Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 12:23 am GMT

PDB ID	:	5M22
Title	:	Crystal structure of hydroquinone 1,2-dioxygenase from Sphingomonas sp. TTNP3
Authors	:	Ferraroni, M.; Da Vela, S.; Scozzafava, A.; Kolvenbach, B.; Corvini, P.F.X.
Deposited on	:	2016-10-11
Resolution	:	2.40 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:

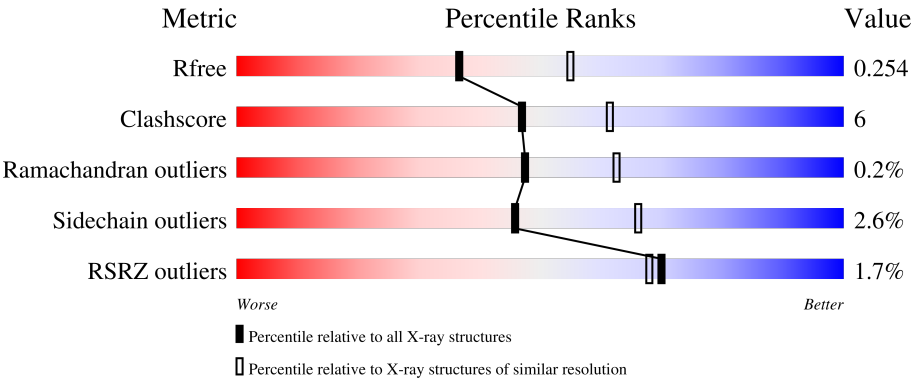
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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% 88% 9% • •
1	C	170	% 88% 10% •
1	E	170	4% 86% 11% • •
1	G	170	% 84% 12% • •
2	B	341	89% 6% • 5%

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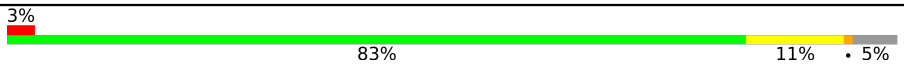
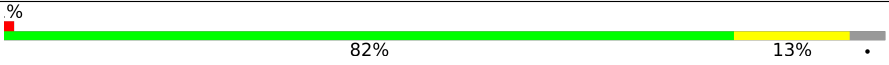
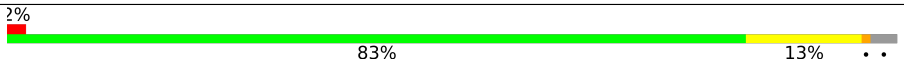
Mol	Chain	Length	Quality of chain
2	D	341	
2	F	341	
2	H	341	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15986 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
			1271	806	216	243	6			
1	C	166	Total	C	N	O	S	0	0	0
			1282	811	216	249	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
			1248	793	210	239	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	0	0
			2558	1623	447	474	14			
2	D	325	Total	C	N	O	S	0	0	0
			2536	1602	442	478	14			
2	F	326	Total	C	N	O	S	0	1	0
			2558	1619	448	476	15			
2	H	331	Total	C	N	O	S	0	0	0
			2577	1632	451	480	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		

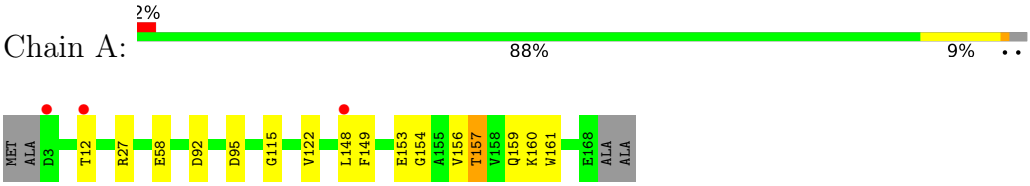
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	50	Total O 50 50	0	0
4	B	126	Total O 126 126	0	0
4	C	59	Total O 59 59	0	0
4	D	126	Total O 126 126	0	0
4	E	52	Total O 52 52	0	0
4	F	109	Total O 109 109	0	0
4	G	29	Total O 29 29	0	0
4	H	126	Total O 126 126	0	0

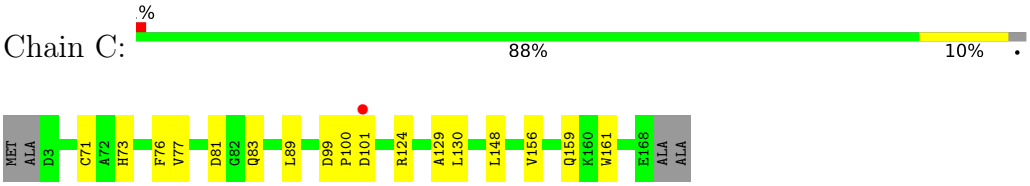
3 Residue-property plots (i)

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.

