Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2024 – 03:57 pm BST

PDB ID	:	5M4O
Title	:	Crystal structure of hydroquinone 1,2-dioxygenase from Sphingomonas sp. TTNP3 in complex with 4-nitrophenol
Authors	:	Ferraroni, M.; Da Vela, S.; Scozzafava, A.; Kolvenbach, B.; Corvini, P.F.X.
Deposited on	:	2016-10-18
Resolution	:	2.10 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

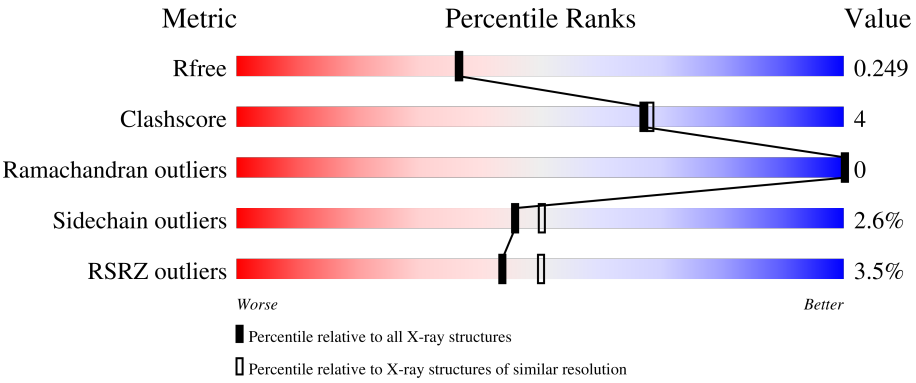
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.10 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.



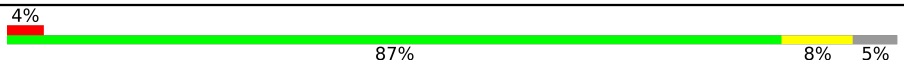
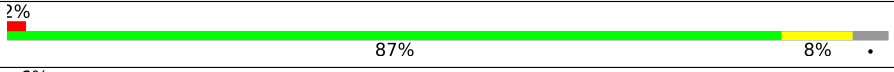
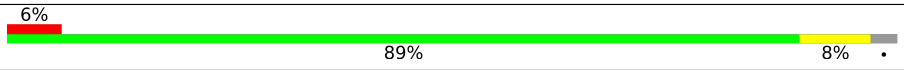
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	170	2% 84% 13% • •
1	C	170	2% 91% 8% •
1	E	170	5% 92% 6% •
1	G	170	6% 85% 11% •
2	B	341	87% 7% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	341	
2	F	341	
2	H	341	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16487 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 Hydroquinone dioxygenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1275	808	216	245	6			
1	C	167	Total	C	N	O	S	0	0	0
			1284	813	217	248	6			
1	E	167	Total	C	N	O	S	0	0	0
			1275	808	213	248	6			
1	G	164	Total	C	N	O	S	0	0	0
			1253	796	211	240	6			

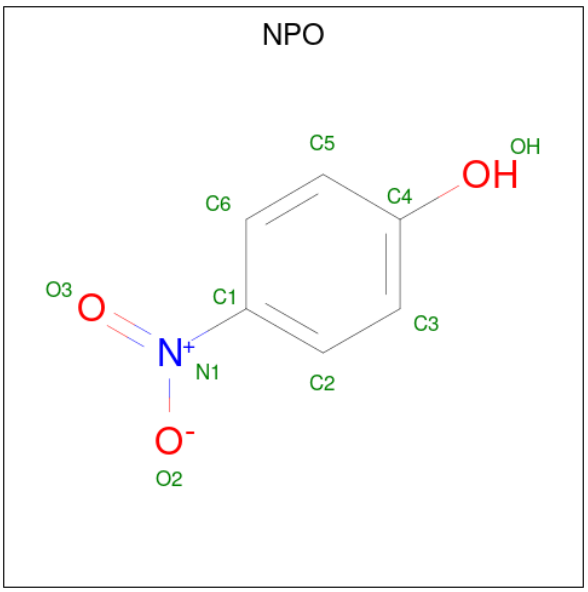
- Molecule 2 is a protein called Hydroquinone dioxygenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	325	Total	C	N	O	S	0	2	0
			2573	1630	448	481	14			
2	D	324	Total	C	N	O	S	0	0	0
			2533	1603	441	475	14			
2	F	326	Total	C	N	O	S	0	4	0
			2579	1633	450	480	16			
2	H	332	Total	C	N	O	S	0	2	0
			2595	1642	453	486	14			

