



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:22 AM GMT

PDB ID : 4B5K
Title : Probing the active center of catalase-phenol oxidase from *Scytalidium thermophilum*
Authors : Yuzugullu, Y.; Trinh, C.H.; Pearson, A.R.; Ogel, Z.B.; McPherson, M.J.
Deposited on : 2012-08-03
Resolution : 1.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

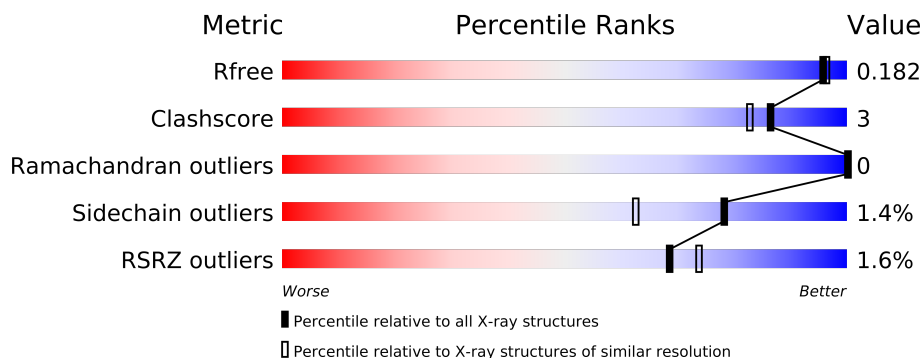
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.70 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}	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	719	
1	B	719	
1	C	719	
1	D	719	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CA	B	1699	-	X
3	CA	B	1701	-	X
3	CA	C	1699	-	X
3	CA	D	1699	-	X

2 Entry composition i

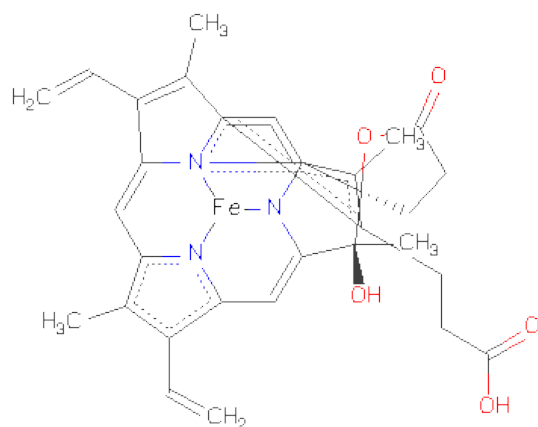
There are 4 unique types of molecules in this entry. The entry contains 24385 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CATALASE-PHENOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	46	0
			5580	3520	976	1071	13			
1	B	673	Total	C	N	O	S	0	43	0
			5559	3507	975	1065	12			
1	C	672	Total	C	N	O	S	0	43	0
			5538	3495	970	1059	14			
1	D	671	Total	C	N	O	S	0	38	0
			5504	3476	964	1050	14			

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	B	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	
			44	34	1	4	5	
2	D	1	Total	C	Fe	N	O	
			44	34	1	4	5	

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca		
			3	3	0	0
3	A	2	Total	Ca		
			2	2	0	0
3	D	2	Total	Ca		
			2	2	0	0
3	C	2	Total	Ca		
			2	2	0	0

- Molecule 4 is water.

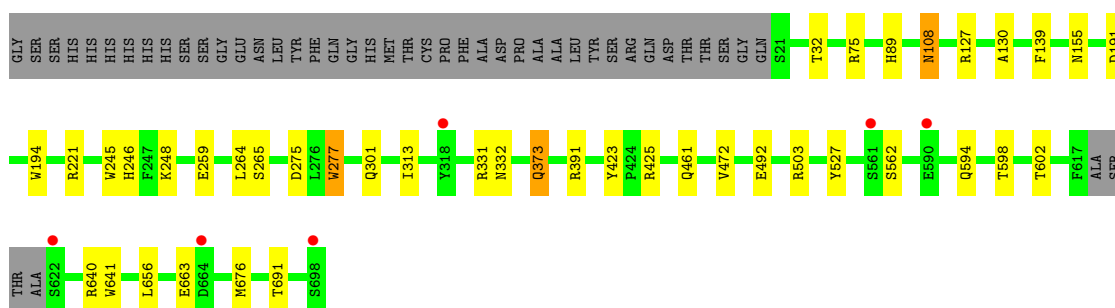
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	648	Total	O		
			648	648	0	0
4	B	564	Total	O		
			564	564	0	0
4	C	423	Total	O		
			423	423	0	0
4	D	384	Total	O		
			384	384	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

