Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:19 AM GMT

PDB ID	:	3HYW
Title	:	3-D X-Ray structure of the sulfide:quinone oxidoreductase of the hyperthermophilic bacterium Aquifex aeolicus in complex with decylubiquinone
Authors	:	Marcia, M.; Ermler, U.; Peng, G.H.; Michel, H.
Deposited on	:	2009-06-23
Resolution	:	2.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

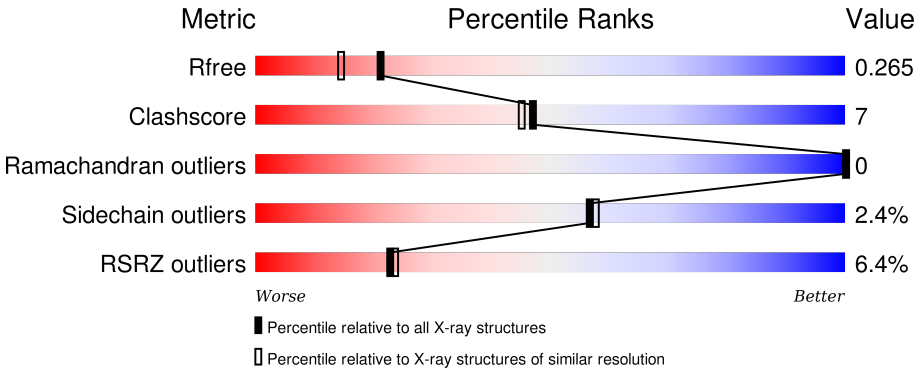
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 <=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	430	7% 88% 11%
1	B	430	5% 88% 11%
1	C	430	7% 91% 8%
1	D	430	8% 85% 14%
1	E	430	7% 86% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	430	5% 87% 12%

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
3	DCQ	A	500	-	-	X	X
3	DCQ	B	500	-	-	X	X
3	DCQ	C	500	-	-	X	X
3	DCQ	D	500	-	-	X	X
3	DCQ	E	500	-	-	X	X
3	DCQ	F	500	-	-	X	X
4	LMT	A	600	-	-	-	X
4	LMT	B	600	-	-	-	X
4	LMT	C	600	-	-	-	X
4	LMT	D	600	-	-	-	X
4	LMT	E	600	-	-	-	X
4	LMT	F	600	-	-	-	X
6	PS9	A	800	-	-	X	X
6	PS9	B	802[B]	-	-	-	X
6	PS9	C	800	-	-	X	X
6	PS9	D	800	-	-	X	X
6	PS9	D	802	-	-	X	-
6	PS9	E	800	-	-	X	X
6	PS9	F	800	-	-	X	X
7	SO4	A	433	-	-	-	X
7	SO4	B	433	-	-	-	X
7	SO4	C	434	-	-	X	-
7	SO4	F	434	-	-	X	-

2 Entry composition

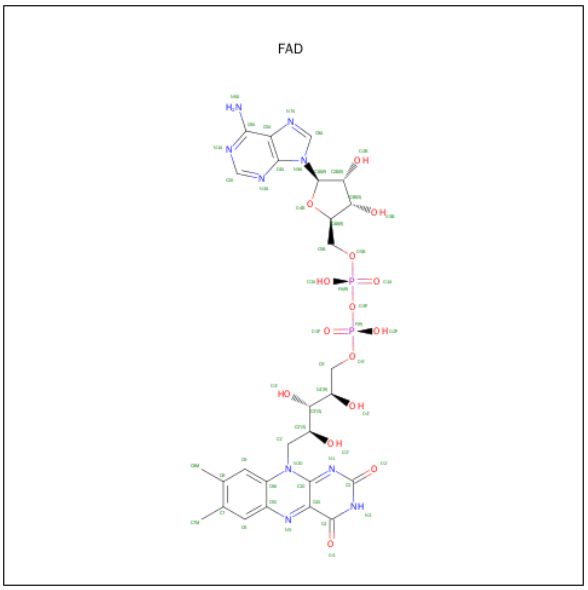
There are 8 unique types of molecules in this entry. The entry contains 22002 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sulfide-quinone reductase.

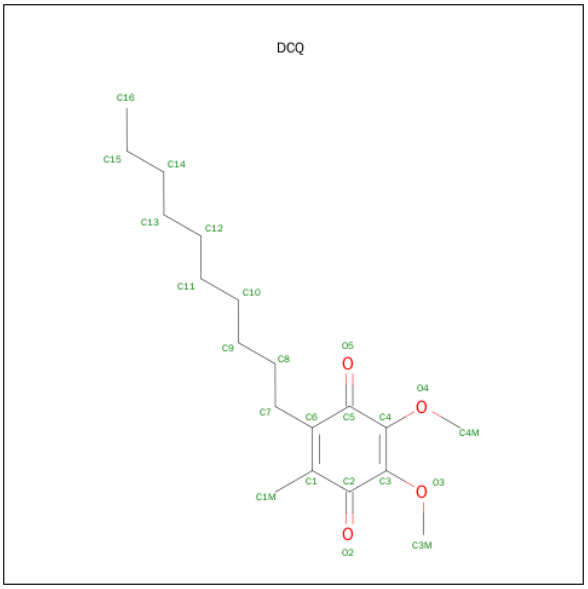
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	3	0
			3339	2161	553	602	23			
1	B	429	Total	C	N	O	S	0	3	0
			3340	2161	553	602	24			
1	C	429	Total	C	N	O	S	0	3	0
			3339	2161	553	602	23			
1	D	429	Total	C	N	O	S	0	3	0
			3340	2161	553	602	24			
1	E	429	Total	C	N	O	S	0	3	0
			3339	2161	553	602	23			
1	F	429	Total	C	N	O	S	0	3	0
			3339	2161	553	602	23			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is 2-DECYL-5,6-DIMETHOXY-3-METHYLCYCLOHEXA-2,5-DIENE-1,4-DIONE (three-letter code: DCQ) (formula: $C_{19}H_{30}O_4$).



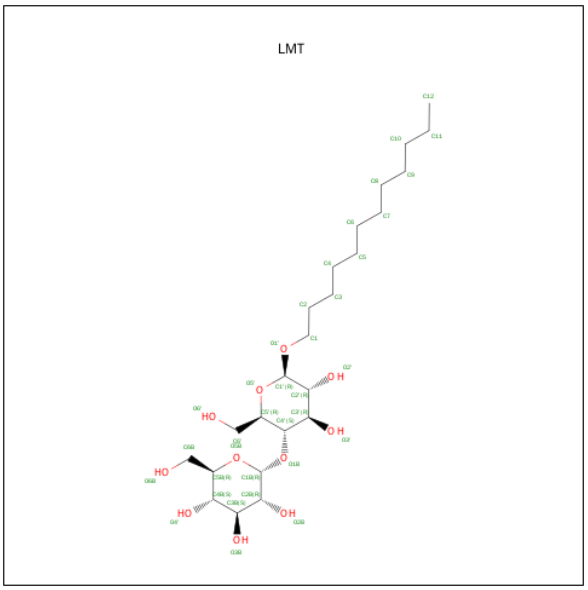
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	19	4		
3	B	1	Total	C	O	0	0
			23	19	4		
3	C	1	Total	C	O	0	0
			23	19	4		
3	D	1	Total	C	O	0	0
			23	19	4		
3	E	1	Total	C	O	0	0
			23	19	4		

Continued on next page...

Continued from previous page...

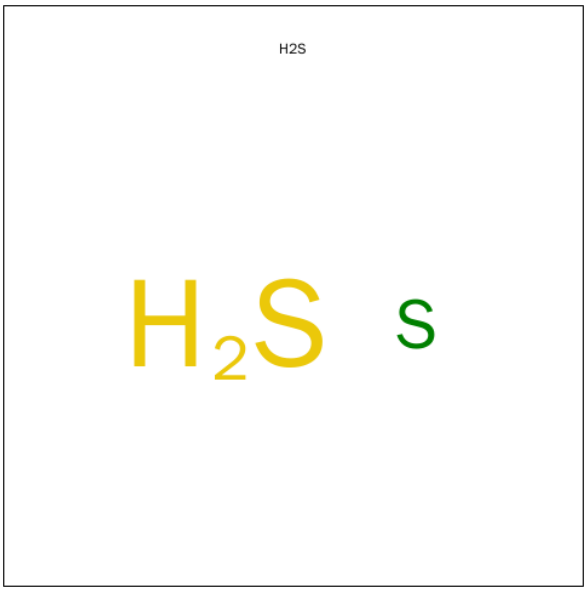
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 23 19 4	0	0

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



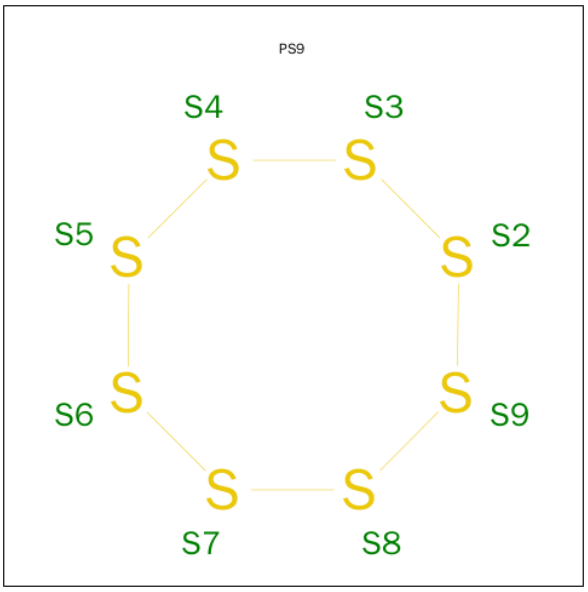
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 35 24 11	0	0
4	B	1	Total C O 35 24 11	0	0
4	C	1	Total C O 35 24 11	0	0
4	D	1	Total C O 35 24 11	0	0
4	E	1	Total C O 35 24 11	0	0
4	F	1	Total C O 35 24 11	0	0

- Molecule 5 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H_2S).



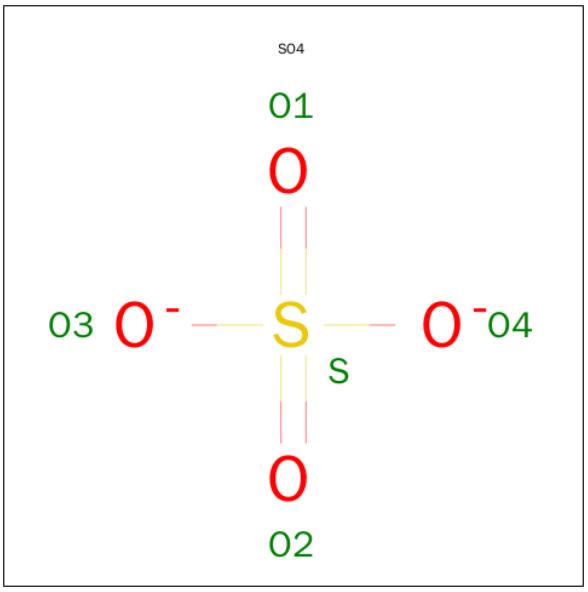
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total S 1 1	0	0
5	B	1	Total S 1 1	0	0
5	C	1	Total S 1 1	0	0
5	D	1	Total S 1 1	0	0
5	E	1	Total S 1 1	0	0
5	F	1	Total S 1 1	0	0

- Molecule 6 is OCTATHIOCANE (three-letter code: PS9) (formula: S_8).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total S 8 8	0	0
6	B	1	Total S 1 1	0	0
6	B	1	Total S 3 3	0	1
6	C	1	Total S 6 6	0	0
6	D	1	Total S 2 2	0	0
6	D	1	Total S 1 1	0	0
6	E	1	Total S 8 8	0	0
6	F	1	Total S 8 8	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	F	1	Total O S 5 4 1	0	0
7	F	1	Total O S 5 4 1	0	0
7	F	1	Total O S 5 4 1	0	0
7	F	1	Total O S 5 4 1	0	0

- Molecule 8 is water.