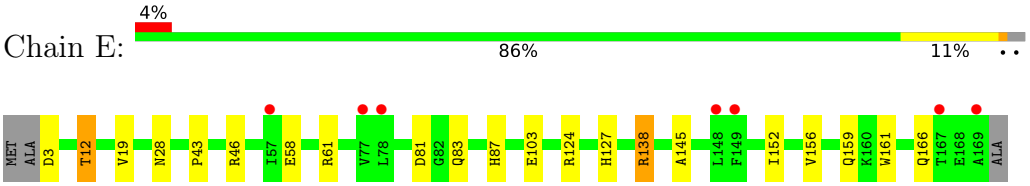
• Molecule 1: Hydroquinone dioxygenase small subunit



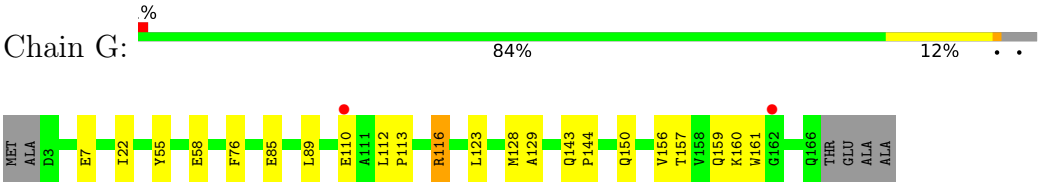
• Molecule 1: Hydroquinone dioxygenase small subunit



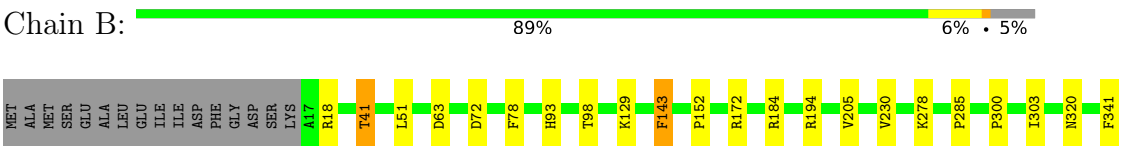
• Molecule 1: Hydroquinone dioxygenase small subunit



