



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:03 PM GMT

PDB ID : 1N9G
Title : Mitochondrial 2-enoyl thioester reductase Etr1p/Etr2p heterodimer from *Candida tropicalis*
Authors : Torkko, J.M.; Koivuranta, K.T.; Kastaniotis, A.J.; Airenne, T.T.; Glumoff, T.; Ilves, M.; Hartig, A.; Gurvitz, A.; Hiltunen, J.K.
Deposited on : 2002-11-25
Resolution : 1.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

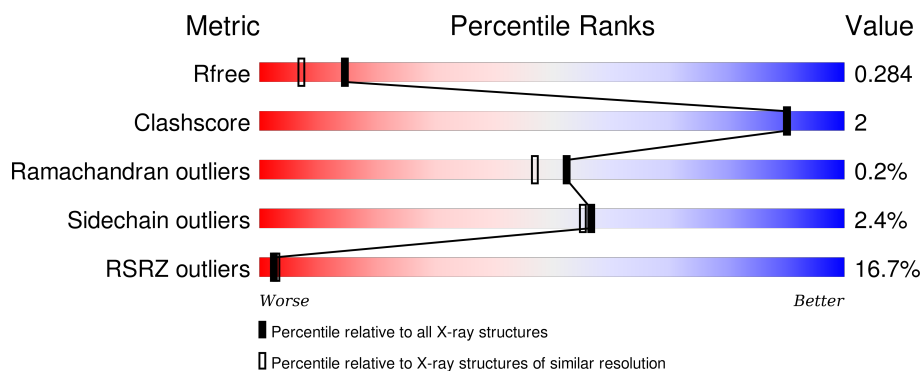
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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	386	<div> <div>3%</div> <div>91%</div> <div>6%</div> </div>
1	C	386	<div> <div>42%</div> <div>80%</div> <div>14%</div> <div>6%</div> </div>
1	F	386	<div> <div>10%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
2	B	386	<div> <div>12%</div> <div>89%</div> <div>5%</div> <div>6%</div> </div>
2	D	386	<div> <div>10%</div> <div>89%</div> <div>5%</div> <div>6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	386	

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	SO4	A	1532	-	-	X	X
3	SO4	B	1535	-	X	-	X
4	NAP	A	2387	-	-	-	X
4	NAP	E	4387	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18417 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 2,4-dienoyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	4	0	0
			2785	1768	464	547	6			
1	C	364	Total	C	N	O	S	0	0	0
			2785	1768	464	547	6			
1	F	364	Total	C	N	O	S	0	0	0
			2785	1768	464	547	6			

- Molecule 2 is a protein called 2,4-dienoyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	364	Total	C	N	O	S	4	0	0
			2788	1768	466	548	6			
2	D	364	Total	C	N	O	S	0	0	0
			2787	1767	466	548	6			
2	E	364	Total	C	N	O	S	0	0	0
			2788	1768	466	548	6			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	2	0
			5	4	1		
3	E	1	Total	O	S	1	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

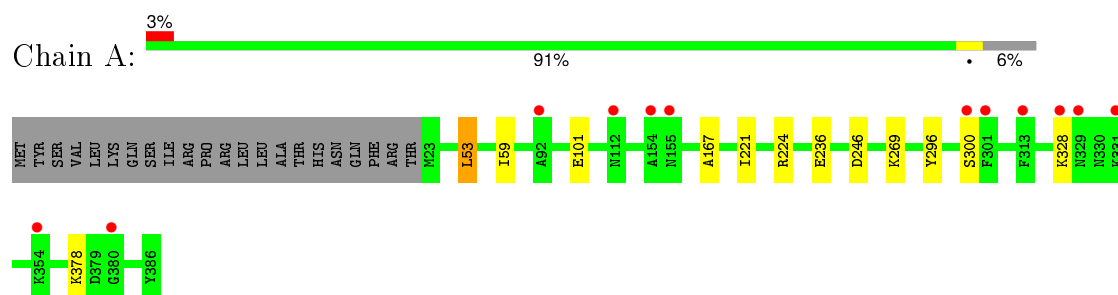
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	296	Total	O	0	0
			296	296		
5	B	234	Total	O	0	0
			234	234		
5	C	183	Total	O	0	0
			183	183		
5	D	318	Total	O	2	0
			318	318		
5	E	206	Total	O	0	0
			206	206		
5	F	283	Total	O	2	0
			283	283		

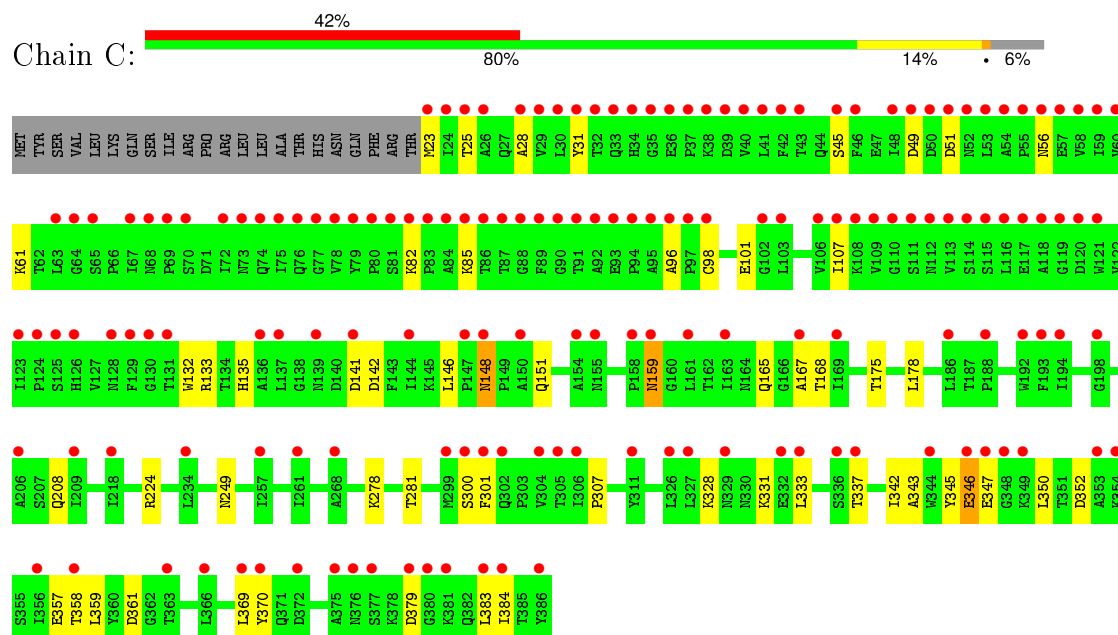
3 Residue-property plots [i](#)