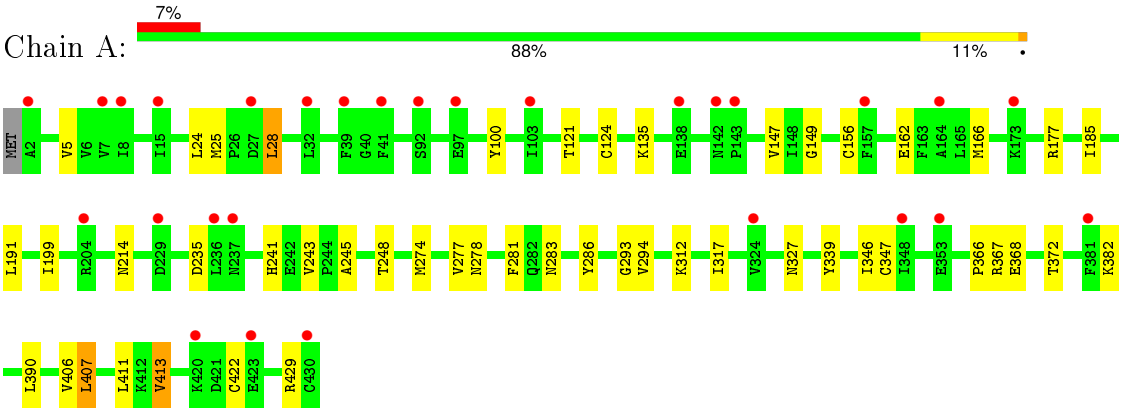
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	214	Total O 214 214	0	0
8	B	197	Total O 197 197	0	0
8	C	189	Total O 189 189	0	0
8	D	160	Total O 160 160	0	0
8	E	179	Total O 179 179	0	0
8	F	198	Total O 198 198	0	0

3 Residue-property plots (i)

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.

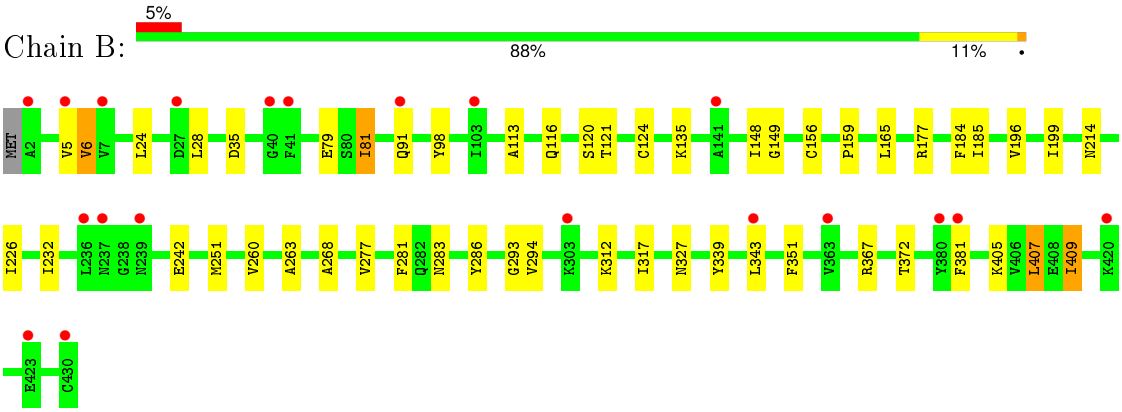
- Molecule 1: Sulfide-quinone reductase

Chain A:



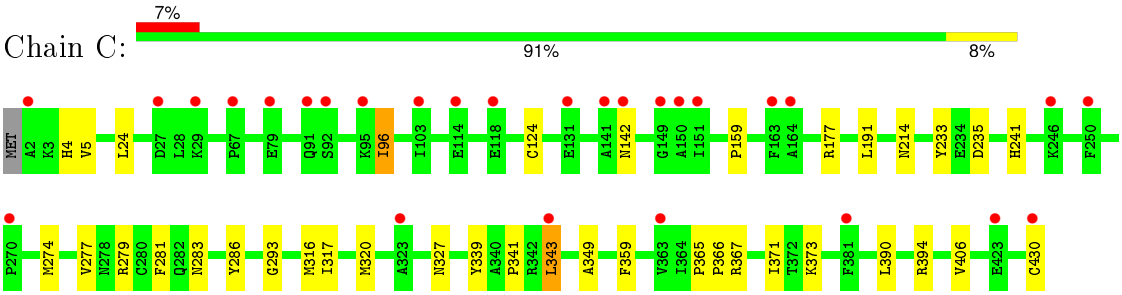
- Molecule 1: Sulfide-quinone reductase

Chain B:



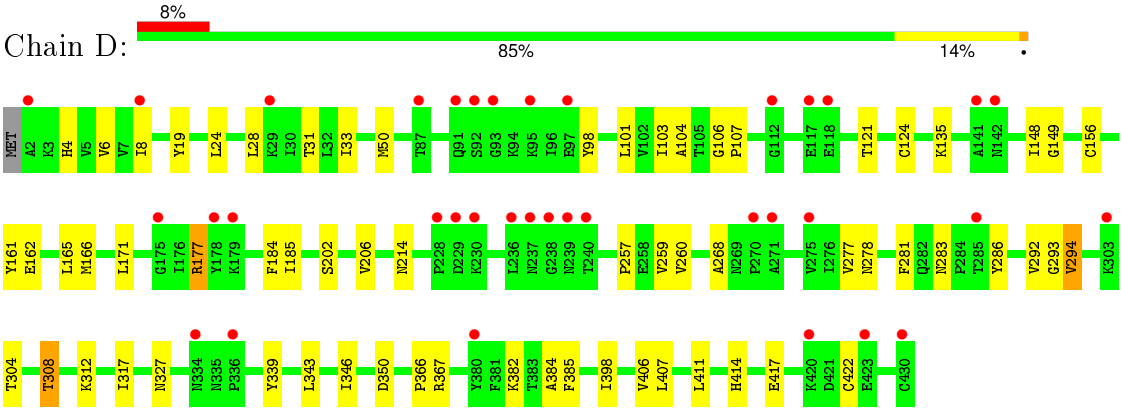
- Molecule 1: Sulfide-quinone reductase

Chain C:



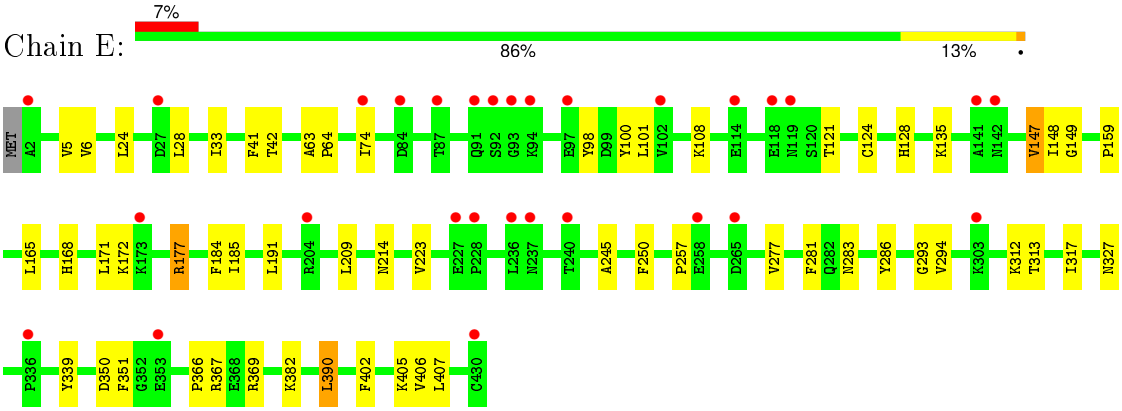
• Molecule 1: Sulfide-quinone reductase

Chain D:



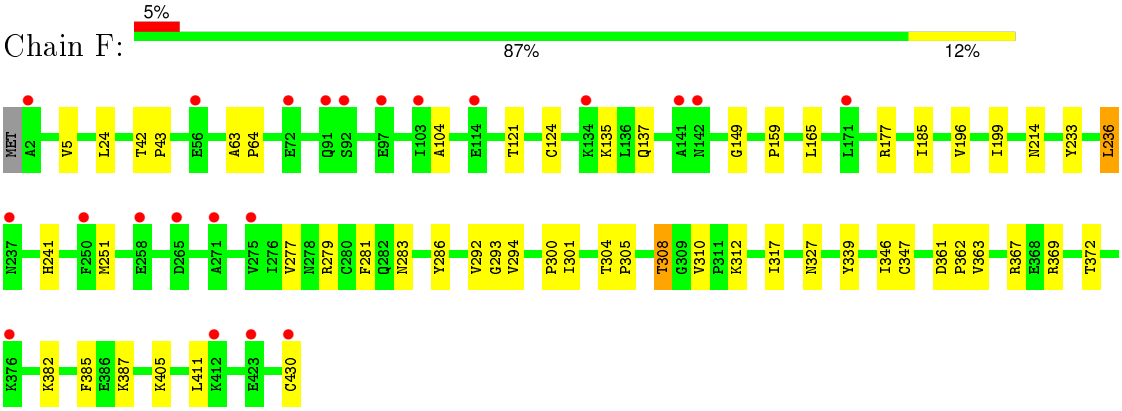
• Molecule 1: Sulfide-quinone reductase

Chain E:



• Molecule 1: Sulfide-quinone reductase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	110.78Å 154.01Å 175.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.45 – 2.00 20.45 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (20.45-2.00) 96.2 (20.45-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.236 0.232 , 0.265	Depositor DCC
R_{free} test set	9757 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 194316 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22002	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: LMT, H2S, PS9, SO4, FAD, CSS, DCQ

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	0.41	0/3417	0.54	0/4637
1	B	0.40	0/3417	0.54	0/4637
1	C	0.40	0/3417	0.54	0/4637
1	D	0.39	0/3417	0.52	0/4637
1	E	0.39	0/3417	0.53	0/4637
1	F	0.39	0/3417	0.53	0/4637
All	All	0.40	0/20502	0.53	0/27822