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Fe	0	0
			1	1		
3	D	1	Total	Fe	0	0
			1	1		
3	F	1	Total	Fe	0	0
			1	1		
3	H	1	Total	Fe	0	0
			1	1		

- Molecule 4 is P-NITROPHENOL (three-letter code: NPO) (formula: $C_6H_5NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 10 6 1 3	0	0
4	D	1	Total C N O 10 6 1 3	0	0
4	F	1	Total C N O 10 6 1 3	0	0
4	H	1	Total C N O 10 6 1 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	88	Total O 88 88	0	0
5	B	241	Total O 241 241	0	0
5	C	101	Total O 101 101	0	0
5	D	197	Total O 197 197	0	0
5	E	71	Total O 71 71	0	0
5	F	161	Total O 161 161	0	0
5	G	37	Total O 37 37	0	0

Continued on next page...

Continued from previous page...

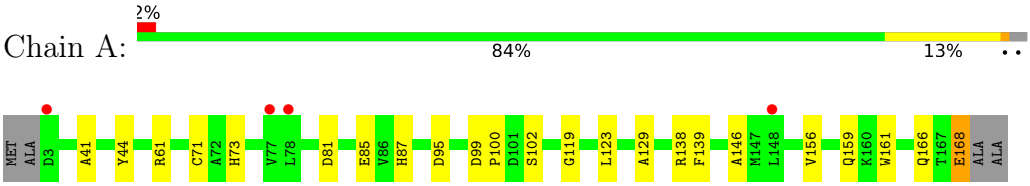
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	180	Total 180	O 180	0	0

3 Residue-property plots (i)

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

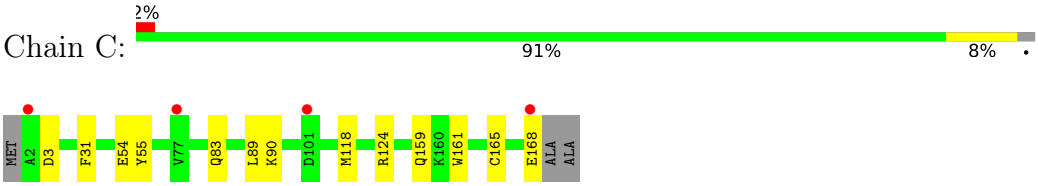
• Molecule 1: Hydroquinone dioxygenase small subunit

Chain A:



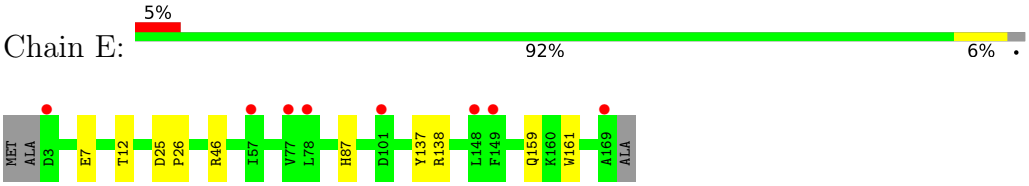
• Molecule 1: Hydroquinone dioxygenase small subunit

Chain C:



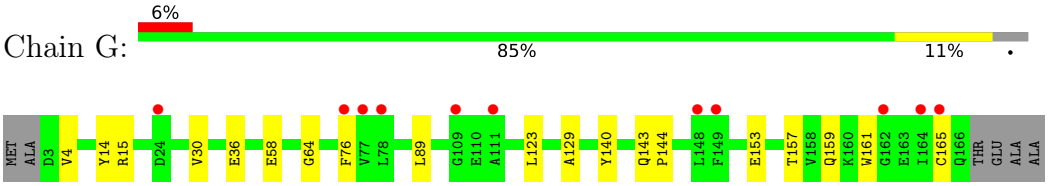
• Molecule 1: Hydroquinone dioxygenase small subunit

