0	0	0
All	All	18226	18	15415	204	2

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 6.

All (204) 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:C:62:PRO:HD2	3:C:65:MET:HE2	1.19	1.10
1:D:299:ILE:HD11	1:D:324:ILE:CD1	1.90	1.00
1:D:415[B]:GLU:OE2	10:D:996:HOH:O	1.84	0.95
2:E:198:GLY:O	10:E:622:HOH:O	1.84	0.94
3:C:62:PRO:HD2	3:C:65:MET:CE	1.99	0.92
1:A:386:ASP:OD2	10:A:601:HOH:O	1.88	0.91
1:D:78:ARG:NH1	10:D:834:HOH:O	1.81	0.91
1:A:295:TYR:CE2	1:A:324:ILE:HD11	2.07	0.89
1:D:304:ARG:HB3	4:H:109:LYS:HE3	1.54	0.88
3:C:65:MET:HG3	3:C:69:GLU:HG3	1.54	0.88
2:B:38[B]:ASN:ND2	10:B:982:HOH:O	2.07	0.87
4:H:12[B]:ILE:HD11	4:H:20:PHE:CE2	2.09	0.87
2:B:10[B]:ARG:NH1	10:B:1065:HOH:O	2.07	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:THR:HG23	1:A:466:GLY:H	1.42	0.83
4:H:77[A]:HIS:ND1	10:H:301:HOH:O	2.10	0.83
1:D:232:SER:OG	10:D:927:HOH:O	1.98	0.80
2:B:70:ASP:OD1	10:B:828:HOH:O	2.01	0.78
1:D:410:ASP:OD1	10:D:926:HOH:O	2.02	0.77
1:A:147:GLU:OE1	10:A:942:HOH:O	2.02	0.77
2:E:188:GLU:HG2	2:E:192:LYS:NZ	1.99	0.77
4:H:27:GLU:OE2	10:H:428:HOH:O	2.01	0.77
2:E:48:ASP:OD2	10:E:623:HOH:O	2.03	0.77
2:E:201:GLU:N	10:E:622:HOH:O	2.16	0.76
2:B:212:TRP:HE1	6:B:401:ACT:H3	1.52	0.75
1:D:299:ILE:HD11	1:D:324:ILE:HD13	1.70	0.74
2:E:120:ARG:HD3	10:E:662:HOH:O	1.88	0.73
2:B:279[A]:HIS:NE2	2:B:283:GLU:OE2	2.22	0.73
4:H:77[A]:HIS:CE1	10:H:301:HOH:O	2.41	0.73
1:D:308:ASP:OD2	10:D:601:HOH:O	2.07	0.71
2:B:112:GLU:OE1	10:B:801:HOH:O	2.09	0.70
1:A:418:SER:OG	10:A:950:HOH:O	2.09	0.70
4:H:109:LYS:HD2	10:H:430:HOH:O	1.91	0.70
1:A:465:GLU:OE2	1:A:469:LYS:HE3	1.92	0.70
2:E:188:GLU:HG2	2:E:192:LYS:HZ3	1.53	0.69
4:I:28:VAL:HG23	4:I:30:ILE:CD1	2.23	0.69
2:B:40:ASP:HB3	10:B:1099:HOH:O	1.93	0.68
2:E:70:ASP:OD1	10:E:423:HOH:O	2.12	0.68
2:B:64:LEU:O	6:B:401:ACT:H1	1.95	0.67
1:D:304:ARG:CB	4:H:109:LYS:HE3	2.26	0.66
4:H:111:HIS:O	4:H:112[B]:SER:HB2	1.96	0.65
1:D:197:GLU:OE2	10:D:950:HOH:O	2.13	0.64
3:C:66:THR:OG1	3:C:69:GLU:HG2	1.98	0.64
1:D:340[A]:THR:HG22	10:D:886:HOH:O	1.98	0.62
3:C:21:VAL:HG11	3:C:30:VAL:HG13	1.81	0.62
