



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:14 PM GMT

PDB ID : 4KX6
Title : Plasticity of the quinone-binding site of the complex II homolog
quinol:fumarate reductase
Authors : Singh, P.K.; Sarwar, M.; Maklashina, E.; Kotlyar, V.; Rajagukguk, S.;
Tomasiak, T.M.; Cecchini, G.; Iverson, T.M.
Deposited on : 2013-05-24
Resolution : 2.95 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

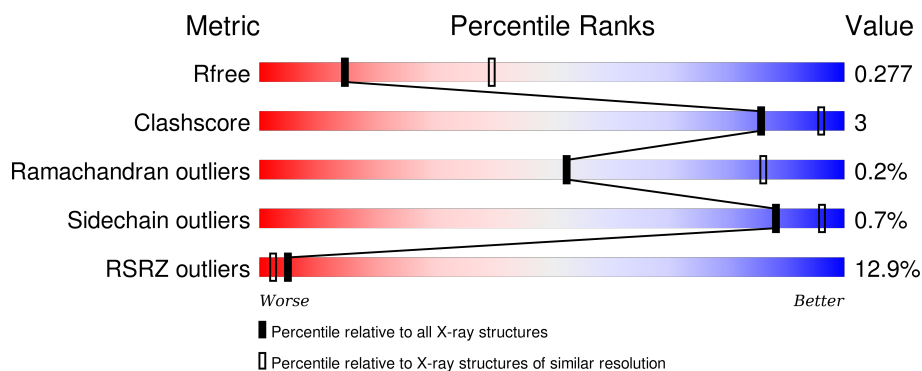
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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. 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	577	<div> <div style="width: 93%;"></div> <div style="width: 7%;"></div> </div>
1	M	577	<div> <div style="width: 33%;"></div> <div style="width: 93%;"></div> <div style="width: 7%;"></div> </div>
2	B	243	<div> <div style="width: 2%;"></div> <div style="width: 92%;"></div> <div style="width: 8%;"></div> </div>
2	N	243	<div> <div style="width: 18%;"></div> <div style="width: 93%;"></div> <div style="width: 6%;"></div> </div>
3	C	130	<div> <div style="width: 6%;"></div> <div style="width: 88%;"></div> <div style="width: 12%;"></div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	O	130	
4	D	119	
4	P	119	

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
9	MQ7	D	701	-	-	-	X
9	MQ7	N	304	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16828 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 Fumarate reductase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4448	2775	802	840	31			
1	M	577	Total	C	N	O	S	0	0	0
			4448	2775	802	840	31			

- Molecule 2 is a protein called Fumarate reductase (Anaerobic), Fe-S subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1887	1189	323	356	19			
2	N	243	Total	C	N	O	S	0	0	0
			1887	1189	323	356	19			

- Molecule 3 is a protein called Fumarate reductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	130	Total	C	N	O	S	0	0	0
			1057	721	166	167	3			
3	O	130	Total	C	N	O	S	0	0	0
			1057	721	166	167	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	29	LEU	GLU	ENGINEERED MUTATION	UNP C9QU46
O	29	LEU	GLU	ENGINEERED MUTATION	UNP C9QU46

- Molecule 4 is a protein called Fumarate reductase subunit D.

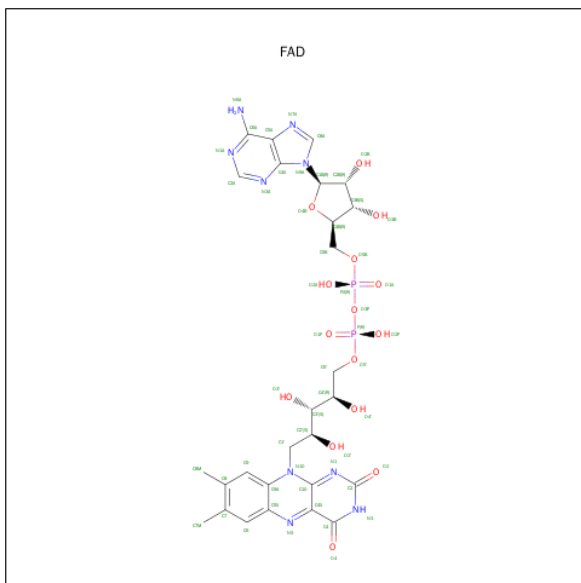
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

Continued on next page...

Continued from previous page...

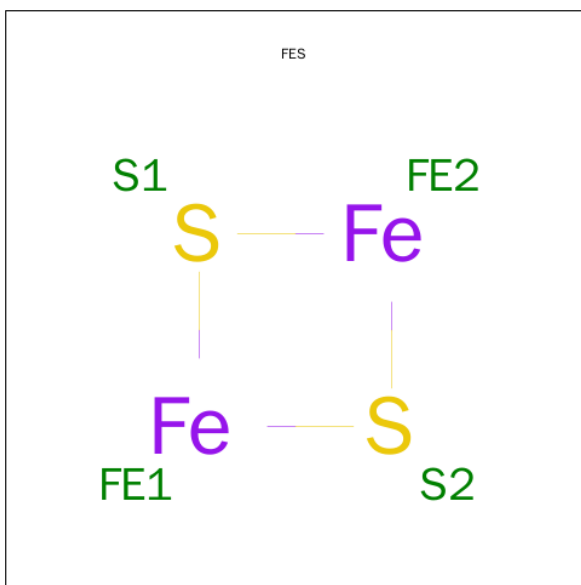
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	M	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