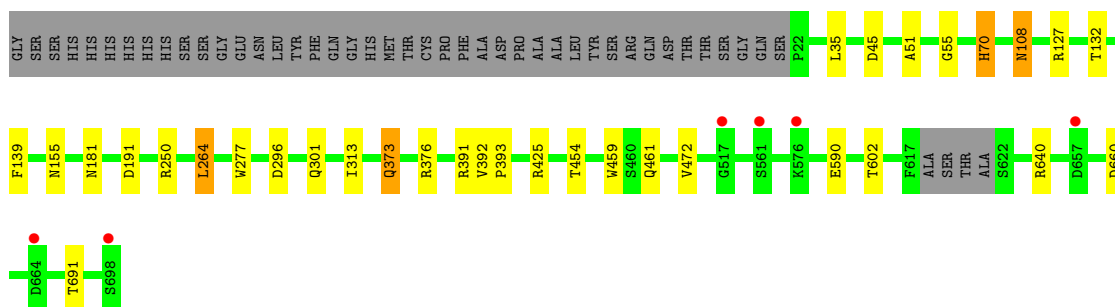
• Molecule 1: CATALASE-PHENOL OXIDASE

Chain A: 



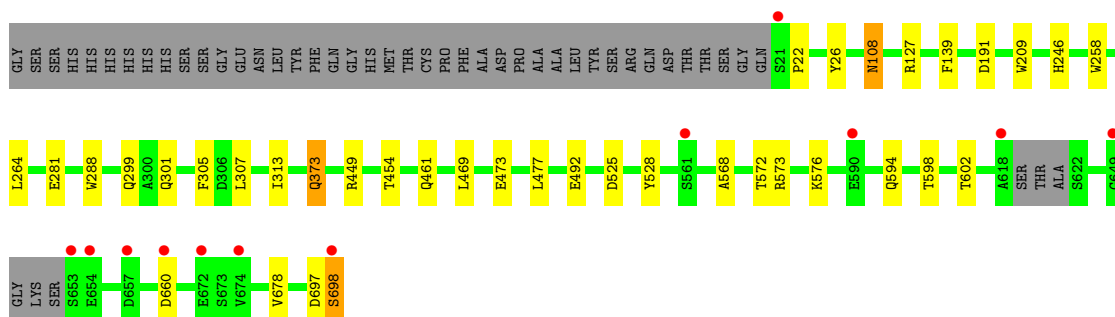
• Molecule 1: CATALASE-PHENOL OXIDASE

Chain B: 



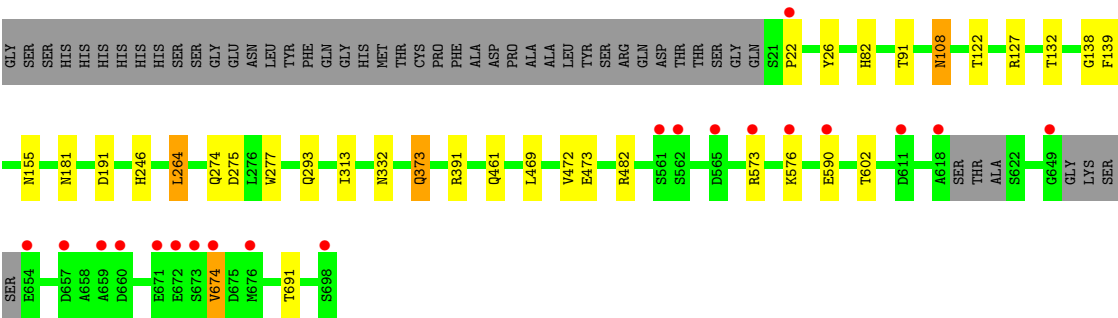
• Molecule 1: CATALASE-PHENOL OXIDASE

Chain C: 



