



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2017 – 07:57 PM EDT

PDB ID : 5VPN
Title : E. coli Quinol fumarate reductase FrdA E245Q mutation
Authors : Starbird, C.A.; Maklashina, E.; Sharma, P.; Qualls-Histed, S.; Cecchini, G.; Iverson, T.M.
Deposited on : unknown
Resolution : 4.22 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029824

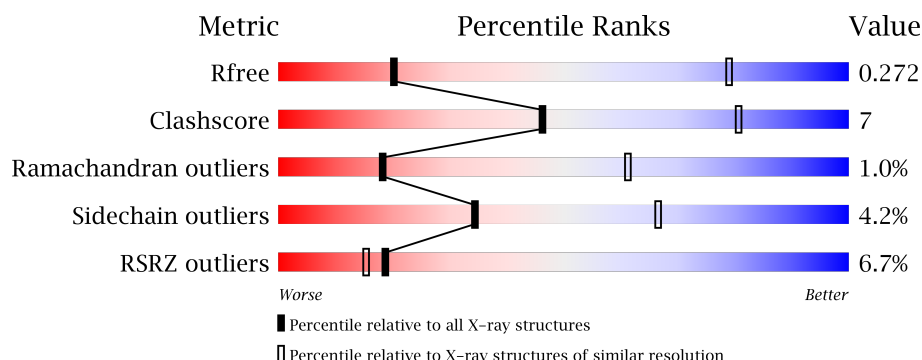
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.22 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.



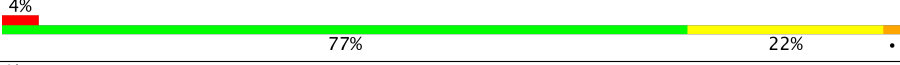
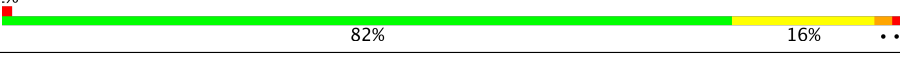

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1180 (4.84-3.60)
Clashscore	112137	1027 (4.76-3.66)
Ramachandran outliers	110173	1006 (4.80-3.64)
Sidechain outliers	110143	1015 (4.80-3.62)
RSRZ outliers	101464	1003 (4.80-3.62)

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	585	<div> <div>12%</div> <div>83%</div> <div>15%</div> <div>..</div> </div>
1	E	585	<div> <div>9%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>
2	B	243	<div> <div>2%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
2	F	243	<div> <div>0%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>
3	C	130	<div> <div>4%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	130	
4	D	119	
4	H	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
5	FAD	A	601	-	-	-	X
5	FAD	E	601	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16845 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	803	839	31			
1	E	585	Total	C	N	O	S	0	0	0
			4509	2813	815	850	31			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	245	GLN	GLU	engineered mutation	UNP P00363
E	245	GLN	GLU	engineered mutation	UNP P00363

- Molecule 2 is a protein called Fumarate reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			
2	F	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	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
			1058	720	166	169	3			
3	G	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			

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

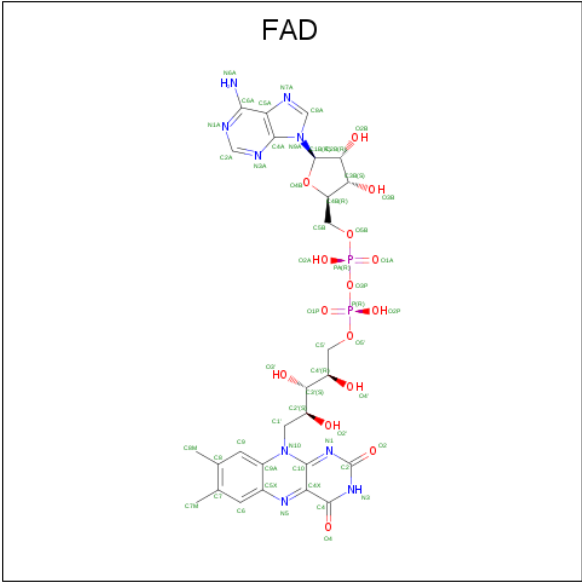
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	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: C₂₇H₃₃N₉O₁₅P₂).



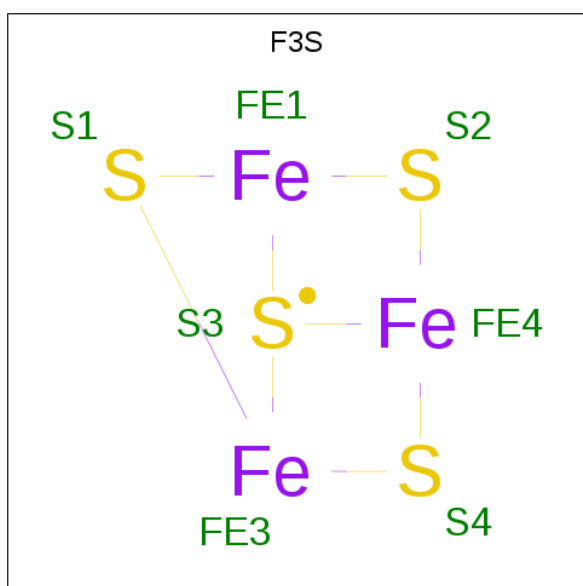
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



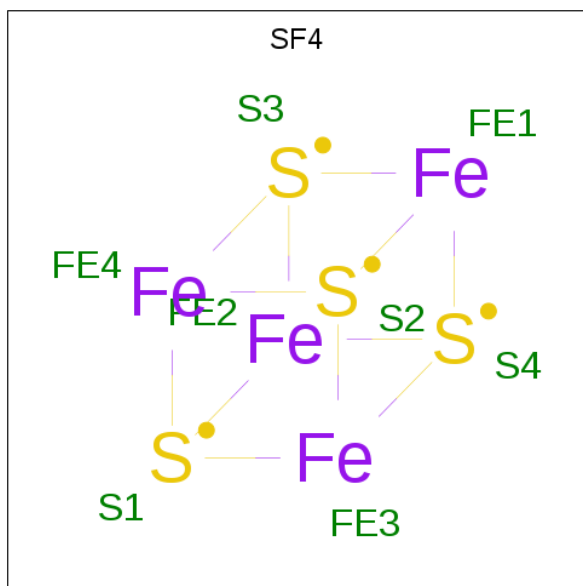
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			4	2	2		
6	F	1	Total	Fe	S	0	0
			4	2	2		