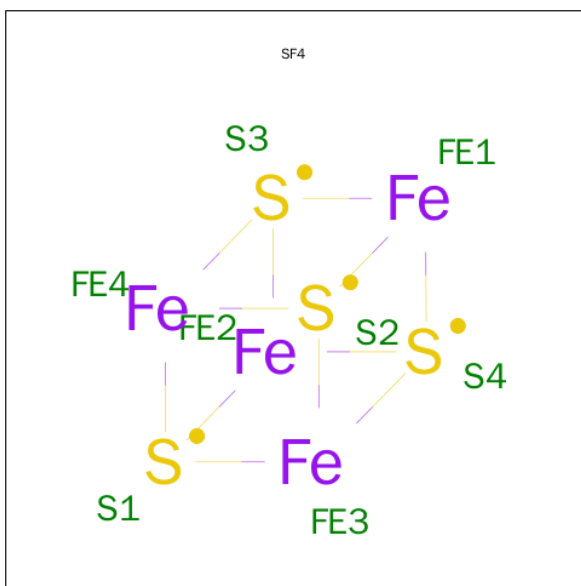
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			4	2	2		
6	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 7 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



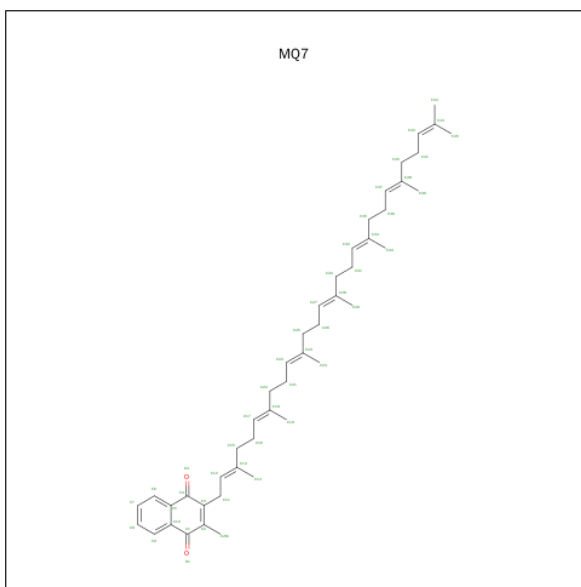
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			7	3	4		
7	N	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		
8	N	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $\text{C}_{46}\text{H}_{64}\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			24	22	2		

Continued on next page...

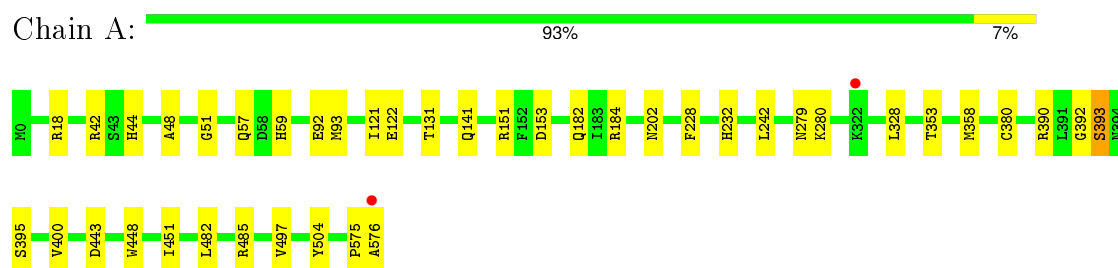
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	N	1	24	22	2	0	0

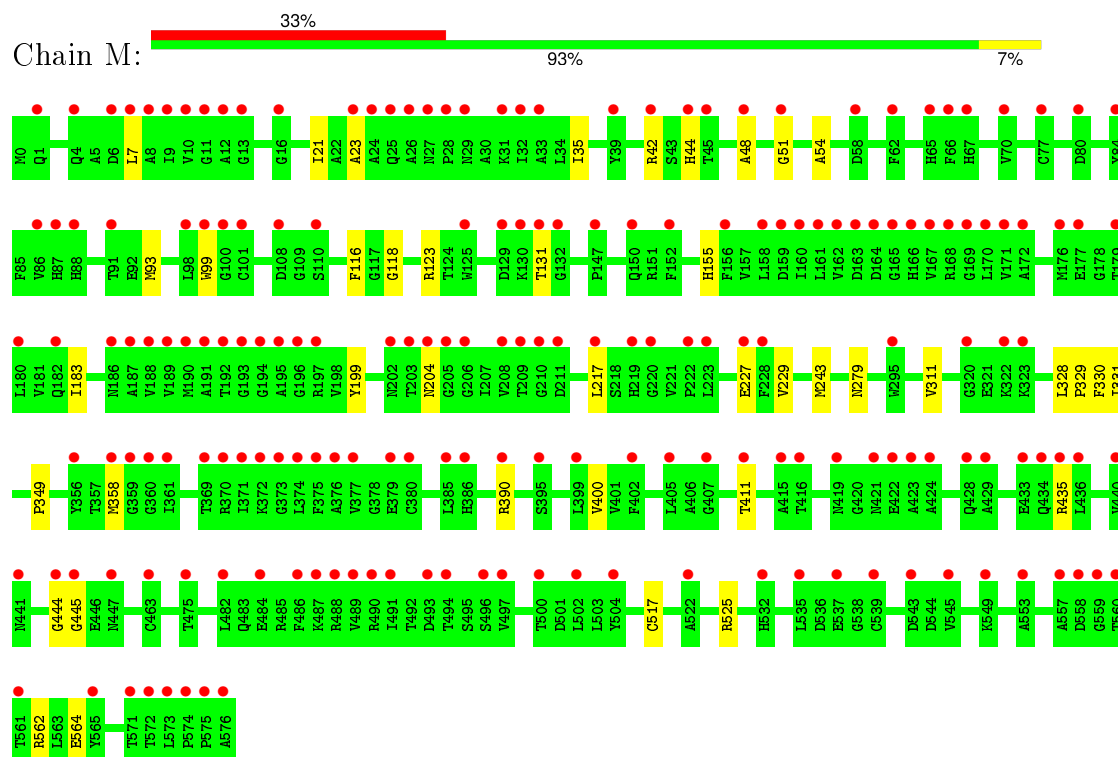
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Fumarate reductase flavoprotein subunit