● Molecule 1: CATALASE-PHENOL OXIDASE

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	201.39Å 122.00Å 125.67Å 90.00° 115.48° 90.00°	Depositor
Resolution (Å)	28.92 – 1.70 29.26 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (28.92-1.70) 99.1 (29.26-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.153 , 0.180 0.156 , 0.182	Depositor DCC
R_{free} test set	14885 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 297331 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	24385	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.63 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0725e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.74	4/5784 (0.1%)	0.76	2/7847 (0.0%)
1	B	0.70	1/5751 (0.0%)	0.73	0/7804
1	C	0.74	3/5744 (0.1%)	0.77	1/7793 (0.0%)
1	D	0.71	0/5692	0.74	1/7724 (0.0%)
All	All	0.72	8/22971 (0.0%)	0.75	4/31168 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	258	TRP	CD2-CE2	5.56	1.48	1.41
1	C	288	TRP	CD2-CE2	5.52	1.48	1.41
1	A	245	TRP	CD2-CE2	5.40	1.47	1.41
1	A	194	TRP	CD2-CE2	5.34	1.47	1.41
1	C	209	TRP	CD2-CE2	5.29	1.47	1.41
1	A	641	TRP	CD2-CE2	5.28	1.47	1.41
1	B	459	TRP	CD2-CE2	5.13	1.47	1.41
1	A	277	TRP	CD2-CE2	5.03	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	449	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	D	482	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	221	ARG	NE-CZ-NH2	-5.21	117.69	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5580	0	5391	29	0
1	B	5559	0	5370	33	0
1	C	5538	0	5357	26	0
1	D	5504	0	5320	30	0
2	A	44	0	31	2	0
2	B	44	0	31	1	0
2	C	44	0	31	0	0
2	D	44	0	31	2	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	648	0	0	14	0
4	B	564	0	0	17	0
4	C	423	0	0	5	0
4	D	384	0	0	4	0
All	All	24385	0	21562	115	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (115) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:2095:HOH:O	1:C:127[B]:ARG:NH2	1.87	1.06
1:A:127[A]:ARG:NH2	4:A:2164:HOH:O	1.88	1.05
4:A:2095:HOH:O	1:C:127[B]:ARG:NH1	1.90	1.04
1:A:259[A]:GLU:HG3	4:A:2300:HOH:O	1.54	1.04
4:B:2089:HOH:O	1:D:127[B]:ARG:NH1	1.84	0.99
1:A:127[A]:ARG:NH1	4:A:2164:HOH:O	1.96	0.97
1:B:127[A]:ARG:NH2	4:B:2144:HOH:O	1.88	0.94
1:D:313:ILE:H	1:D:461:GLN:HE22	1.15	0.94
1:B:313:ILE:H	1:B:461:GLN:HE22	1.15	0.93
1:C:313:ILE:H	1:C:461:GLN:HE22	1.16	0.92
1:A:127[A]:ARG:CZ	4:A:2164:HOH:O	2.13	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:91[B]:THR:HG22	4:D:2042:HOH:O	1.72	0.90
1:A:313:ILE:H	1:A:461:GLN:HE22	1.22	0.88
4:B:2089:HOH:O	1:D:127[B]:ARG:NH2	2.09	0.85
4:B:2142:HOH:O	1:D:127[A]:ARG:NH1	2.10	0.84
4:B:2089:HOH:O	1:D:127[B]:ARG:CZ	2.21	0.84
4:A:2095:HOH:O	1:C:127[B]:ARG:CZ	2.13	0.82
1:B:70:HIS:CE1	4:B:2067:HOH:O	2.33	0.81
1:A:656:LEU:HD12	1:A:663[A]:GLU:HG3	1.65	0.78
1:D:264:LEU:HG	1:D:602:THR:HB	1.64	0.78
1:B:127[A]:ARG:NH1	4:B:2144:HOH:O	2.15	0.78
1:C:281[B]:GLU:O	1:C:281[B]:GLU:HG3	1.82	0.78
1:B:127[A]:ARG:CZ	4:B:2144:HOH:O	2.28	0.76
1:C:264:LEU:HG	1:C:602:THR:HB	1.66	0.76
1:B:70:HIS:HE1	4:B:2067:HOH:O	1.70	0.75
1:A:425[B]:ARG:CZ	4:A:2457:HOH:O	2.34	0.75
1:A:656:LEU:CD1	1:A:663[A]:GLU:HG3	2.19	0.71
1:B:425[B]:ARG:CZ	4:B:2401:HOH:O	2.38	0.71
1:B:264:LEU:HG	1:B:602:THR:HB	1.72	0.70
1:A:264:LEU:HG	1:A:602:THR:HB	1.74	0.69
1:C:573[A]:ARG:HG3	1:C:678:VAL:HG11	1.74	0.68
1:C:576:LYS:HG3	4:C:2386:HOH:O	1.93	0.67
1:D:373:GLN:HA	1:D:373:GLN:HE21	1.60	0.66
1:A:32:THR:HG22	4:A:2011:HOH:O	1.96	0.64
1:B:640[B]:ARG:HG2	4:B:2263:HOH:O	1.96	0.64
1:D:391[B]:ARG:NE	4:D:2246:HOH:O	2.30	0.64
1:B:127[B]:ARG:NH1	4:B:2147:HOH:O	2.31	0.64
1:B:313:ILE:N	1:B:461:GLN:HE22	1.93	0.59
1:C:301:GLN:HE22	1:C:454:THR:HG21	1.67	0.59
1:B:425[B]:ARG:NE	4:B:2401:HOH:O	2.35	0.59
1:B:373:GLN:HA	1:B:373:GLN:HE21	1.68	0.59
1:B:472[B]:VAL:HG23	4:B:2450:HOH:O	2.03	0.59