2:E:10:ARG:HG2	4:I:13:TRP:CH2	2.35	0.61
1:D:165:ASN:ND2	10:D:885:HOH:O	2.33	0.61
2:E:202:LEU:N	10:E:622:HOH:O	1.91	0.61
4:H:12[B]:ILE:HD11	4:H:20:PHE:CZ	2.35	0.60
4:H:12[B]:ILE:HD11	4:H:20:PHE:HE2	1.63	0.60
4:H:77[A]:HIS:CD2	4:H:78:GLY:N	2.69	0.59
4:H:2:SER:N	10:H:303:HOH:O	2.35	0.59
1:D:388:VAL:HG12	1:D:388:VAL:O	2.03	0.58
3:F:11:GLU:O	3:F:12:LYS:HB2	2.03	0.58
1:D:299:ILE:HD11	1:D:324:ILE:HD11	1.79	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:287:GLU:OE1	2:E:287:GLU:HA	2.03	0.58
2:B:290:ARG:NH2	10:B:1004:HOH:O	2.33	0.57
3:C:11:GLU:O	3:C:12:LYS:HB2	2.04	0.57
3:F:55:HIS:CD2	3:F:56:ARG:HG2	2.40	0.57
1:A:402:ILE:CG2	1:A:403:PRO:HD2	2.35	0.57
1:A:47:TYR:CE2	1:A:240:PRO:HB2	2.40	0.56
2:B:10[A]:ARG:HD2	10:B:1067:HOH:O	2.04	0.56
4:H:77[A]:HIS:HD2	4:H:78:GLY:N	2.03	0.56
3:C:62:PRO:CD	3:C:65:MET:HE2	2.13	0.56
1:D:415[B]:GLU:HG2	1:D:417:PHE:CE1	2.41	0.56
3:C:27:MET:SD	3:C:52:VAL:HB	2.46	0.56
2:E:240:TRP:HA	10:E:594:HOH:O	2.06	0.55
1:D:402:ILE:CG2	1:D:403:PRO:HD2	2.36	0.55
1:A:463:THR:CG2	1:A:466:GLY:H	2.17	0.55
1:A:469:LYS:HD2	2:B:3:PHE:CZ	2.42	0.55
1:D:344:TRP:O	1:D:346:PRO:HD3	2.07	0.54
4:I:90:PRO:HD3	4:I:105:ILE:CD1	2.38	0.54
1:A:77:GLU:OE2	10:A:964:HOH:O	2.18	0.54
2:E:283:GLU:O	2:E:287:GLU:HG2	2.07	0.54
2:E:305:SER:HB3	10:E:626:HOH:O	2.08	0.54
1:A:314:PRO:HD2	1:A:317:TRP:CE3	2.42	0.53
2:B:212:TRP:HE1	6:B:401:ACT:CH3	2.21	0.53
1:D:301:GLN:HB2	10:D:827:HOH:O	2.08	0.53
4:I:28:VAL:HG23	4:I:30:ILE:HD11	1.90	0.53
1:A:288:GLN:HE22	1:A:297:TRP:HE1	1.57	0.53
4:H:96:ASP:OD1	10:H:439:HOH:O	2.18	0.53
2:B:290:ARG:HB2	2:B:291:PRO:HD3	1.91	0.52
2:B:104:ARG:NH1	10:B:1119:HOH:O	2.41	0.52
1:A:469:LYS:HD2	2:B:3:PHE:CE2	2.45	0.52
1:D:367:LYS:HD2	1:D:371:ARG:NH2	2.25	0.51
2:B:290:ARG:CB	2:B:291:PRO:HD3	2.41	0.50
1:A:321:LEU:O	1:A:324:ILE:HG12	2.11	0.50
3:C:53:ARG:HG3	3:C:54:LYS:O	2.12	0.50
3:C:61:PHE:HD1	3:C:65:MET:HE1	1.76	0.50
1:D:435:TRP:O	1:D:439:GLN:HG2	2.12	0.50
2:E:91:GLU:O	2:E:95:GLN:HG2	2.12	0.49
3:C:2:SER:HG	3:C:22:ASP:CG	2.15	0.49
2:B:20:LYS:HE3	4:H:34:GLU:OE1	2.12	0.49
1:D:55:TYR:HB3	1:D:56:PRO:HD3	1.94	0.49