- Molecule 1: Fumarate reductase flavoprotein subunit

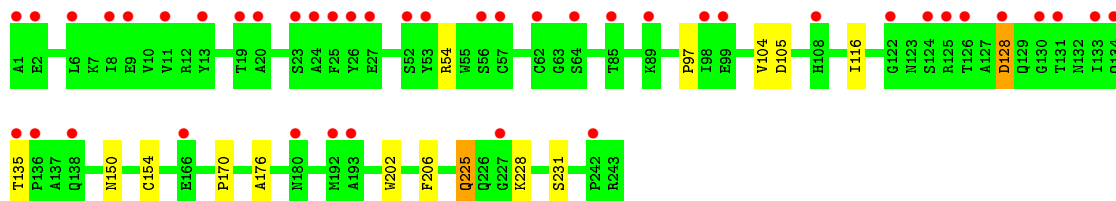


- Molecule 2: Fumarate reductase (Anaerobic), Fe-S subunit

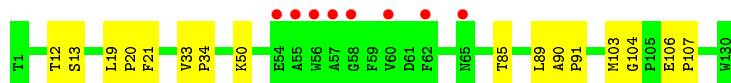
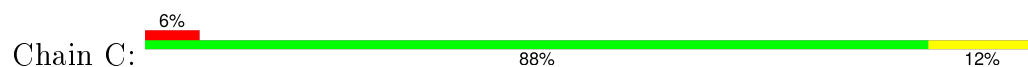




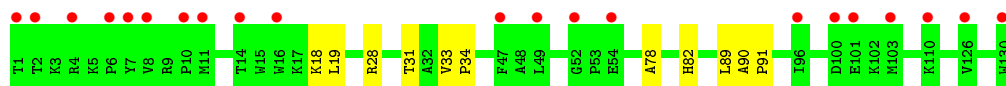
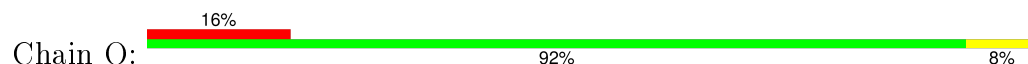
- Molecule 2: Fumarate reductase (Anaerobic), Fe-S subunit



- Molecule 3: Fumarate reductase subunit C



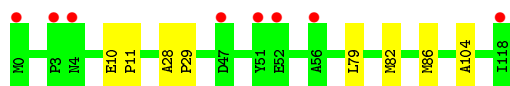
- Molecule 3: Fumarate reductase subunit C



- Molecule 4: Fumarate reductase subunit D



- Molecule 4: Fumarate reductase subunit D



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.09Å 138.62Å 273.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.80 – 2.95 48.65 – 2.95	Depositor EDS
% Data completeness (in resolution range)	95.8 (47.80-2.95) 95.8 (48.65-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.240 , 0.280 0.243 , 0.277	Depositor DCC
R_{free} test set	1348 reflections (1.83%)	DCC
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 77286 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16828	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SF4, F3S, FES, MQ7, FAD

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	0.33	0/4540	0.54	0/6139
1	M	0.32	0/4540	0.50	0/6139
2	B	0.32	0/1930	0.53	0/2617
2	N	0.33	0/1930	0.51	0/2617
3	C	0.31	0/1093	0.48	0/1495
3	O	0.31	0/1093	0.44	0/1495
4	D	0.29	0/956	0.42	0/1303
4	P	0.30	0/956	0.42	0/1303
All	All	0.32	0/17038	0.50	0/23108

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	4448	0	4335	26	0
1	M	4448	0	4335	22	0
2	B	1887	0	1837	11	0
2	N	1887	0	1837	13	0
3	C	1057	0	1113	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	1057	0	1113	8	0
4	D	926	0	971	3	0
4	P	926	0	971	6	0
5	A	53	0	31	7	0
5	M	53	0	31	2	0
6	B	4	0	0	0	0
6	N	4	0	0	0	0
7	B	7	0	0	0	0
7	N	7	0	0	0	0
8	B	8	0	0	0	0
8	N	8	0	0	0	0
9	D	24	0	23	3	0
9	N	24	0	23	1	0
All	All	16828	0	16620	95	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 3.