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.

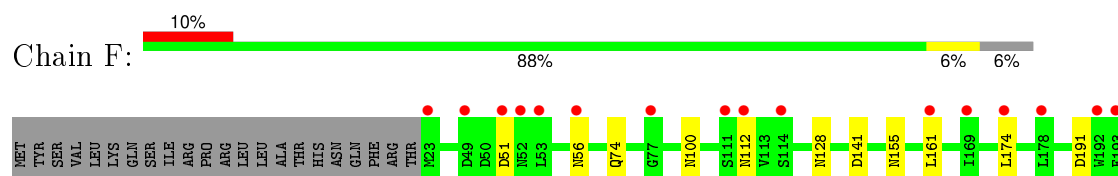
- Molecule 1: 2,4-dienoyl-CoA reductase

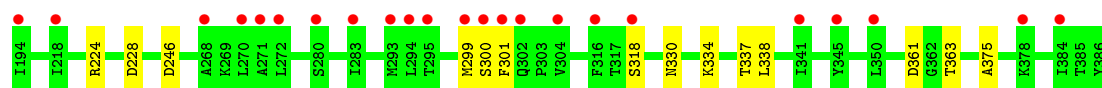


- Molecule 1: 2,4-dienoyl-CoA reductase

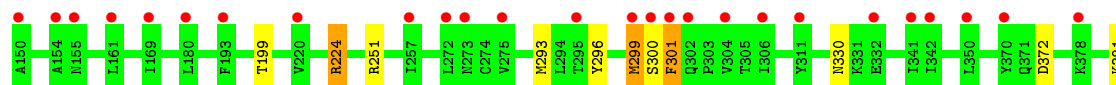
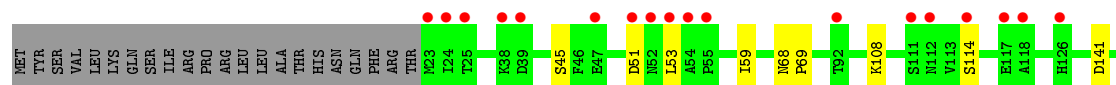
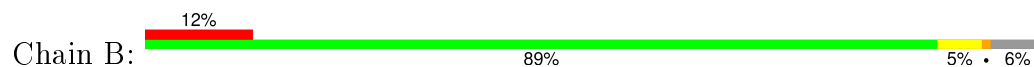


- Molecule 1: 2,4-dienoyl-CoA reductase

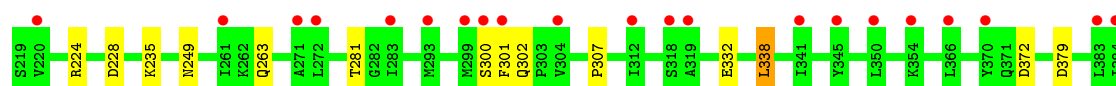
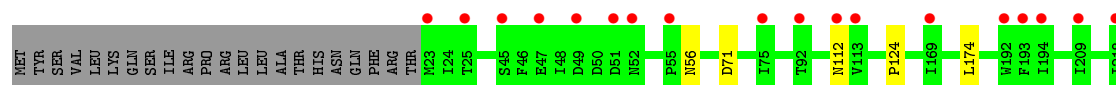
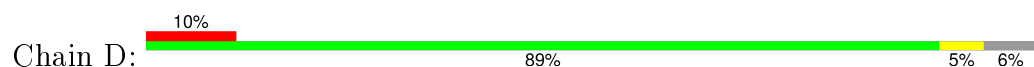




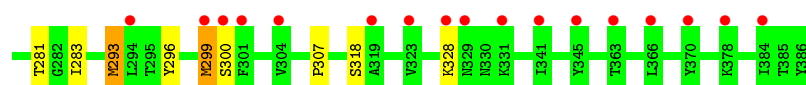
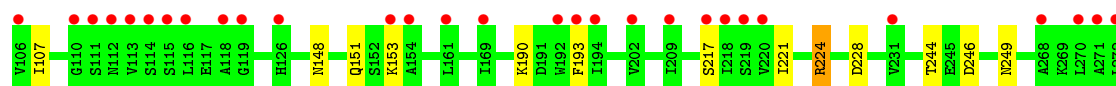
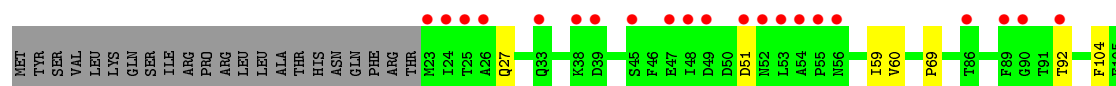
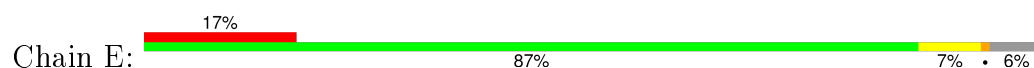
- Molecule 2: 2,4-dienoyl-CoA reductase