- 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	F	1	Total	Fe	S	0	0
			7	3	4		

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

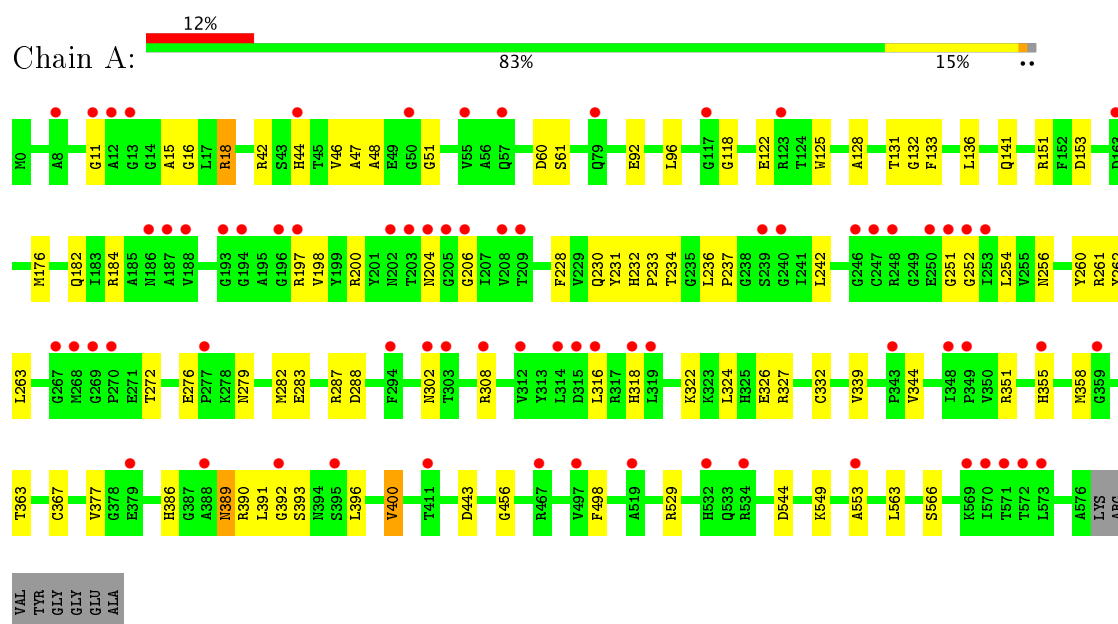


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		
8	F	1	Total	Fe	S	0	0
			8	4	4		

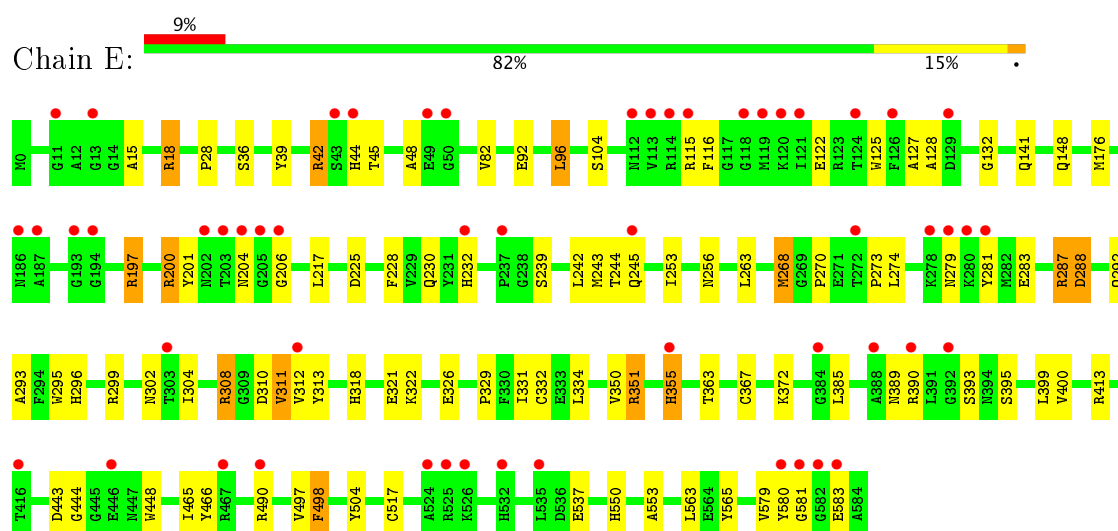
3 Residue-property plots

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.

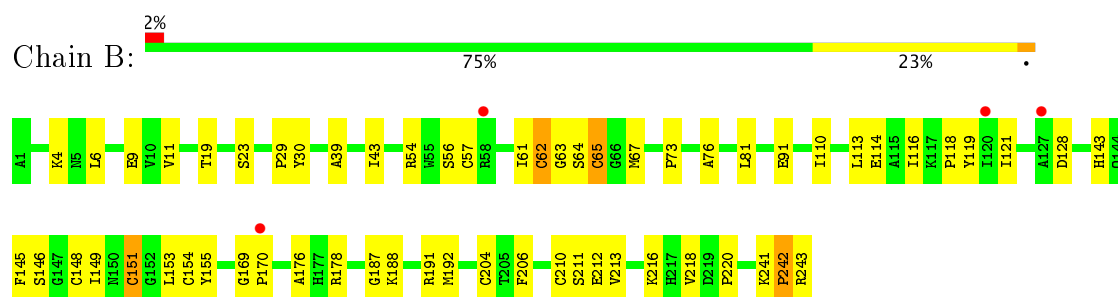
• Molecule 1: Fumarate reductase flavoprotein subunit



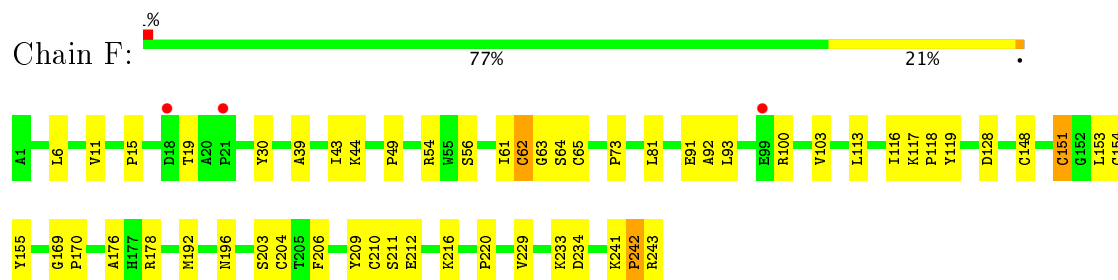
• Molecule 1: Fumarate reductase flavoprotein subunit