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	3339	0	3338	34	0
1	B	3340	0	3338	33	0
1	C	3339	0	3338	28	0
1	D	3340	0	3338	54	0
1	E	3339	0	3338	43	0
1	F	3339	0	3338	50	0
2	A	53	0	29	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	29	0	0
2	C	53	0	29	0	0
2	D	53	0	29	6	0
2	E	53	0	29	0	0
2	F	53	0	29	7	0
3	A	23	0	30	16	0
3	B	23	0	30	23	0
3	C	23	0	30	32	0
3	D	23	0	29	34	0
3	E	23	0	30	18	0
3	F	23	0	30	19	0
4	A	35	0	46	2	0
4	B	35	0	46	6	0
4	C	35	0	46	5	0
4	D	35	0	44	1	0
4	E	35	0	46	4	0
4	F	35	0	46	6	0
5	A	1	0	0	1	0
5	B	1	0	0	1	0
5	C	1	0	0	1	0
5	D	1	0	0	1	0
5	E	1	0	0	1	0
5	F	1	0	0	1	0
6	A	8	0	0	2	0
6	B	4	0	0	1	0
6	C	6	0	0	2	0
6	D	3	0	0	3	0
6	E	8	0	0	2	0
6	F	8	0	0	2	0
7	A	25	0	0	0	0
7	B	20	0	0	0	0
7	C	20	0	0	5	0
7	D	20	0	0	0	0
7	E	15	0	0	1	0
7	F	20	0	0	4	0
8	A	214	0	0	1	0
8	B	197	0	0	0	0
8	C	189	0	0	2	0
8	D	160	0	0	1	0
8	E	179	0	0	1	0
8	F	198	0	0	2	0
All	All	22002	0	20655	310	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 (310) 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:500:DCQ:C15	3:D:500:DCQ:H12	1.19	1.59
3:C:500:DCQ:H15	3:D:500:DCQ:C12	1.29	1.55
3:C:500:DCQ:C16	3:D:500:DCQ:H12	1.52	1.37
3:C:500:DCQ:H15	3:D:500:DCQ:C13	1.52	1.34
3:C:500:DCQ:H15	3:D:500:DCQ:C14	1.56	1.34
3:C:500:DCQ:C14	3:D:500:DCQ:H14	1.57	1.32
3:C:500:DCQ:C15	3:D:500:DCQ:H14A	1.60	1.31
3:C:500:DCQ:C15	3:D:500:DCQ:C14	2.10	1.27
3:C:500:DCQ:C14	3:D:500:DCQ:C14	2.12	1.26
1:A:347[B]:CSS:SG	6:A:800:PS9:S5	2.33	1.25
3:A:500:DCQ:C13	3:B:500:DCQ:H16A	1.66	1.24
3:E:500:DCQ:H14A	3:F:500:DCQ:C13	1.71	1.19
3:C:500:DCQ:C15	3:D:500:DCQ:C12	2.02	1.16
3:E:500:DCQ:C14	3:F:500:DCQ:H13	1.77	1.15
3:B:500:DCQ:H15A	4:B:600:LMT:H112	1.11	1.10
3:E:500:DCQ:H14A	3:F:500:DCQ:H13	1.18	1.09
3:A:500:DCQ:H16A	3:B:500:DCQ:H13A	1.27	1.08
3:E:500:DCQ:H12	3:F:500:DCQ:H15	1.18	1.08
3:B:500:DCQ:C8	3:B:500:DCQ:H1M	1.84	1.08
3:B:500:DCQ:H15A	4:B:600:LMT:C11	1.84	1.06
1:C:327:ASN:HD21	1:C:339:TYR:H	1.05	1.03
3:E:500:DCQ:H12	3:F:500:DCQ:C15	1.88	1.03
3:A:500:DCQ:H13A	3:B:500:DCQ:C16	1.89	1.02
3:C:500:DCQ:H14A	3:D:500:DCQ:H14	1.02	1.01
3:E:500:DCQ:C12	3:F:500:DCQ:C15	2.39	1.01
3:C:500:DCQ:C16	3:D:500:DCQ:C12	2.29	1.00
3:B:500:DCQ:H8A	3:B:500:DCQ:C1M	1.88	1.00
3:E:500:DCQ:H12A	3:F:500:DCQ:H15A	1.44	0.98
1:A:327:ASN:HD21	1:A:339:TYR:H	1.09	0.97
1:D:8:ILE:HD11	2:D:441:FAD:C2A	1.95	0.97
3:E:500:DCQ:C12	3:F:500:DCQ:H15	1.95	0.96
3:A:500:DCQ:H13A	3:B:500:DCQ:H16A	0.97	0.96
1:E:283:ASN:HD22	1:E:286:TYR:H	1.13	0.95
3:B:500:DCQ:H8A	3:B:500:DCQ:H1M	0.97	0.95
3:C:500:DCQ:C13	3:D:500:DCQ:C14	2.45	0.94
1:E:327:ASN:HD21	1:E:339:TYR:H	1.13	0.94
1:B:327:ASN:HD21	1:B:339:TYR:H	1.11	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:ASN:HD21	1:D:339:TYR:H	1.12	0.92
3:C:500:DCQ:H16	3:D:500:DCQ:H12	1.51	0.92
3:C:500:DCQ:C14	3:D:500:DCQ:H14A	1.92	0.91
1:F:327:ASN:HD21	1:F:339:TYR:H	1.14	0.90
3:C:500:DCQ:H16B	3:D:500:DCQ:H11A	1.52	0.90
3:C:500:DCQ:C16	3:D:500:DCQ:H11A	2.02	0.89
3:E:500:DCQ:C12	3:F:500:DCQ:H15A	2.01	0.89
3:C:500:DCQ:C13	3:D:500:DCQ:H14A	2.04	0.87
1:D:283:ASN:HD22	1:D:286:TYR:H	1.22	0.87
6:D:800:PS9:S3	6:D:802:PS9:S2	2.72	0.87
3:A:500:DCQ:C16	3:B:500:DCQ:H13A	2.03	0.86
1:B:196:VAL:HG22	1:B:367:ARG:NH1	1.92	0.85
1:E:293:GLY:HA2	1:E:317:ILE:HD12	1.57	0.85
6:D:800:PS9:S2	6:D:802:PS9:S2	2.75	0.84
3:B:500:DCQ:C15	4:B:600:LMT:H112	2.04	0.84
3:C:500:DCQ:C16	3:D:500:DCQ:C11	2.55	0.84
1:D:367:ARG:H	1:F:214:ASN:HD22	1.26	0.83
3:A:500:DCQ:C12	3:B:500:DCQ:H16A	2.09	0.83
4:C:600:LMT:H6'2	7:C:434:SO4:O3	1.79	0.82
4:C:600:LMT:H5B	7:C:434:SO4:O1	1.80	0.81
3:E:500:DCQ:C15	3:F:500:DCQ:H13	2.11	0.80
1:F:283:ASN:HD22	1:F:286:TYR:H	1.27	0.80
1:A:283:ASN:HD22	1:A:286:TYR:H	1.28	0.79
1:C:283:ASN:HD22	1:C:286:TYR:H	1.31	0.78
3:E:500:DCQ:H14A	3:F:500:DCQ:C15	2.12	0.77
1:A:274:MET:SD	8:A:1113:HOH:O	2.42	0.77
1:B:196:VAL:HG22	1:B:367:ARG:HH11	1.50	0.77
3:C:500:DCQ:H13	3:D:500:DCQ:H16B	1.66	0.76
3:C:500:DCQ:C13	3:D:500:DCQ:H14	2.14	0.76
1:E:313:THR:O	1:E:317:ILE:HG12	1.85	0.75
1:F:346:ILE:HG22	3:F:500:DCQ:H4MA	1.69	0.74
3:C:500:DCQ:H14A	3:D:500:DCQ:C14	1.89	0.74
1:E:283:ASN:ND2	1:E:286:TYR:H	1.87	0.73
1:B:283:ASN:HD22	1:B:286:TYR:H	1.34	0.72
1:F:347[A]:CSS:HB2	6:F:800:PS9:S6	2.30	0.72
3:C:500:DCQ:H16	3:D:500:DCQ:C12	2.14	0.71
3:C:500:DCQ:H15	3:D:500:DCQ:H14A	1.34	0.71
1:F:42:THR:HG21	2:F:441:FAD:O4'	1.90	0.71
1:B:327:ASN:HD21	1:B:339:TYR:N	1.87	0.71
3:E:500:DCQ:H14A	3:F:500:DCQ:C14	2.21	0.70
3:C:500:DCQ:H16B	3:D:500:DCQ:C11	2.17	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124[A]:CYS:SG	5:A:700:H2S:S	2.69	0.69
1:A:147:VAL:HG13	1:A:248:THR:HG22	1.74	0.69
1:B:367:ARG:H	1:D:214:ASN:HD22	1.39	0.68
1:E:327:ASN:HD21	1:E:339:TYR:N	1.89	0.68
1:D:367:ARG:H	1:F:214:ASN:ND2	1.92	0.68
3:A:500:DCQ:H11	3:B:500:DCQ:C16	2.24	0.67
1:F:42:THR:HG21	2:F:441:FAD:H3'	1.75	0.67
3:C:500:DCQ:H13A	3:D:500:DCQ:H14A	1.77	0.67
3:C:500:DCQ:H15A	3:D:500:DCQ:H14A	1.68	0.67
1:F:300:PRO:HA	1:F:310:VAL:HG23	1.76	0.66
1:F:347[B]:CSS:SG	6:F:800:PS9:S6	2.93	0.66
3:A:500:DCQ:C11	3:B:500:DCQ:C16	2.74	0.65
1:C:214:ASN:HD22	1:E:367:ARG:H	1.45	0.65
1:F:137:GLN:NE2	8:F:572:HOH:O	2.29	0.65
1:E:350:ASP:HB2	1:E:382:LYS:HD3	1.79	0.65
1:F:385:PHE:CE2	3:F:500:DCQ:H3MB	2.32	0.64
1:F:293:GLY:HA2	1:F:317:ILE:HG12	1.79	0.64
1:C:327:ASN:HD21	1:C:339:TYR:N	1.87	0.64
1:A:346:ILE:HD11	1:A:411:LEU:CD1	2.28	0.64
1:D:106:GLY:HA2	1:D:294:VAL:HG13	1.79	0.64
1:B:124[A]:CYS:SG	5:B:700:H2S:S	2.74	0.64
3:E:500:DCQ:H12A	3:F:500:DCQ:C15	2.15	0.63
1:D:294:VAL:HA	1:D:312:LYS:HD3	1.80	0.63
1:C:214:ASN:ND2	1:E:367:ARG:H	1.96	0.63
4:F:600:LMT:H5B	7:F:434:SO4:S	2.38	0.63
3:E:500:DCQ:H15	3:F:500:DCQ:H13	1.79	0.63
1:C:124[A]:CYS:SG	5:C:700:H2S:S	2.82	0.63
1:E:121:THR:CG2	1:E:135:LYS:HD3	2.29	0.63
1:B:327:ASN:ND2	1:B:339:TYR:H	1.91	0.62
1:B:232:ILE:HG12	1:B:242:GLU:HG2	1.81	0.62
1:B:159:PRO:HB2	1:B:251:MET:HE1	1.81	0.62
1:F:124[A]:CYS:SG	5:F:700:H2S:S	2.64	0.62
1:D:162:GLU:HG3	1:D:350:ASP:O	2.00	0.61
3:A:500:DCQ:H14	3:B:500:DCQ:H14	1.82	0.61
1:C:327:ASN:ND2	1:C:339:TYR:H	1.88	0.61
1:F:196:VAL:HG22	1:F:367:ARG:HH11	1.66	0.61
1:C:235:ASP:OD2	1:C:241:HIS:HE1	1.84	0.60
4:F:600:LMT:H3B	7:F:434:SO4:O1	2.02	0.60
1:A:283:ASN:ND2	1:A:286:TYR:H	2.00	0.60
1:D:414:HIS:HE1	1:D:417:GLU:OE2	1.84	0.60
1:E:121:THR:HG22	1:E:135:LYS:HD3	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:327:ASN:HD21	1:F:339:TYR:N	1.93	0.59
1:A:367:ARG:H	1:E:214:ASN:HD22	1.48	0.59
1:B:79:GLU:HG3	1:B:91:GLN:HA	1.84	0.59
1:F:196:VAL:HG22	1:F:367:ARG:NH1	2.18	0.58
1:E:327:ASN:ND2	1:E:339:TYR:H	1.94	0.58
1:E:293:GLY:HA2	1:E:317:ILE:CD1	2.31	0.58
1:F:283:ASN:ND2	1:F:286:TYR:H	2.00	0.58
1:D:4:HIS:NE2	1:D:31:THR:HG22	2.17	0.58
1:A:199:ILE:O	1:A:372:THR:HG21	2.03	0.58
1:A:214:ASN:HD22	1:C:367:ARG:H	1.50	0.58
1:E:6:VAL:HG12	1:E:98:TYR:HB3	1.86	0.57
1:C:4:HIS:HE1	1:C:96:ILE:HD11	1.69	0.57
4:A:600:LMT:H112	4:B:600:LMT:H101	1.87	0.57
3:A:500:DCQ:C11	3:B:500:DCQ:H16A	2.34	0.56
1:B:367:ARG:H	1:D:214:ASN:ND2	2.02	0.56
3:C:500:DCQ:H16	3:D:500:DCQ:H11A	1.83	0.56
3:A:500:DCQ:H11	3:B:500:DCQ:H16	1.88	0.56
1:F:279:ARG:HD3	1:F:430:CYS:HB3	1.87	0.56
3:A:500:DCQ:C12	3:B:500:DCQ:C16	2.82	0.56
1:D:149:GLY:HA3	1:D:185:ILE:O	2.06	0.56
1:A:293:GLY:HA2	1:A:317:ILE:HG12	1.87	0.55
1:D:8:ILE:HD11	2:D:441:FAD:H2A	1.83	0.55
3:C:500:DCQ:H13	3:D:500:DCQ:C14	2.34	0.55
1:F:159:PRO:HB2	1:F:251:MET:HE3	1.88	0.55
1:D:107:PRO:HD3	1:D:294:VAL:HG11	1.89	0.54
3:A:500:DCQ:H13	4:A:600:LMT:H111	1.90	0.54
1:D:346:ILE:HD11	1:D:411:LEU:CD1	2.37	0.54
1:B:214:ASN:HD22	1:F:367:ARG:H	1.56	0.54
1:B:199:ILE:O	1:B:372:THR:HG21	2.07	0.54
1:D:304:THR:OG1	1:D:308:THR:HB	2.08	0.54
1:F:104:ALA:HB2	1:F:292:VAL:CG1	2.38	0.54
4:F:600:LMT:H5B	7:F:434:SO4:O1	2.08	0.54
3:C:500:DCQ:H13	3:D:500:DCQ:C16	2.38	0.53
1:E:405:LYS:HD3	1:F:387:LYS:HD2	1.90	0.53
1:B:156[A]:CSS:SG	6:B:800:PS9:S2	3.05	0.53
1:D:293:GLY:HA2	1:D:317:ILE:HG12	1.90	0.53
3:E:500:DCQ:C14	3:F:500:DCQ:C15	2.85	0.53
4:C:600:LMT:C6B	7:C:434:SO4:O3	2.53	0.53
1:C:279:ARG:HD3	1:C:430:CYS:HB3	1.90	0.53
1:F:304:THR:OG1	1:F:308:THR:HB	2.07	0.53
1:F:42:THR:CG2	1:F:43:PRO:HD3	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:ARG:NH2	8:D:1251:HOH:O	2.43	0.52
1:F:42:THR:HG23	1:F:43:PRO:HD3	1.92	0.52
1:E:5:VAL:HG22	1:E:100:TYR:HB2	1.90	0.52
1:B:293:GLY:HA2	1:B:317:ILE:HG12	1.92	0.52
1:A:367:ARG:H	1:E:214:ASN:ND2	2.07	0.51
1:D:104:ALA:HB2	1:D:292:VAL:CG2	2.39	0.51
1:D:283:ASN:ND2	1:D:286:TYR:H	2.01	0.51
1:E:41:PHE:HB2	1:E:390:LEU:HD11	1.92	0.51
1:E:6:VAL:HG12	1:E:98:TYR:CB	2.41	0.51
1:E:159:PRO:HD3	6:E:800:PS9:S3	2.51	0.51
1:B:277:VAL:HB	1:B:281:PHE:HA	1.92	0.51
1:F:346:ILE:HD11	1:F:411:LEU:CD1	2.41	0.51
1:C:274:MET:HE1	8:C:501:HOH:O	2.10	0.50
1:C:283:ASN:ND2	1:C:286:TYR:H	2.04	0.50
1:F:382:LYS:NZ	2:F:441:FAD:O4	2.44	0.50
1:D:8:ILE:HD12	1:D:33:ILE:O	2.11	0.50
1:D:50:MET:HG3	1:D:166:MET:HE2	1.94	0.50
1:B:121:THR:CG2	1:B:135:LYS:HD3	2.42	0.50
3:C:500:DCQ:H16	3:D:500:DCQ:C11	2.32	0.50
1:B:149:GLY:HA3	1:B:185:ILE:O	2.12	0.50
1:C:214:ASN:HD21	1:E:366:PRO:HA	1.76	0.49
3:A:500:DCQ:H11	3:B:500:DCQ:H16A	1.94	0.49
1:F:327:ASN:ND2	1:F:339:TYR:H	1.96	0.49
1:F:121:THR:CG2	1:F:135:LYS:HD3	2.42	0.49
1:B:6:VAL:HG13	1:B:98:TYR:HB3	1.94	0.49
1:E:149:GLY:HA3	1:E:185:ILE:O	2.12	0.49
1:A:156[A]:CSS:SG	6:A:800:PS9:S2	3.10	0.49
1:F:405:LYS:HE2	8:F:481:HOH:O	2.13	0.49
1:B:283:ASN:ND2	1:B:286:TYR:H	2.09	0.49
1:F:104:ALA:HB2	1:F:292:VAL:HG13	1.95	0.48
1:D:366:PRO:HA	1:F:214:ASN:HD21	1.78	0.48
1:D:385:PHE:CE2	3:D:500:DCQ:H3MB	2.48	0.48
1:F:149:GLY:HA3	1:F:185:ILE:O	2.14	0.48
1:A:406:VAL:HG21	3:A:500:DCQ:H14A	1.95	0.48
1:B:294:VAL:HA	1:B:312:LYS:HD3	1.96	0.48
1:D:327:ASN:ND2	1:D:339:TYR:H	1.94	0.47
1:D:327:ASN:HD21	1:D:339:TYR:N	1.95	0.47
4:E:600:LMT:C6B	4:F:600:LMT:H1'	2.45	0.47
1:C:394:ARG:NH2	8:C:858:HOH:O	2.47	0.47
1:F:277:VAL:HB	1:F:281:PHE:HA	1.96	0.47
1:A:407:LEU:HB3	1:A:413:VAL:HG13	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:SER:O	1:D:206:VAL:HG23	2.15	0.47
1:C:293:GLY:HA2	1:C:317:ILE:HG12	1.96	0.46
1:E:128:HIS:HE1	8:E:469:HOH:O	1.96	0.46
1:E:147:VAL:CG1	1:E:245:ALA:HB2	2.46	0.46
1:C:277:VAL:HB	1:C:281:PHE:HA	1.97	0.46
1:D:260:VAL:HG12	1:D:268:ALA:HB2	1.96	0.46
1:E:124[A]:CYS:SG	5:E:700:H2S:S	3.04	0.46
3:B:500:DCQ:C15	4:B:600:LMT:C11	2.75	0.46
1:D:8:ILE:HG22	1:D:103:ILE:HA	1.98	0.46
1:D:6:VAL:HG13	1:D:101:LEU:HD12	1.98	0.46
1:E:406:VAL:HG11	3:E:500:DCQ:H13A	1.97	0.46
1:F:385:PHE:HE2	3:F:500:DCQ:H3MB	1.79	0.46
2:A:441:FAD:H9	2:A:441:FAD:H1'1	1.80	0.45
1:F:42:THR:CG2	2:F:441:FAD:H3'	2.45	0.45
1:D:6:VAL:HG13	1:D:101:LEU:CD1	2.46	0.45
1:A:121:THR:CG2	1:A:135:LYS:HD3	2.46	0.45
1:B:381:PHE:HE1	4:B:600:LMT:H61	1.82	0.45
1:C:394:ARG:NH1	7:C:432:SO4:O1	2.49	0.45
1:A:366:PRO:O	1:A:429:ARG:NH1	2.50	0.45
3:A:500:DCQ:H1M	3:A:500:DCQ:H7	1.76	0.45
1:F:196:VAL:HG21	1:F:363:VAL:HG13	1.99	0.45
1:D:148:ILE:O	1:D:184:PHE:HA	2.17	0.45
1:A:149:GLY:HA3	1:A:185:ILE:O	2.17	0.44
1:D:19:TYR:CD2	1:D:398:ILE:HG12	2.53	0.44
1:A:214:ASN:HD21	1:C:365:PRO:HB3	1.82	0.44
1:C:316:MET:O	1:C:320:MET:HG3	2.17	0.44
1:A:382:LYS:NZ	2:A:441:FAD:O4	2.49	0.44
1:F:233:TYR:CZ	1:F:241:HIS:HB2	2.52	0.44
1:C:406:VAL:HG22	1:D:384:ALA:HB1	1.99	0.44
1:B:165:LEU:HD13	1:B:351:PHE:CD1	2.52	0.44
1:D:161:TYR:CE1	1:D:206:VAL:HG11	2.52	0.44
1:F:294:VAL:HA	1:F:312:LYS:HD3	1.98	0.44
1:D:346:ILE:O	3:D:500:DCQ:H4MB	2.18	0.44
1:B:381:PHE:HE2	3:B:500:DCQ:H1MB	1.83	0.44
1:D:8:ILE:CD1	2:D:441:FAD:C2A	2.84	0.44
3:C:500:DCQ:H7	3:C:500:DCQ:H1M	1.79	0.44
4:E:600:LMT:H3B	7:E:434:SO4:O2	2.17	0.44
1:E:6:VAL:HG13	1:E:101:LEU:CD1	2.47	0.44
1:F:199:ILE:O	1:F:372:THR:HG21	2.17	0.44
1:A:277:VAL:HB	1:A:281:PHE:HA	1.98	0.44
1:B:148:ILE:O	1:B:184:PHE:HA	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:600:LMT:H1'	4:D:600:LMT:O2B	2.16	0.44
2:F:441:FAD:H1'1	2:F:441:FAD:H9	1.79	0.44
1:B:113:ALA:HB3	1:B:116:GLN:HB2	1.99	0.44
1:B:407:LEU:HD21	3:B:500:DCQ:H8	1.98	0.43
1:D:8:ILE:HD11	2:D:441:FAD:N1A	2.28	0.43
1:E:209:LEU:HD21	1:E:351:PHE:CE2	2.53	0.43
3:B:500:DCQ:O2	3:B:500:DCQ:H3MB	2.18	0.43
1:D:6:VAL:HG12	1:D:98:TYR:HB3	1.99	0.43
1:E:294:VAL:HA	1:E:312:LYS:HD3	2.00	0.43
1:E:108:LYS:HD2	1:E:257:PRO:HA	1.99	0.43
1:A:214:ASN:ND2	1:C:366:PRO:HA	2.33	0.43
1:D:6:VAL:HG12	1:D:98:TYR:CB	2.48	0.43
1:F:236:LEU:HD11	1:F:305:PRO:HB3	2.00	0.43
1:E:402:PHE:HE2	3:E:500:DCQ:H13	1.84	0.43
1:D:8:ILE:CG2	1:D:103:ILE:HA	2.48	0.43
1:D:19:TYR:HD2	1:D:398:ILE:HG12	1.84	0.43
1:B:120:SER:HB2	1:B:226:ILE:HG21	2.01	0.43
1:A:346:ILE:HD11	1:A:411:LEU:HD12	1.98	0.43
4:E:600:LMT:H6'2	4:F:600:LMT:H1'	2.00	0.43
1:D:277:VAL:HB	1:D:281:PHE:HA	2.01	0.43
1:A:278:ASN:HB2	1:A:422:CYS:O	2.19	0.43
1:A:368:GLU:O	1:E:172:LYS:HE3	2.19	0.43
1:A:235:ASP:OD2	1:A:241:HIS:HE1	2.00	0.43
1:D:124[A]:CYS:SG	5:D:700:H2S:S	3.07	0.43
1:D:382:LYS:NZ	2:D:441:FAD:O4	2.47	0.42
1:F:42:THR:HG21	2:F:441:FAD:C4'	2.48	0.42
1:A:147:VAL:HG12	1:A:245:ALA:HB2	2.00	0.42
3:E:500:DCQ:C14	3:F:500:DCQ:H15	2.48	0.42
1:F:196:VAL:HG23	1:F:301:ILE:CD1	2.49	0.42
1:D:121:THR:CG2	1:D:135:LYS:HD3	2.48	0.42
1:D:278:ASN:HB2	1:D:422:CYS:O	2.19	0.42
1:E:168:HIS:ND1	1:E:177:ARG:HD3	2.35	0.42
1:B:81:ILE:HG23	1:B:263:ALA:HB2	2.00	0.42
1:B:405:LYS:O	1:B:409:ILE:HG23	2.19	0.42
1:E:148:ILE:O	1:E:184:PHE:HA	2.19	0.42
1:D:156[A]:CSS:SG	6:D:800:PS9:S2	3.17	0.42
1:F:42:THR:HG21	2:F:441:FAD:C3'	2.44	0.42
4:E:600:LMT:O5B	4:F:600:LMT:H3'	2.19	0.42
1:E:283:ASN:HD22	1:E:286:TYR:N	1.97	0.42
1:C:349:ALA:HB2	6:C:800:PS9:S6	2.59	0.42
1:E:6:VAL:HG13	1:E:101:LEU:HD13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:369:ARG:NH1	7:F:431:SO4:O3	2.52	0.42
1:C:373:LYS:NZ	4:C:600:LMT:H11	2.35	0.42
1:A:25:MET:SD	1:A:28:LEU:HG	2.60	0.42
1:D:257:PRO:HB2	1:D:259:VAL:HG12	2.02	0.41
1:B:214:ASN:ND2	1:F:367:ARG:H	2.16	0.41
1:C:233:TYR:CZ	1:C:241:HIS:HB2	2.56	0.41
1:D:257:PRO:HG2	1:D:260:VAL:HG23	2.01	0.41
1:E:277:VAL:HB	1:E:281:PHE:HA	2.03	0.41
1:B:260:VAL:HG12	1:B:268:ALA:HB2	2.01	0.41
1:E:223:VAL:HG21	1:E:250:PHE:CE1	2.55	0.41
1:A:327:ASN:HD21	1:A:339:TYR:N	1.94	0.41
1:D:406:VAL:HG21	3:D:500:DCQ:H15A	2.02	0.41
1:E:159:PRO:HD3	6:E:800:PS9:S4	2.61	0.41
1:C:159:PRO:HD3	6:C:800:PS9:S2	2.61	0.41
1:A:162:GLU:O	1:A:166:MET:HG3	2.20	0.41
1:D:294:VAL:HG12	2:D:441:FAD:O2P	2.21	0.41
1:D:366:PRO:HA	1:F:214:ASN:ND2	2.35	0.41
1:F:361:ASP:HA	1:F:362:PRO:HA	1.93	0.41
1:E:63:ALA:HB3	1:E:64:PRO:HD3	2.03	0.41
1:E:33:ILE:HG12	1:E:74:ILE:CG2	2.51	0.41
1:F:63:ALA:HB3	1:F:64:PRO:HD3	2.03	0.40
1:A:147:VAL:CG1	1:A:245:ALA:HB2	2.52	0.40
7:C:431:SO4:O4	1:E:369:ARG:NH1	2.55	0.40
1:A:5:VAL:HG22	1:A:100:TYR:HB2	2.04	0.40
1:C:359:PHE:HB3	1:C:371:ILE:HB	2.04	0.40
1:C:341:PRO:HB2	1:C:343:LEU:HD13	2.02	0.40
1:A:294:VAL:HA	1:A:312:LYS:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/430 (99%)	419 (98%)	7 (2%)	0	100	100
1	B	426/430 (99%)	417 (98%)	9 (2%)	0	100	100
1	C	426/430 (99%)	419 (98%)	7 (2%)	0	100	100
1	D	426/430 (99%)	421 (99%)	5 (1%)	0	100	100
1	E	426/430 (99%)	417 (98%)	9 (2%)	0	100	100
1	F	426/430 (99%)	419 (98%)	7 (2%)	0	100	100
All	All	2556/2580 (99%)	2512 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	355/355 (100%)	347 (98%)	8 (2%)	58	60
1	B	355/355 (100%)	345 (97%)	10 (3%)	51	50
1	C	355/355 (100%)	347 (98%)	8 (2%)	58	60
1	D	355/355 (100%)	346 (98%)	9 (2%)	55	55
1	E	355/355 (100%)	345 (97%)	10 (3%)	51	50
1	F	355/355 (100%)	349 (98%)	6 (2%)	68	71
All	All	2130/2130 (100%)	2079 (98%)	51 (2%)	57	58