All (95) 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)
2:B:44:LYS:HA	2:B:48:ALA:O	1.83	0.77
9:D:701:MQ7:H12	9:D:701:MQ7:O4	1.84	0.76
3:O:31:THR:HG21	3:O:82:HIS:HB2	1.66	0.76
1:A:44:HIS:NE2	5:A:601:FAD:C8M	2.55	0.70
1:A:44:HIS:NE2	5:A:601:FAD:HM82	2.07	0.69
1:A:182:GLN:OE1	1:A:184:ARG:NH1	2.30	0.63
3:C:85:THR:O	3:C:89:LEU:HG	2.02	0.60
2:N:54:ARG:NH2	2:N:104:VAL:O	2.33	0.60
9:D:701:MQ7:C12	9:D:701:MQ7:O4	2.51	0.59
1:A:44:HIS:CE1	5:A:601:FAD:HM82	2.38	0.58
2:B:206:PHE:HE2	3:C:89:LEU:HD22	1.70	0.57
4:P:79:LEU:HD23	4:P:82:MET:HE3	1.86	0.56
2:B:62:CYS:SG	2:B:64:SER:OG	2.63	0.56
1:A:44:HIS:NE2	5:A:601:FAD:HM81	2.21	0.55
2:B:151:CYS:SG	2:B:153:LEU:HG	2.46	0.55
1:M:93:MET:CE	1:M:400:VAL:HG21	2.37	0.55
2:N:206:PHE:CE1	3:O:89:LEU:HG	2.43	0.54
3:C:19:LEU:HD12	3:C:20:PRO:HD2	1.89	0.54
1:A:151:ARG:NH1	1:A:153:ASP:OD2	2.40	0.54
3:C:103:MET:HG2	3:C:104:GLY:N	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:LYS:HE3	4:D:117:THR:HG22	1.89	0.53
1:A:390:ARG:HD2	1:A:395:SER:HB2	1.90	0.53
4:P:79:LEU:HD23	4:P:82:MET:CE	2.39	0.53
3:O:33:VAL:HB	3:O:34:PRO:HD3	1.91	0.53
1:M:227:GLU:OE2	1:M:525:ARG:NE	2.42	0.52
3:O:90:ALA:N	3:O:91:PRO:HD2	2.26	0.51
1:M:118:GLY:HA2	1:M:279:ASN:HD21	1.76	0.51
2:B:57:CYS:HB3	2:B:62:CYS:HB3	1.93	0.51
2:N:225:GLN:OE1	2:N:228:LYS:HD2	2.11	0.50
3:C:50:LYS:CE	4:D:117:THR:HG22	2.42	0.49
1:M:311:VAL:HG11	1:M:349:PRO:CB	2.43	0.49
1:M:51:GLY:HA2	1:M:131:THR:HG21	1.95	0.48
4:P:28:ALA:N	4:P:29:PRO:HD2	2.29	0.48
4:P:10:GLU:N	4:P:11:PRO:CD	2.76	0.48
2:N:154:CYS:SG	2:N:170:PRO:HG2	2.53	0.48
2:N:116:ILE:CG2	2:N:176:ALA:HB2	2.44	0.48
3:C:33:VAL:HB	3:C:34:PRO:HD3	1.95	0.48
2:N:206:PHE:HD1	2:N:206:PHE:O	1.97	0.47
4:D:20:GLY:HA2	4:D:73:LEU:HB3	1.97	0.47
2:N:202:TRP:HE1	2:N:231:SER:HG	1.62	0.47
1:A:141:GLN:HB3	2:B:118:PRO:O	2.13	0.47
1:M:44:HIS:NE2	5:M:601:FAD:HM82	2.29	0.47
1:M:183:ILE:HD12	1:M:183:ILE:N	2.29	0.47
1:M:243:MET:HE3	1:M:331:ILE:HG23	1.96	0.47
2:N:225:GLN:OE1	2:N:225:GLN:HA	2.15	0.47
1:A:51:GLY:HA2	1:A:131:THR:HG21	1.97	0.46
1:A:443:ASP:C	1:A:443:ASP:OD1	2.53	0.46
1:M:35:ILE:HD11	1:M:155:HIS:HB3	1.97	0.46
9:D:701:MQ7:H193	9:D:701:MQ7:H151	1.97	0.46
1:A:448:TRP:CH2	1:A:504:TYR:HB3	2.51	0.46
1:A:242:LEU:CD2	5:A:601:FAD:HM73	2.46	0.46
2:B:212:GLU:HG3	3:C:21:PHE:CE2	2.50	0.46
1:A:202:ASN:HA	1:A:353:THR:HG22	1.98	0.46
1:A:575:PRO:O	1:A:576:ALA:HB3	2.15	0.46
1:A:242:LEU:HD23	5:A:601:FAD:HM73	1.98	0.45
1:A:451:ILE:HG23	1:A:482:LEU:HD22	1.98	0.45
1:A:18:ARG:HG2	1:A:400:VAL:HA	1.98	0.45
2:N:206:PHE:CD1	2:N:206:PHE:O	2.70	0.45
1:A:232:HIS:CD2	1:A:242:LEU:CD1	3.00	0.44
4:P:79:LEU:HD13	4:P:104:ALA:HB2	1.99	0.44
1:M:7:LEU:HD12	1:M:23:ALA:HB1	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:42:ARG:NH2	2:N:150:ASN:O	2.50	0.44
1:M:48:ALA:HA	5:M:601:FAD:C6	2.48	0.44
3:O:18:LYS:HB3	3:O:19:LEU:HD23	2.00	0.43
2:N:97:PRO:HG2	2:N:105:ASP:HB3	2.00	0.43
2:B:167:PHE:CD1	2:B:203:SER:HB2	2.53	0.43
3:C:12:THR:HG22	3:C:13:SER:N	2.33	0.43
1:A:497:VAL:HG21	2:B:15:PRO:HG2	2.00	0.43
3:C:90:ALA:N	3:C:91:PRO:HD2	2.33	0.43
1:M:562:ARG:NH1	1:M:564:GLU:OE2	2.52	0.43
1:A:18:ARG:NH1	1:A:92:GLU:OE1	2.52	0.43
1:M:328:LEU:N	1:M:329:PRO:CD	2.81	0.43
1:M:21:ILE:HG21	1:M:99:TRP:CH2	2.53	0.43
3:O:31:THR:HG23	3:O:78:ALA:HB1	2.00	0.43
4:P:82:MET:O	4:P:86:MET:HG2	2.19	0.42
1:M:54:ALA:O	1:M:123:ARG:HB2	2.18	0.42
1:M:7:LEU:HD21	1:M:411:THR:HA	2.00	0.42
2:N:128:ASP:OD1	2:N:128:ASP:N	2.45	0.42
3:O:31:THR:HG21	3:O:82:HIS:CB	2.45	0.42
1:A:228:PHE:O	1:A:358:MET:HB2	2.20	0.42
3:C:106:GLU:N	3:C:107:PRO:CD	2.83	0.41
9:N:304:MQ7:H2M2	3:O:28:ARG:NH1	2.35	0.41
1:M:199:TYR:CE1	1:M:229:VAL:HG11	2.56	0.41
1:A:59:HIS:CE1	1:A:121:ILE:HG23	2.56	0.41
1:A:279:ASN:O	1:A:280:LYS:HB2	2.21	0.41
1:M:358:MET:SD	1:M:390:ARG:N	2.94	0.41
1:A:48:ALA:HA	5:A:601:FAD:C6	2.50	0.41
2:N:116:ILE:HG21	2:N:176:ALA:HB2	2.02	0.41
1:M:217:LEU:HD21	1:M:517:CYS:SG	2.61	0.41
1:A:57:GLN:NE2	1:A:122:GLU:HG2	2.36	0.41
1:A:392:GLY:O	1:A:393:SER:CB	2.69	0.41
1:M:44:HIS:NE2	1:M:204:ASN:HA	2.36	0.40
2:B:100:ARG:O	2:B:101:ASP:C	2.59	0.40
2:B:206:PHE:CD2	3:C:89:LEU:HD13	2.57	0.40
1:M:358:MET:HG2	1:M:390:ARG:HB2	2.03	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	575/577 (100%)	556 (97%)	17 (3%)	2 (0%)	46	81
1	M	575/577 (100%)	540 (94%)	33 (6%)	2 (0%)	46	81
2	B	241/243 (99%)	232 (96%)	8 (3%)	1 (0%)	39	78
2	N	241/243 (99%)	227 (94%)	14 (6%)	0	100	100
3	C	128/130 (98%)	125 (98%)	3 (2%)	0	100	100
3	O	128/130 (98%)	120 (94%)	8 (6%)	0	100	100
4	D	117/119 (98%)	112 (96%)	5 (4%)	0	100	100
4	P	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
All	All	2122/2138 (99%)	2023 (95%)	94 (4%)	5 (0%)	52	86