1:A:253:GLU:N	1:A:253:GLU:OE1	2.43	0.49
1:A:295:TYR:CE2	1:A:324:ILE:CD1	2.91	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:ARG:HH11	2:B:290:ARG:HG3	1.78	0.49
3:C:67:ILE:O	3:C:70:SER:OG	2.13	0.49
3:C:49:VAL:HG11	3:C:83:GLU:OE1	2.11	0.49
2:E:237:GLN:NE2	2:E:241:GLU:OE2	2.33	0.49
2:E:111:ARG:HH21	2:E:242:ASN:HA	1.78	0.49
4:I:28:VAL:CG2	4:I:30:ILE:HD11	2.43	0.49
2:E:290:ARG:HB3	2:E:291:PRO:HD3	1.94	0.49
1:A:2:ALA:N	2:B:102:ASN:HD22	2.11	0.49
2:B:123[A]:SER:OG	2:B:124:PRO:HD3	2.13	0.48
2:B:40:ASP:CB	10:B:1099:HOH:O	2.58	0.48
1:D:20:PRO:HA	2:E:204:GLU:OE2	2.14	0.48
2:E:126:ARG:HB2	2:E:163:LEU:HD13	1.96	0.48
2:B:123[A]:SER:N	2:B:124:PRO:CD	2.77	0.47
1:D:402:ILE:HG23	1:D:403:PRO:HD2	1.96	0.47
1:A:402:ILE:HG22	1:A:403:PRO:HD2	1.96	0.47
1:A:78:ARG:HB2	10:A:930:HOH:O	2.15	0.47
2:E:111:ARG:NH2	2:E:111:ARG:HB2	2.30	0.47
2:E:279[B]:HIS:HB2	10:E:635:HOH:O	2.14	0.47
2:E:290:ARG:N	2:E:291:PRO:CD	2.78	0.47
1:A:344:TRP:O	1:A:346:PRO:HD3	2.15	0.47
2:E:233:LYS:HB2	2:E:234:PRO:HD3	1.96	0.47
2:B:120:ARG:HH12	2:B:306:SER:HG	1.63	0.46
3:C:83:GLU:C	10:C:145:HOH:O	2.53	0.46
2:E:83:TYR:CZ	2:E:87:GLN:HG3	2.51	0.46
2:B:123[B]:SER:N	2:B:124:PRO:CD	2.79	0.46
2:E:188:GLU:HG2	2:E:192:LYS:HZ1	1.77	0.46
3:F:39:VAL:O	3:F:40:ASN:HB2	2.14	0.46
2:E:188:GLU:CG	2:E:192:LYS:NZ	2.76	0.46
3:F:23:LEU:HD12	3:F:68:ALA:HB2	1.97	0.46
3:C:65:MET:SD	3:C:70:SER:HA	2.55	0.46
1:A:49:GLU:HG2	1:A:49:GLU:O	2.15	0.46
1:A:6:ARG:HA	1:A:9:TRP:CE2	2.51	0.46
1:A:313:LYS:NZ	10:A:824:HOH:O	2.41	0.45
4:I:30:ILE:N	4:I:30:ILE:HD12	2.30	0.45
1:A:20:PRO:HA	2:B:204:GLU:OE2	2.17	0.45
1:A:177:ASP:HA	1:A:181:THR:OG1	2.15	0.45
1:D:314:PRO:HD2	1:D:317:TRP:CE3	2.51	0.45
1:D:144:PHE:N	1:D:145:PRO:HD2	2.32	0.45
1:A:78:ARG:HG2	1:A:78:ARG:HH11	1.82	0.45
2:E:224:LYS:N	2:E:225:PRO:CD	2.79	0.45
2:E:201:GLU:CA	10:E:622:HOH:O	2.63	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:HG23	1:A:403:PRO:HD2	1.99	0.44
1:A:136:ARG:HB2	2:B:80:TYR:CZ	2.52	0.44
1:D:159:TRP:CE2	2:E:14:HIS:CD2	3.06	0.44
3:C:39:VAL:O	3:C:40:ASN:HB2	2.17	0.44