1:D:472[A]:VAL:HG11	1:D:691:THR:HB	1.85	0.58
1:D:22:PRO:O	1:D:26:TYR:HD2	1.86	0.58
1:D:313:ILE:N	1:D:461:GLN:HE22	1.96	0.57
1:D:108:ASN:HD22	1:D:108:ASN:C	2.08	0.57
1:A:373:GLN:HE21	1:A:373:GLN:HA	1.70	0.56
1:C:246[A]:HIS:CE1	4:C:2173:HOH:O	2.57	0.56
1:A:155:ASN:CG	2:A:900:HDD:HMB2	2.26	0.55
1:C:697:ASP:O	1:C:698:SER:HB2	2.06	0.55
1:A:391[A]:ARG:HH11	1:A:391[A]:ARG:HG3	1.72	0.55
1:B:132:THR:HG21	1:B:264:LEU:HD13	1.89	0.54
1:B:640[B]:ARG:CG	4:B:2263:HOH:O	2.53	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:472[B]:VAL:HG23	4:D:2308:HOH:O	2.07	0.54
4:A:2162:HOH:O	1:C:127[A]:ARG:NH1	2.41	0.54
1:B:301:GLN:HE22	1:B:454:THR:HG21	1.75	0.52
1:A:503[B]:ARG:HH21	1:A:527:TYR:HE2	1.58	0.52
1:A:423:TYR:CE1	1:A:425[A]:ARG:HD2	2.45	0.51
1:D:246[A]:HIS:CE1	1:D:293:GLN:OE1	2.64	0.51
1:A:127[B]:ARG:NH1	4:A:2166:HOH:O	2.43	0.51
1:B:250:ARG:HD3	4:B:2295:HOH:O	2.09	0.51
1:B:108:ASN:HD22	1:B:108:ASN:C	2.14	0.50
1:C:22:PRO:O	1:C:26:TYR:HD2	1.94	0.50
1:A:492[B]:GLU:HG2	4:A:2523:HOH:O	2.12	0.50
1:D:469:LEU:HB3	1:D:473:GLU:HB3	1.94	0.49
1:C:373:GLN:HE21	1:C:373:GLN:HA	1.77	0.49
1:A:89:HIS:HB2	1:A:331:ARG:HB3	1.93	0.49
1:B:181:ASN:HB3	1:D:277:TRP:CE3	2.47	0.49
1:D:274[B]:GLN:CD	4:D:2187:HOH:O	2.51	0.49
1:C:568:ALA:O	1:C:572:THR:HG23	2.13	0.48
1:D:573:ARG:HH11	1:D:573:ARG:HG3	1.77	0.48
1:A:640[A]:ARG:HG2	4:A:2304:HOH:O	2.13	0.48
1:A:248[A]:LYS:HG2	4:A:2288:HOH:O	2.13	0.48
1:D:132:THR:HG21	1:D:264:LEU:HD13	1.96	0.47
1:D:573:ARG:HE	1:D:674:VAL:HB	1.79	0.47
1:B:472[A]:VAL:HG11	1:B:691:THR:HB	1.95	0.47
1:B:301:GLN:NE2	1:B:454:THR:HG21	2.30	0.47
1:C:108:ASN:HD22	1:C:108:ASN:C	2.18	0.47
1:A:155:ASN:ND2	2:A:900:HDD:HMB2	2.29	0.47
1:A:108:ASN:HD22	1:A:108:ASN:C	2.18	0.46
1:B:391[B]:ARG:C	1:B:392[B]:VAL:HG23	2.35	0.46
1:D:472[B]:VAL:HG11	1:D:691:THR:HB	1.98	0.46
1:A:130:ALA:CB	1:A:265[B]:SER:HB2	2.45	0.46
1:A:594[A]:GLN:HG3	1:A:598:THR:OG1	2.16	0.45
1:C:305:PHE:CE1	1:C:307:LEU:HD23	2.53	0.44
1:D:155:ASN:CG	2:D:900:HDD:HMB2	2.37	0.44
1:B:181:ASN:HB3	1:D:277:TRP:CZ3	2.52	0.44
1:C:492[A]:GLU:HG2	4:C:2341:HOH:O	2.17	0.44
1:C:313:ILE:N	1:C:461:GLN:HE22	1.98	0.44
1:B:155:ASN:CG	2:B:900:HDD:HMB2	2.38	0.43
1:D:277:TRP:CH2	1:D:332:ASN:HB3	2.53	0.43
1:A:246[B]:HIS:CE1	1:A:248[B]:LYS:HD3	2.54	0.43
1:B:392[B]:VAL:CG1	1:B:393:PRO:HD2	2.50	0.42
1:A:277:TRP:CZ3	1:A:332:ASN:HB3	2.54	0.42
1:C:477:LEU:C	1:C:477:LEU:HD23	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:108:ASN:ND2	1:D:108:ASN:C	2.72	0.42
1:B:35:LEU:HD21	1:B:45:ASP:HB3	2.01	0.42
1:D:138:GLY:HA3	2:D:900:HDD:HMA2	2.01	0.42
1:B:425[A]:ARG:NH2	4:B:2405:HOH:O	2.53	0.42
1:C:594[A]:GLN:HG3	1:C:598:THR:OG1	2.20	0.41
1:D:82:HIS:HA	1:D:122:THR:O	2.19	0.41
1:C:469:LEU:HB3	1:C:473:GLU:HB3	2.03	0.41
1:C:525:ASP:HA	1:C:528:TYR:CD2	2.56	0.41
1:A:472[A]:VAL:HG11	1:A:691:THR:HB	2.02	0.41
1:B:51:ALA:O	1:B:55:GLY:HA3	2.20	0.41
1:D:313:ILE:H	1:D:461:GLN:NE2	1.98	0.41
1:B:373:GLN:NE2	1:B:376:ARG:HD3	2.36	0.41
1:C:299[A]:GLN:OE1	4:C:2213:HOH:O	2.22	0.41
1:B:373:GLN:CA	1:B:373:GLN:HE21	2.34	0.41
1:B:373:GLN:HA	1:B:373:GLN:NE2	2.34	0.40
1:A:391[A]:ARG:HH11	1:A:391[A]:ARG:CG	2.34	0.40
1:C:301:GLN:NE2	1:C:454:THR:HG21	2.36	0.40
1:C:492[A]:GLU:CG	4:C:2341:HOH:O	2.69	0.40
1:B:277:TRP:CZ3	1:D:181:ASN:HB3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	716/719 (100%)	701 (98%)	15 (2%)	0	100	100
1	B	712/719 (99%)	696 (98%)	16 (2%)	0	100	100
1	C	709/719 (99%)	693 (98%)	16 (2%)	0	100	100
1	D	703/719 (98%)	688 (98%)	15 (2%)	0	100	100
All	All	2840/2876 (99%)	2778 (98%)	62 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	605/596 (102%)	597 (99%)	8 (1%)	80	66
1	B	601/596 (101%)	591 (98%)	10 (2%)	73	55
1	C	600/596 (101%)	594 (99%)	6 (1%)	85	76
1	D	594/596 (100%)	584 (98%)	10 (2%)	73	55
All	All	2400/2384 (101%)	2366 (99%)	34 (1%)	78	62