• Molecule 1: Hydroquinone dioxygenase small subunit

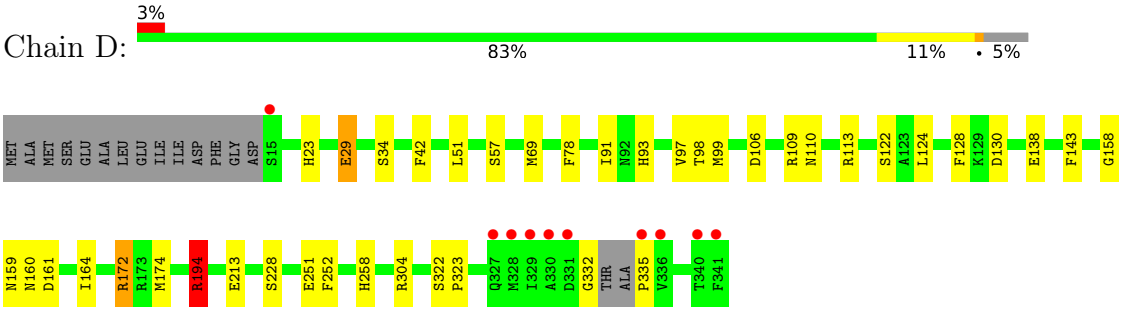


• Molecule 2: Hydroquinone dioxygenase large subunit



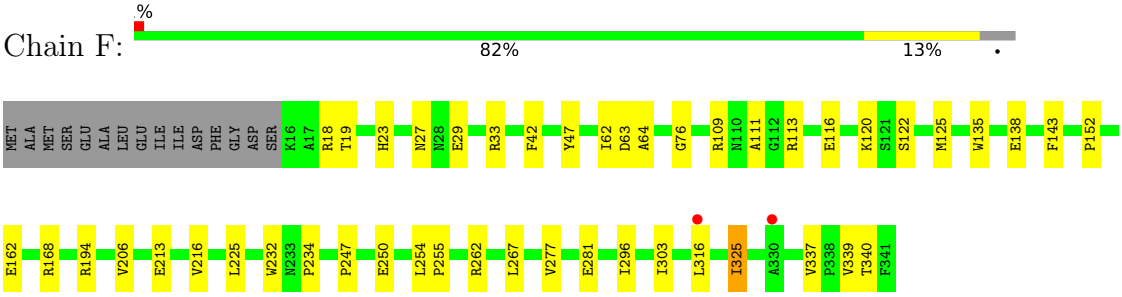
• Molecule 2: Hydroquinone dioxygenase large subunit

Chain D:



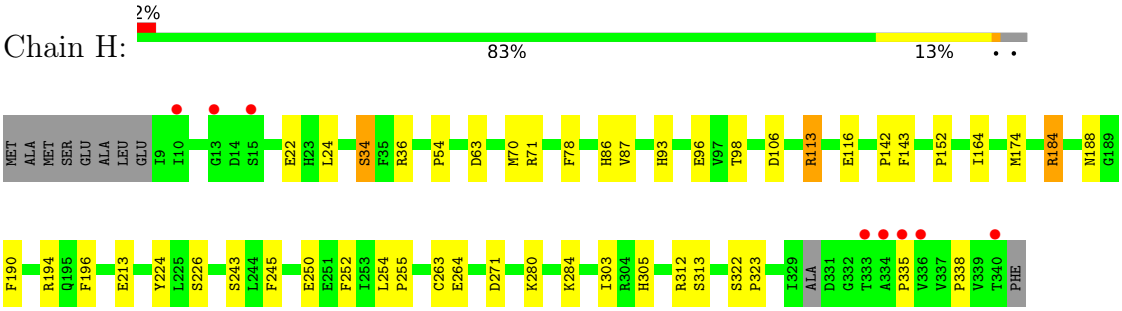
• Molecule 2: Hydroquinone dioxygenase large subunit

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	89.33Å 126.09Å 92.97Å 90.00° 105.02° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-2.40) 97.4 (29.98-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.178 , 0.254 0.178 , 0.254	Depositor DCC
R_{free} test set	3643 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15986	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: 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	0.59	0/1298	0.75	0/1761
1	C	0.62	0/1309	0.78	0/1775
1	E	0.63	0/1302	0.77	1/1768 (0.1%)
1	G	0.56	0/1275	0.74	1/1730 (0.1%)
2	B	0.64	0/2631	0.79	2/3578 (0.1%)
2	D	0.64	0/2607	0.80	1/3546 (0.0%)
2	F	0.62	0/2633	0.76	0/3580
2	H	0.63	0/2649	0.77	0/3602
All	All	0.62	0/15704	0.77	5/21340 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	194	ARG	NE-CZ-NH1	7.21	123.90	120.30
2	B	184	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	G	89	LEU	CA-CB-CG	5.69	128.38	115.30
2	B	72	ASP	CB-CG-OD1	5.56	123.31	118.30
1	E	138	ARG	NE-CZ-NH2	-5.38	117.61	120.30

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	1271	0	1216	14	0
1	C	1282	0	1226	19	0
1	E	1275	0	1209	15	0
1	G	1248	0	1186	24	0
2	B	2558	0	2419	14	0
2	D	2536	0	2358	44	0
2	F	2558	0	2408	28	0
2	H	2577	0	2396	51	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	1	0
4	A	50	0	0	0	0
4	B	126	0	0	5	0
4	C	59	0	0	1	0
4	D	126	0	0	7	0
4	E	52	0	0	3	0
4	F	109	0	0	6	0
4	G	29	0	0	2	0
4	H	126	0	0	7	0
All	All	15986	0	14418	183	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 6.