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	393	SER
1	M	444	GLY
2	B	56	SER
1	M	445	GLY
1	A	328	LEU

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	460/460 (100%)	456 (99%)	4 (1%)	84	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	460/460 (100%)	457 (99%)	3 (1%)	88	96
2	B	205/205 (100%)	202 (98%)	3 (2%)	72	91
2	N	205/205 (100%)	202 (98%)	3 (2%)	72	91
3	C	111/111 (100%)	111 (100%)	0	100	100
3	O	111/111 (100%)	111 (100%)	0	100	100
4	D	97/97 (100%)	97 (100%)	0	100	100
4	P	97/97 (100%)	97 (100%)	0	100	100
All	All	1746/1746 (100%)	1733 (99%)	13 (1%)	88	96

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	93	MET
1	A	380	CYS
1	A	485	ARG
2	B	65	CYS
2	B	113	LEU
2	B	178	ARG
1	M	116	PHE
1	M	330	PHE
1	M	435	ARG
2	N	128	ASP
2	N	135	THR
2	N	225	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	87	HIS
1	A	141	GLN
1	A	232	HIS
1	A	279	ASN
1	A	292	GLN
1	A	409	GLN
2	B	134	GLN
2	B	194	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	51	ASN
3	C	64	GLN
1	M	88	HIS
1	M	182	GLN
1	M	279	ASN
1	M	292	GLN
1	M	366	ASN
1	M	434	GLN
2	N	95	ASN
3	O	72	ASN

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 ⓘ

10 ligands are modelled in this entry.