- Molecule 2: 2,4-dienoyl-CoA reductase



- Molecule 2: 2,4-dienoyl-CoA reductase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.45Å 95.50Å 164.23Å 90.00° 124.71° 90.00°	Depositor
Resolution (Å)	19.43 – 1.98 19.41 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.43-1.98) 99.8 (19.41-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.97Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.235 0.260 , 0.284	Depositor DCC
R_{free} test set	10101 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 202007 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18417	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, SO4

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	0.58	2/2844 (0.1%)	0.74	1/3865 (0.0%)
1	C	0.58	0/2844	0.76	7/3865 (0.2%)
1	F	0.58	0/2844	0.75	5/3865 (0.1%)
2	B	0.61	2/2847 (0.1%)	0.74	5/3870 (0.1%)
2	D	0.60	0/2846	0.78	4/3869 (0.1%)
2	E	0.55	1/2847 (0.0%)	0.76	4/3870 (0.1%)
All	All	0.58	5/17072 (0.0%)	0.75	26/23204 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	B	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	199	THR	CB-OG1	-14.07	1.15	1.43
1	A	296	TYR	C-O	-8.21	1.07	1.23
2	E	293	MET	SD-CE	-6.81	1.39	1.77
1	A	269	LYS	C-O	-5.43	1.13	1.23
2	B	293	MET	SD-CE	-5.14	1.49	1.77

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	372	ASP	CB-CG-OD2	9.18	126.56	118.30
1	C	141	ASP	CB-CG-OD2	8.68	126.11	118.30
2	E	228	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	246	ASP	CB-CG-OD2	6.78	124.40	118.30
2	E	246	ASP	CB-CG-OD2	6.13	123.82	118.30
1	C	352	ASP	CB-CG-OD2	6.05	123.75	118.30
1	F	246	ASP	CB-CG-OD2	6.02	123.72	118.30
1	C	379	ASP	CB-CG-OD2	6.00	123.70	118.30
2	B	372	ASP	CB-CG-OD2	5.92	123.63	118.30
1	C	49	ASP	CB-CG-OD2	5.80	123.52	118.30
2	B	199	THR	CA-CB-OG1	5.79	121.17	109.00
2	B	141	ASP	CB-CG-OD2	5.64	123.38	118.30
2	E	224	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	C	51	ASP	CB-CG-OD2	5.53	123.27	118.30
1	F	191	ASP	CB-CG-OD2	5.51	123.26	118.30
2	B	224	ARG	NE-CZ-NH2	-5.47	117.57	120.30
2	D	228	ASP	CB-CG-OD2	5.45	123.20	118.30
1	F	228	ASP	CB-CG-OD2	5.40	123.16	118.30
1	F	51	ASP	CB-CG-OD2	5.37	123.13	118.30
2	B	51	ASP	CB-CG-OD2	5.29	123.06	118.30
2	D	379	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	361	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	142	ASP	CB-CG-OD2	5.19	122.97	118.30
2	E	224	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	D	71	ASP	CB-CG-OD2	5.06	122.85	118.30
1	F	141	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	299	MET	Peptide
1	C	346	GLU	Peptide

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	2785	0	2767	4	0
1	C	2785	0	2767	30	0
1	F	2785	0	2767	11	0
2	B	2788	0	2767	6	0
2	D	2787	0	2764	8	0
2	E	2788	0	2767	17	0
3	A	5	0	0	2	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
3	E	5	0	0	1	0
3	F	5	0	0	0	0
4	A	48	0	25	1	0
4	B	48	0	25	4	0
4	E	48	0	25	6	0
5	A	296	0	0	1	0
5	B	234	0	0	1	0
5	C	183	0	0	9	0
5	D	318	0	0	4	0
5	E	206	0	0	1	0
5	F	283	0	0	3	0
All	All	18417	0	16674	77	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 2.