All (183) 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:H:106:ASP:HB3	4:H:586:HOH:O	1.33	1.26
1:C:76:PHE:HD2	2:D:174:MET:HE2	1.23	1.02
1:G:76:PHE:CD1	2:H:174:MET:CE	2.46	0.98
1:C:76:PHE:CD2	2:D:174:MET:HE2	1.99	0.97
2:F:281:GLU:HG3	4:F:599:HOH:O	1.66	0.93
1:E:159:GLN:HE21	1:E:161:TRP:HE1	0.98	0.93
1:G:116:ARG:HH11	1:G:116:ARG:HG3	1.32	0.93
1:A:159:GLN:HE21	1:A:161:TRP:HE1	1.10	0.93
1:C:76:PHE:HD2	2:D:174:MET:CE	1.84	0.90
1:G:58:GLU:OE2	1:G:157:THR:HG22	1.72	0.90
2:D:109:ARG:HD2	4:D:578:HOH:O	1.73	0.88
1:C:76:PHE:CD2	2:D:174:MET:CE	2.57	0.85
1:G:76:PHE:HD1	2:H:174:MET:CE	1.85	0.85
2:F:116:GLU:HG2	4:F:577:HOH:O	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:THR:HB	4:E:225:HOH:O	1.76	0.83
1:G:76:PHE:CD1	2:H:174:MET:HE3	2.15	0.81
1:E:87:HIS:HD2	4:E:247:HOH:O	1.64	0.80
2:D:109:ARG:CD	4:D:578:HOH:O	2.28	0.80
1:G:76:PHE:CD1	2:H:174:MET:HE2	2.15	0.80
1:A:154:GLY:H	1:A:157:THR:CG2	1.96	0.79
1:E:43:PRO:HD3	1:E:61:ARG:NH2	1.98	0.78
1:E:19:VAL:H	1:E:166:GLN:HE22	1.31	0.77
2:B:129:LYS:HE2	4:B:604:HOH:O	1.85	0.77
2:H:93:HIS:HE1	2:H:98:THR:OG1	1.68	0.77
1:A:95:ASP:OD2	2:D:323:PRO:HG3	1.85	0.76
1:E:159:GLN:NE2	1:E:161:TRP:HE1	1.81	0.75
2:D:99:MET:HE2	2:D:128:PHE:CZ	2.23	0.74
1:A:159:GLN:NE2	1:A:161:TRP:HE1	1.84	0.73
1:G:143:GLN:HG3	1:G:144:PRO:HD2	1.69	0.73
1:G:76:PHE:CE1	2:H:174:MET:CE	2.73	0.72
1:G:58:GLU:OE2	1:G:157:THR:CG2	2.38	0.71
2:H:263:CYS:SG	2:H:338:PRO:HD3	2.30	0.71
4:F:584:HOH:O	2:H:284:LYS:CD	2.39	0.71
2:F:339:VAL:HG12	2:F:340:THR:H	1.56	0.70
2:D:99:MET:HE2	2:D:128:PHE:HZ	1.54	0.70
2:H:70:MET:HE2	2:H:164:ILE:HG22	1.73	0.70
2:B:93:HIS:HE1	2:B:98:THR:OG1	1.74	0.70
1:G:156:VAL:CB	4:G:226:HOH:O	2.39	0.69
1:C:159:GLN:HE21	1:C:161:TRP:HE1	1.39	0.69
2:F:339:VAL:HG12	2:F:340:THR:N	2.07	0.69
2:D:99:MET:CE	2:D:128:PHE:CZ	2.76	0.68
1:C:130:LEU:N	2:D:174:MET:HE1	2.08	0.68
1:C:76:PHE:CE2	2:D:174:MET:HE3	2.30	0.67
2:H:254:LEU:HD12	2:H:255:PRO:HD2	1.77	0.66
1:G:76:PHE:CE1	2:H:174:MET:HE3	2.29	0.66
2:H:70:MET:HE1	2:H:164:ILE:HA	1.78	0.66
2:H:113:ARG:NH2	4:H:501:HOH:O	2.25	0.65
2:B:278:LYS:HG2	2:B:285:PRO:HA	1.79	0.64
1:G:116:ARG:HH11	1:G:116:ARG:CG	2.10	0.64
2:H:184:ARG:HG3	2:H:224:TYR:CD1	2.33	0.64
2:B:172:ARG:HH12	2:D:172:ARG:HH22	1.48	0.62
2:D:99:MET:HE1	2:D:124:LEU:HD11	1.82	0.61
2:D:99:MET:CE	2:D:128:PHE:HZ	2.13	0.61
1:G:76:PHE:CE1	2:H:174:MET:HE2	2.32	0.61
1:G:85:GLU:HG3	4:G:216:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLU:OE2	1:A:157:THR:HB	2.00	0.61
2:H:70:MET:CE	2:H:142:PRO:HG2	2.31	0.60
1:A:153:GLU:HA	1:A:157:THR:HG21	1.83	0.60
2:D:106:ASP:HB3	4:D:593:HOH:O	2.03	0.59
2:B:93:HIS:CE1	2:B:98:THR:OG1	2.56	0.59
2:F:225:LEU:HD21	2:F:247:PRO:HB2	1.84	0.59
2:H:113:ARG:CG	2:H:113:ARG:HH21	2.16	0.59
2:H:264:GLU:OE1	3:H:401:FE:FE	1.53	0.59
2:D:93:HIS:HE1	2:D:98:THR:OG1	1.85	0.58