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	$\# Z > 2$
5	FAD	A	601	-	48,58,58	1.30	6 (12%)	54,89,89	2.17	10 (18%)
6	FES	B	301	2	0,4,4	0.00	-	0,4,4	0.00	-
7	F3S	B	302	2	0,9,9	0.00	-	0,15,15	0.00	-
8	SF4	B	303	2	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MQ7	D	701	-	25,25,49	1.79	2 (8%)	33,34,63	1.22	4 (12%)
5	FAD	M	601	-	48,58,58	1.38	6 (12%)	54,89,89	2.16	10 (18%)
6	FES	N	301	2	0,4,4	0.00	-	0,4,4	0.00	-
7	F3S	N	302	2	0,9,9	0.00	-	0,15,15	0.00	-
8	SF4	N	303	2	0,12,12	0.00	-	0,24,24	0.00	-
9	MQ7	N	304	-	25,25,49	1.80	2 (8%)	33,34,63	1.67	7 (21%)

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
5	FAD	A	601	-	-	0/30/50/50	0/6/6/6
6	FES	B	301	2	-	0/0/4/4	0/1/1/1
7	F3S	B	302	2	-	0/0/24/24	0/0/3/3
8	SF4	B	303	2	-	0/0/48/48	0/6/5/5
9	MQ7	D	701	-	-	0/13/33/61	0/2/2/2
5	FAD	M	601	-	-	0/30/50/50	0/6/6/6
6	FES	N	301	2	-	0/0/4/4	0/1/1/1
7	F3S	N	302	2	-	0/0/24/24	0/0/3/3
8	SF4	N	303	2	-	0/0/48/48	0/6/5/5
9	MQ7	N	304	-	-	0/13/33/61	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	FAD	C9A-N10	2.21	1.41	1.38
5	M	601	FAD	C9A-N10	2.44	1.42	1.38
5	A	601	FAD	C8-C7	2.46	1.47	1.41
5	A	601	FAD	C5A-C4A	2.72	1.46	1.40
5	M	601	FAD	C8-C7	3.05	1.49	1.41
5	M	601	FAD	C5A-C4A	3.06	1.47	1.40
5	A	601	FAD	C4-C4X	3.33	1.47	1.41
5	M	601	FAD	C9A-C5X	3.65	1.50	1.42
5	A	601	FAD	C4X-C10	3.66	1.47	1.41
5	A	601	FAD	C9A-C5X	3.70	1.50	1.42
5	M	601	FAD	C4-C4X	3.80	1.48	1.41
5	M	601	FAD	C4X-C10	3.99	1.48	1.41
9	D	701	MQ7	C10-C5	5.51	1.49	1.40
9	N	304	MQ7	C10-C5	5.60	1.49	1.40
9	N	304	MQ7	C3-C2	6.23	1.50	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	701	MQ7	C3-C2	6.32	1.50	1.35