Chain E:



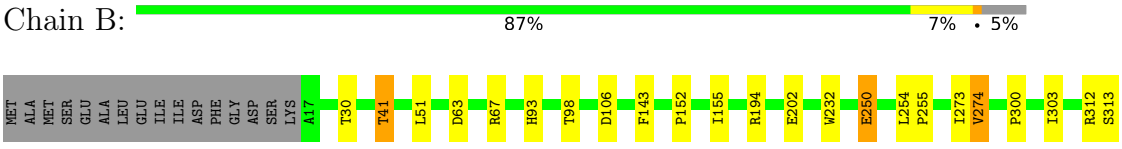
• Molecule 1: Hydroquinone dioxygenase small subunit

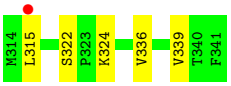
Chain G:



• Molecule 2: Hydroquinone dioxygenase large subunit

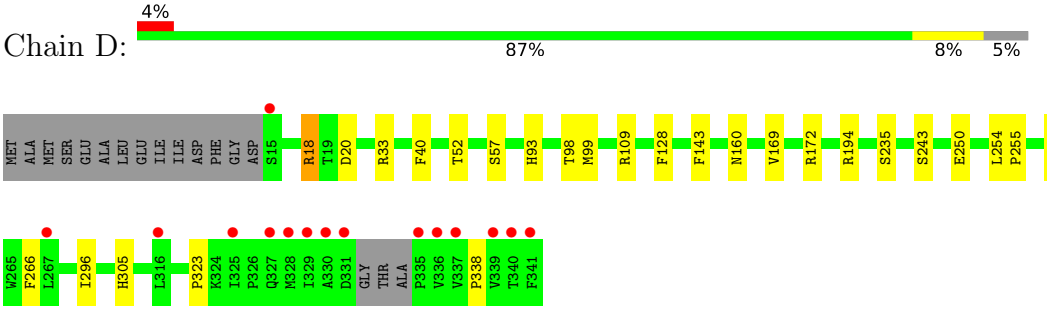
Chain B:





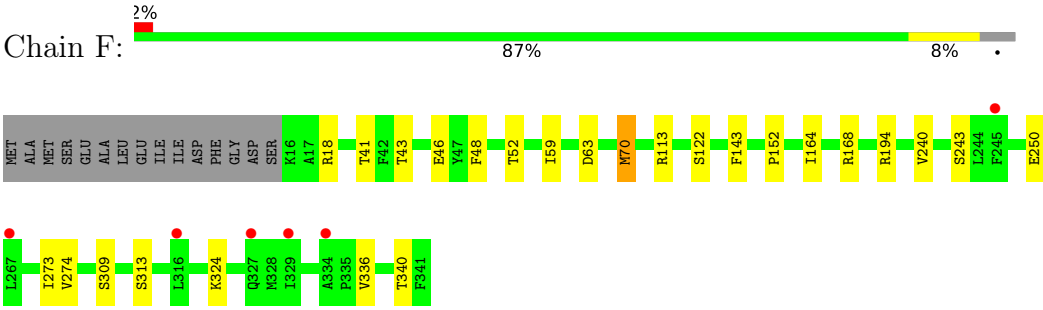
• Molecule 2: Hydroquinone dioxygenase large subunit

Chain D:



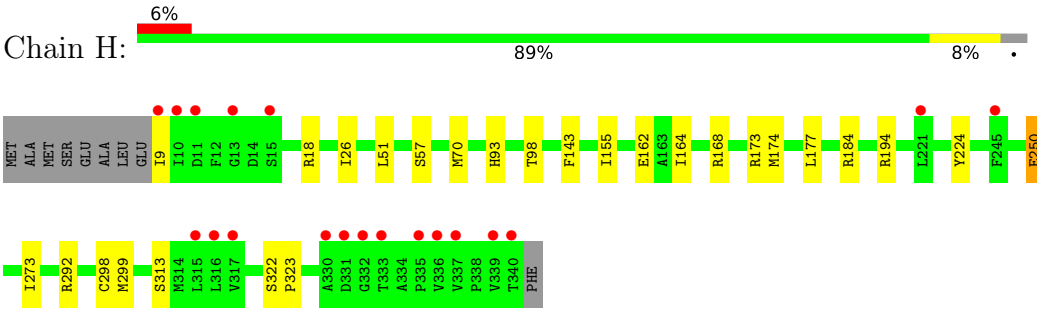
• Molecule 2: Hydroquinone dioxygenase large subunit