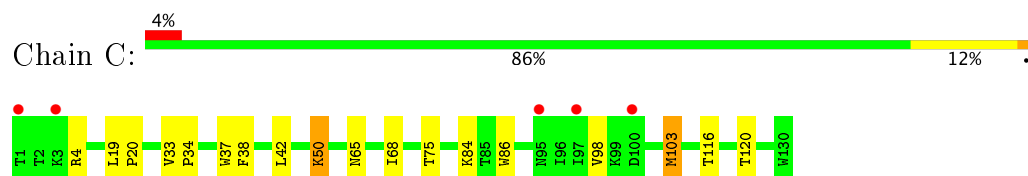
• Molecule 2: Fumarate reductase iron-sulfur subunit



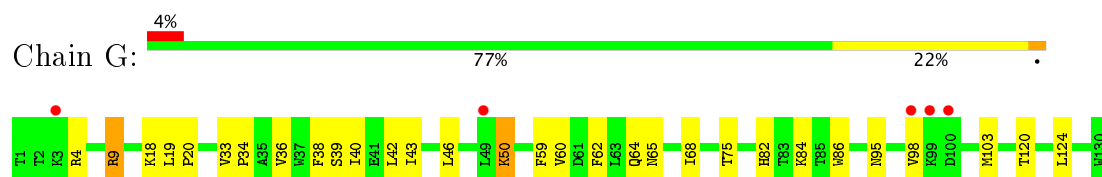
• Molecule 2: Fumarate reductase iron-sulfur subunit



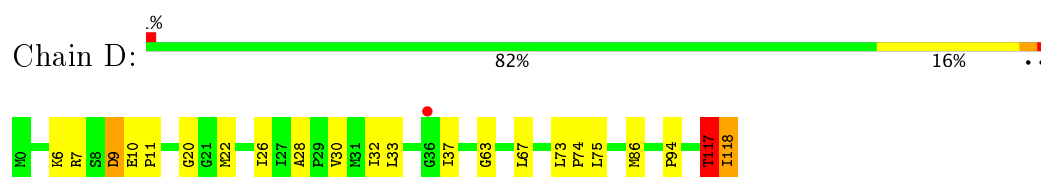
• Molecule 3: Fumarate reductase subunit C



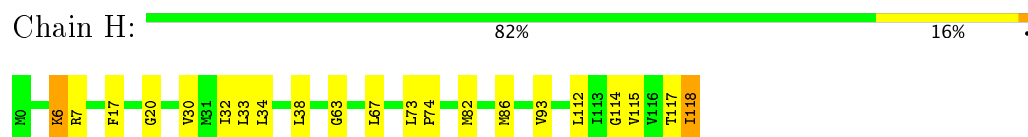
• Molecule 3: Fumarate reductase subunit C



• 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	133.56Å 138.13Å 220.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.96 – 4.22 50.29 – 4.21	Depositor EDS
% Data completeness (in resolution range)	95.9 (22.96-4.22) 80.5 (50.29-4.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.215 , 0.270 0.208 , 0.272	Depositor DCC
R_{free} test set	1191 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	140.8	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 144.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	16845	wwPDB-VP
Average B, all atoms (Å ²)	214.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: SF4, F3S, FES, 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	0.26	0/4540	0.45	0/6139
1	E	0.27	0/4602	0.46	0/6221
2	B	0.27	0/1931	0.44	0/2617
2	F	0.27	0/1931	0.45	0/2617
3	C	0.28	0/1094	0.43	0/1496
3	G	0.28	0/1094	0.47	0/1496
4	D	0.27	0/956	0.41	0/1303
4	H	0.30	0/956	0.42	0/1303
All	All	0.27	0/17104	0.45	0/23192

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

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	4337	57	0
1	E	4509	0	4398	75	0
2	B	1888	0	1848	37	0
2	F	1888	0	1847	34	0
3	C	1058	0	1108	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1058	0	1108	24	0
4	D	926	0	971	17	0
4	H	926	0	971	15	0
5	A	53	0	31	5	0
5	E	53	0	31	11	0
6	B	4	0	0	0	0
6	F	4	0	0	0	0
7	B	7	0	0	0	0
7	F	7	0	0	0	0
8	B	8	0	0	0	0
8	F	8	0	0	0	0
All	All	16845	0	16650	240	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 7.