All (77) 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:C:159:ASN:HB2	1:C:346:GLU:HB3	1.59	0.85
2:B:300:SER:HB3	5:B:3487:HOH:O	1.80	0.82
2:B:296:TYR:O	4:B:3387:NAP:H2N	1.85	0.76
2:B:69:PRO:HG2	4:B:3387:NAP:H52N	1.68	0.74
2:D:56:ASN:HD21	2:D:112:ASN:HD22	1.36	0.73
1:C:82:LYS:NZ	5:C:1591:HOH:O	2.25	0.69
1:A:221:ILE:HA	3:A:1532:SO4:O3	1.93	0.69
1:C:175:THR:OG1	5:C:1624:HOH:O	2.12	0.68
1:F:334:LYS:CD	5:F:1784:HOH:O	2.44	0.66
1:F:334:LYS:HD3	5:F:1784:HOH:O	1.96	0.66
1:A:236:GLU:OE1	5:A:2472:HOH:O	2.14	0.64
1:C:208:GLN:NE2	5:C:1668:HOH:O	2.31	0.64
3:B:1535:SO4:O2	4:B:3387:NAP:O3B	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:LEU:HD21	1:C:337:THR:HG21	1.83	0.59
1:F:100:ASN:HD22	1:F:128:ASN:H	1.50	0.59
1:F:56:ASN:HD21	1:F:112:ASN:HD22	1.51	0.58
1:C:56:ASN:N	5:C:1556:HOH:O	2.20	0.58
2:E:69:PRO:HG2	4:E:4387:NAP:H52N	1.87	0.57
2:D:302:GLN:NE2	5:D:1623:HOH:O	2.29	0.57
2:E:221:ILE:O	2:E:244:THR:HA	2.05	0.57
1:F:174:LEU:HD22	1:F:337:THR:HG22	1.85	0.57
1:C:61:LYS:HG2	1:C:135:HIS:CD2	2.40	0.56
1:C:333:LEU:O	1:C:337:THR:HG23	2.05	0.56
2:E:299:MET:HE2	4:E:4387:NAP:O4B	2.06	0.55
2:E:249:ASN:ND2	5:E:4531:HOH:O	2.30	0.55
1:C:98:CYS:HB3	1:C:132:TRP:CE3	2.43	0.54
1:A:53:LEU:HD11	1:A:59:ILE:HG23	1.89	0.54
1:F:74:GLN:HE22	1:F:100:ASN:HD21	1.56	0.53
1:C:249:ASN:ND2	5:C:1604:HOH:O	2.29	0.53
2:E:283:ILE:HG13	2:E:293:MET:CE	2.39	0.53
1:A:101:GLU:HG2	1:A:167:ALA:O	2.09	0.52
1:C:383:LEU:HD13	5:C:1639:HOH:O	2.10	0.52
2:D:249:ASN:ND2	5:D:1704:HOH:O	2.28	0.51
2:E:59:ILE:HG22	2:E:107:ILE:HD11	1.93	0.51
2:E:296:TYR:O	4:E:4387:NAP:H2N	2.11	0.50
2:B:68:ASN:HD22	2:B:381:LYS:NZ	2.11	0.49
2:E:281:THR:HG23	2:E:307:PRO:HD3	1.94	0.49
2:D:174:LEU:HD21	2:D:338:LEU:HD13	1.94	0.49
1:F:375:ALA:O	5:F:1798:HOH:O	2.20	0.49
1:C:281:THR:HG23	1:C:307:PRO:HD3	1.94	0.48
2:B:296:TYR:O	4:B:3387:NAP:C2N	2.59	0.47
2:E:299:MET:HG2	4:E:4387:NAP:C5A	2.44	0.47
1:C:345:TYR:CE2	1:C:350:LEU:HD12	2.49	0.46
2:D:281:THR:HG23	2:D:307:PRO:HD3	1.98	0.46
2:D:124:PRO:HD2	5:D:1721:HOH:O	2.16	0.45
1:F:100:ASN:ND2	1:F:128:ASN:H	2.12	0.45
2:E:148:ASN:H	2:E:151:GLN:NE2	2.15	0.45
2:E:60:VAL:HB	2:E:104:PHE:HB3	1.98	0.44
1:C:28:ALA:HA	1:C:133:ARG:HB3	2.00	0.44
1:C:31:TYR:CZ	1:C:96:ALA:HB3	2.52	0.44
1:C:357:GLU:HA	1:C:383:LEU:O	2.17	0.44
1:C:101:GLU:HG2	1:C:167:ALA:O	2.17	0.44
2:D:235:LYS:CE	5:D:1554:HOH:O	2.66	0.43
1:C:148:ASN:HD22	1:C:148:ASN:C	2.22	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:318:SER:HB3	1:F:318:SER:HB3	2.01	0.43
1:C:383:LEU:HD21	5:C:1587:HOH:O	2.19	0.43
1:C:165:GLN:HG2	1:C:345:TYR:CE2	2.54	0.43
1:C:343:ALA:O	1:C:347:GLU:HB2	2.19	0.43
3:A:1532:SO4:O1	4:A:2387:NAP:O2B	2.36	0.42
1:C:148:ASN:ND2	1:C:151:GLN:H	2.17	0.42
1:C:148:ASN:HD22	1:C:151:GLN:H	1.66	0.42
2:E:193:PHE:CE2	2:E:217:SER:HB3	2.54	0.42
2:E:299:MET:CE	4:E:4387:NAP:O4B	2.68	0.42
2:E:283:ILE:HG13	2:E:293:MET:HE2	2.02	0.42
1:C:25:THR:HG23	5:C:1628:HOH:O	2.19	0.42
2:E:148:ASN:H	2:E:151:GLN:HE21	1.68	0.42
1:F:361:ASP:HB3	1:F:363:THR:HG23	2.02	0.41
2:B:53:LEU:HD21	2:B:59:ILE:CD1	2.51	0.41
2:E:283:ILE:HG13	2:E:293:MET:HE1	2.03	0.41
1:F:56:ASN:ND2	1:F:112:ASN:HD22	2.17	0.41
1:C:146:LEU:CD2	1:C:342:ILE:HD11	2.51	0.41
1:C:45:SER:HB3	5:C:1628:HOH:O	2.21	0.40
1:C:159:ASN:C	1:C:346:GLU:HB3	2.42	0.40
1:C:369:LEU:HB3	1:C:384:ILE:HD12	2.02	0.40
1:C:278:LYS:NZ	2:D:263:GLN:O	2.54	0.40
3:E:1536:SO4:S	4:E:4387:NAP:O2B	2.78	0.40
1:C:370:TYR:CE2	1:C:384:ILE:HG13	2.57	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	362/386 (94%)	354 (98%)	8 (2%)	0	100	100
1	C	362/386 (94%)	350 (97%)	11 (3%)	1 (0%)	46	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	362/386 (94%)	351 (97%)	10 (3%)	1 (0%)	46	39
2	B	362/386 (94%)	353 (98%)	8 (2%)	1 (0%)	46	39
2	D	362/386 (94%)	351 (97%)	10 (3%)	1 (0%)	46	39
2	E	362/386 (94%)	350 (97%)	11 (3%)	1 (0%)	46	39
All	All	2172/2316 (94%)	2109 (97%)	58 (3%)	5 (0%)	52	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	300	SER
2	E	300	SER
1	F	300	SER
2	B	301	PHE
1	C	300	SER