1:E:83:GLN:HE21	1:E:124:ARG:HH11	1.51	0.58
2:H:264:GLU:OE1	2:H:305:HIS:NE2	2.36	0.58
1:G:116:ARG:HG3	1:G:116:ARG:NH1	2.12	0.58
2:D:159:ASN:HB2	4:D:529:HOH:O	2.05	0.57
2:B:63:ASP:HB3	2:B:152:PRO:HG3	1.86	0.56
1:C:159:GLN:HG2	1:C:161:TRP:NE1	2.20	0.56
1:C:76:PHE:CD2	2:D:174:MET:HE3	2.38	0.56
2:D:332:GLY:HA2	2:D:335:PRO:HD3	1.88	0.56
2:B:18:ARG:HD2	4:B:599:HOH:O	2.06	0.56
2:F:281:GLU:CG	4:F:599:HOH:O	2.39	0.55
1:A:154:GLY:H	1:A:157:THR:HG21	1.70	0.55
2:D:194:ARG:NH2	2:D:251:GLU:OE1	2.39	0.55
1:C:76:PHE:CE2	2:D:174:MET:CE	2.89	0.55
2:B:41:THR:HG22	4:B:519:HOH:O	2.07	0.54
1:C:99:ASP:OD1	1:C:100:PRO:O	2.25	0.54
1:A:95:ASP:OD2	2:D:323:PRO:CG	2.56	0.54
1:A:154:GLY:H	1:A:157:THR:HG23	1.70	0.53
1:G:76:PHE:HD1	2:H:174:MET:HE3	1.59	0.53
2:B:129:LYS:CE	4:B:604:HOH:O	2.52	0.53
2:H:70:MET:HE3	2:H:142:PRO:HG2	1.91	0.52
2:F:19:THR:HG22	2:F:120:LYS:HG3	1.91	0.51
2:H:184:ARG:HD3	4:H:605:HOH:O	2.09	0.51
1:E:124:ARG:HB2	1:E:127:HIS:CE1	2.46	0.51
2:H:116:GLU:HG3	4:H:593:HOH:O	2.10	0.51
2:H:113:ARG:HH21	2:H:113:ARG:HG2	1.75	0.51
2:D:99:MET:CE	2:D:128:PHE:CE1	2.94	0.50
2:F:27:ASN:OD1	2:F:29:GLU:HG3	2.11	0.50
1:C:76:PHE:HE2	2:D:174:MET:HE3	1.76	0.50
2:H:184:ARG:HG3	2:H:224:TYR:CE1	2.47	0.50
2:H:113:ARG:NH2	2:H:113:ARG:CG	2.74	0.49
1:E:81:ASP:O	1:E:145:ALA:HB1	2.13	0.49
2:H:188:ASN:HB2	4:H:521:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:LEU:HD12	1:G:113:PRO:HD2	1.95	0.49
2:D:23:HIS:HE1	2:D:130:ASP:OD2	1.95	0.49
1:E:28:ASN:N	1:E:28:ASN:HD22	2.11	0.48
1:G:128:MET:HG2	1:G:129:ALA:N	2.28	0.48
2:F:339:VAL:CG1	2:F:340:THR:N	2.76	0.48
2:D:91:ILE:O	2:D:97:VAL:HG23	2.13	0.48
2:F:47:TYR:O	2:F:62:ILE:HG22	2.13	0.48
1:A:58:GLU:O	1:A:148:LEU:HA	2.12	0.48
2:B:300:PRO:O	2:B:303:ILE:HG13	2.13	0.48
1:A:27:ARG:HG2	2:B:341:PHE:CE2	2.48	0.48
4:B:619:HOH:O	2:D:172:ARG:HB2	2.13	0.48
2:F:339:VAL:CG1	2:F:340:THR:H	2.25	0.47
2:F:42:PHE:HB3	2:F:135:TRP:CH2	2.49	0.47
2:H:70:MET:HE2	2:H:142:PRO:HG2	1.96	0.47
1:C:71:CYS:SG	1:C:73:HIS:CE1	3.07	0.47
2:D:99:MET:HE1	2:D:128:PHE:CE1	2.50	0.47
2:H:250:GLU:O	2:H:312:ARG:HA	2.15	0.47
1:E:83:GLN:NE2	1:E:124:ARG:HH11	2.13	0.47
2:H:196:PHE:HB3	2:H:226:SER:HB2	1.97	0.46
1:C:100:PRO:O	1:C:101:ASP:HB2	2.15	0.46
2:D:138:GLU:HG3	2:D:158:GLY:HA3	1.97	0.46
1:G:123:LEU:HD21	1:G:129:ALA:HB2	1.97	0.46
2:H:93:HIS:CE1	2:H:98:THR:OG1	2.58	0.46
2:B:143:PHE:CD1	2:B:230:VAL:HB	2.51	0.46
2:H:271:ASP:HB2	2:H:313:SER:HB3	1.97	0.46
2:D:258:HIS:O	2:D:304:ARG:HA	2.16	0.46
2:F:138:GLU:HB3	4:F:527:HOH:O	2.16	0.46
2:H:322:SER:HA	2:H:323:PRO:HD3	1.84	0.45
1:G:159:GLN:HE21	1:G:161:TRP:HE1	1.64	0.45
2:H:184:ARG:HB3	2:H:190:PHE:HB2	1.98	0.45
1:C:83:GLN:NE2	1:C:124:ARG:NH1	2.63	0.45
1:E:46:ARG:HD2	1:E:58:GLU:OE1	2.17	0.45
2:H:86:HIS:CD2	2:H:87:VAL:HG23	2.52	0.45
2:H:213:GLU:H	2:H:213:GLU:CD	2.19	0.45
1:A:122:VAL:HB	2:B:205:VAL:HB	1.99	0.45