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	FAD	N3A-C2A-N1A	-8.09	122.70	128.89
5	M	601	FAD	N3A-C2A-N1A	-7.62	123.06	128.89
5	A	601	FAD	C4-C4X-C10	-5.39	116.49	119.94
5	M	601	FAD	C4-C4X-C10	-4.65	116.97	119.94
9	N	304	MQ7	C15-C13-C12	-3.82	113.80	121.05
5	M	601	FAD	P-O3P-PA	-3.79	122.09	132.73
5	M	601	FAD	C4X-C4-N3	-3.75	118.46	123.59
5	M	601	FAD	C4A-C5A-N7A	-3.51	106.25	109.48
5	A	601	FAD	C4X-C4-N3	-3.44	118.88	123.59
5	A	601	FAD	C4A-C5A-N7A	-3.43	106.33	109.48
9	D	701	MQ7	C16-C17-C18	-3.05	121.12	127.76
5	A	601	FAD	P-O3P-PA	-2.57	125.51	132.73
5	M	601	FAD	C1B-N9A-C4A	-2.57	123.07	126.94
9	D	701	MQ7	C11-C12-C13	-2.50	122.46	126.70
5	A	601	FAD	C1B-N9A-C4A	-2.50	123.17	126.94
9	N	304	MQ7	C16-C17-C18	-2.24	122.89	127.76
9	N	304	MQ7	C2M-C2-C3	-2.16	119.49	124.10
9	N	304	MQ7	C15-C16-C17	-2.01	106.43	111.69
9	D	701	MQ7	C2M-C2-C1	2.14	119.74	116.27
5	A	601	FAD	C4-C4X-N5	2.25	121.45	118.72
9	N	304	MQ7	C2M-C2-C1	2.38	120.13	116.27
9	N	304	MQ7	C19-C18-C20	2.56	118.58	115.68
5	M	601	FAD	C4-C4X-N5	2.63	121.91	118.72
5	A	601	FAD	C4X-N5-C5X	2.71	119.88	116.76
9	D	701	MQ7	C19-C18-C20	3.28	119.39	115.68
5	M	601	FAD	C4X-N5-C5X	3.55	120.84	116.76
5	M	601	FAD	C1'-N10-C9A	3.61	122.92	118.86
5	A	601	FAD	C1'-N10-C9A	4.56	123.98	118.86
9	N	304	MQ7	C14-C13-C15	5.88	124.38	115.41
5	A	601	FAD	C4-N3-C2	7.41	121.65	115.25
5	M	601	FAD	C4-N3-C2	7.77	121.97	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	FAD	7	0
9	D	701	MQ7	3	0
5	M	601	FAD	2	0
9	N	304	MQ7	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	577/577 (100%)	-0.07	2 (0%) 94 87	29, 40, 64, 95	0
1	M	577/577 (100%)	1.62	188 (32%) 1 0	72, 113, 147, 165	0
2	B	243/243 (100%)	-0.03	4 (1%) 74 55	30, 45, 64, 123	0
2	N	243/243 (100%)	1.06	43 (17%) 2 1	63, 97, 134, 141	0
3	C	130/130 (100%)	0.12	8 (6%) 24 13	50, 61, 92, 95	0
3	O	130/130 (100%)	0.63	21 (16%) 3 1	56, 79, 115, 145	0
4	D	119/119 (100%)	-0.23	2 (1%) 73 53	48, 63, 86, 95	0
4	P	119/119 (100%)	0.15	8 (6%) 21 11	63, 77, 101, 140	0
All	All	2138/2138 (100%)	0.58	276 (12%) 5 2	29, 71, 132, 165	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	165	GLY	12.7
1	M	411	THR	8.7
1	M	163	ASP	7.5
3	O	1	THR	7.4
1	M	169	GLY	7.3
1	M	188	VAL	7.2
1	M	161	LEU	6.9
1	M	6	ASP	6.7
1	M	376	ALA	6.3
1	M	574	PRO	6.2
1	M	189	VAL	5.7
1	M	560	THR	5.5
2	B	1	ALA	5.5
1	M	172	ALA	5.5
1	M	24	ALA	5.4
1	M	77	CYS	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	380	CYS	5.4
1	M	170	LEU	5.4
1	M	162	VAL	5.4
1	M	159	ASP	5.4
2	N	20	ALA	5.2
1	M	375	PHE	5.2
2	N	19	THR	5.2
1	M	8	ALA	5.1
1	M	573	LEU	5.0
1	M	28	PRO	5.0
1	M	484	GLU	5.0
1	M	4	GLN	5.0
1	M	486	PHE	4.9
1	M	164	ASP	4.9
2	N	133	ILE	4.9
2	N	98	ILE	4.8
1	M	424	ALA	4.8
1	M	176	MET	4.7
1	M	576	ALA	4.7
1	M	160	ILE	4.6
2	N	126	THR	4.6
2	N	136	PRO	4.5
1	M	32	ILE	4.4
1	M	220	GLY	4.3
1	M	373	GLY	4.3
1	M	167	VAL	4.2
1	M	490	ARG	4.2
4	D	118	ILE	4.2
1	M	84	TYR	4.1
1	M	571	THR	4.1
1	M	219	HIS	4.0
1	M	386	HIS	4.0
1	M	180	LEU	3.9
1	M	419	ASN	3.9
1	M	192	THR	3.9
1	M	489	VAL	3.8
1	M	405	LEU	3.8
1	M	11	GLY	3.8
2	N	128	ASP	3.8
1	M	27	ASN	3.8
2	N	1	ALA	3.8
1	M	7	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	206	GLY	3.7
1	M	31	LYS	3.7
1	M	210	GLY	3.7
1	M	370	ARG	3.7
1	M	445	GLY	3.6
1	M	222	PRO	3.6
2	N	27	GLU	3.6
1	M	374	LEU	3.5
2	N	122	GLY	3.5
2	N	26	TYR	3.5
3	O	10	PRO	3.5
3	O	130	TRP	3.5
2	N	11	VAL	3.5
1	M	385	LEU	3.4
4	P	3	PRO	3.4
1	M	402	PHE	3.4
2	N	25	PHE	3.4
3	O	2	THR	3.4
1	M	557	ALA	3.4
1	M	395	SER	3.4
1	M	44	HIS	3.4
3	O	4	ARG	3.3
1	M	66	PHE	3.3
1	M	125	TRP	3.3
1	M	360	GLY	3.3
1	M	493	ASP	3.3
3	O	103	MET	3.3
1	M	168	ARG	3.3
3	O	100	ASP	3.3
1	M	422	GLU	3.3
1	M	9	ILE	3.3
3	O	47	PHE	3.3
1	M	561	THR	3.2
4	P	51	TYR	3.2
4	P	4	ASN	3.2
2	N	52	SER	3.2