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	28	LEU
1	A	177	ARG
1	A	191	LEU
1	A	243	VAL
1	A	390	LEU
1	A	407	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	413	VAL
1	B	5	VAL
1	B	6	VAL
1	B	24	LEU
1	B	28	LEU
1	B	35	ASP
1	B	81	ILE
1	B	177	ARG
1	B	343	LEU
1	B	407	LEU
1	B	409	ILE
1	C	5	VAL
1	C	24	LEU
1	C	96	ILE
1	C	142	ASN
1	C	177	ARG
1	C	191	LEU
1	C	343	LEU
1	C	390	LEU
1	D	24	LEU
1	D	28	LEU
1	D	165	LEU
1	D	171	LEU
1	D	177	ARG
1	D	294	VAL
1	D	308	THR
1	D	343	LEU
1	D	407	LEU
1	E	24	LEU
1	E	28	LEU
1	E	42	THR
1	E	147	VAL
1	E	165	LEU
1	E	171	LEU
1	E	177	ARG
1	E	191	LEU
1	E	390	LEU
1	E	407	LEU
1	F	5	VAL
1	F	24	LEU
1	F	165	LEU
1	F	177	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	236	LEU
1	F	308	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	214	ASN
1	A	237	ASN
1	A	241	HIS
1	A	283	ASN
1	A	327	ASN
1	A	379	HIS
1	A	395	ASN
1	B	23	ASN
1	B	119	ASN
1	B	128	HIS
1	B	214	ASN
1	B	241	HIS
1	B	283	ASN
1	B	327	ASN
1	B	334	ASN
1	B	379	HIS
1	B	395	ASN
1	C	23	ASN
1	C	128	HIS
1	C	214	ASN
1	C	237	ASN
1	C	241	HIS
1	C	283	ASN
1	C	327	ASN
1	C	379	HIS
1	C	395	ASN
1	D	128	HIS
1	D	214	ASN
1	D	237	ASN
1	D	241	HIS
1	D	283	ASN
1	D	326	HIS
1	D	327	ASN
1	D	379	HIS
1	D	395	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	414	HIS
1	E	23	ASN
1	E	128	HIS
1	E	133	GLN
1	E	137	GLN
1	E	214	ASN
1	E	237	ASN
1	E	241	HIS
1	E	283	ASN
1	E	327	ASN
1	E	379	HIS
1	E	395	ASN
1	F	23	ASN
1	F	128	HIS
1	F	214	ASN
1	F	283	ASN
1	F	327	ASN
1	F	379	HIS
1	F	395	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