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	306/327 (94%)	301 (98%)	5 (2%)	70	71
1	C	306/327 (94%)	294 (96%)	12 (4%)	39	32
1	F	306/327 (94%)	299 (98%)	7 (2%)	58	57
2	B	307/328 (94%)	298 (97%)	9 (3%)	50	46
2	D	306/328 (93%)	302 (99%)	4 (1%)	76	77
2	E	307/328 (94%)	299 (97%)	8 (3%)	54	51
All	All	1838/1965 (94%)	1793 (98%)	45 (2%)	57	55

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	224	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	300	SER
1	A	328	LYS
1	A	378	LYS
2	B	45	SER
2	B	108	LYS
2	B	114	SER
2	B	224	ARG
2	B	251	ARG
2	B	299	MET
2	B	301	PHE
2	B	330	ASN
2	B	384	ILE
1	C	23	MET
1	C	85	LYS
1	C	107	ILE
1	C	148	ASN
1	C	159	ASN
1	C	168	THR
1	C	224	ARG
1	C	301	PHE
1	C	328	LYS
1	C	331	LYS
1	C	358	THR
1	C	359	LEU
2	D	224	ARG
2	D	301	PHE
2	D	332	GLU
2	D	338	LEU
2	E	27	GLN
2	E	51	ASP
2	E	92	THR
2	E	153	LYS
2	E	190	LYS
2	E	224	ARG
2	E	299	MET
2	E	328	LYS
1	F	155	ASN
1	F	161	LEU
1	F	224	ARG
1	F	299	MET
1	F	301	PHE
1	F	330	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	338	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	73	ASN
1	A	155	ASN
1	A	249	ASN
2	B	68	ASN
2	B	135	HIS
2	B	376	ASN
1	C	148	ASN
1	C	159	ASN
1	C	249	ASN
1	C	340	GLN
2	D	56	ASN
2	D	139	ASN
2	E	27	GLN
2	E	139	ASN
2	E	151	GLN
1	F	56	ASN
1	F	100	ASN
1	F	249	ASN
1	F	330	ASN
1	F	376	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	SO4	A	1532	-	4,4,4	0.56	0	6,6,6	0.35	0
4	NAP	A	2387	1	42,52,52	1.54	3 (7%)	54,80,80	2.01	3 (5%)
3	SO4	B	1535	4	4,4,4	9.11	4 (100%)	6,6,6	4.20	5 (83%)
4	NAP	B	3387	3	42,52,52	1.74	4 (9%)	54,80,80	2.16	9 (16%)
3	SO4	C	1534	-	4,4,4	0.59	0	6,6,6	0.32	0
3	SO4	D	1531	-	4,4,4	0.32	0	6,6,6	0.33	0
3	SO4	D	1533	-	4,4,4	0.55	0	6,6,6	0.42	0
3	SO4	E	1536	4	4,4,4	3.19	1 (25%)	6,6,6	1.81	2 (33%)
4	NAP	E	4387	3	42,52,52	1.59	3 (7%)	54,80,80	2.07	11 (20%)
3	SO4	F	1537	-	4,4,4	0.62	0	6,6,6	0.22	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
3	SO4	A	1532	-	-	0/0/0/0	0/0/0/0
4	NAP	A	2387	1	-	0/27/67/67	0/5/5/5
3	SO4	B	1535	4	-	0/0/0/0	0/0/0/0
4	NAP	B	3387	3	-	0/27/67/67	0/5/5/5
3	SO4	C	1534	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1531	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1533	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1536	4	-	0/0/0/0	0/0/0/0
4	NAP	E	4387	3	-	0/27/67/67	0/5/5/5
3	SO4	F	1537	-	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1535	SO4	O4-S	-14.48	0.95	1.47
3	B	1535	SO4	O2-S	-7.53	1.21	1.47
3	B	1535	SO4	O3-S	-6.63	1.23	1.47