1:A:467:ALA:O	1:A:471:MET:HG3	2.18	0.44
2:E:247:LEU:N	2:E:248:PRO:CD	2.81	0.44
2:E:123:SER:OG	2:E:124:PRO:HD3	2.18	0.43
2:E:163:LEU:HD12	2:E:163:LEU:O	2.18	0.43
4:I:90:PRO:HD3	4:I:105:ILE:HD13	2.00	0.43
2:E:123:SER:N	2:E:124:PRO:CD	2.81	0.43
3:C:55:HIS:CG	3:C:56:ARG:HG2	2.53	0.43
1:A:461:PRO:HG2	1:A:463:THR:HG22	2.01	0.43
1:D:183:ARG:HB2	10:D:973:HOH:O	2.19	0.43
3:C:61:PHE:HB3	3:C:65:MET:HE3	2.01	0.43
1:A:50:PRO:HD2	1:A:236:GLN:OE1	2.19	0.43
1:A:299:ILE:HD13	1:A:321:LEU:HD23	2.00	0.43
1:D:78:ARG:HG2	10:D:716:HOH:O	2.18	0.43
1:D:6:ARG:HA	1:D:9:TRP:CE2	2.54	0.43
2:E:10:ARG:CG	4:I:13:TRP:CZ3	3.02	0.43
1:A:270:ALA:O	1:A:275:PRO:HD3	2.19	0.42
2:B:247:LEU:N	2:B:248:PRO:CD	2.82	0.42
1:D:39:ILE:HA	1:D:40:PRO:HD3	1.79	0.42
1:A:435:TRP:O	1:A:439:GLN:HG2	2.19	0.42
2:B:198:GLY:HA3	2:B:296:ALA:HA	2.01	0.42
3:C:66:THR:H	3:C:69:GLU:CG	2.31	0.42
1:D:376:ILE:O	1:D:380:VAL:HG23	2.18	0.42
1:D:338:TRP:CE2	1:D:394:PRO:HD3	2.54	0.42
3:F:55:HIS:CG	3:F:56:ARG:HG2	2.54	0.42
1:A:388:VAL:HG12	1:A:388:VAL:O	2.20	0.42
4:H:77[A]:HIS:CD2	4:H:78:GLY:O	2.73	0.42
1:D:47:TYR:CE2	1:D:240:PRO:HB2	2.55	0.42
1:A:144:PHE:N	1:A:145:PRO:HD2	2.35	0.42
1:D:468:LEU:HD13	1:D:479:MET:SD	2.60	0.42
1:D:49:GLU:HG2	1:D:49:GLU:O	2.20	0.42
2:E:188:GLU:CG	2:E:192:LYS:HZ3	2.29	0.42
4:H:12[B]:ILE:CD1	4:H:20:PHE:HE2	2.32	0.42
4:I:22:THR:OG1	4:I:26:THR:HB	2.19	0.42
2:E:124:PRO:HB2	2:E:196:TRP:CZ2	2.55	0.42
4:H:12[A]:ILE:HD11	4:H:17:MET:HA	2.01	0.42
2:E:138:TYR:CZ	2:E:142:MET:HG3	2.55	0.42
1:A:432:VAL:O	1:A:436:VAL:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123[B]:SER:HB2	2:B:124:PRO:HD3	2.02	0.41
2:B:247:LEU:HB3	2:B:248:PRO:HD3	2.02	0.41
1:D:467:ALA:O	1:D:471:MET:HG3	2.20	0.41
1:A:460:GLN:HA	1:A:461:PRO:C	2.39	0.41
1:A:400:SER:O	1:A:401:GLN:HB2	2.19	0.41
1:A:469:LYS:CD	2:B:3:PHE:CZ	3.03	0.41
2:E:261:HIS:HA	2:E:264:TRP:CD1	2.56	0.41
1:D:107:ALA:HA	1:D:180:ILE:HG21	2.02	0.41
2:B:138:TYR:O	2:B:141:GLN:HG2	2.21	0.41
2:B:91:GLU:O	2:B:95:GLN:HG2	2.20	0.41
2:E:59:ARG:HD2	10:E:464:HOH:O	2.20	0.41
1:A:55:TYR:HB3	1:A:56:PRO:HD3	2.01	0.41