All (240) 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:E:96:LEU:HD11	1:E:400:VAL:HG11	1.54	0.87
3:G:65:ASN:HB3	3:G:68:ILE:H	1.50	0.76
2:B:62:CYS:SG	2:B:63:GLY:N	2.60	0.74
1:E:28:PRO:HA	1:E:148:GLN:HE21	1.52	0.74
1:E:176:MET:HB3	3:G:4:ARG:HD3	1.69	0.74
1:A:96:LEU:HD11	1:A:400:VAL:HG11	1.71	0.72
3:C:65:ASN:HB3	3:C:68:ILE:H	1.55	0.72
4:D:20:GLY:HA2	4:D:73:LEU:HB3	1.72	0.71
1:A:288:ASP:OD1	1:A:389:ASN:ND2	2.23	0.71
1:A:324:LEU:HD13	1:A:344:VAL:HA	1.71	0.70
3:C:98:VAL:HG22	3:C:103:MET:HB3	1.74	0.70
3:G:19:LEU:HD12	3:G:20:PRO:HD2	1.73	0.70
1:E:293:ALA:HA	1:E:296:HIS:HD1	1.58	0.69
1:E:393:SER:HA	5:E:601:FAD:HN3	1.59	0.68
1:E:197:ARG:HD2	1:E:206:GLY:HA2	1.77	0.67
1:E:48:ALA:HB3	1:E:132:GLY:HA3	1.77	0.67
1:E:281:TYR:HE1	1:E:583:GLU:HB2	1.59	0.66
1:A:197:ARG:HD2	1:A:206:GLY:HA2	1.79	0.64
2:F:93:LEU:O	3:G:9:ARG:NH2	2.31	0.64
1:A:151:ARG:NH1	1:A:153:ASP:OD2	2.31	0.63
1:E:395:SER:HG	5:E:601:FAD:HO3'	1.46	0.63
3:C:120:THR:HG23	4:D:30:VAL:HB	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:PRO:HD2	1:E:281:TYR:HE2	1.65	0.62
1:E:18:ARG:NH1	1:E:92:GLU:OE1	2.34	0.61
1:A:529:ARG:NH2	1:A:544:ASP:OD1	2.32	0.60
2:F:44:LYS:NZ	2:F:49:PRO:O	2.31	0.60
4:H:34:LEU:HD23	4:H:38:LEU:HD12	1.82	0.60
3:G:75:THR:HG22	4:H:32:ILE:HD13	1.82	0.59
4:H:20:GLY:HA2	4:H:73:LEU:HB3	1.84	0.59
3:C:33:VAL:HB	3:C:34:PRO:HD3	1.84	0.59
1:A:251:GLY:O	1:A:318:HIS:NE2	2.29	0.59
3:C:50:LYS:HB3	4:D:118:ILE:HG22	1.84	0.58
3:G:120:THR:HG23	4:H:30:VAL:HB	1.85	0.58
1:A:18:ARG:NH1	1:A:92:GLU:OE1	2.36	0.58
1:A:242:LEU:HD22	5:A:601:FAD:HM73	1.85	0.58
1:E:281:TYR:CE1	1:E:583:GLU:HB2	2.38	0.58
2:F:62:CYS:SG	2:F:63:GLY:N	2.77	0.58
1:A:230:GLN:OE1	1:A:390:ARG:NH2	2.35	0.58
1:A:18:ARG:HG2	1:A:400:VAL:HA	1.86	0.58
2:F:54:ARG:HB3	2:F:64:SER:HB2	1.87	0.57
3:G:98:VAL:HG22	3:G:103:MET:HB3	1.87	0.57
1:A:11:GLY:HA2	5:A:601:FAD:H1B	1.87	0.57
2:F:192:MET:O	2:F:196:ASN:ND2	2.38	0.57
1:E:390:ARG:HD2	1:E:395:SER:HB2	1.86	0.57
1:E:256:ASN:HD22	1:E:302:ASN:HB3	1.68	0.56
1:A:390:ARG:NH1	1:A:391:LEU:O	2.38	0.56
2:B:54:ARG:HB3	2:B:64:SER:HB2	1.86	0.56
3:C:75:THR:HG22	4:D:32:ILE:HD13	1.86	0.56
1:E:355:HIS:HE1	5:E:601:FAD:C8	2.19	0.56
2:F:11:VAL:HG21	2:F:91:GLU:HG2	1.88	0.56
2:B:143:HIS:O	2:B:146:SER:OG	2.23	0.55
2:F:6:LEU:HD23	2:F:81:LEU:HD13	1.88	0.55
2:B:30:TYR:HB3	2:B:81:LEU:HD12	1.89	0.55
2:F:30:TYR:HB3	2:F:81:LEU:HD12	1.88	0.55
2:F:211:SER:HA	2:F:220:PRO:HD2	1.89	0.54
1:E:292:GLN:HA	1:E:465:ILE:HG21	1.89	0.54
3:G:33:VAL:HB	3:G:34:PRO:HD3	1.90	0.54
1:A:237:PRO:HB2	1:A:308:ARG:HB2	1.89	0.54
2:B:210:CYS:SG	2:B:220:PRO:HG2	2.48	0.54
1:E:45:THR:OG1	5:E:601:FAD:O2A	2.19	0.54
1:E:393:SER:HA	5:E:601:FAD:N3	2.23	0.53
1:A:393:SER:HA	5:A:601:FAD:HN3	1.72	0.53
2:F:73:PRO:HB2	2:F:153:LEU:HD22	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:295:TRP:HE1	1:E:299:ARG:NE	2.07	0.53
1:A:176:MET:HG3	3:C:4:ARG:HD3	1.91	0.53
1:E:82:VAL:HG22	1:E:385:LEU:HD12	1.91	0.53
1:E:44:HIS:CE1	1:E:204:ASN:HA	2.43	0.53
2:F:155:TYR:CE2	2:F:169:GLY:HA3	2.43	0.53
1:E:253:ILE:HG12	1:E:318:HIS:HE1	1.74	0.53
1:E:232:HIS:HB2	1:E:355:HIS:HD2	1.73	0.53
1:E:141:GLN:HB3	2:F:118:PRO:O	2.08	0.53
2:F:234:ASP:OD1	4:H:7:ARG:NH2	2.42	0.52
2:B:11:VAL:HG21	2:B:91:GLU:HG2	1.92	0.52
4:D:6:LYS:HE2	4:H:6:LYS:HB2	1.90	0.52
2:F:210:CYS:SG	2:F:220:PRO:HG2	2.50	0.52
3:G:46:LEU:HD21	4:H:114:GLY:HA3	1.92	0.52
3:C:50:LYS:HG3	4:D:118:ILE:H	1.75	0.51
1:A:254:LEU:HD12	1:A:263:LEU:HD11	1.91	0.51
2:F:151:CYS:SG	2:F:153:LEU:HG	2.50	0.51
1:A:393:SER:HA	5:A:601:FAD:N3	2.25	0.51
1:E:295:TRP:CD1	1:E:466:TYR:HD1	2.29	0.51
2:B:154:CYS:SG	2:B:170:PRO:HG2	2.51	0.51