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	139	PHE
1	A	191	ASP
1	A	275	ASP
1	A	373	GLN
1	A	562	SER
1	A	676[A]	MET
1	A	676[B]	MET
1	B	70	HIS
1	B	108	ASN
1	B	139	PHE
1	B	191	ASP
1	B	264	LEU
1	B	296	ASP
1	B	373	GLN
1	B	590[A]	GLU
1	B	590[B]	GLU
1	B	660	ASP
1	C	108	ASN
1	C	139	PHE
1	C	191	ASP
1	C	373	GLN
1	C	660	ASP
1	C	698	SER
1	D	108	ASN
1	D	139	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	191	ASP
1	D	264	LEU
1	D	275	ASP
1	D	373	GLN
1	D	576	LYS
1	D	590[A]	GLU
1	D	590[B]	GLU
1	D	674	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	167	GLN
1	A	373	GLN
1	A	375	ASN
1	A	461	GLN
1	B	108	ASN
1	B	301	GLN
1	B	373	GLN
1	B	375	ASN
1	B	430	ASN
1	B	461	GLN
1	C	108	ASN
1	C	167	GLN
1	C	301	GLN
1	C	373	GLN
1	C	375	ASN
1	C	461	GLN
1	D	108	ASN
1	D	301	GLN
1	D	373	GLN
1	D	375	ASN
1	D	461	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 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	$\# Z > 2$
2	HDD	A	900	1,4	52,52,52	2.18	18 (34%)	70,89,89	3.28	24 (34%)
2	HDD	B	900	1,4	52,52,52	2.18	18 (34%)	70,89,89	3.33	27 (38%)
2	HDD	C	900	1,4	52,52,52	2.07	17 (32%)	70,89,89	3.10	27 (38%)
2	HDD	D	900	1,4	52,52,52	2.06	17 (32%)	70,89,89	2.99	25 (35%)