3	E	1536	SO4	O4-S	-6.35	1.24	1.47
4	B	3387	NAP	O4D-C1D	2.31	1.44	1.41
4	E	4387	NAP	C2A-N1A	2.40	1.38	1.33
4	A	2387	NAP	C2A-N1A	2.54	1.38	1.33
4	B	3387	NAP	C2A-N1A	2.77	1.39	1.33
4	E	4387	NAP	C2A-N3A	3.76	1.38	1.32
4	A	2387	NAP	C2A-N3A	3.77	1.38	1.32
4	B	3387	NAP	C2A-N3A	3.91	1.39	1.32
3	B	1535	SO4	O1-S	4.65	1.63	1.47
4	E	4387	NAP	O7N-C7N	7.57	1.40	1.24
4	A	2387	NAP	O7N-C7N	7.61	1.40	1.24
4	B	3387	NAP	O7N-C7N	8.47	1.42	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2387	NAP	N3A-C2A-N1A	-11.81	119.85	128.89
4	E	4387	NAP	N3A-C2A-N1A	-11.60	120.01	128.89
4	B	3387	NAP	N3A-C2A-N1A	-11.55	120.05	128.89
3	B	1535	SO4	O2-S-O1	-6.44	89.08	109.50
4	B	3387	NAP	O7N-C7N-C3N	-4.97	114.16	119.59
4	E	4387	NAP	PN-O3-PA	-3.08	124.07	132.73
4	E	4387	NAP	C5D-C4D-C3D	-2.90	103.68	115.21
3	B	1535	SO4	O4-S-O2	-2.71	84.95	110.19
4	B	3387	NAP	O5D-PN-O1N	-2.55	99.71	109.62
4	E	4387	NAP	O5D-PN-O1N	-2.39	100.35	109.62
4	E	4387	NAP	O7N-C7N-C3N	-2.38	116.99	119.59
4	A	2387	NAP	O7N-C7N-C3N	-2.36	117.01	119.59
4	E	4387	NAP	C3B-C2B-C1B	-2.31	98.26	102.73
4	E	4387	NAP	O3B-C3B-C4B	-2.31	104.13	111.05
4	E	4387	NAP	C5N-C4N-C3N	-2.28	117.47	120.33
4	B	3387	NAP	C5D-C4D-C3D	-2.20	106.47	115.21
3	B	1535	SO4	O4-S-O1	-2.20	89.70	110.19
3	E	1536	SO4	O4-S-O2	-2.19	89.81	110.19
4	B	3387	NAP	O4B-C1B-C2B	-2.13	102.74	106.60
4	E	4387	NAP	C4A-C5A-N7A	-2.02	107.62	109.48
3	B	1535	SO4	O3-S-O2	2.18	130.52	110.19
4	E	4387	NAP	O7N-C7N-N7N	2.20	125.69	122.59
4	E	4387	NAP	C2B-C3B-C4B	2.42	107.57	101.85
4	B	3387	NAP	O5D-C5D-C4D	2.58	118.63	109.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3387	NAP	O5B-C5B-C4B	2.73	119.18	109.12
4	B	3387	NAP	C3N-C7N-N7N	3.13	121.24	117.82
4	B	3387	NAP	O4D-C1D-N1N	3.44	111.91	108.13
3	E	1536	SO4	O4-S-O3	3.83	124.57	108.98
4	A	2387	NAP	O4D-C1D-N1N	4.37	112.93	108.13
3	B	1535	SO4	O4-S-O3	6.86	136.89	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1532	SO4	2	0
4	A	2387	NAP	1	0
3	B	1535	SO4	1	0
4	B	3387	NAP	4	0
3	E	1536	SO4	1	0
4	E	4387	NAP	6	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	364/386 (94%)	0.11	12 (3%) 50 54	11, 18, 28, 44	12 (3%)
1	C	364/386 (94%)	2.22	162 (44%) 0 1	11, 32, 59, 70	13 (3%)
1	F	364/386 (94%)	0.69	39 (10%) 8 10	13, 29, 43, 71	3 (0%)
2	B	364/386 (94%)	0.78	45 (12%) 5 6	12, 27, 51, 62	8 (2%)
2	D	364/386 (94%)	0.73	39 (10%) 8 10	12, 27, 41, 60	4 (1%)
2	E	364/386 (94%)	1.09	67 (18%) 2 2	11, 29, 50, 60	4 (1%)
All	All	2184/2316 (94%)	0.94	364 (16%) 2 3	11, 27, 50, 71	44 (2%)