Chain F:



• Molecule 2: Hydroquinone dioxygenase large subunit

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.99Å 125.98Å 92.33Å 90.00° 105.14° 90.00°	Depositor
Resolution (Å)	29.70 – 2.10 29.79 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.70-2.10) 98.3 (29.79-2.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.188 , 0.249 0.192 , 0.249	Depositor DCC
R_{free} test set	6331 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16487	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0/1302	0.57	0/1766
1	C	0.41	0/1311	0.61	0/1778
1	E	0.39	0/1302	0.59	0/1768
1	G	0.37	0/1280	0.57	0/1737
2	B	0.44	0/2652	0.63	0/3606
2	D	0.44	0/2605	0.59	0/3543
2	F	0.40	0/2660	0.57	0/3615
2	H	0.41	0/2674	0.59	0/3638
All	All	0.41	0/15786	0.59	0/21451

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	1275	0	1220	17	0
1	C	1284	0	1229	6	0
1	E	1275	0	1209	6	0
1	G	1253	0	1196	17	0
2	B	2573	0	2437	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2533	0	2353	23	0
2	F	2579	0	2438	18	0
2	H	2595	0	2423	22	0
3	B	1	0	0	0	0
3	D	1	0	0	1	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
4	B	10	0	5	1	0
4	D	10	0	4	0	0
4	F	10	0	4	1	0
4	H	10	0	4	0	0
5	A	88	0	0	1	0
5	B	241	0	0	5	0
5	C	101	0	0	1	0
5	D	197	0	0	5	0
5	E	71	0	0	2	0
5	F	161	0	0	5	0
5	G	37	0	0	1	0
5	H	180	0	0	6	0
All	All	16487	0	14522	117	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 4.