1:E:232:HIS:HB2	1:E:355:HIS:CD2	2.46	0.51
2:B:149:ILE:HG13	2:B:151:CYS:HB3	1.92	0.51
4:D:94:PRO:HA	2:F:242:PRO:HA	1.91	0.51
1:E:104:SER:OG	1:E:127:ALA:O	2.26	0.50
2:F:210:CYS:SG	2:F:211:SER:N	2.84	0.50
1:A:51:GLY:HA2	1:A:131:THR:HG21	1.93	0.50
2:B:151:CYS:SG	2:B:153:LEU:HG	2.51	0.50
3:C:19:LEU:HD12	3:C:20:PRO:HD2	1.93	0.50
1:E:18:ARG:HG2	1:E:400:VAL:HA	1.92	0.50
1:A:15:ALA:HB1	1:A:377:VAL:HG13	1.93	0.50
1:E:310:ASP:O	1:E:351:ARG:NH1	2.42	0.50
1:A:42:ARG:NH2	2:B:63:GLY:O	2.45	0.49
2:B:155:TYR:CZ	2:B:169:GLY:HA3	2.46	0.49
3:G:50:LYS:HB3	4:H:118:ILE:HG22	1.95	0.49
3:C:116:THR:HA	4:D:26:ILE:HG23	1.94	0.49
4:D:73:LEU:HB2	4:D:74:PRO:HD3	1.95	0.49
2:B:210:CYS:SG	2:B:211:SER:N	2.86	0.49
1:E:232:HIS:HE1	1:E:245:GLN:HG3	1.78	0.49
1:A:390:ARG:HH12	1:A:392:GLY:HA2	1.77	0.49
1:E:115:ARG:HD3	1:E:279:ASN:ND2	2.28	0.49
1:A:237:PRO:HG2	1:A:308:ARG:HD2	1.94	0.49
1:E:395:SER:N	5:E:601:FAD:O2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:TYR:CE2	2:B:169:GLY:HA3	2.47	0.49
3:G:38:PHE:O	3:G:42:LEU:HG	2.13	0.48
4:D:33:LEU:HA	4:D:37:ILE:HD12	1.95	0.48
1:E:288:ASP:CG	1:E:389:ASN:HD21	2.16	0.48
1:E:116:PHE:CE2	1:E:245:GLN:HB2	2.49	0.48
1:E:372:LYS:HE3	1:E:413:ARG:HD2	1.95	0.47
3:G:33:VAL:HA	4:H:82:MET:HE3	1.96	0.47
1:E:497:VAL:HG21	2:F:15:PRO:HG2	1.96	0.47
1:E:331:ILE:HD13	1:E:334:LEU:HD12	1.96	0.47
2:F:92:ALA:O	3:G:9:ARG:NH1	2.36	0.47
1:A:48:ALA:HB3	1:A:132:GLY:HA3	1.95	0.47
1:A:236:LEU:HD13	1:A:339:VAL:HG13	1.96	0.47
3:C:38:PHE:O	3:C:42:LEU:HG	2.14	0.47
1:E:242:LEU:HB3	5:E:601:FAD:HM73	1.95	0.47
3:G:36:VAL:O	3:G:40:ILE:HG12	2.15	0.47
1:E:253:ILE:HA	1:E:283:GLU:HG2	1.97	0.47
1:E:263:LEU:HD22	1:E:268:MET:HE3	1.96	0.47
2:F:154:CYS:SG	2:F:170:PRO:HG2	2.55	0.47
3:G:50:LYS:HD2	4:H:118:ILE:O	2.15	0.46
2:B:145:PHE:HA	2:B:218:VAL:HG13	1.97	0.46
1:E:497:VAL:HG13	3:G:4:ARG:HG2	1.96	0.46
1:E:200:ARG:NH1	1:E:201:TYR:OH	2.48	0.46
2:B:6:LEU:HB2	2:B:30:TYR:CE2	2.51	0.46
3:G:59:PHE:O	3:G:62:PHE:HB3	2.15	0.46
1:A:322:LYS:O	1:A:326:GLU:HB3	2.15	0.46
3:G:60:VAL:O	3:G:64:GLN:HG3	2.15	0.46
1:A:141:GLN:HB3	2:B:118:PRO:O	2.16	0.46
2:B:73:PRO:HG2	2:B:213:VAL:HG11	1.96	0.46
1:E:295:TRP:CE3	1:E:465:ILE:HB	2.51	0.46
1:E:448:TRP:CH2	1:E:504:TYR:HB3	2.51	0.46
3:G:50:LYS:HD3	3:G:50:LYS:O	2.16	0.46
4:D:9:ASP:N	4:D:9:ASP:OD1	2.36	0.45
1:A:42:ARG:HG3	2:B:62:CYS:SG	2.56	0.45
2:B:67:MET:SD	2:B:76:ALA:HB2	2.56	0.45
1:A:252:GLY:HA3	1:A:316:LEU:HD23	1.96	0.45
2:B:113:LEU:HD23	2:B:118:PRO:HG3	1.97	0.45
2:B:188:LYS:O	2:B:192:MET:HG2	2.16	0.45
1:E:253:ILE:HG12	1:E:318:HIS:CE1	2.52	0.45
1:E:48:ALA:HA	5:E:601:FAD:C6	2.46	0.45
4:H:73:LEU:HB2	4:H:74:PRO:HD3	1.98	0.45
3:C:50:LYS:HD2	4:D:117:THR:HG23	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:443:ASP:HA	1:E:490:ARG:HG3	1.97	0.45
1:A:11:GLY:O	1:A:16:GLY:HA3	2.16	0.45
1:E:15:ALA:HB2	1:E:399:LEU:HD22	1.99	0.45
1:E:550:HIS:O	1:E:565:TYR:HA	2.17	0.45
3:G:39:SER:O	3:G:43:ILE:HG13	2.16	0.45
1:E:39:TYR:HB2	1:E:42:ARG:HD3	1.97	0.45
1:E:36:SER:HA	5:E:601:FAD:N3A	2.31	0.45
2:F:116:ILE:HB	2:F:176:ALA:HB2	1.99	0.45
2:B:65:CYS:SG	2:B:76:ALA:HB3	2.57	0.44
3:C:86:TRP:HE1	4:D:22:MET:HE2	1.83	0.44
1:E:304:ILE:HG13	1:E:313:TYR:CE2	2.51	0.44
2:F:154:CYS:HB2	2:F:210:CYS:HB2	1.98	0.44
1:A:198:VAL:O	1:A:456:GLY:HA2	2.18	0.44
1:E:295:TRP:HE1	1:E:299:ARG:HE	1.64	0.44
1:E:256:ASN:HB2	1:E:302:ASN:HB3	2.00	0.44
1:E:42:ARG:HG3	2:F:62:CYS:SG	2.58	0.44
1:A:182:GLN:OE1	1:A:184:ARG:NH1	2.44	0.44
2:B:110:ILE:O	2:B:114:GLU:HG3	2.18	0.44
1:A:133:PHE:CE1	2:B:149:ILE:HG22	2.53	0.44
1:A:47:ALA:O	5:A:601:FAD:HM72	2.18	0.43
1:E:311:VAL:HG23	1:E:350:VAL:O	2.18	0.43
2:B:119:TYR:O	2:B:191:ARG:NH2	2.51	0.43