3	C	58	GLY	3.2
1	M	191	ALA	3.2
1	A	322	LYS	3.2
1	M	190	MET	3.2
1	M	187	ALA	3.2
1	M	553	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	P	56	ALA	3.2
1	M	482	LEU	3.1
2	B	243	ARG	3.1
1	M	322	LYS	3.1
1	M	436	LEU	3.1
1	M	559	GLY	3.1
1	M	129	ASP	3.1
1	M	33	ALA	3.1
1	M	204	ASN	3.1
1	M	444	GLY	3.1
1	M	323	LYS	3.0
1	M	399	LEU	3.0
1	M	147	PRO	3.0
1	M	500	THR	3.0
1	M	166	HIS	3.0
1	M	25	GLN	3.0
3	C	65	ASN	3.0
2	B	2	GLU	3.0
2	N	2	GLU	3.0
2	N	193	ALA	2.9
1	M	428	GLN	2.9
3	C	54	GLU	2.9
1	M	23	ALA	2.9
1	M	65	HIS	2.9
1	M	549	LYS	2.9
1	M	535	LEU	2.9
1	M	415	ALA	2.9
3	O	126	VAL	2.9
4	P	47	ASP	2.9
1	M	152	PHE	2.9
1	M	572	THR	2.9
1	M	10	VAL	2.9
3	O	6	PRO	2.9
1	M	211	ASP	2.8
1	M	223	LEU	2.8
1	M	491	ILE	2.8
3	O	49	LEU	2.8
4	P	0	MET	2.8
1	M	377	VAL	2.8
3	O	96	ILE	2.8
1	M	193	GLY	2.8
1	M	447	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	99	GLU	2.8
1	M	202	ASN	2.8
1	M	203	THR	2.8
3	C	56	TRP	2.8
2	N	8	ILE	2.7
2	B	241	LYS	2.7
2	N	134	GLN	2.7
3	O	101	GLU	2.7
1	M	171	VAL	2.7
1	M	407	GLY	2.7
3	C	62	PHE	2.7
1	M	108	ASP	2.7
1	M	177	GLU	2.7
1	M	158	LEU	2.7
1	M	80	ASP	2.7
1	M	13	GLY	2.7
2	N	166	GLU	2.7
2	N	130	GLY	2.7
2	N	180	ASN	2.6
1	M	502	LEU	2.6
4	P	118	ILE	2.6
1	M	441	ASN	2.6
1	M	320	GLY	2.6
2	N	62	CYS	2.6
1	M	558	ASP	2.6
1	M	12	ALA	2.6
1	M	475	THR	2.6
3	O	110	LYS	2.6
1	M	371	ILE	2.6
1	M	91	THR	2.6
1	M	217	LEU	2.6
2	N	131	THR	2.6
2	N	23	SER	2.6
2	N	64	SER	2.6
1	A	576	ALA	2.6
3	O	11	MET	2.5
1	M	62	PHE	2.5
1	M	372	LYS	2.5
2	N	192	MET	2.5
1	M	156	PHE	2.5
1	M	433	GLU	2.5
1	M	39	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	361	ILE	2.5
3	O	14	THR	2.5
1	M	51	GLY	2.5
1	M	295	TRP	2.5
1	M	194	GLY	2.5
1	M	421	ASN	2.4
3	O	7	TYR	2.4
1	M	87	HIS	2.4
1	M	86	VAL	2.4
1	M	99	TRP	2.4
1	M	369	THR	2.4
2	N	24	ALA	2.4
1	M	390	ARG	2.4
1	M	463	CYS	2.4
1	M	1	GLN	2.4
2	N	13	TYR	2.4
2	N	53	TYR	2.4
1	M	88	HIS	2.4
4	D	0	MET	2.4
1	M	150	GLN	2.4
1	M	429	ALA	2.4
1	M	209	THR	2.4
1	M	440	VAL	2.4
1	M	487	LYS	2.4
1	M	195	ALA	2.4
2	N	9	GLU	2.3
1	M	494	THR	2.3
1	M	358	MET	2.3
3	C	55	ALA	2.3
1	M	228	PHE	2.3
1	M	67	HIS	2.3
1	M	131	THR	2.3
3	O	54	GLU	2.3
1	M	29	ASN	2.3
1	M	48	ALA	2.3
1	M	132	GLY	2.3
1	M	359	GLY	2.3
1	M	16	GLY	2.3
1	M	100	GLY	2.3
1	M	545	VAL	2.3
1	M	58	ASP	2.3
1	M	197	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	57	CYS	2.3
1	M	565	TYR	2.3
1	M	497	VAL	2.3
2	N	125	ARG	2.3
4	P	52	GLU	2.3
1	M	543	ASP	2.2
3	O	52	GLY	2.3
1	M	423	ALA	2.2
1	M	435	ARG	2.2
2	N	85	THR	2.2
1	M	208	VAL	2.2
1	M	488	ARG	2.2
1	M	186	ASN	2.2
1	M	70	VAL	2.2
1	M	537	GLU	2.2
1	M	130	LYS	2.2
2	N	89	LYS	2.2
1	M	26	ALA	2.2
1	M	416	THR	2.2
1	M	179	THR	2.2
1	M	522	ALA	2.2
2	N	242	PRO	2.1
1	M	182	GLN	2.1
2	N	108	HIS	2.1
1	M	196	GLY	2.1
1	M	101	CYS	2.1
2	N	124	SER	2.1
1	M	42	ARG	2.1
1	M	539	CYS	2.1
2	N	6	LEU	2.1
3	C	60	VAL	2.1
1	M	532	HIS	2.1
1	M	356	TYR	2.1
2	N	135	THR	2.1
1	M	227	GLU	2.1
1	M	379	GLU	2.1
1	M	45	THR	2.1
2	N	227	GLY	2.0
3	O	8	VAL	2.0
1	M	575	PRO	2.0
1	M	434	GLN	2.0
1	M	504	TYR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	56	SER	2.0
2	N	138	GLN	2.0
3	C	57	ALA	2.0
3	O	16	TRP	2.0
1	M	98	LEU	2.0
1	M	205	GLY	2.0
1	M	110	SER	2.0
1	M	496	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
9	MQ7	D	701	24/48	0.69	0.57	10.54	43,45,46,47	24
9	MQ7	N	304	24/48	0.49	0.63	7.27	60,63,66,67	24
5	FAD	A	601	53/53	0.97	0.18	-1.07	17,19,22,22	0
5	FAD	M	601	53/53	0.84	0.29	-1.09	41,61,89,91	0
8	SF4	B	303	8/8	0.97	0.15	-1.23	23,24,24,25	0
7	F3S	N	302	7/7	0.96	0.10	-1.89	48,50,55,55	0
7	F3S	B	302	7/7	0.97	0.11	-1.94	27,28,29,30	0
6	FES	B	301	4/4	0.99	0.16	-2.14	19,20,20,20	0
8	SF4	N	303	8/8	0.95	0.12	-2.69	40,42,43,44	0
6	FES	N	301	4/4	0.98	0.13	-3.95	40,40,41,44	0

6.5 Other polymers

There are no such residues in this entry.