All (117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:250[B]:GLU:OE1	2:F:313[B]:SER:HB2	1.37	1.21
2:D:172:ARG:HB2	5:D:676:HOH:O	1.48	1.10
1:G:58:GLU:OE2	1:G:157:THR:HG22	1.59	1.02
1:A:159:GLN:HE21	1:A:161:TRP:HE1	1.02	0.94
2:D:99:MET:HE2	2:D:128:PHE:HZ	1.35	0.91
1:E:159:GLN:HE21	1:E:161:TRP:HE1	1.20	0.89
2:D:305:HIS:HE1	5:D:526:HOH:O	1.57	0.87
2:F:41:THR:HG22	2:F:52:THR:OG1	1.75	0.87
2:B:250[B]:GLU:OE2	2:B:313[B]:SER:HB2	1.77	0.84
2:H:250[B]:GLU:CD	2:H:273:ILE:HD11	1.99	0.84
2:H:250[B]:GLU:OE1	2:H:313[B]:SER:OG	1.96	0.83
2:D:305:HIS:CE1	5:D:526:HOH:O	2.30	0.82
2:H:70:MET:HE1	2:H:164:ILE:HG22	1.61	0.81
2:D:99:MET:CE	2:D:128:PHE:HZ	1.97	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:260:ASN:HB2	5:D:526:HOH:O	1.82	0.78
1:G:159:GLN:HE21	1:G:161:TRP:HE1	1.27	0.78
2:D:99:MET:HE2	2:D:128:PHE:CZ	2.19	0.77
2:D:99:MET:CE	2:D:128:PHE:CZ	2.68	0.76
2:H:93:HIS:HE1	2:H:98:THR:OG1	1.71	0.73
1:G:89:LEU:HG	5:G:220:HOH:O	1.89	0.72
2:D:18:ARG:HD3	2:D:20:ASP:OD1	1.90	0.72
1:A:100:PRO:HG3	2:D:323:PRO:HG2	1.73	0.70
2:H:250[B]:GLU:CD	2:H:313[B]:SER:OG	2.29	0.70
1:C:159:GLN:HE21	1:C:161:TRP:HE1	1.40	0.69
2:B:93:HIS:HE1	2:B:98:THR:OG1	1.77	0.68
2:H:263:CYS:HB3	5:H:570:HOH:O	1.93	0.68
2:F:250[B]:GLU:CD	2:F:273:ILE:HD11	2.14	0.68
2:B:202:GLU:HB2	5:B:663:HOH:O	1.95	0.67
2:H:250[B]:GLU:OE2	2:H:313[B]:SER:OG	2.11	0.67
1:G:143:GLN:HG3	1:G:144:PRO:HD2	1.78	0.66
2:D:264:GLU:OE1	3:D:401:FE:FE	1.49	0.66
1:E:87:HIS:HE1	5:E:821:HOH:O	1.80	0.64
1:A:95:ASP:OD2	2:D:323:PRO:HG3	1.99	0.62
1:G:159:GLN:NE2	1:G:161:TRP:HE1	1.99	0.59
2:H:9:ILE:HA	5:H:659:HOH:O	2.02	0.59
1:C:168:GLU:HB3	5:C:284:HOH:O	2.03	0.59
2:D:99:MET:HE1	2:D:128:PHE:CZ	2.38	0.58
2:F:41:THR:HG23	5:F:506:HOH:O	2.02	0.58
2:F:70[A]:MET:HE1	2:F:164:ILE:HG22	1.86	0.58
2:B:41:THR:HG22	5:B:521:HOH:O	2.03	0.58
1:G:76:PHE:CD1	2:H:174:MET:CE	2.88	0.57
2:F:240:VAL:HG13	2:F:243:SER:HB3	1.87	0.56
1:G:76:PHE:HD1	2:H:174:MET:CE	2.18	0.56
2:F:18:ARG:HD2	5:F:604:HOH:O	2.05	0.56
1:A:123:LEU:HD21	1:A:129:ALA:HB2	1.87	0.54
2:B:250[B]:GLU:CD	2:B:273:ILE:HD11	2.28	0.54
2:B:322:SER:OG	2:B:324:LYS:HG2	2.06	0.54
2:H:184:ARG:HG3	2:H:224:TYR:CE1	2.43	0.54
1:E:87:HIS:HD2	5:E:866:HOH:O	1.90	0.53
2:H:250[B]:GLU:OE2	2:H:273:ILE:HD11	2.09	0.53
2:F:70[A]:MET:CE	2:F:164:ILE:HA	2.39	0.53
1:G:76:PHE:CD1	2:H:174:MET:HE3	2.43	0.53
2:B:274:VAL:HG22	5:B:535:HOH:O	2.08	0.53
1:C:55:TYR:CD1	2:D:243:SER:HB2	2.44	0.53
2:F:168:ARG:HG2	5:F:650:HOH:O	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:VAL:HG12	5:A:230:HOH:O	2.10	0.52
1:C:83:GLN:HE21	1:C:124:ARG:HD2	1.74	0.52
1:G:76:PHE:HD1	2:H:174:MET:HE3	1.74	0.52
2:D:263:CYS:SG	2:D:338:PRO:HD3	2.50	0.51
2:H:266:PHE:CE2	2:H:299:MET:HG3	2.45	0.51
1:A:81:ASP:HB3	1:A:146:ALA:H	1.76	0.50
1:A:87:HIS:ND1	1:A:138:ARG:NH1	2.60	0.50
2:F:113:ARG:HD2	5:F:631:HOH:O	2.11	0.50
1:G:15:ARG:O	2:H:292:ARG:HD2	2.11	0.50
1:E:25:ASP:OD1	1:E:26:PRO:HD2	2.11	0.50
2:B:41:THR:CG2	5:B:521:HOH:O	2.58	0.49
1:C:31:PHE:O	1:C:165:CYS:HA	2.12	0.49