24 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSS	A	156[A]	-	4,5,7	1.22	0	3,5,8	1.38	1 (33%)
1	CSS	A	156[B]	6	4,6,7	0.96	0	3,6,8	2.48	2 (66%)
1	CSS	A	347[A]	-	4,5,7	1.33	1 (25%)	3,5,8	1.92	2 (66%)
1	CSS	A	347[B]	-	4,5,7	1.26	1 (25%)	3,5,8	2.00	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	CSS	B	156[A]	-	4,5,7	1.21	0	3,5,8	1.61	0
1	CSS	B	156[B]	6	4,6,7	0.94	0	3,6,8	2.39	1 (33%)
1	CSS	B	347[A]	-	4,5,7	1.29	1 (25%)	3,5,8	1.46	0
1	CSS	B	347[B]	6	4,6,7	0.96	0	3,6,8	2.47	1 (33%)
1	CSS	C	156[A]	-	4,5,7	1.20	0	3,5,8	1.59	1 (33%)
1	CSS	C	156[B]	6	4,6,7	0.91	0	3,6,8	2.04	2 (66%)
1	CSS	C	347[A]	-	4,5,7	1.34	1 (25%)	3,5,8	1.84	2 (66%)
1	CSS	C	347[B]	-	4,5,7	1.20	0	3,5,8	1.82	2 (66%)
1	CSS	D	156[A]	-	4,5,7	1.25	0	3,5,8	1.80	2 (66%)
1	CSS	D	156[B]	6	4,6,7	0.94	0	3,6,8	2.90	2 (66%)
1	CSS	D	347[A]	-	4,5,7	1.19	0	3,5,8	1.68	2 (66%)
1	CSS	D	347[B]	6	4,6,7	0.88	0	3,6,8	2.22	2 (66%)
1	CSS	E	156[A]	-	4,5,7	1.26	1 (25%)	3,5,8	1.44	1 (33%)
1	CSS	E	156[B]	6	4,6,7	0.91	0	3,6,8	1.94	2 (66%)
1	CSS	E	347[A]	-	4,5,7	1.25	0	3,5,8	1.67	1 (33%)
1	CSS	E	347[B]	-	4,5,7	1.22	0	3,5,8	1.78	2 (66%)
1	CSS	F	156[A]	-	4,5,7	1.23	0	3,5,8	1.80	1 (33%)
1	CSS	F	156[B]	6	4,6,7	0.85	0	3,6,8	1.85	2 (66%)
1	CSS	F	347[A]	-	4,5,7	1.40	1 (25%)	3,5,8	1.84	1 (33%)
1	CSS	F	347[B]	-	4,5,7	1.20	0	3,5,8	1.80	1 (33%)

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
1	CSS	A	156[A]	-	-	0/1/4/7	0/0/0/0
1	CSS	A	156[B]	6	-	0/1/5/7	0/0/0/0
1	CSS	A	347[A]	-	-	0/1/4/7	0/0/0/0
1	CSS	A	347[B]	-	-	0/1/4/7	0/0/0/0
1	CSS	B	156[A]	-	-	0/1/4/7	0/0/0/0
1	CSS	B	156[B]	6	-	0/1/5/7	0/0/0/0
1	CSS	B	347[A]	-	-	0/1/4/7	0/0/0/0
1	CSS	B	347[B]	6	-	0/1/5/7	0/0/0/0
1	CSS	C	156[A]	-	-	0/1/4/7	0/0/0/0
1	CSS	C	156[B]	6	-	0/1/5/7	0/0/0/0
1	CSS	C	347[A]	-	-	0/1/4/7	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSS	C	347[B]	-	-	0/1/4/7	0/0/0/0
1	CSS	D	156[A]	-	-	0/1/4/7	0/0/0/0
1	CSS	D	156[B]	6	-	0/1/5/7	0/0/0/0
1	CSS	D	347[A]	-	-	0/1/4/7	0/0/0/0
1	CSS	D	347[B]	6	-	0/1/5/7	0/0/0/0
1	CSS	E	156[A]	-	-	0/1/4/7	0/0/0/0
1	CSS	E	156[B]	6	-	0/1/5/7	0/0/0/0
1	CSS	E	347[A]	-	-	0/1/4/7	0/0/0/0
1	CSS	E	347[B]	-	-	0/1/4/7	0/0/0/0
1	CSS	F	156[A]	-	-	0/1/4/7	0/0/0/0
1	CSS	F	156[B]	6	-	0/1/5/7	0/0/0/0
1	CSS	F	347[A]	-	-	0/1/4/7	0/0/0/0
1	CSS	F	347[B]	-	-	0/1/4/7	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	347[A]	CSS	CB-SG	-2.32	1.76	1.81
1	A	347[A]	CSS	CB-SG	-2.19	1.76	1.81
1	C	347[A]	CSS	CB-SG	-2.15	1.76	1.81
1	B	347[A]	CSS	CB-SG	-2.06	1.76	1.81
1	E	156[A]	CSS	CB-SG	-2.06	1.76	1.81
1	A	347[B]	CSS	CB-SG	-2.03	1.76	1.81