1:E:232:HIS:CE1	1:E:245:GLN:HG3	2.53	0.43
1:E:553:ALA:HA	1:E:563:LEU:HD23	2.00	0.43
1:A:386:HIS:CE1	1:A:390:ARG:HG3	2.53	0.43
4:H:63:GLY:O	4:H:67:LEU:HD23	2.18	0.43
1:A:308:ARG:HH12	1:A:339:VAL:HA	1.83	0.43
1:E:225:ASP:HB3	1:E:228:PHE:HD1	1.83	0.43
3:G:9:ARG:HE	3:G:9:ARG:HB2	1.48	0.43
1:E:42:ARG:N	1:E:42:ARG:HD2	2.33	0.43
1:E:42:ARG:NH2	2:F:63:GLY:O	2.52	0.43
2:B:116:ILE:HB	2:B:176:ALA:HB2	2.00	0.43
2:F:113:LEU:HD23	2:F:118:PRO:HG3	2.00	0.43
3:G:82:HIS:O	3:G:86:TRP:HB2	2.19	0.43
2:B:216:LYS:HA	2:B:216:LYS:HE2	2.00	0.43
2:B:6:LEU:HD22	2:B:81:LEU:HB3	2.01	0.43
1:E:270:PRO:HD2	1:E:281:TYR:CE2	2.49	0.43
2:F:229:VAL:HG12	2:F:233:LYS:HE3	2.00	0.43
1:E:217:LEU:HD11	1:E:517:CYS:SG	2.59	0.43
1:A:272:THR:H	1:A:282:MET:HG3	1.84	0.43
2:F:117:LYS:HD2	2:F:119:TYR:OH	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:TYR:O	1:A:287:ARG:HD3	2.19	0.42
1:A:260:TYR:O	1:A:262:TYR:N	2.52	0.42
3:C:34:PRO:HA	3:C:37:TRP:HB3	2.01	0.42
4:D:63:GLY:O	4:D:67:LEU:HD23	2.19	0.42
1:E:287:ARG:HG2	1:E:288:ASP:N	2.34	0.42
1:E:363:THR:HB	1:E:367:CYS:HA	2.01	0.42
2:F:39:ALA:O	2:F:43:ILE:HG13	2.20	0.42
1:E:148:GLN:OE1	1:E:148:GLN:N	2.41	0.42
1:A:256:ASN:HB2	1:A:302:ASN:O	2.20	0.42
1:A:327:ARG:HD3	1:A:327:ARG:HA	1.84	0.42
1:A:236:LEU:HD22	1:A:339:VAL:HG11	2.02	0.42
2:B:9:GLU:HG3	2:B:23:SER:HB3	2.02	0.42
3:G:34:PRO:HB3	3:G:75:THR:HA	2.02	0.42
1:A:46:VAL:HB	1:A:136:LEU:HD23	2.02	0.41
4:D:10:GLU:N	4:D:11:PRO:HD2	2.35	0.41
2:F:155:TYR:CZ	2:F:169:GLY:HA3	2.54	0.41
1:A:228:PHE:O	1:A:358:MET:HB2	2.19	0.41
4:D:75:LEU:HA	4:D:75:LEU:HD23	1.90	0.41
1:A:396:LEU:HA	1:A:396:LEU:HD23	1.81	0.41
1:A:44:HIS:CE1	1:A:204:ASN:HA	2.56	0.41
4:H:112:LEU:HA	4:H:115:VAL:HG22	2.03	0.41
1:A:553:ALA:HA	1:A:563:LEU:HD23	2.03	0.41
1:E:498:PHE:CD2	2:F:103:VAL:HG21	2.56	0.41
1:E:399:LEU:HD11	5:E:601:FAD:H4'	2.02	0.41
2:B:116:ILE:H	2:B:116:ILE:HG13	1.70	0.41
1:E:395:SER:OG	5:E:601:FAD:O3'	2.23	0.41
2:B:39:ALA:O	2:B:43:ILE:HG13	2.21	0.41
2:F:241:LYS:HA	2:F:242:PRO:HD3	1.80	0.41
1:A:125:TRP:CD1	1:A:125:TRP:N	2.89	0.41
1:A:230:GLN:HB2	1:A:358:MET:SD	2.61	0.41
1:A:60:ASP:OD2	1:A:61:SER:N	2.51	0.41
3:C:98:VAL:HG23	3:C:98:VAL:O	2.21	0.41
1:E:217:LEU:HA	1:E:217:LEU:HD23	1.96	0.41
1:A:118:GLY:HA2	1:A:279:ASN:HD21	1.86	0.41
1:A:549:LYS:HB2	1:A:566:SER:O	2.21	0.41
2:B:4:LYS:O	2:B:29:PRO:HA	2.21	0.41
1:E:308:ARG:HD2	1:E:308:ARG:N	2.36	0.41
1:A:282:MET:HB3	1:A:283:GLU:OE1	2.21	0.40
1:A:308:ARG:NH1	1:A:339:VAL:HG12	2.37	0.40
1:A:363:THR:HB	1:A:367:CYS:HA	2.01	0.40
2:B:121:ILE:HB	2:B:187:GLY:HA3	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:28:ALA:O	4:D:32:ILE:HG13	2.20	0.40
2:B:154:CYS:HG	2:B:155:TYR:HD1	1.67	0.40
1:E:230:GLN:CD	1:E:287:ARG:HD3	2.42	0.40
1:E:42:ARG:HG2	2:F:64:SER:HB3	2.04	0.40
1:E:497:VAL:O	2:F:100:ARG:NH1	2.51	0.40
2:F:216:LYS:HE2	2:F:216:LYS:HA	2.03	0.40
3:G:124:LEU:HD21	4:H:33:LEU:HD23	2.02	0.40
1:A:232:HIS:H	1:A:355:HIS:HB2	1.86	0.40
1:A:392:GLY:O	1:A:393:SER:OG	2.32	0.40
2:B:241:LYS:HA	2:B:242:PRO:HD3	1.88	0.40
2:B:57:CYS:HB3	2:B:62:CYS:HB3	2.03	0.40
1:E:125:TRP:N	1:E:125:TRP:CD1	2.88	0.40
2:B:242:PRO:HB3	4:H:93:VAL:C	2.41	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	575/585 (98%)	540 (94%)	31 (5%)	4 (1%)	25	68
1	E	583/585 (100%)	538 (92%)	37 (6%)	8 (1%)	13	54
2	B	241/243 (99%)	225 (93%)	13 (5%)	3 (1%)	15	58
2	F	241/243 (99%)	230 (95%)	8 (3%)	3 (1%)	15	58
3	C	128/130 (98%)	122 (95%)	6 (5%)	0	100	100
3	G	128/130 (98%)	121 (94%)	6 (5%)	1 (1%)	22	66
4	D	117/119 (98%)	110 (94%)	6 (5%)	1 (1%)	20	63
4	H	117/119 (98%)	111 (95%)	5 (4%)	1 (1%)	20	63
All	All	2130/2154 (99%)	1997 (94%)	112 (5%)	21 (1%)	18	61