2:H:184:ARG:HD3	5:H:653:HOH:O	2.11	0.49
2:B:232:TRP:HA	4:B:402:NPO:OH	2.12	0.49
1:G:153:GLU:HA	1:G:157:THR:HG21	1.93	0.49
2:D:93:HIS:HE1	2:D:98:THR:OG1	1.95	0.48
2:F:63:ASP:HB3	2:F:152:PRO:HG3	1.94	0.48
2:H:18:ARG:HD2	5:H:596:HOH:O	2.14	0.47
1:G:76:PHE:CD1	2:H:174:MET:HE2	2.50	0.47
2:H:173:ARG:HD3	2:H:177:LEU:HD13	1.96	0.47
2:H:322:SER:HA	2:H:323:PRO:HD3	1.81	0.46
1:A:159:GLN:NE2	1:A:161:TRP:HE1	1.87	0.46
1:G:123:LEU:HD21	1:G:129:ALA:HB2	1.98	0.46
2:B:30:THR:HA	2:B:155:ILE:HG22	1.97	0.46
2:F:70[A]:MET:HE1	2:F:164:ILE:HA	1.98	0.46
1:G:64:GLY:O	1:G:140:TYR:HA	2.16	0.46
2:D:99:MET:HE1	2:D:128:PHE:CE1	2.51	0.45
2:F:324:LYS:HA	5:F:651:HOH:O	2.16	0.45
2:F:48:PHE:HB3	2:F:59:ILE:HG23	1.97	0.45
2:F:250[B]:GLU:OE1	2:F:273:ILE:HD11	2.15	0.45
2:B:250[B]:GLU:OE2	2:B:273:ILE:HD11	2.17	0.45
1:G:14:TYR:OH	1:G:36:GLU:HG3	2.17	0.45
1:A:100:PRO:HG3	2:D:323:PRO:CG	2.45	0.45
1:E:87:HIS:O	1:E:137:TYR:HA	2.18	0.44
2:F:274:VAL:CG2	5:H:504:HOH:O	2.64	0.44
1:A:119:GLY:HA2	5:B:558:HOH:O	2.16	0.44
1:A:161:TRP:CD2	2:B:339:VAL:HG11	2.52	0.44
2:B:250[A]:GLU:OE2	2:B:315:LEU:HD23	2.18	0.44
2:H:70:MET:CE	2:H:164:ILE:HA	2.48	0.43
2:B:106:ASP:OD1	2:B:106:ASP:N	2.52	0.43
2:D:169:VAL:HG23	2:D:235:SER:OG	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:CYS:SG	1:A:73:HIS:CE1	3.11	0.43
1:C:90:LYS:HB2	1:C:118:MET:HG3	2.00	0.43
2:F:46:GLU:HG3	5:H:508:HOH:O	2.19	0.43
1:A:166:GLN:HE21	1:A:168:GLU:HB2	1.84	0.43
2:F:266:PHE:HZ	4:F:402:NPO:O3	2.01	0.42
2:B:67:ARG:HB3	2:B:255:PRO:HB3	2.00	0.42
2:D:40:PHE:HA	2:D:52:THR:O	2.20	0.42
2:B:300:PRO:O	2:B:303:ILE:HG13	2.21	0.41
1:A:85:GLU:O	1:A:139:PHE:HA	2.20	0.41
2:B:254:LEU:HA	2:B:255:PRO:HD3	1.90	0.41
1:G:58:GLU:OE2	1:G:157:THR:CG2	2.48	0.41
2:D:33:ARG:NE	5:D:509:HOH:O	2.54	0.41
1:E:46:ARG:NH1	1:E:137:TYR:OH	2.44	0.41
1:G:30:VAL:HG12	1:G:165:CYS:SG	2.60	0.41
2:B:63:ASP:HB3	2:B:152:PRO:HG3	2.02	0.40
2:D:254:LEU:HA	2:D:255:PRO:HD3	1.86	0.40
1:A:99:ASP:HB3	1:A:102:SER:HB3	2.03	0.40
1:A:41:ALA:O	1:A:61:ARG:NH1	2.47	0.40
1:A:44:TYR:CE1	1:A:139:PHE:HB2	2.56	0.40
2:D:266:PHE:O	2:D:296:ILE:HA	2.22	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	164/170 (96%)	157 (96%)	7 (4%)	0	100	100
1	C	165/170 (97%)	155 (94%)	10 (6%)	0	100	100
1	E	165/170 (97%)	159 (96%)	6 (4%)	0	100	100
1	G	162/170 (95%)	152 (94%)	10 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	325/341 (95%)	310 (95%)	15 (5%)	0	100	100
2	D	320/341 (94%)	306 (96%)	14 (4%)	0	100	100
2	F	328/341 (96%)	311 (95%)	17 (5%)	0	100	100
2	H	332/341 (97%)	316 (95%)	16 (5%)	0	100	100
All	All	1961/2044 (96%)	1866 (95%)	95 (5%)	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	128/131 (98%)	127 (99%)	1 (1%)	81	86
1	C	129/131 (98%)	126 (98%)	3 (2%)	50	55
1	E	127/131 (97%)	124 (98%)	3 (2%)	49	53
1	G	125/131 (95%)	124 (99%)	1 (1%)	81	86
2	B	271/284 (95%)	263 (97%)	8 (3%)	41	44
2	D	261/284 (92%)	254 (97%)	7 (3%)	44	48
2	F	269/284 (95%)	259 (96%)	10 (4%)	34	35
2	H	267/284 (94%)	256 (96%)	11 (4%)	30	31
All	All	1577/1660 (95%)	1533 (97%)	44 (3%)	46	47