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	156[B]	CSS	CB-SG-SD	-4.51	95.10	103.94
1	B	156[B]	CSS	CB-SG-SD	-3.67	96.75	103.94
1	A	156[B]	CSS	CB-SG-SD	-3.65	96.78	103.94
1	B	347[B]	CSS	CB-SG-SD	-3.48	97.11	103.94
1	D	347[B]	CSS	CB-SG-SD	-2.96	98.13	103.94
1	C	156[B]	CSS	CB-SG-SD	-2.91	98.23	103.94
1	E	156[B]	CSS	CB-SG-SD	-2.55	98.94	103.94
1	A	347[B]	CSS	CA-CB-SG	-2.50	108.74	114.48
1	F	347[B]	CSS	O-C-CA	-2.42	119.20	125.49
1	F	347[A]	CSS	O-C-CA	-2.42	119.20	125.49
1	F	156[B]	CSS	O-C-CA	-2.36	119.34	125.49
1	F	156[A]	CSS	O-C-CA	-2.36	119.34	125.49
1	A	347[A]	CSS	CA-CB-SG	-2.30	109.22	114.48
1	A	156[A]	CSS	O-C-CA	-2.23	119.68	125.49
1	A	156[B]	CSS	O-C-CA	-2.23	119.68	125.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	156[A]	CSS	O-C-CA	-2.22	119.71	125.49
1	D	156[B]	CSS	O-C-CA	-2.22	119.71	125.49
1	E	347[A]	CSS	O-C-CA	-2.18	119.81	125.49
1	E	347[B]	CSS	O-C-CA	-2.18	119.81	125.49
1	F	156[B]	CSS	CB-SG-SD	-2.16	99.71	103.94
1	C	347[B]	CSS	O-C-CA	-2.15	119.89	125.49
1	C	347[A]	CSS	O-C-CA	-2.15	119.89	125.49
1	A	347[A]	CSS	O-C-CA	-2.12	119.97	125.49
1	A	347[B]	CSS	O-C-CA	-2.12	119.97	125.49
1	C	347[A]	CSS	CA-CB-SG	-2.11	109.65	114.48
1	E	156[A]	CSS	O-C-CA	-2.11	120.00	125.49
1	E	156[B]	CSS	O-C-CA	-2.11	120.00	125.49
1	E	347[B]	CSS	CA-CB-SG	-2.09	109.69	114.48
1	D	347[A]	CSS	CA-CB-SG	-2.05	109.78	114.48
1	C	347[B]	CSS	CA-CB-SG	-2.05	109.78	114.48
1	D	156[A]	CSS	CA-CB-SG	-2.05	109.79	114.48
1	D	347[A]	CSS	O-C-CA	-2.03	120.19	125.49
1	D	347[B]	CSS	O-C-CA	-2.03	120.19	125.49
1	C	156[B]	CSS	O-C-CA	-2.00	120.28	125.49
1	C	156[A]	CSS	O-C-CA	-2.00	120.28	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	156[A]	CSS	1	0
1	A	347[B]	CSS	1	0
1	B	156[A]	CSS	1	0
1	D	156[A]	CSS	1	0
1	F	347[A]	CSS	1	0
1	F	347[B]	CSS	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 57 ligands modelled in this entry, 8 are modelled with single atom - leaving 49 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	$\#\|Z\| > 2$
7	SO4	A	431	-	4,4,4	0.24	0	6,6,6	0.10	0
7	SO4	A	432	-	4,4,4	0.34	0	6,6,6	0.13	0
7	SO4	A	433	-	4,4,4	0.29	0	6,6,6	0.30	0
7	SO4	A	434	-	4,4,4	0.20	0	6,6,6	0.11	0
7	SO4	A	435	-	4,4,4	0.25	0	6,6,6	0.09	0
2	FAD	A	441	5	48,58,58	1.09	2 (4%)	54,89,89	2.00	7 (12%)
3	DCQ	A	500	-	23,23,23	2.12	6 (26%)	26,29,29	0.86	0
4	LMT	A	600	-	36,36,36	0.47	0	47,47,47	0.70	1 (2%)
6	PS9	A	800	1	8,8,8	0.71	0	8,8,8	0.89	0
7	SO4	B	431	-	4,4,4	0.24	0	6,6,6	0.07	0
7	SO4	B	432	-	4,4,4	0.33	0	6,6,6	0.19	0
7	SO4	B	433	-	4,4,4	0.24	0	6,6,6	0.09	0
7	SO4	B	434	-	4,4,4	0.24	0	6,6,6	0.14	0
2	FAD	B	441	5	48,58,58	1.05	2 (4%)	54,89,89	1.93	6 (11%)
3	DCQ	B	500	-	23,23,23	2.18	7 (30%)	26,29,29	0.73	0
4	LMT	B	600	-	36,36,36	0.49	0	47,47,47	0.77	1 (2%)
6	PS9	B	802[A]	-	0,1,8	0.00	-	0,0,8	0.00	-
6	PS9	B	802[B]	-	0,1,8	0.00	-	0,0,8	0.00	-
7	SO4	C	431	-	4,4,4	0.24	0	6,6,6	0.08	0
7	SO4	C	432	-	4,4,4	0.32	0	6,6,6	0.15	0
7	SO4	C	433	-	4,4,4	0.23	0	6,6,6	0.38	0
7	SO4	C	434	-	4,4,4	0.23	0	6,6,6	0.07	0
2	FAD	C	441	5	48,58,58	1.11	2 (4%)	54,89,89	2.13	10 (18%)
3	DCQ	C	500	-	23,23,23	2.13	6 (26%)	26,29,29	0.88	0
4	LMT	C	600	-	36,36,36	0.53	1 (2%)	47,47,47	0.75	1 (2%)
6	PS9	C	800	1	3,5,8	1.58	0	2,4,8	0.80	0
7	SO4	D	431	-	4,4,4	0.25	0	6,6,6	0.06	0
7	SO4	D	432	-	4,4,4	0.28	0	6,6,6	0.09	0
7	SO4	D	433	-	4,4,4	0.23	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	SO4	D	434	-	4,4,4	0.21	0	6,6,6	0.13	0
2	FAD	D	441	5	48,58,58	1.09	2 (4%)	54,89,89	2.01	9 (16%)
3	DCQ	D	500	-	23,23,23	2.13	6 (26%)	26,29,29	0.95	1 (3%)
4	LMT	D	600	-	36,36,36	0.48	0	47,47,47	0.89	1 (2%)
6	PS9	D	800	1	0,1,8	0.00	-	0,0,8	0.00	-
7	SO4	E	432	-	4,4,4	0.32	0	6,6,6	0.13	0
7	SO4	E	433	-	4,4,4	0.23	0	6,6,6	0.26	0
7	SO4	E	434	-	4,4,4	0.18	0	6,6,6	0.07	0
2	FAD	E	441	5	48,58,58	1.12	2 (4%)	54,89,89	2.06	10 (18%)
3	DCQ	E	500	-	23,23,23	2.12	6 (26%)	26,29,29	0.91	0
4	LMT	E	600	-	36,36,36	0.50	0	47,47,47	0.93	2 (4%)
6	PS9	E	800	1	8,8,8	0.72	0	8,8,8	0.75	0
7	SO4	F	431	-	4,4,4	0.25	0	6,6,6	0.18	0
7	SO4	F	432	-	4,4,4	0.32	0	6,6,6	0.09	0
7	SO4	F	433	-	4,4,4	0.22	0	6,6,6	0.25	0
7	SO4	F	434	-	4,4,4	0.20	0	6,6,6	0.15	0
2	FAD	F	441	5	48,58,58	1.11	2 (4%)	54,89,89	2.02	6 (11%)
3	DCQ	F	500	-	23,23,23	2.24	7 (30%)	26,29,29	0.97	1 (3%)
4	LMT	F	600	-	36,36,36	0.53	0	47,47,47	0.86	1 (2%)
6	PS9	F	800	1	8,8,8	0.68	0	8,8,8	0.99	0