2:D:34:SER:HB2	2:D:42:PHE:O	2.17	0.45
2:D:110:ASN:CG	4:D:534:HOH:O	2.54	0.45
2:D:213:GLU:H	2:D:213:GLU:CD	2.20	0.45
2:H:22:GLU:HG2	2:H:36:ARG:HE	1.81	0.45
1:A:92:ASP:OD1	1:A:115:GLY:HA2	2.17	0.44
2:F:213:GLU:H	2:F:213:GLU:CD	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:143:GLN:HG3	1:G:144:PRO:CD	2.45	0.44
2:H:280:LYS:HE3	4:H:565:HOH:O	2.17	0.44
2:H:63:ASP:HB3	2:H:152:PRO:HG3	1.99	0.44
1:G:150:GLN:HB2	2:H:245:PHE:CZ	2.53	0.43
1:C:129:ALA:C	2:D:174:MET:HE1	2.38	0.43
1:A:58:GLU:HB2	1:A:149:PHE:HB2	2.01	0.43
2:D:109:ARG:HD3	4:D:578:HOH:O	2.03	0.43
2:F:76:GLY:HA2	2:F:125:MET:HE3	2.01	0.43
2:F:63:ASP:OD1	2:F:64:ALA:N	2.47	0.43
1:E:156:VAL:HG22	4:E:223:HOH:O	2.19	0.43
2:D:113:ARG:NE	4:D:504:HOH:O	2.51	0.43
2:F:262:ARG:HB2	2:F:325:ILE:HG21	2.01	0.42
2:F:23:HIS:HB3	2:F:33:ARG:HD3	2.01	0.42
2:H:24:LEU:HD12	2:H:34:SER:OG	2.18	0.42
2:D:322:SER:HA	2:D:323:PRO:HD3	1.75	0.42
2:H:71:ARG:HG2	2:H:255:PRO:HG2	2.01	0.42
2:B:320:ASN:OD1	2:B:320:ASN:C	2.58	0.42
2:F:109:ARG:C	2:F:111:ALA:H	2.23	0.42
1:E:43:PRO:HD3	1:E:61:ARG:HH22	1.82	0.42
2:F:113:ARG:HD3	1:G:22:ILE:HA	2.01	0.42
2:D:42:PHE:CD2	2:D:51:LEU:HD22	2.55	0.41
2:F:206:VAL:HG13	2:F:216:VAL:HG12	2.01	0.41
2:D:93:HIS:CE1	2:D:98:THR:OG1	2.70	0.41
2:H:113:ARG:HD2	2:H:113:ARG:HA	1.82	0.41
2:F:232:TRP:HA	2:F:250:GLU:OE1	2.20	0.41
1:G:55:TYR:CD1	2:H:243:SER:HB2	2.56	0.41
2:H:70:MET:CE	2:H:164:ILE:HA	2.49	0.41
1:E:103:GLU:HB3	1:E:152:ILE:HG21	2.02	0.41
2:F:168:ARG:NH1	2:F:234:PRO:O	2.54	0.41
2:H:93:HIS:HB2	2:H:96:GLU:O	2.21	0.41
2:F:277:VAL:HG13	2:F:303:ILE:HD13	2.03	0.41
1:C:156:VAL:HG22	4:C:209:HOH:O	2.20	0.41
2:D:29:GLU:H	2:D:29:GLU:CD	2.24	0.41
2:D:99:MET:HE2	2:D:128:PHE:CE1	2.55	0.41
2:F:267:LEU:HB3	2:F:316:LEU:HB3	2.03	0.40
2:H:106:ASP:CB	4:H:586:HOH:O	2.20	0.40
1:C:77:VAL:HA	1:C:148:LEU:O	2.22	0.40
2:D:69:MET:SD	2:D:128:PHE:CD2	3.15	0.40
2:F:267:LEU:HD13	2:F:296:ILE:HB	2.02	0.40
2:H:196:PHE:CD2	2:H:226:SER:HA	2.57	0.40
1:C:159:GLN:NE2	1:C:161:TRP:HE1	2.15	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:161:ASP:HA	2:D:164:ILE:HG12	2.02	0.40
2:F:162:GLU:HB2	4:F:574:HOH:O	2.20	0.40
2:F:254:LEU:HA	2:F:255:PRO:HD3	1.93	0.40
2:H:263:CYS:SG	2:H:338:PRO:CD	3.05	0.40
2:H:303:ILE:HD12	2:H:303:ILE:C	2.42	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%)	154 (94%)	10 (6%)	0	100	100
1	C	164/170 (96%)	151 (92%)	12 (7%)	1 (1%)	25	36
1	E	165/170 (97%)	157 (95%)	8 (5%)	0	100	100
1	G	162/170 (95%)	152 (94%)	10 (6%)	0	100	100
2	B	323/341 (95%)	309 (96%)	14 (4%)	0	100	100
2	D	321/341 (94%)	298 (93%)	22 (7%)	1 (0%)	41	55
2	F	325/341 (95%)	306 (94%)	19 (6%)	0	100	100
2	H	327/341 (96%)	306 (94%)	19 (6%)	2 (1%)	25	36
All	All	1951/2044 (96%)	1833 (94%)	114 (6%)	4 (0%)	47	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	252	PHE
2	H	54	PRO
1	C	81	ASP
2	H	252	PHE