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	PRO
1	E	579	VAL
1	A	261	ARG
2	B	242	PRO
1	E	329	PRO
2	F	242	PRO
1	A	128	ALA
1	A	234	THR
4	D	117	THR
3	G	18	LYS
4	H	117	THR
1	E	128	ALA
1	E	273	PRO
1	E	322	LYS
2	F	56	SER
2	B	56	SER
1	E	312	VAL
2	B	61	ILE
2	F	61	ILE
1	E	444	GLY
1	E	581	GLY

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	460/465 (99%)	450 (98%)	10 (2%)	57	80
1	E	465/465 (100%)	442 (95%)	23 (5%)	29	63
2	B	205/205 (100%)	194 (95%)	11 (5%)	26	61
2	F	205/205 (100%)	192 (94%)	13 (6%)	21	55
3	C	111/111 (100%)	108 (97%)	3 (3%)	50	75
3	G	111/111 (100%)	107 (96%)	4 (4%)	40	70
4	D	97/97 (100%)	92 (95%)	5 (5%)	27	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	97/97 (100%)	93 (96%)	4 (4%)	35	67
All	All	1751/1756 (100%)	1678 (96%)	73 (4%)	34	66

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	122	GLU
1	A	200	ARG
1	A	276	GLU
1	A	332	CYS
1	A	351	ARG
1	A	389	ASN
1	A	400	VAL
1	A	443	ASP
1	A	498	PHE
2	B	19	THR
2	B	62	CYS
2	B	65	CYS
2	B	128	ASP
2	B	148	CYS
2	B	151	CYS
2	B	178	ARG
2	B	204	CYS
2	B	206	PHE
2	B	212	GLU
2	B	243	ARG
3	C	50	LYS
3	C	84	LYS
3	C	103	MET
4	D	7	ARG
4	D	9	ASP
4	D	86	MET
4	D	117	THR
4	D	118	ILE
1	E	18	ARG
1	E	42	ARG
1	E	96	LEU
1	E	122	GLU
1	E	197	ARG
1	E	200	ARG
1	E	239	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	243	MET
1	E	244	THR
1	E	268	MET
1	E	274	LEU
1	E	287	ARG
1	E	288	ASP
1	E	308	ARG
1	E	311	VAL
1	E	321	GLU
1	E	326	GLU
1	E	332	CYS
1	E	351	ARG
1	E	355	HIS
1	E	498	PHE
1	E	537	GLU
1	E	580	TYR
2	F	19	THR
2	F	62	CYS
2	F	65	CYS
2	F	128	ASP
2	F	148	CYS
2	F	151	CYS
2	F	178	ARG
2	F	203	SER
2	F	204	CYS
2	F	206	PHE
2	F	209	TYR
2	F	212	GLU
2	F	243	ARG
3	G	9	ARG
3	G	50	LYS
3	G	84	LYS
3	G	95	ASN
4	H	6	LYS
4	H	17	PHE
4	H	86	MET
4	H	118	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	150	ASN
1	E	204	ASN
1	E	230	GLN
1	E	232	HIS
1	E	389	ASN
3	G	95	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 ⓘ