2:E:127:TYR:OH	2:E:187:ARG:HB2	2.21	0.41
2:B:120:ARG:HD3	10:B:927:HOH:O	2.21	0.41
2:B:279[A]:HIS:CE1	2:B:283:GLU:OE2	2.73	0.41
1:A:277:MET:HE2	1:A:290:PHE:HA	2.03	0.41
4:H:67:HIS:HB2	9:H:201:FES:S2	2.61	0.41
1:A:358:LEU:HD13	1:A:365:TRP:CZ2	2.56	0.40
1:A:491:LYS:NZ	10:A:1050:HOH:O	2.53	0.40
1:A:49:GLU:HA	1:A:50:PRO:HD3	1.90	0.40
1:A:412:TRP:CE3	3:C:11:GLU:HG3	2.57	0.40
2:E:126:ARG:HB2	2:E:163:LEU:CD1	2.51	0.40
3:F:65:MET:SD	3:F:70:SER:HA	2.62	0.40
1:A:97:TYR:CD2	1:A:145:PRO:HB3	2.56	0.40
1:A:465:GLU:OE2	1:A:469:LYS:CE	2.66	0.40
2:B:10[A]:ARG:NH1	4:H:10:ASP:O	2.44	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:818:HOH:O	10:F:110:HOH:O[1_655]	1.91	0.29
10:B:813:HOH:O	10:E:408:HOH:O[5_665]	2.19	0.01

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	491/490 (100%)	476 (97%)	15 (3%)	0	100	100
1	D	492/490 (100%)	477 (97%)	15 (3%)	0	100	100
2	B	308/305 (101%)	302 (98%)	6 (2%)	0	100	100
2	E	306/305 (100%)	300 (98%)	6 (2%)	0	100	100
3	C	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
3	F	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
4	H	111/111 (100%)	107 (96%)	4 (4%)	0	100	100
4	I	109/111 (98%)	104 (95%)	5 (5%)	0	100	100
All	All	1977/1976 (100%)	1919 (97%)	58 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	418/415 (101%)	414 (99%)	4 (1%)	76	75
1	D	419/415 (101%)	416 (99%)	3 (1%)	84	84
2	B	281/276 (102%)	280 (100%)	1 (0%)	91	91
2	E	279/276 (101%)	276 (99%)	3 (1%)	73	73
3	C	73/73 (100%)	73 (100%)	0	100	100
3	F	73/73 (100%)	72 (99%)	1 (1%)	67	65
4	H	96/93 (103%)	93 (97%)	3 (3%)	40	33
4	I	93/93 (100%)	92 (99%)	1 (1%)	73	73
All	All	1732/1714 (101%)	1716 (99%)	16 (1%)	78	79

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLU
1	A	78	ARG
1	A	123	ASN
1	A	323	ASP
2	B	76	ASP
1	D	78	ARG
1	D	123	ASN
1	D	323	ASP
2	E	2	SER
2	E	76	ASP
2	E	163	LEU
3	F	23	LEU
4	H	10	ASP
4	H	12[A]	ILE
4	H	12[B]	ILE
4	I	103	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	ACT	D	504	-	1,3,3	0.60	0	0,3,3	0.00	-
8	PEG	D	503	-	6,6,6	0.62	0	5,5,5	0.76	0
6	ACT	A	505	-	1,3,3	0.71	0	0,3,3	0.00	-