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
2	HDD	A	900	1,4	-	0/5/89/89	0/1/9/9
2	HDD	B	900	1,4	-	0/5/89/89	0/1/9/9
2	HDD	C	900	1,4	-	0/5/89/89	0/1/9/9
2	HDD	D	900	1,4	-	0/5/89/89	0/1/9/9

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	HDD	C1C-C2C	6.15	1.47	1.40
2	C	900	HDD	C1C-C2C	5.83	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	HDD	C4A-C3A	5.69	1.47	1.40
2	D	900	HDD	C1C-C2C	5.34	1.46	1.40
2	A	900	HDD	C4A-C3A	5.10	1.46	1.40
2	A	900	HDD	C3C-C4C	4.99	1.48	1.40
2	D	900	HDD	C4A-C3A	4.80	1.46	1.40
2	B	900	HDD	C4B-C3B	4.77	1.47	1.41
2	B	900	HDD	C1C-C2C	4.71	1.46	1.40
2	C	900	HDD	C4A-C3A	4.66	1.46	1.40
2	C	900	HDD	C4B-C3B	4.49	1.47	1.41
2	B	900	HDD	O1D-CGD	4.17	1.43	1.35
2	A	900	HDD	C4B-C3B	3.91	1.46	1.41
2	C	900	HDD	C3C-C4C	3.90	1.46	1.40
2	A	900	HDD	FE-NB	3.78	2.08	1.92
2	B	900	HDD	C3C-C4C	3.78	1.46	1.40
2	D	900	HDD	FE-NB	3.76	2.08	1.92
2	C	900	HDD	O1D-CGD	3.71	1.42	1.35
2	B	900	HDD	FE-NB	3.69	2.08	1.92
2	A	900	HDD	C3B-C2B	3.63	1.47	1.41
2	C	900	HDD	FE-NB	3.63	2.08	1.92
2	D	900	HDD	FE-NC	3.55	2.07	1.92
2	B	900	HDD	FE-NA	3.53	2.07	1.92
2	B	900	HDD	FE-NC	3.48	2.07	1.92
2	D	900	HDD	O1D-CGD	3.47	1.41	1.35
2	D	900	HDD	C4B-C3B	3.41	1.45	1.41
2	A	900	HDD	FE-NC	3.39	2.07	1.92
2	C	900	HDD	FE-NC	3.38	2.06	1.92
2	B	900	HDD	C3B-C2B	3.38	1.47	1.41
2	D	900	HDD	C1A-CHA	3.34	1.49	1.39
2	A	900	HDD	O1D-CGD	3.30	1.41	1.35
2	D	900	HDD	C3C-C4C	3.24	1.45	1.40
2	D	900	HDD	FE-NA	3.22	2.06	1.92
2	D	900	HDD	C4B-CHC	3.11	1.48	1.38
2	C	900	HDD	FE-NA	3.09	2.05	1.92
2	D	900	HDD	C1B-CHB	3.06	1.47	1.38
2	C	900	HDD	C1A-CHA	3.06	1.48	1.39
2	B	900	HDD	C1A-C2A	3.03	1.48	1.43
2	A	900	HDD	C4B-CHC	2.99	1.47	1.38
2	C	900	HDD	C3B-C2B	2.99	1.46	1.41
2	B	900	HDD	C4B-CHC	2.95	1.47	1.38
2	B	900	HDD	C2A-C3A	2.95	1.46	1.37
2	D	900	HDD	C3B-C2B	2.90	1.46	1.41
2	A	900	HDD	FE-NA	2.84	2.04	1.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	900	HDD	C4C-CHD	2.82	1.47	1.39
2	A	900	HDD	C1A-C2A	2.79	1.48	1.43
2	C	900	HDD	C4B-CHC	2.78	1.46	1.38
2	C	900	HDD	C2A-C3A	2.76	1.45	1.37
2	A	900	HDD	C1B-CHB	2.74	1.46	1.38
2	C	900	HDD	C1B-CHB	2.69	1.46	1.38
2	B	900	HDD	C1A-CHA	2.67	1.47	1.39
2	D	900	HDD	C2A-C3A	2.66	1.45	1.37
2	A	900	HDD	C1C-CHC	2.61	1.47	1.39
2	A	900	HDD	C1A-CHA	2.59	1.47	1.39
2	B	900	HDD	C3C-C2C	2.59	1.45	1.41
2	C	900	HDD	C3C-C2C	2.54	1.45	1.41
2	D	900	HDD	C1A-C2A	2.47	1.47	1.43
2	B	900	HDD	C4A-CHB	2.46	1.46	1.39
2	A	900	HDD	C4C-CHD	2.45	1.46	1.39
2	B	900	HDD	C1B-CHB	2.41	1.45	1.38
2	A	900	HDD	OND-C2D	2.36	1.47	1.42
2	D	900	HDD	C4A-CHB	2.31	1.46	1.39
2	B	900	HDD	C4C-CHD	2.30	1.46	1.39
2	D	900	HDD	C1C-CHC	2.25	1.46	1.39
2	A	900	HDD	C2A-C3A	2.24	1.44	1.37
2	A	900	HDD	C4A-CHB	2.22	1.46	1.39
2	B	900	HDD	C1C-CHC	2.21	1.45	1.39
2	C	900	HDD	C1A-C2A	2.18	1.47	1.43
2	C	900	HDD	C4A-CHB	2.15	1.45	1.39
2	C	900	HDD	C1C-CHC	2.14	1.45	1.39