8 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	-	51,58,58	0.91	4 (7%)	54,89,89	2.24	6 (11%)
6	FES	B	301	-	0,4,4	0.00	-	0,4,4	0.00	-
7	F3S	B	302	-	0,9,9	0.00	-	0,15,15	0.00	-
8	SF4	B	303	-	0,12,12	0.00	-	0,24,24	0.00	-
5	FAD	E	601	-	51,58,58	0.90	5 (9%)	54,89,89	2.27	6 (11%)
6	FES	F	301	-	0,4,4	0.00	-	0,4,4	0.00	-
7	F3S	F	302	-	0,9,9	0.00	-	0,15,15	0.00	-
8	SF4	F	303	2	0,12,12	0.00	-	0,24,24	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
5	FAD	A	601	-	-	0/28/50/50	0/6/6/6
6	FES	B	301	-	-	0/0/4/4	0/1/1/1
7	F3S	B	302	-	-	0/0/24/24	0/0/3/3
8	SF4	B	303	-	-	0/0/48/48	0/6/5/5
5	FAD	E	601	-	-	0/28/50/50	0/6/6/6
6	FES	F	301	-	-	0/0/4/4	0/1/1/1
7	F3S	F	302	-	-	0/0/24/24	0/0/3/3
8	SF4	F	303	2	-	0/0/48/48	0/6/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	601	FAD	C4X-C10	2.01	1.44	1.41
5	E	601	FAD	C9A-N10	2.03	1.41	1.38
5	A	601	FAD	C9A-N10	2.08	1.41	1.38
5	A	601	FAD	C4-C4X	2.14	1.45	1.41
5	E	601	FAD	C4-N3	2.22	1.37	1.33
5	E	601	FAD	C4-C4X	2.27	1.45	1.41
5	E	601	FAD	C5X-N5	2.39	1.39	1.35
5	A	601	FAD	C5X-N5	2.55	1.39	1.35
5	A	601	FAD	C4-N3	2.80	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	601	FAD	C4X-C4-N3	-6.80	113.81	123.48
5	A	601	FAD	C4X-C4-N3	-6.68	113.97	123.48
5	A	601	FAD	C4X-C10-N10	-5.53	116.68	120.52
5	E	601	FAD	C4X-C10-N10	-5.40	116.77	120.52
5	A	601	FAD	C4-C4X-C10	-3.08	117.47	119.96
5	E	601	FAD	C4-C4X-C10	-3.06	117.48	119.96
5	A	601	FAD	C1'-N10-C9A	2.40	120.54	118.35
5	E	601	FAD	C1'-N10-C9A	2.63	120.76	118.35
5	E	601	FAD	C10-C4X-N5	3.38	124.48	120.59
5	A	601	FAD	C10-C4X-N5	3.40	124.51	120.59
5	A	601	FAD	C4-N3-C2	12.59	126.17	115.16
5	E	601	FAD	C4-N3-C2	12.77	126.33	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	FAD	5	0
5	E	601	FAD	11	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	577/585 (98%)	0.60	71 (12%) 5 7	155, 242, 339, 446	0
1	E	585/585 (100%)	0.43	54 (9%) 10 9	140, 249, 328, 385	0
2	B	243/243 (100%)	0.02	4 (1%) 72 64	125, 175, 237, 294	0
2	F	243/243 (100%)	0.04	3 (1%) 79 72	125, 179, 248, 287	0
3	C	130/130 (100%)	-0.19	5 (3%) 41 33	103, 157, 240, 295	0
3	G	130/130 (100%)	-0.21	5 (3%) 41 33	92, 167, 271, 403	0
4	D	119/119 (100%)	-0.36	1 (0%) 86 80	101, 146, 221, 276	0
4	H	119/119 (100%)	-0.42	0 100 100	93, 141, 206, 279	0
All	All	2146/2154 (99%)	0.22	143 (6%) 19 15	92, 209, 318, 446	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	GLY	8.2
1	A	187	ALA	7.5
1	E	186	ASN	7.1
1	E	583	GLU	6.5
1	E	582	GLY	6.3
1	A	251	GLY	5.9
1	A	204	ASN	5.6
1	E	581	GLY	5.6
1	A	205	GLY	5.2
1	A	379	GLU	5.2
1	A	318	HIS	5.1
1	E	467	ARG	5.0
1	A	268	MET	5.0
1	E	355	HIS	5.0
1	A	269	GLY	4.8
1	A	270	PRO	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	525	ARG	4.7
3	G	98	VAL	4.6
1	A	319	LEU	4.6
1	E	113	VAL	4.5
1	A	250	GLU	4.5
1	A	316	LEU	4.3
1	A	193	GLY	4.2
1	A	569	LYS	4.2
1	E	112	ASN	4.1
1	E	115	ARG	4.1
1	A	571	THR	4.0
1	E	49	GLU	4.0
1	A	208	VAL	3.9
1	A	252	GLY	3.9
1	E	278	LYS	3.9
1	A	202	ASN	3.8
3	C	1	THR	3.7
1	E	280	LYS	3.7
1	E	526	LYS	3.7
3	G	99	LYS	3.6
1	A	197	ARG	3.6
1	E	392	GLY	3.6
1	A	572	THR	3.6
1	E	388	ALA	3.6
1	A	123	ARG	3.6
1	A	55	VAL	3.6
1	A	303	THR	3.5
1	E	303	THR	3.5
1	E	187	ALA	3.5
1	A	467	ARG	3.4
1	A	79	GLN	3.4
1	E	43	SER	3.4
1	A	163	ASP	3.4
3	C	3	LYS	3.3
1	E	279	ASN	3.3
1	A	50	GLY	3.2
1	A	188	VAL	3.1
2	F	18	ASP	3.1
1	A	247	CYS	3.1
1	A	117	GLY	3.1
1	A	44	HIS	3.1
1	E	120	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	204	ASN	3.0
1	A	388	ALA	3.0
1	A	206	GLY	3.0
1	A	315	ASP	2.9
1	E	50	GLY	2.9
1	A	302	ASN	2.9
1	E	114	ARG	2.9
1	A	209	THR	2.9
1	A	573	LEU	2.8
2	B	58	ARG	2.8
1	A	253	ILE	2.8
1	A	277	PRO	2.8
1	A	355	HIS	2.8
3	G	3	LYS	2.8
1	A	314	LEU	2.8
1	E	532	HIS	2.7
1	A	239	SER	2.7
1	E	126	PHE	2.7
3	C	100	ASP	2.7
1	A	248	ARG	2.7
1	A	349	PRO	2.7
1	E	446	GLU	2.7
1	A	534	ARG	2.6
1	A	343	PRO	2.6
1	E	13	GLY	2.6
1	A	13	GLY	2.6
1	A	359	GLY	2.6
1	E	203	THR	2.6
1	A	348	ILE	2.6
1	E	232	HIS	2.6
2	B	127	ALA	2.5
1	E	129	ASP	2.5
3	C	95	ASN	2.5
1	E	193	GLY	2.5
1	E	237	PRO	2.5
1	E	272	THR	2.5
1	E	124	THR	2.5
1	A	11	GLY	2.5
1	E	384	GLY	2.5
1	E	11	GLY	2.5
1	E	416	THR	2.4
1	A	186	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	570	ILE	2.4
2	B	120	ILE	2.4
1	E	205	GLY	2.4
1	A	57	GLN	2.3
1	E	390	ARG	2.3
1	A	395	SER	2.3
1	E	119	MET	2.3
1	A	308	ARG	2.3
1	A	392	GLY	2.3
1	E	44	HIS	2.3
1	A	312	VAL	2.3
2	F	21	PRO	2.3
1	E	206	GLY	2.2
1	E	580	TYR	2.2
4	D	36	GLY	2.2
1	A	12	ALA	2.2
1	A	203	THR	2.2
1	E	535	LEU	2.2
1	E	118	GLY	2.2
1	E	245	GLN	2.2
2	F	99	GLU	2.2
1	A	196	GLY	2.2
3	G	49	LEU	2.1
3	C	97	ILE	2.1
1	A	497	VAL	2.1
1	A	240	GLY	2.1
1	A	267	GLY	2.1
1	A	411	THR	2.1
1	A	532	HIS	2.1
1	A	246	GLY	2.1
1	E	490	ARG	2.1
1	E	194	GLY	2.1
1	E	312	VAL	2.1
1	A	294	PHE	2.1
1	E	202	ASN	2.1
1	E	281	TYR	2.0
3	G	100	ASP	2.0
2	B	170	PRO	2.0
1	A	8	ALA	2.0
1	A	553	ALA	2.0
1	E	121	ILE	2.0
1	A	519	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	524	ALA	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(\AA^2)	Q<0.9
5	FAD	E	601	53/53	0.88	0.70	0.69	188,233,295,298	0
5	FAD	A	601	53/53	0.82	0.71	0.41	185,237,298,299	0
6	FES	F	301	4/4	0.97	0.37	-0.21	142,149,154,158	0
6	FES	B	301	4/4	0.98	0.40	-0.40	146,147,156,162	0
8	SF4	F	303	8/8	0.99	0.22	-0.97	127,147,160,162	0
7	F3S	B	302	7/7	0.97	0.22	-1.05	120,157,185,189	0
8	SF4	B	303	8/8	0.99	0.23	-1.43	131,137,151,162	0
7	F3S	F	302	7/7	0.99	0.14	-2.46	101,175,201,217	0

6.5 Other polymers [i](#)

There are no such residues in this entry.