All (364) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	301	PHE	22.8
1	F	301	PHE	12.9
1	C	41	LEU	10.2
2	D	301	PHE	9.9
1	C	52	ASN	7.7
1	C	301	PHE	7.5
2	B	301	PHE	7.5
1	C	84	ALA	7.4
1	C	55	PRO	7.3
1	C	32	THR	7.2
1	C	112	ASN	7.0
1	F	300	SER	6.7
1	C	92	ALA	6.6
1	C	78	VAL	6.6
1	C	88	GLY	6.6
1	A	300	SER	6.5
1	C	95	ALA	6.4
2	E	23	MET	6.3
1	C	94	PRO	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	111	SER	6.3
1	C	90	GLY	6.3
1	C	56	ASN	6.2
1	C	154	ALA	6.1
1	C	300	SER	6.0
2	E	53	LEU	6.0
1	C	35	GLY	6.0
1	C	48	ILE	5.9
1	C	25	THR	5.9
1	C	354	LYS	5.8
1	C	53	LEU	5.8
1	C	118	ALA	5.8
2	E	111	SER	5.8
2	E	52	ASN	5.6
1	C	87	THR	5.5
1	C	89	PHE	5.5
2	E	112	ASN	5.5
1	C	69	PRO	5.5
1	C	23	MET	5.5
1	C	86	THR	5.4
1	C	375	ALA	5.4
1	C	75	ILE	5.3
1	C	26	ALA	5.3
1	C	379	ASP	5.2
1	C	24	ILE	5.2
1	C	46	PHE	5.1
1	C	79	TYR	5.1
1	C	37	PRO	5.1
1	C	34	HIS	5.0
1	C	131	THR	5.0
2	D	92	THR	4.9
2	E	55	PRO	4.9
2	D	23	MET	4.9
1	C	51	ASP	4.9
1	C	148	ASN	4.9
1	C	54	ALA	4.9
1	C	70	SER	4.9
1	C	380	GLY	4.8
1	C	114	SER	4.7
2	D	52	ASN	4.7
1	C	58	VAL	4.7
1	C	117	GLU	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	114	SER	4.7
1	A	329	ASN	4.6
2	B	23	MET	4.6
1	A	301	PHE	4.6
1	C	363	THR	4.6
1	C	60	VAL	4.5
2	D	300	SER	4.5
2	E	54	ALA	4.5
1	C	43	THR	4.5
2	E	25	THR	4.5
2	E	113	VAL	4.5
1	C	42	PHE	4.4
1	C	39	ASP	4.4
2	E	329	ASN	4.3
1	F	299	MET	4.3
2	B	300	SER	4.3
2	E	116	LEU	4.3
1	C	59	ILE	4.3
1	C	377	SER	4.2
1	C	83	PRO	4.2
1	C	333	LEU	4.2
2	E	51	ASP	4.2
1	C	40	VAL	4.1
1	C	370	TYR	4.1
1	C	109	VAL	4.1
2	B	304	VAL	4.0
2	E	118	ALA	4.0
1	C	299	MET	4.0
1	C	110	GLY	3.9
2	E	300	SER	3.9
1	C	158	PRO	3.9
1	C	85	LYS	3.9
1	C	80	PRO	3.9
2	E	90	GLY	3.8
1	C	50	ASP	3.8
1	C	120	ASP	3.8
2	B	257	ILE	3.8
1	C	125	SER	3.7
1	C	150	ALA	3.7
1	C	31	TYR	3.7
2	D	112	ASN	3.7
1	C	91	THR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	192	TRP	3.7
1	A	354	LYS	3.6
1	C	36	GLU	3.6
2	B	24	ILE	3.6
1	C	349	LYS	3.6
1	C	103	LEU	3.6
1	C	72	ILE	3.6
1	C	348	GLY	3.5
2	D	51	ASP	3.5
1	C	356	ILE	3.5
1	C	38	LYS	3.5
2	E	24	ILE	3.5
1	C	77	GLY	3.5
2	E	56	ASN	3.5
2	E	218	ILE	3.5
2	D	55	PRO	3.5
2	B	111	SER	3.5
1	C	82	LYS	3.5
1	C	107	ILE	3.4
1	C	193	PHE	3.4
2	D	271	ALA	3.4
1	C	113	VAL	3.4
1	F	111	SER	3.4
1	C	108	LYS	3.4
2	E	194	ILE	3.4
1	C	128	ASN	3.4
1	C	366	LEU	3.4
2	D	370	TYR	3.4
1	C	68	ASN	3.4
1	F	378	LYS	3.4
1	C	384	ILE	3.3
2	E	154	ALA	3.3
2	E	47	GLU	3.3
2	D	384	ILE	3.3
2	E	331	LYS	3.3
1	C	49	ASP	3.3
1	C	163	ILE	3.3
1	C	93	GLU	3.3
1	C	304	VAL	3.3
1	C	115	SER	3.3
1	F	112	ASN	3.2
1	C	130	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	304	VAL	3.2
2	B	114	SER	3.2
1	F	52	ASN	3.2
1	C	119	GLY	3.1
2	E	92	THR	3.1
1	C	306	ILE	3.1
1	C	116	LEU	3.1
1	C	76	GLN	3.1
1	F	270	LEU	3.1
1	C	64	GLY	3.1
1	C	358	THR	3.1
2	D	299	MET	3.1
2	B	54	ALA	3.1
1	C	376	ASN	3.1
1	C	327	LEU	3.0
1	C	33	GLN	3.0
2	B	370	TYR	3.0
1	C	346	GLU	3.0
2	B	180	LEU	3.0
1	C	102	GLY	3.0
2	E	304	VAL	3.0
2	E	370	TYR	3.0
2	D	192	TRP	3.0
2	E	115	SER	3.0
2	B	55	PRO	3.0
2	E	345	TYR	3.0
1	C	57	GLU	3.0
2	E	378	LYS	3.0
1	F	23	MET	3.0
1	F	194	ILE	3.0
1	F	384	ILE	3.0
2	D	194	ILE	3.0
1	C	194	ILE	3.0
1	F	193	PHE	2.9
1	C	126	HIS	2.9
1	F	271	ALA	2.9
1	A	155	ASN	2.9
1	F	345	TYR	2.9
1	F	280	SER	2.9
2	D	218	ILE	2.9
1	C	74	GLN	2.9
1	C	311	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	110	GLY	2.9
1	C	141	ASP	2.9
2	D	169	ILE	2.9
2	D	341	ILE	2.8
1	C	159	ASN	2.8
1	F	293	MET	2.8
1	C	369	LEU	2.8
1	C	67	ILE	2.8
1	F	350	LEU	2.8
1	C	65	SER	2.8
2	E	366	LEU	2.8