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	127/131 (97%)	123 (97%)	4 (3%)	40	60
1	C	130/131 (99%)	129 (99%)	1 (1%)	81	91
1	E	127/131 (97%)	124 (98%)	3 (2%)	49	68
1	G	124/131 (95%)	120 (97%)	4 (3%)	39	59
2	B	266/284 (94%)	261 (98%)	5 (2%)	57	75
2	D	262/284 (92%)	253 (97%)	9 (3%)	37	56
2	F	266/284 (94%)	259 (97%)	7 (3%)	46	66
2	H	262/284 (92%)	255 (97%)	7 (3%)	44	65
All	All	1564/1660 (94%)	1524 (97%)	40 (3%)	46	66

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	156	VAL
1	A	157	THR
1	A	160	LYS
2	B	41	THR
2	B	51	LEU
2	B	78	PHE
2	B	143	PHE
2	B	194	ARG
1	C	89	LEU
2	D	29	GLU
2	D	57	SER
2	D	78	PHE
2	D	122	SER
2	D	143	PHE
2	D	160	ASN
2	D	172	ARG
2	D	194	ARG
2	D	228	SER

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Mol	Chain	Res	Type
1	E	3	ASP
1	E	12	THR
1	E	138	ARG
2	F	18	ARG
2	F	122	SER
2	F	143	PHE
2	F	152	PRO
2	F	194	ARG
2	F	325	ILE
2	F	337	VAL
1	G	7	GLU
1	G	110	GLU
1	G	116	ARG
1	G	160	LYS
2	H	34	SER
2	H	78	PHE
2	H	113	ARG
2	H	143	PHE
2	H	184	ARG
2	H	194	ARG
2	H	335	PRO