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	GLU
2	B	41	THR
2	B	51	LEU
2	B	143	PHE
2	B	194	ARG
2	B	250[A]	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	250[B]	GLU
2	B	274	VAL
2	B	336	VAL
1	C	3	ASP
1	C	54	GLU
1	C	89	LEU
2	D	18	ARG
2	D	57	SER
2	D	109	ARG
2	D	143	PHE
2	D	160	ASN
2	D	194	ARG
2	D	250	GLU
1	E	7	GLU
1	E	12	THR
1	E	138	ARG
2	F	43	THR
2	F	70[A]	MET
2	F	70[B]	MET
2	F	122	SER
2	F	143	PHE
2	F	194	ARG
2	F	262	ARG
2	F	309	SER
2	F	336	VAL
2	F	340	THR
1	G	4	VAL
2	H	26	ILE
2	H	51	LEU
2	H	57	SER
2	H	143	PHE
2	H	155	ILE
2	H	162	GLU
2	H	168	ARG
2	H	194	ARG
2	H	250[A]	GLU
2	H	250[B]	GLU
2	H	298	CYS

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

Mol	Chain	Res	Type
1	A	28	ASN
1	A	83	GLN
1	A	159	GLN
2	B	83	ASN
2	B	93	HIS
1	C	28	ASN
1	C	40	ASN
1	C	83	GLN
1	C	159	GLN
2	D	83	ASN
2	D	93	HIS
2	D	160	ASN
2	D	203	GLN
1	E	28	ASN
1	E	40	ASN
1	E	83	GLN
1	E	87	HIS
1	E	159	GLN
1	G	40	ASN
1	G	159	GLN
2	H	28	ASN
2	H	93	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
4	NPO	H	402	3	9,10,10	3.27	1 (11%)	11,13,13	1.07	1 (9%)
4	NPO	D	402	3	9,10,10	3.32	2 (22%)	11,13,13	1.21	1 (9%)
4	NPO	B	402	3	9,10,10	3.33	1 (11%)	11,13,13	0.81	1 (9%)
4	NPO	F	402	3	9,10,10	3.17	2 (22%)	11,13,13	0.89	1 (9%)