1	F	114	SER	2.8
1	C	155	ASN	2.7
2	B	112	ASN	2.7
1	C	123	ILE	2.7
2	D	283	ILE	2.7
2	E	48	ILE	2.7
2	D	220	VAL	2.7
2	E	126	HIS	2.7
2	B	118	ALA	2.7
1	C	257	ILE	2.7
1	F	51	ASP	2.7
1	A	313	PHE	2.7
1	C	129	PHE	2.7
1	F	272	LEU	2.7
1	C	96	ALA	2.7
2	D	49	ASP	2.7
2	E	328	LYS	2.7
1	C	45	SER	2.7
2	E	270	LEU	2.7
1	C	97	PRO	2.6
2	D	261	ILE	2.6
2	B	378	LYS	2.6
1	C	81	SER	2.6
2	E	45	SER	2.6
1	C	124	PRO	2.6
1	C	261	ILE	2.6
2	E	220	VAL	2.6
1	C	121	TRP	2.6
1	C	161	LEU	2.6
2	B	272	LEU	2.6
2	D	193	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	304	VAL	2.6
2	D	366	LEU	2.6
1	C	218	ILE	2.5
1	A	92	ALA	2.5
1	C	28	ALA	2.5
2	E	271	ALA	2.5
2	E	49	ASP	2.5
1	C	336	SER	2.5
2	E	217	SER	2.5
1	F	283	ILE	2.5
2	D	75	ILE	2.5
1	C	353	ALA	2.5
1	C	329	ASN	2.5
1	F	318	SER	2.5
2	D	45	SER	2.5
1	F	316	PHE	2.5
2	E	119	GLY	2.5
1	F	218	ILE	2.5
2	B	53	LEU	2.5
1	C	63	LEU	2.5
2	B	384	ILE	2.4
2	B	299	MET	2.4
2	D	354	LYS	2.4
2	E	89	PHE	2.4
2	B	275	VAL	2.4
1	F	49	ASP	2.4
1	C	209	ILE	2.4
1	C	169	ILE	2.4
2	D	318	SER	2.4
1	A	331	LYS	2.4
1	C	136	ALA	2.4
1	C	332	GLU	2.4
2	B	52	ASN	2.4
2	E	219	SER	2.4
2	B	306	ILE	2.3
1	F	295	THR	2.3
1	C	73	ASN	2.3
1	F	341	ILE	2.3
1	C	186	LEU	2.3
2	E	38	LYS	2.3
1	F	77	GLY	2.3
2	D	209	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	169	ILE	2.3
2	E	341	ILE	2.3
2	B	38	LYS	2.3
1	C	344	TRP	2.3
1	C	206	ALA	2.3
1	F	53	LEU	2.3
1	F	294	LEU	2.3
2	D	25	THR	2.3
2	B	341	ILE	2.3
2	B	51	ASP	2.3
1	C	386	TYR	2.3
2	B	25	THR	2.3
2	E	363	THR	2.3
1	F	161	LEU	2.3
1	C	98	CYS	2.3
2	B	193	PHE	2.3
1	C	144	ILE	2.3
2	B	150	ALA	2.3
1	C	30	LEU	2.2
1	C	347	GLU	2.2
2	D	113	VAL	2.2
2	E	231	VAL	2.2
1	C	268	ALA	2.2
2	B	126	HIS	2.2
2	D	293	MET	2.2
2	E	299	MET	2.2
2	E	161	LEU	2.2
2	E	202	VAL	2.2
1	A	112	ASN	2.2
2	E	39	ASP	2.2
2	E	268	ALA	2.2
1	C	326	LEU	2.2
2	D	272	LEU	2.2
1	C	29	VAL	2.2
1	C	167	ALA	2.2
2	E	193	PHE	2.2
1	C	188	PRO	2.2
2	B	342	ILE	2.2
2	B	155	ASN	2.2
2	B	273	ASN	2.2
1	F	178	LEU	2.2
2	E	272	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	302	GLN	2.2
1	C	305	THR	2.2
1	C	106	VAL	2.2
1	C	147	PRO	2.2
2	B	302	GLN	2.2
2	B	154	ALA	2.1
2	E	33	GLN	2.1
2	D	312	ILE	2.1
2	E	384	ILE	2.1
2	B	92	THR	2.1
1	F	56	ASN	2.1
1	C	372	ASP	2.1
1	F	192	TRP	2.1
2	D	47	GLU	2.1
1	C	337	THR	2.1
1	F	169	ILE	2.1
2	E	209	ILE	2.1
1	C	137	LEU	2.1
1	A	380	GLY	2.1
2	E	26	ALA	2.1
2	B	220	VAL	2.1
2	B	47	GLU	2.1
2	B	332	GLU	2.1
2	E	86	THR	2.1
2	B	169	ILE	2.1
2	B	161	LEU	2.1
2	D	350	LEU	2.1
2	E	319	ALA	2.1
2	B	117	GLU	2.1
2	B	295	THR	2.1
2	E	192	TRP	2.1
1	A	154	ALA	2.1
1	C	234	LEU	2.1
2	B	39	ASP	2.1
2	B	350	LEU	2.1
2	D	345	TYR	2.1
2	D	383	LEU	2.1
2	E	294	LEU	2.1
2	E	153	LYS	2.0
1	C	139	ASN	2.0
2	D	319	ALA	2.0
1	C	383	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	106	VAL	2.0
1	A	328	LYS	2.0
1	C	381	LYS	2.0
1	C	198	GLY	2.0
1	F	174	LEU	2.0
2	B	311	TYR	2.0
2	E	323	VAL	2.0
1	F	268	ALA	2.0
1	F	302	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	B	1535	5/5	0.97	0.33	5.12	30,30,40,66	2
4	NAP	E	4387	48/48	0.82	0.29	2.79	21,43,46,47	41
3	SO4	A	1532	5/5	0.98	0.18	2.40	43,45,48,49	0
4	NAP	A	2387	48/48	0.89	0.28	2.19	6,16,21,22	41
4	NAP	B	3387	48/48	0.86	0.23	1.32	22,48,53,54	41
3	SO4	C	1534	5/5	0.93	0.17	0.50	60,61,62,63	0
3	SO4	F	1537	5/5	0.99	0.10	-1.04	38,39,41,41	0
3	SO4	D	1533	5/5	0.99	0.10	-1.15	38,39,39,40	0
3	SO4	E	1536	5/5	0.99	0.09	-1.87	30,57,60,61	1
3	SO4	D	1531	5/5	0.90	0.25	-	60,62,63,63	0

6.5 Other polymers

There are no such residues in this entry.