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	HDD	C3C-C2C-C1C	-11.04	100.54	107.00
2	D	900	HDD	C3C-C2C-C1C	-10.51	100.85	107.00
2	A	900	HDD	C1B-C2B-C3B	-10.48	100.10	107.07
2	B	900	HDD	C1B-C2B-C3B	-10.47	100.11	107.07
2	C	900	HDD	C1B-C2B-C3B	-10.16	100.31	107.07
2	C	900	HDD	C2B-C1B-NB	9.81	116.81	109.41
2	A	900	HDD	C2B-C1B-NB	9.80	116.81	109.41
2	C	900	HDD	C3C-C2C-C1C	-9.04	101.71	107.00
2	B	900	HDD	C2B-C1B-NB	8.83	116.08	109.41
2	B	900	HDD	C2C-C1C-NC	8.26	115.65	109.41
2	A	900	HDD	C3C-C2C-C1C	-8.26	102.16	107.00
2	D	900	HDD	C1B-C2B-C3B	-8.10	101.68	107.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	HDD	C3A-C4A-NA	7.98	115.44	109.41
2	B	900	HDD	C3A-C4A-NA	7.88	115.36	109.41
2	D	900	HDD	C2C-C1C-NC	7.55	115.11	109.41
2	D	900	HDD	C2B-C1B-NB	7.33	114.94	109.41
2	A	900	HDD	C2C-C1C-NC	7.31	114.93	109.41
2	A	900	HDD	C4A-C3A-C2A	-6.96	102.16	107.00
2	C	900	HDD	C2C-C1C-NC	6.82	114.56	109.41
2	B	900	HDD	C4A-C3A-C2A	-6.60	102.40	107.00
2	B	900	HDD	C2D-C1D-ND	6.04	116.29	105.53
2	A	900	HDD	C4D-ND-C1D	-5.99	103.89	107.94
2	D	900	HDD	C3A-C4A-NA	5.96	113.91	109.41
2	A	900	HDD	C3D-C4D-ND	5.88	115.75	105.75
2	A	900	HDD	C2D-C1D-ND	5.71	115.69	105.53
2	C	900	HDD	C3D-C4D-ND	5.48	115.07	105.75
2	D	900	HDD	C2D-C1D-ND	5.37	115.10	105.53
2	C	900	HDD	C2D-C1D-ND	5.36	115.07	105.53
2	A	900	HDD	CMB-C2B-C3B	5.18	133.13	124.97
2	C	900	HDD	C3A-C4A-NA	5.00	113.19	109.41
2	C	900	HDD	C4D-ND-C1D	-5.00	104.55	107.94
2	B	900	HDD	C3C-CAC-CBC	-4.99	115.61	125.95
2	B	900	HDD	C3D-C4D-ND	4.95	114.17	105.75
2	C	900	HDD	C4A-C3A-C2A	-4.87	103.61	107.00
2	D	900	HDD	C3D-C4D-ND	4.84	113.97	105.75
2	B	900	HDD	CMC-C2C-C3C	4.60	132.22	124.97
2	B	900	HDD	C4D-ND-C1D	-4.41	104.95	107.94
2	B	900	HDD	C3B-CAB-CBB	-4.16	117.33	125.95
2	C	900	HDD	CMC-C2C-C3C	4.13	131.48	124.97
2	D	900	HDD	O1D-C3D-CAD	-4.05	102.55	105.29
2	A	900	HDD	C3A-C4A-CHB	-3.96	118.50	126.00
2	D	900	HDD	C4D-ND-C1D	-3.93	105.28	107.94
2	A	900	HDD	C3C-C4C-NC	3.91	112.44	108.64
2	D	900	HDD	C3B-CAB-CBB	-3.84	117.99	125.95
2	D	900	HDD	CMB-C2B-C3B	3.78	130.92	124.97
2	D	900	HDD	C4A-C3A-C2A	-3.71	104.42	107.00
2	D	900	HDD	CMC-C2C-C3C	3.71	130.81	124.97
2	D	900	HDD	C2C-C1C-CHC	-3.67	119.04	126.00
2	C	900	HDD	CMB-C2B-C3B	3.66	130.74	124.97
2	D	900	HDD	C4B-CHC-C1C	-3.62	122.71	127.47
2	A	900	HDD	C3C-CAC-CBC	-3.60	118.49	125.95
2	B	900	HDD	CMB-C2B-C3B	3.59	130.63	124.97
2	D	900	HDD	C4C-CHD-C1D	-3.54	122.70	130.06
2	C	900	HDD	O1D-C3D-CAD	-3.51	102.91	105.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	HDD	C1A-CHA-C4D	-3.49	122.79	130.06
2	A	900	HDD	OND-C2D-CMD	-3.44	103.60	109.57
2	D	900	HDD	C3C-C4C-NC	3.41	111.96	108.64
2	D	900	HDD	C1A-C2A-C3A	-3.41	103.39	106.92
2	C	900	HDD	C3B-CAB-CBB	-3.39	118.92	125.95
2	C	900	HDD	C3C-CAC-CBC	-3.39	118.94	125.95
2	A	900	HDD	CMC-C2C-C3C	3.35	130.24	124.97
2	C	900	HDD	C2C-C1C-CHC	-3.30	119.75	126.00
2	C	900	HDD	OND-C2D-CMD	-3.28	103.87	109.57
2	B	900	HDD	C3C-C4C-NC	3.22	111.78	108.64
2	B	900	HDD	C2C-C1C-CHC	-3.22	119.89	126.00
2	B	900	HDD	C1A-C2A-C3A	-3.21	103.60	106.92
2	D	900	HDD	CAA-CBA-CGA	-3.15	103.34	113.47
2	C	900	HDD	C3C-C4C-NC	3.09	111.65	108.64
2	A	900	HDD	C4C-CHD-C1D	-3.08	123.65	130.06
2	C	900	HDD	C3A-C4A-CHB	-3.07	120.17	126.00
2	D	900	HDD	C3C-CAC-CBC	-3.03	119.68	125.95