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
7	SO4	A	431	-	-	0/0/0/0	0/0/0/0
7	SO4	A	432	-	-	0/0/0/0	0/0/0/0
7	SO4	A	433	-	-	0/0/0/0	0/0/0/0
7	SO4	A	434	-	-	0/0/0/0	0/0/0/0
7	SO4	A	435	-	-	0/0/0/0	0/0/0/0
2	FAD	A	441	5	-	0/30/50/50	0/6/6/6
3	DCQ	A	500	-	-	0/14/38/38	0/1/1/1
4	LMT	A	600	-	-	0/21/61/61	0/2/2/2
6	PS9	A	800	1	-	0/0/8/8	0/1/1/1
7	SO4	B	431	-	-	0/0/0/0	0/0/0/0
7	SO4	B	432	-	-	0/0/0/0	0/0/0/0
7	SO4	B	433	-	-	0/0/0/0	0/0/0/0
7	SO4	B	434	-	-	0/0/0/0	0/0/0/0
2	FAD	B	441	5	-	0/30/50/50	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DCQ	B	500	-	-	0/14/38/38	0/1/1/1
4	LMT	B	600	-	-	0/21/61/61	0/2/2/2
6	PS9	B	802[A]	-	-	0/0/0/8	0/0/0/1
6	PS9	B	802[B]	-	-	0/0/0/8	0/0/0/1
7	SO4	C	431	-	-	0/0/0/0	0/0/0/0
7	SO4	C	432	-	-	0/0/0/0	0/0/0/0
7	SO4	C	433	-	-	0/0/0/0	0/0/0/0
7	SO4	C	434	-	-	0/0/0/0	0/0/0/0
2	FAD	C	441	5	-	0/30/50/50	0/6/6/6
3	DCQ	C	500	-	-	0/14/38/38	0/1/1/1
4	LMT	C	600	-	-	0/21/61/61	0/2/2/2
6	PS9	C	800	1	-	0/3/3/8	0/0/0/1
7	SO4	D	431	-	-	0/0/0/0	0/0/0/0
7	SO4	D	432	-	-	0/0/0/0	0/0/0/0
7	SO4	D	433	-	-	0/0/0/0	0/0/0/0
7	SO4	D	434	-	-	0/0/0/0	0/0/0/0
2	FAD	D	441	5	-	0/30/50/50	0/6/6/6
3	DCQ	D	500	-	-	0/14/38/38	0/1/1/1
4	LMT	D	600	-	-	0/21/61/61	0/2/2/2
6	PS9	D	800	1	-	0/0/0/8	0/0/0/1
7	SO4	E	432	-	-	0/0/0/0	0/0/0/0
7	SO4	E	433	-	-	0/0/0/0	0/0/0/0
7	SO4	E	434	-	-	0/0/0/0	0/0/0/0
2	FAD	E	441	5	-	0/30/50/50	0/6/6/6
3	DCQ	E	500	-	-	0/14/38/38	0/1/1/1
4	LMT	E	600	-	-	0/21/61/61	0/2/2/2
6	PS9	E	800	1	-	0/0/8/8	0/1/1/1
7	SO4	F	431	-	-	0/0/0/0	0/0/0/0
7	SO4	F	432	-	-	0/0/0/0	0/0/0/0
7	SO4	F	433	-	-	0/0/0/0	0/0/0/0
7	SO4	F	434	-	-	0/0/0/0	0/0/0/0
2	FAD	F	441	5	-	0/30/50/50	0/6/6/6
3	DCQ	F	500	-	-	0/14/38/38	0/1/1/1
4	LMT	F	600	-	-	0/21/61/61	0/2/2/2
6	PS9	F	800	1	-	0/0/8/8	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	441	FAD	C10-N10	-3.70	1.34	1.39
3	B	500	DCQ	C3-C2	-3.40	1.39	1.48
2	E	441	FAD	C10-N10	-3.38	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	500	DCQ	C3-C2	-3.36	1.39	1.48
3	D	500	DCQ	C3-C2	-3.36	1.39	1.48
3	F	500	DCQ	C3-C2	-3.31	1.39	1.48
3	E	500	DCQ	C3-C2	-3.31	1.39	1.48
3	F	500	DCQ	C4-C5	-3.29	1.39	1.48
3	B	500	DCQ	C4-C5	-3.29	1.39	1.48
3	A	500	DCQ	C3-C2	-3.29	1.39	1.48
2	F	441	FAD	C10-N10	-3.26	1.35	1.39
3	A	500	DCQ	C4-C5	-3.25	1.39	1.48
3	E	500	DCQ	C4-C5	-3.24	1.39	1.48
3	C	500	DCQ	C4-C5	-3.19	1.39	1.48
3	D	500	DCQ	C4-C5	-3.11	1.40	1.48
2	D	441	FAD	C10-N10	-2.89	1.35	1.39
2	A	441	FAD	C10-N10	-2.46	1.36	1.39
2	B	441	FAD	C10-N10	-2.35	1.36	1.39
3	A	500	DCQ	C6-C5	-2.28	1.39	1.46
3	E	500	DCQ	C6-C5	-2.25	1.39	1.46
3	F	500	DCQ	C6-C5	-2.24	1.39	1.46
3	D	500	DCQ	C6-C5	-2.18	1.39	1.46
3	C	500	DCQ	C6-C5	-2.16	1.40	1.46
3	B	500	DCQ	C6-C5	-2.12	1.40	1.46
3	B	500	DCQ	C1-C2	-2.02	1.39	1.47
3	A	500	DCQ	C6-C1	2.01	1.40	1.35
3	C	500	DCQ	C6-C1	2.02	1.40	1.35
4	C	600	LMT	O1'-C1'	2.03	1.43	1.40
3	D	500	DCQ	C6-C1	2.10	1.40	1.35
3	E	500	DCQ	C6-C1	2.11	1.40	1.35
3	F	500	DCQ	C6-C1	2.15	1.40	1.35
3	B	500	DCQ	C6-C1	2.31	1.40	1.35
3	F	500	DCQ	C16-C15	2.64	1.72	1.49
2	C	441	FAD	O4-C4	4.52	1.35	1.24
2	D	441	FAD	O4-C4	4.64	1.35	1.24
2	B	441	FAD	O4-C4	4.73	1.36	1.24
2	F	441	FAD	O4-C4	4.80	1.36	1.24
2	E	441	FAD	O4-C4	4.83	1.36	1.24
2	A	441	FAD	O4-C4	5.15	1.37	1.24
3	D	500	DCQ	O2-C2	5.68	1.36	1.23
3	F	500	DCQ	O2-C2	5.68	1.36	1.23
3	A	500	DCQ	O2-C2	5.71	1.36	1.23
3	C	500	DCQ	O2-C2	5.72	1.36	1.23
3	E	500	DCQ	O5-C5	5.73	1.36	1.23
3	E	500	DCQ	O2-C2	5.74	1.36	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	DCQ	O5-C5	5.83	1.36	1.23
3	B	500	DCQ	O2-C2	5.83	1.36	1.23
3	C	500	DCQ	O5-C5	5.88	1.36	1.23
3	D	500	DCQ	O5-C5	5.89	1.36	1.23
3	F	500	DCQ	O5-C5	5.89	1.36	1.23
3	B	500	DCQ	O5-C5	6.00	1.37	1.23

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	441	FAD	N3A-C2A-N1A	-11.22	120.31	128.89
2	E	441	FAD	N3A-C2A-N1A	-10.95	120.51	128.89
2	A	441	FAD	N3A-C2A-N1A	-10.68	120.72	128.89
2	F	441	FAD	N3A-C2A-N1A	-10.60	120.78	128.89
2	B	441	FAD	N3A-C2A-N1A	-10.42	120.91	128.89
2	D	441	FAD	N3A-C2A-N1A	-10.07	121.18	128.89
2	A	441	FAD	C4X-C4-N3	-2.93	119.58	123.59
2	C	441	FAD	C4A-C5A-N7A	-2.70	107.00	109.48
2	C	441	FAD	C4X-C4-N3	-2.60	120.03	123.59
2	D	441	FAD	P-O3P-PA	-2.55	125.57	132.73
2	E	441	FAD	C4X-C4-N3	-2.51	120.16	123.59
2	C	441	FAD	C1B-N9A-C4A	-2.45	123.24	126.94
2	B	441	FAD	C4X-C4-N3	-2.45	120.24	123.59
2	D	441	FAD	C4X-C4-N3	-2.44	120.25	123.59
2	F	441	FAD	C4X-C4-N3	-2.41	120.29	123.59
2	F	441	FAD	P-O3P-PA	-2.41	125.96	132.73
2	C	441	FAD	P-O3P-PA	-2.38	126.05	132.73
2	B	441	FAD	C4A-C5A-N7A	-2.29	107.37	109.48
2	E	441	FAD	P-O3P-PA	-2.28	126.33	132.73
4	B	600	LMT	C1B-O1B-C4'	-2.19	112.29	118.01
2	E	441	FAD	C1B-N9A-C4A	-2.18	123.65	126.94
4	A	600	LMT	C1B-O1B-C4'	-2.15	112.40	118.01
2	E	441	FAD	C4A-C5A-N7A	-2.09	107.55	109.48
2	D	441	FAD	C4A-C5A-N7A	-2.06	107.58	109.48
2	A	441	FAD	C4A-C5A-N7A	-2.05	107.59	109.48
2	A	441	FAD	C1B-N9A-C4A	-2.04	123.86	126.94
2	E	441	FAD	C1'-N10-C9A	2.02	121.13	118.86
2	E	441	FAD	C6-C5X-C9A	2.03	121.66	118.98
2	D	441	FAD	C2B-C1B-N9A	2.06	117.44	114.29
2	D	441	FAD	C4X-N5-C5X	2.12	119.20	116.76
3	D	500	DCQ	C3M-O3-C3	2.14	124.22	116.61
2	C	441	FAD	C4X-N5-C5X	2.17	119.26	116.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	441	FAD	C4X-N5-C5X	2.24	119.34	116.76
2	C	441	FAD	C2B-C1B-N9A	2.30	117.80	114.29
3	F	500	DCQ	C3M-O3-C3	2.32	124.86	116.61
4	D	600	LMT	C1B-O5B-C5B	2.49	118.57	113.75
2	D	441	FAD	C1'-N10-C9A	2.51	121.68	118.86
2	F	441	FAD	C4X-N5-C5X	2.57	119.72	116.76
4	E	600	LMT	O1B-C4'-C5'	2.62	116.21	109.32
2	E	441	FAD	C4X-N5-C5X	2.68	119.85	116.76
4	E	600	LMT	O1B-C4'-C3'	2.74	114.25	107.17
4	F	600	LMT	O1B-C1B-C2B	2.76	114.82	108.10
2	C	441	FAD	C1'-N10-C9A	2.90	122.11	118.86
4	C	600	LMT	O1B-C4'-C3'	3.08	115.13	107.17
2	A	441	FAD	C4X-N5-C5X	3.10	120.33	116.76
2	C	441	FAD	C5X-C9A-N10	3.33	120.15	117.62
2	D	441	FAD	C5X-C9A-N10	3.61	120.36	117.62
2	E	441	FAD	C5X-C9A-N10	3.63	120.37	117.62
2	A	441	FAD	C5X-C9A-N10	3.67	120.41	117.62
2	B	441	FAD	C5X-C9A-N10	3.85	120.54	117.62
2	F	441	FAD	C5X-C9A-N10	4.01	120.66	117.62
2	B	441	FAD	C4-N3-C2	4.98	119.55	115.25
2	F	441	FAD	C4-N3-C2	5.37	119.89	115.25
2	A	441	FAD	C4-N3-C2	5.53	120.02	115.25
2	C	441	FAD	C4-N3-C2	5.89	120.34	115.25
2	E	441	FAD	C4-N3-C2	5.95	120.39	115.25
2	D	441	FAD	C4-N3-C2	6.17	120.58	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