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	40	ASN
1	A	83	GLN
1	A	159	GLN
2	B	83	ASN
2	B	93	HIS
1	C	28	ASN
1	C	83	GLN
1	C	159	GLN
2	D	23	HIS
2	D	93	HIS
2	D	160	ASN
1	E	28	ASN
1	E	83	GLN
1	E	87	HIS
1	E	159	GLN
1	E	166	GLN

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Mol	Chain	Res	Type
2	F	28	ASN
1	G	28	ASN
1	G	40	ASN
1	G	159	GLN
2	H	93	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	166/170 (97%)	-0.23	3 (1%) 68 66	19, 28, 42, 58	0
1	C	166/170 (97%)	-0.26	1 (0%) 89 88	20, 28, 56, 70	0
1	E	167/170 (98%)	-0.07	7 (4%) 36 35	19, 29, 49, 74	0
1	G	164/170 (96%)	0.03	2 (1%) 79 77	25, 39, 57, 79	0
2	B	325/341 (95%)	-0.46	0 100 100	15, 24, 37, 58	0
2	D	325/341 (95%)	-0.31	10 (3%) 49 47	17, 26, 55, 98	0
2	F	326/341 (95%)	-0.31	2 (0%) 89 88	17, 27, 53, 73	0
2	H	331/341 (97%)	-0.25	8 (2%) 59 57	17, 28, 65, 95	0
All	All	1970/2044 (96%)	-0.27	33 (1%) 70 68	15, 27, 51, 98	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	341	PHE	5.1
1	E	169	ALA	5.0
2	D	331	ASP	3.6
2	H	335	PRO	3.6
2	H	13	GLY	3.5
1	E	148	LEU	3.5
2	H	336	VAL	3.5
1	G	162	GLY	3.5
1	C	101	ASP	3.2
2	D	340	THR	3.2
1	A	12	THR	3.1
2	D	327	GLN	3.0
2	D	335	PRO	2.9
2	H	334	ALA	2.8
1	E	167	THR	2.8
1	E	78	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	329	ILE	2.6
1	E	57	ILE	2.6
2	H	340	THR	2.4
2	D	330	ALA	2.4
2	H	10	ILE	2.4
2	F	330	ALA	2.4
2	D	328	MET	2.3
2	D	336	VAL	2.3
2	H	333	THR	2.3
1	E	77	VAL	2.2
2	D	15	SER	2.2
2	H	15	SER	2.1
1	E	149	PHE	2.1
1	A	148	LEU	2.0
2	F	316	LEU	2.0
1	A	3	ASP	2.0
1	G	110	GLU	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
3	FE	F	401	1/1	0.99	0.11	24,24,24,24	0
3	FE	H	401	1/1	0.99	0.12	25,25,25,25	0
3	FE	B	401	1/1	1.00	0.13	24,24,24,24	0
3	FE	D	401	1/1	1.00	0.13	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.