2	A	900	HDD	C2C-C1C-CHC	-3.00	120.30	126.00
2	B	900	HDD	C2A-C1A-NA	2.98	113.88	109.73
2	B	900	HDD	OND-C2D-CMD	-2.91	104.52	109.57
2	C	900	HDD	C4B-CHC-C1C	-2.91	123.65	127.47
2	B	900	HDD	CMA-C3A-C2A	2.81	130.24	124.94
2	B	900	HDD	O1D-C3D-CAD	-2.78	103.41	105.29
2	B	900	HDD	C3A-C4A-CHB	-2.73	120.82	126.00
2	A	900	HDD	CBA-CAA-C2A	-2.73	107.89	112.69
2	A	900	HDD	C3B-CAB-CBB	-2.72	120.32	125.95
2	D	900	HDD	C2A-C1A-NA	2.72	113.51	109.73
2	B	900	HDD	C4B-CHC-C1C	-2.67	123.95	127.47
2	A	900	HDD	CAA-CBA-CGA	-2.67	104.89	113.47
2	A	900	HDD	CMA-C3A-C2A	2.61	129.87	124.94
2	C	900	HDD	CAA-CBA-CGA	-2.53	105.35	113.47
2	A	900	HDD	C1A-CHA-C4D	-2.52	124.82	130.06
2	A	900	HDD	C4B-CHC-C1C	-2.51	124.17	127.47
2	C	900	HDD	C4C-CHD-C1D	-2.45	124.97	130.06
2	C	900	HDD	CBD-CAD-C3D	2.39	108.73	105.00
2	C	900	HDD	C1A-C2A-C3A	-2.35	104.48	106.92
2	A	900	HDD	C2D-C1D-CHD	-2.25	117.45	123.22
2	B	900	HDD	CBD-CAD-C3D	2.24	108.50	105.00
2	B	900	HDD	O1D-CGD-O2D	2.24	123.02	120.81
2	B	900	HDD	CAA-CBA-CGA	-2.21	106.37	113.47
2	D	900	HDD	C2D-C1D-CHD	-2.20	117.60	123.22
2	D	900	HDD	OND-C2D-CMD	-2.19	105.76	109.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	HDD	CAD-C3D-C2D	2.12	118.43	116.32
2	C	900	HDD	CBA-CAA-C2A	-2.10	108.98	112.69
2	B	900	HDD	C4C-CHD-C1D	-2.05	125.79	130.06
2	D	900	HDD	C3A-C4A-CHB	-2.05	122.11	126.00
2	C	900	HDD	C4B-NB-C1B	-2.04	102.52	105.58
2	B	900	HDD	C2D-C1D-CHD	-2.04	117.99	123.22
2	D	900	HDD	CBA-CAA-C2A	-2.00	109.16	112.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	674/719 (93%)	-0.48	6 (0%) 81 86	9, 16, 27, 42	0
1	B	673/719 (93%)	-0.37	6 (0%) 81 86	10, 18, 32, 46	0
1	C	672/719 (93%)	-0.38	12 (1%) 65 71	9, 17, 37, 71	0
1	D	671/719 (93%)	-0.32	20 (2%) 48 53	10, 18, 41, 76	0
All	All	2690/2876 (93%)	-0.39	44 (1%) 68 74	9, 17, 34, 76	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	672	GLU	5.4
1	C	698	SER	4.9
1	D	654	GLU	4.7
1	D	672	GLU	4.7
1	C	618	ALA	3.9
1	C	654	GLU	3.8
1	B	517	GLY	3.7
1	D	618	ALA	3.5
1	A	698	SER	3.3
1	D	576	LYS	3.2
1	D	590[A]	GLU	3.2
1	D	657	ASP	3.0
1	D	565	ASP	2.9
1	A	622	SER	2.9
1	C	649	GLY	2.8
1	D	561	SER	2.8
1	D	674	VAL	2.8
1	D	22	PRO	2.8
1	D	649	GLY	2.7
1	D	660	ASP	2.7
1	C	590[A]	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	561	SER	2.7
1	D	698	SER	2.7
1	D	673	SER	2.6
1	B	698	SER	2.5
1	D	676[A]	MET	2.5
1	C	561	SER	2.5
1	C	674	VAL	2.4
1	B	576[A]	LYS	2.4
1	D	671	GLU	2.4
1	B	657	ASP	2.3
1	B	561	SER	2.3
1	C	21	SER	2.3
1	A	664	ASP	2.2
1	C	660	ASP	2.2
1	D	611	ASP	2.2
1	A	318	TYR	2.1
1	C	653	SER	2.1
1	D	573	ARG	2.1
1	A	590[A]	GLU	2.0
1	D	562	SER	2.0
1	D	659	ALA	2.0
1	B	664	ASP	2.0
1	C	657	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CA	B	1701	1/1	0.08	10.69	22,22,22,22	1
3	CA	C	1699	1/1	0.09	6.94	11,11,11,11	1
3	CA	B	1699	1/1	0.10	3.37	15,15,15,15	1
3	CA	D	1699	1/1	0.10	3.27	15,15,15,15	1
3	CA	A	1700	1/1	0.10	1.89	17,17,17,17	1
3	CA	A	1699	1/1	0.07	1.70	14,14,14,14	1
2	HDD	B	900	44/44	0.07	0.75	12,15,16,18	0
2	HDD	C	900	44/44	0.08	0.36	11,13,17,19	0
2	HDD	D	900	44/44	0.08	0.25	12,14,16,19	0
2	HDD	A	900	44/44	0.07	0.02	10,13,15,16	0
3	CA	B	1700	1/1	0.07	-0.39	27,27,27,27	1
3	CA	D	1700	1/1	0.05	-1.13	26,26,26,26	1
3	CA	C	1700	1/1	0.05	-2.42	21,21,21,21	1

6.5 Other polymers ⓘ

There are no such residues in this entry.