6	ACT	A	503	-	1,3,3	0.52	0	0,3,3	0.00	-
6	ACT	A	504	5	1,3,3	0.29	0	0,3,3	0.00	-
9	FES	H	201	4	0,4,4	0.00	-	-	-	-
6	ACT	D	506	5	1,3,3	0.62	0	0,3,3	0.00	-
9	FES	I	201	4	0,4,4	0.00	-	-	-	-
6	ACT	D	505	-	1,3,3	0.78	0	0,3,3	0.00	-
6	ACT	B	401	-	1,3,3	0.74	0	0,3,3	0.00	-

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
9	FES	H	201	4	-	-	0/1/1/1
8	PEG	D	503	-	-	2/4/4/4	-
9	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 (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	503	PEG	O2-C3-C4-O4
8	D	503	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	H	201	FES	1	0
6	B	401	ACT	3	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	490/490 (100%)	-0.62	0 100 100	13, 25, 43, 63	0
1	D	490/490 (100%)	-0.53	1 (0%) 95 95	14, 24, 44, 72	1 (0%)
2	B	305/305 (100%)	-0.74	0 100 100	15, 27, 45, 74	0
2	E	305/305 (100%)	-0.58	1 (0%) 94 94	15, 29, 52, 71	0
3	C	82/82 (100%)	0.23	9 (10%) 5 5	25, 45, 61, 78	0
3	F	82/82 (100%)	-0.83	0 100 100	21, 32, 44, 62	1 (1%)
4	H	111/111 (100%)	-0.79	0 100 100	16, 22, 39, 45	0
4	I	111/111 (100%)	-0.72	0 100 100	16, 26, 46, 55	0
All	All	1976/1976 (100%)	-0.60	11 (0%) 89 91	13, 26, 49, 78	2 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	2	SER	3.0
3	C	71	GLY	2.6
3	C	59	GLU	2.5
2	E	2	SER	2.5
3	C	23	LEU	2.4
3	C	68	ALA	2.4
1	D	491	LYS	2.3
3	C	62	PRO	2.2
3	C	61	PHE	2.1
3	C	65	MET	2.0
3	C	49	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
6	ACT	B	401	4/4	0.65	0.28	32,39,58,64	0
6	ACT	D	505	4/4	0.78	0.15	58,60,72,72	0
8	PEG	D	503	7/7	0.86	0.13	44,52,66,70	0
6	ACT	D	506	4/4	0.91	0.55	6,12,12,13	4
6	ACT	D	504	4/4	0.91	0.17	33,41,49,49	0
7	NA	A	506	1/1	0.93	0.25	60,60,60,60	0
6	ACT	A	504	4/4	0.93	0.23	17,31,43,43	7
6	ACT	A	503	4/4	0.94	0.19	32,44,53,53	0
6	ACT	A	505	4/4	0.96	0.10	20,25,29,29	0
5	FE	A	502	1/1	0.97	0.08	32,32,32,32	0
5	FE	D	502	1/1	0.98	0.13	31,31,31,31	0
9	FES	I	201	4/4	0.99	0.07	18,19,19,20	0
5	FE	D	501	1/1	0.99	0.12	22,22,22,22	0
5	FE	A	501	1/1	1.00	0.07	23,23,23,23	0
9	FES	H	201	4/4	1.00	0.06	17,17,18,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.