26 monomers are involved in 125 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	441	FAD	2	0
3	A	500	DCQ	16	0
4	A	600	LMT	2	0
6	A	800	PS9	2	0
3	B	500	DCQ	23	0
4	B	600	LMT	6	0
7	C	431	SO4	1	0
7	C	432	SO4	1	0
7	C	434	SO4	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	500	DCQ	32	0
4	C	600	LMT	5	0
6	C	800	PS9	2	0
2	D	441	FAD	6	0
3	D	500	DCQ	34	0
4	D	600	LMT	1	0
6	D	800	PS9	3	0
7	E	434	SO4	1	0
3	E	500	DCQ	18	0
4	E	600	LMT	4	0
6	E	800	PS9	2	0
7	F	431	SO4	1	0
7	F	434	SO4	3	0
2	F	441	FAD	7	0
3	F	500	DCQ	19	0
4	F	600	LMT	6	0
6	F	800	PS9	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	427/430 (99%)	0.58	28 (6%)	22	22	29, 35, 41, 46	0
1	B	427/430 (99%)	0.54	20 (4%)	35	37	29, 35, 41, 47	0
1	C	427/430 (99%)	0.53	28 (6%)	22	22	29, 35, 42, 49	0
1	D	427/430 (99%)	0.60	36 (8%)	14	14	29, 35, 41, 44	0
1	E	427/430 (99%)	0.54	29 (6%)	20	22	29, 35, 42, 45	0
1	F	427/430 (99%)	0.52	22 (5%)	31	33	29, 35, 41, 48	0
All	All	2562/2580 (99%)	0.55	163 (6%)	23	24	29, 35, 42, 49	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	430	CYS	8.8
1	F	430	CYS	7.8
1	B	430	CYS	6.0
1	E	430	CYS	5.7
1	A	430	CYS	4.8
1	D	430	CYS	4.7
1	D	238	GLY	4.7
1	C	2	ALA	4.5
1	A	2	ALA	4.5
1	C	27	ASP	4.3
1	D	236	LEU	4.3
1	B	236	LEU	4.3
1	B	420	LYS	4.1
1	B	237	ASN	4.1
1	E	91	GLN	3.9
1	D	237	ASN	3.9
1	F	141	ALA	3.7
1	A	237	ASN	3.6
1	A	236	LEU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	92	SER	3.6
1	B	91	GLN	3.5
1	E	2	ALA	3.5
1	E	27	ASP	3.4
1	B	2	ALA	3.4
1	E	336	PRO	3.4
1	B	239	ASN	3.4
1	F	91	GLN	3.3
1	D	29	LYS	3.3
1	D	380	TYR	3.3
1	D	2	ALA	3.3
1	D	229	ASP	3.3
1	C	150	ALA	3.2
1	E	74	ILE	3.2
1	D	303	LYS	3.1
1	D	239	ASN	3.1
1	D	142	ASN	3.1
1	E	204	ARG	3.1
1	E	84	ASP	3.1
1	B	27	ASP	3.0
1	D	336	PRO	3.0
1	C	141	ALA	3.0
1	A	420	LYS	3.0
1	A	7	VAL	3.0
1	F	2	ALA	3.0
1	F	423	GLU	2.9
1	C	95	LYS	2.9
1	D	423	GLU	2.9
1	D	91	GLN	2.9
1	C	149	GLY	2.8
1	E	97	GLU	2.8
1	E	236	LEU	2.8
1	E	118	GLU	2.8
1	A	229	ASP	2.8
1	D	93	GLY	2.7
1	D	141	ALA	2.7
1	F	97	GLU	2.7
1	D	228	PRO	2.7
1	D	175	GLY	2.7
1	F	92	SER	2.6
1	B	343	LEU	2.6
1	C	343	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	271	ALA	2.6
1	F	134	LYS	2.6
1	E	228	PRO	2.6
1	E	237	ASN	2.6
1	C	250	PHE	2.6
1	C	103	ILE	2.6
1	B	7	VAL	2.6
1	D	334	ASN	2.6
1	C	67	PRO	2.5
1	C	91	GLN	2.5
1	A	15	ILE	2.5
1	E	265	ASP	2.5
1	B	141	ALA	2.5
1	E	114	GLU	2.5
1	C	92	SER	2.5
1	D	95	LYS	2.5
1	E	353	GLU	2.5
1	B	423	GLU	2.5
1	A	143	PRO	2.5
1	A	142	ASN	2.4
1	B	303	LYS	2.4
1	C	114	GLU	2.4
1	E	141	ALA	2.4
1	A	353	GLU	2.4
1	F	258	GLU	2.4
1	B	381	PHE	2.4
1	A	173	LYS	2.4
1	D	240	THR	2.4
1	E	94	LYS	2.4
1	D	112	GLY	2.4
1	C	270	PRO	2.4
1	C	142	ASN	2.4
1	A	381	PHE	2.4
1	D	92	SER	2.4
1	E	240	THR	2.4
1	F	376	LYS	2.4
1	A	32	LEU	2.4
1	A	8	ILE	2.3
1	A	27	ASP	2.3
1	A	41	PHE	2.3
1	F	265	ASP	2.3
1	E	303	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	178	TYR	2.3
1	A	138	GLU	2.3
1	D	97	GLU	2.3
1	E	227	GLU	2.3
1	A	348	ILE	2.3
1	D	118	GLU	2.3
1	D	117	GLU	2.2
1	E	258	GLU	2.2
1	D	8	ILE	2.2
1	C	381	PHE	2.2
1	D	420	LYS	2.2
1	B	363	VAL	2.2
1	C	164	ALA	2.2
1	D	270	PRO	2.2
1	B	41	PHE	2.2
1	E	173	LYS	2.2
1	F	103	ILE	2.2
1	F	271	ALA	2.2
1	C	29	LYS	2.2
1	C	163	PHE	2.2
1	C	151	ILE	2.2
1	D	285	THR	2.2
1	A	92	SER	2.2
1	C	79	GLU	2.2
1	B	5	VAL	2.2
1	C	363	VAL	2.2
1	F	171	LEU	2.1
1	C	131	GLU	2.1
1	D	87	THR	2.1
1	E	87	THR	2.1
1	B	103	ILE	2.1
1	F	56	GLU	2.1
1	A	157	PHE	2.1
1	B	380	TYR	2.1
1	C	118	GLU	2.1
1	C	323	ALA	2.1
1	A	324	VAL	2.1
1	C	246	LYS	2.1
1	E	93	GLY	2.1
1	A	204	ARG	2.1
1	F	412	LYS	2.1
1	A	164	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	72	GLU	2.1
1	A	97	GLU	2.1
1	B	40	GLY	2.1
1	F	114	GLU	2.1
1	D	230	LYS	2.1
1	D	179	LYS	2.1
1	E	119	ASN	2.1
1	A	39	PHE	2.1
1	F	250	PHE	2.1
1	F	275	VAL	2.1
1	A	423	GLU	2.0
1	C	423	GLU	2.0
1	F	237	ASN	2.0
1	D	275	VAL	2.0
1	E	102	VAL	2.0
1	E	142	ASN	2.0
1	F	142	ASN	2.0
1	A	103	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
1	CSS	B	347[B]	7/8	0.92	0.13	-	43,44,44,45	2
1	CSS	B	347[A]	6/8	0.92	0.13	-	43,44,44,47	1
1	CSS	F	156[B]	7/8	0.95	0.14	-	35,36,37,37	2
1	CSS	F	156[A]	6/8	0.95	0.14	-	35,36,37,39	1
1	CSS	D	156[A]	6/8	0.97	0.08	-	35,35,36,37	1
1	CSS	A	347[A]	6/8	0.84	0.15	-	45,45,46,49	1
1	CSS	A	347[B]	6/8	0.84	0.15	-	45,45,46,47	1
1	CSS	D	156[B]	7/8	0.97	0.08	-	35,35,36,36	2
1	CSS	C	156[B]	7/8	0.95	0.13	-	35,35,36,37	2
1	CSS	C	156[A]	6/8	0.95	0.13	-	35,36,36,40	1
1	CSS	A	156[A]	6/8	0.95	0.18	-	36,36,37,40	1
1	CSS	A	156[B]	7/8	0.95	0.18	-	36,36,38,38	2
1	CSS	F	347[B]	6/8	0.89	0.13	-	44,44,45,45	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	CSS	F	347[A]	6/8	0.89	0.13	-	44,44,45,48	1
1	CSS	B	156[B]	7/8	0.96	0.15	-	33,35,36,36	2
1	CSS	B	156[A]	6/8	0.96	0.15	-	35,35,36,39	1
1	CSS	E	347[A]	6/8	0.84	0.15	-	44,44,44,47	1
1	CSS	E	347[B]	6/8	0.84	0.15	-	44,44,44,45	1
1	CSS	E	156[A]	6/8	0.94	0.13	-	35,36,37,39	1
1	CSS	D	347[A]	6/8	0.89	0.15	-	44,44,44,47	1
1	CSS	E	156[B]	7/8	0.94	0.13	-	35,36,38,38	2
1	CSS	C	347[B]	6/8	0.82	0.17	-	43,43,43,44	1
1	CSS	D	347[B]	7/8	0.89	0.15	-	44,44,44,45	2
1	CSS	C	347[A]	6/8	0.82	0.17	-	43,43,44,47	1

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
6	PS9	B	802[B]	2/8	0.53	1.11	69.97	39,39,39,41	2
3	DCQ	F	500	23/23	0.64	0.78	22.93	52,53,53,54	23
3	DCQ	E	500	23/23	0.67	0.72	22.26	47,48,48,48	23
6	PS9	C	800	6/8	0.49	0.56	21.93	39,40,42,42	6
6	PS9	D	800	2/8	0.46	0.47	19.24	33,33,33,34	2
6	PS9	E	800	8/8	0.47	0.55	18.33	42,43,43,43	8
3	DCQ	D	500	23/23	0.63	0.72	16.14	49,50,51,51	23
3	DCQ	A	500	23/23	0.64	0.69	15.13	46,51,51,51	23
3	DCQ	B	500	23/23	0.69	0.55	15.09	43,48,48,48	23
3	DCQ	C	500	23/23	0.70	0.63	14.47	43,46,47,47	23
6	PS9	F	800	8/8	0.65	0.50	13.75	39,40,41,41	8
6	PS9	A	800	8/8	0.51	0.57	13.05	40,41,41,42	8
4	LMT	E	600	35/35	0.44	0.46	9.63	53,55,58,58	35
4	LMT	C	600	35/35	0.28	0.56	9.56	53,57,59,60	35
4	LMT	F	600	35/35	0.38	0.43	9.16	44,50,54,55	35

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	LMT	A	600	35/35	0.33	0.52	7.19	50,55,57,58	35
4	LMT	B	600	35/35	0.43	0.46	6.35	49,50,52,53	35
4	LMT	D	600	35/35	0.46	0.42	5.80	47,51,53,54	35
7	SO4	A	433	5/5	0.87	0.26	3.65	29,31,32,32	5
7	SO4	B	433	5/5	0.77	0.26	2.32	51,51,52,52	5
7	SO4	D	433	5/5	0.77	0.26	1.46	57,57,57,58	5
7	SO4	C	433	5/5	0.84	0.26	1.17	36,37,37,38	5
7	SO4	E	433	5/5	0.80	0.22	0.30	56,56,56,56	5
7	SO4	F	433	5/5	0.88	0.21	0.21	39,41,41,41	5
2	FAD	D	441	53/53	0.96	0.10	-1.09	23,32,33,33	0
2	FAD	E	441	53/53	0.95	0.10	-1.32	26,29,37,37	0
2	FAD	C	441	53/53	0.95	0.10	-1.35	21,27,30,31	0
5	H2S	E	700	1/1	0.89	0.11	-1.35	32,32,32,32	1
2	FAD	F	441	53/53	0.96	0.09	-1.43	24,28,34,34	0
5	H2S	C	700	1/1	0.96	0.09	-1.63	31,31,31,31	1
5	H2S	B	700	1/1	0.94	0.09	-1.70	28,28,28,28	1
5	H2S	D	700	1/1	0.95	0.07	-2.29	33,33,33,33	1
2	FAD	B	441	53/53	0.96	0.09	-2.40	22,26,28,29	0
2	FAD	A	441	53/53	0.96	0.09	-2.47	20,23,26,26	0
5	H2S	F	700	1/1	0.98	0.07	-2.65	31,31,31,31	1
5	H2S	A	700	1/1	0.99	0.10	-7.14	28,28,28,28	1
6	PS9	B	802[A]	2/8	0.53	1.11	-	41,41,41,41	2
6	PS9	D	802	1/8	0.63	0.63	-	44,44,44,44	1
7	SO4	D	431	5/5	0.74	0.48	-	38,38,38,38	5
7	SO4	B	431	5/5	0.88	0.27	-	37,37,38,38	5
6	PS9	B	800	1/8	0.80	0.77	-	32,32,32,32	1
7	SO4	D	432	5/5	0.93	0.15	-	34,34,34,35	5
7	SO4	D	434	5/5	0.59	0.39	-	54,54,54,55	5
7	SO4	F	432	5/5	0.93	0.19	-	41,42,42,42	5
7	SO4	E	434	5/5	0.86	0.23	-	42,43,43,43	5
7	SO4	C	434	5/5	0.66	0.29	-	60,60,61,61	5
7	SO4	B	432	5/5	0.97	0.14	-	25,26,26,27	5
7	SO4	B	434	5/5	0.78	0.35	-	44,45,45,46	5
7	SO4	A	431	5/5	0.91	0.19	-	39,39,39,39	5
7	SO4	F	434	5/5	0.62	0.39	-	54,54,55,55	5
7	SO4	E	432	5/5	0.94	0.19	-	36,36,36,37	5
7	SO4	A	432	5/5	0.97	0.14	-	30,31,31,31	5
7	SO4	C	431	5/5	0.74	0.38	-	39,39,39,39	5
7	SO4	C	432	5/5	0.91	0.20	-	35,35,36,36	5
7	SO4	A	434	5/5	0.82	0.25	-	47,47,48,48	5
7	SO4	F	431	5/5	0.80	0.28	-	33,34,34,34	5
7	SO4	A	435	5/5	0.71	0.31	-	38,39,39,39	5

6.5 Other polymers (i)

There are no such residues in this entry.