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
4	NPO	H	402	3	-	0/2/4/4	0/1/1/1
4	NPO	D	402	3	-	2/2/4/4	0/1/1/1
4	NPO	B	402	3	-	0/2/4/4	0/1/1/1
4	NPO	F	402	3	-	0/2/4/4	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	NPO	O3-N1	9.69	1.39	1.22
4	H	402	NPO	O3-N1	9.56	1.39	1.22
4	D	402	NPO	O3-N1	9.41	1.38	1.22
4	F	402	NPO	O3-N1	9.15	1.38	1.22
4	D	402	NPO	C1-N1	-3.02	1.37	1.45
4	F	402	NPO	C1-N1	-2.22	1.39	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	402	NPO	C2-C1-N1	3.06	121.68	119.38
4	D	402	NPO	C2-C1-N1	-2.39	117.58	119.38
4	F	402	NPO	O3-N1-C1	2.38	122.17	118.80
4	B	402	NPO	O3-N1-C1	2.27	122.01	118.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	402	NPO	C2-C1-N1-O3
4	D	402	NPO	C6-C1-N1-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	402	NPO	1	0
4	F	402	NPO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	166/170 (97%)	-0.06	4 (2%)	59	64	22, 32, 45, 56	0
1	C	167/170 (98%)	-0.16	4 (2%)	59	64	21, 31, 54, 72	0
1	E	167/170 (98%)	0.19	8 (4%)	30	36	23, 35, 51, 66	0
1	G	164/170 (96%)	0.40	11 (6%)	17	22	29, 44, 63, 78	0
2	B	325/341 (95%)	-0.26	1 (0%)	94	94	20, 27, 40, 55	0
2	D	324/341 (95%)	-0.09	15 (4%)	32	38	19, 29, 50, 97	0
2	F	326/341 (95%)	-0.14	6 (1%)	68	72	22, 32, 52, 69	0
2	H	332/341 (97%)	0.03	19 (5%)	23	29	23, 33, 64, 90	0
All	All	1971/2044 (96%)	-0.04	68 (3%)	44	50	19, 31, 54, 97	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	333	THR	5.9
2	H	330	ALA	5.6
2	D	340	THR	4.9
2	H	9	ILE	4.8
2	H	335	PRO	4.6
2	H	332	GLY	4.2
1	E	169	ALA	4.2
1	E	148	LEU	4.2
2	D	331	ASP	4.0
2	D	329	ILE	4.0
2	H	10	ILE	4.0
1	E	78	LEU	3.8
1	C	2	ALA	3.8
1	A	78	LEU	3.7
2	D	341	PHE	3.6
2	H	316	LEU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	149	PHE	3.6
2	F	267	LEU	3.6
2	D	328	MET	3.4
1	E	57	ILE	3.4
2	D	330	ALA	3.3
1	E	77	VAL	3.3
1	G	78	LEU	3.2
1	A	148	LEU	3.1
2	H	339	VAL	3.0
2	F	245	PHE	3.0
2	D	335	PRO	2.9
2	F	327	GLN	2.8
1	G	77	VAL	2.8
2	H	336	VAL	2.7
1	E	3	ASP	2.7
2	D	336	VAL	2.6
2	H	340	THR	2.6
2	H	245	PHE	2.5
2	H	337	VAL	2.5
1	G	162	GLY	2.5
2	B	315	LEU	2.5
2	F	316	LEU	2.5
2	F	334	ALA	2.5
2	D	316	LEU	2.4
1	G	164	ILE	2.4
1	G	24	ASP	2.4
2	H	331	ASP	2.4
1	G	148	LEU	2.4
1	G	109	GLY	2.4
1	E	101	ASP	2.4
1	A	77	VAL	2.3
1	A	3	ASP	2.3
2	D	339	VAL	2.3
2	H	13	GLY	2.3
1	C	101	ASP	2.3
2	H	15	SER	2.2
2	H	317	VAL	2.2
2	H	11	ASP	2.2
1	G	165	CYS	2.2
1	G	76	PHE	2.2
2	D	337	VAL	2.2
2	D	267	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	15	SER	2.1
2	H	221	LEU	2.1
2	H	315	LEU	2.1
1	G	111	ALA	2.1
2	D	325	ILE	2.1
1	C	77	VAL	2.1
1	C	168	GLU	2.1
2	D	327	GLN	2.1
2	F	329	ILE	2.0
1	G	149	PHE	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
4	NPO	B	402	10/10	0.92	0.16	29,30,33,37	0
4	NPO	D	402	10/10	0.94	0.15	31,33,37,38	0
4	NPO	F	402	10/10	0.95	0.14	31,32,42,43	0
3	FE	H	401	1/1	0.98	0.07	42,42,42,42	0
4	NPO	H	402	10/10	0.98	0.15	37,39,47,48	0
3	FE	F	401	1/1	0.99	0.10	32,32,32,32	0
3	FE	D	401	1/1	0.99	0.07	37,37,37,37	0
3	FE	B	401	1/1	1.00	0.09	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.