



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:03 PM UTC

PDB ID : 5M22 / pdb_00005m22
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

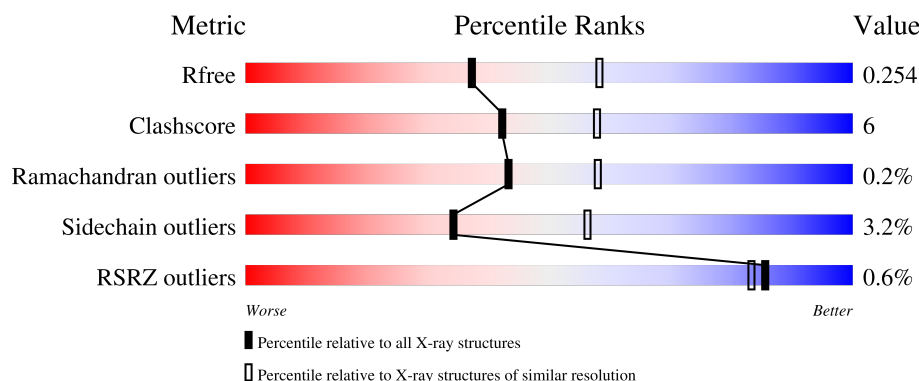
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	170	
1	C	170	
1	E	170	
1	G	170	
2	B	341	

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Mol	Chain	Length	Quality of chain
2	D	341	% 82%11%5%
2	F	341	81%13%. .
2	H	341	% 81%14%. .

2 Entry composition

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 (CCD ID: 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 50	O 50	0	0
4	B	126	Total 126	O 126	0	0
4	C	59	Total 59	O 59	0	0
4	D	126	Total 126	O 126	0	0
4	E	52	Total 52	O 52	0	0
4	F	109	Total 109	O 109	0	0
4	G	29	Total 29	O 29	0	0
4	H	126	Total 126	O 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

Chain A:  87% 10% ..



- Molecule 1: Hydroquinone dioxygenase small subunit

Chain C:  84% 12% ..



- Molecule 1: Hydroquinone dioxygenase small subunit

Chain E:  85% 12% ..



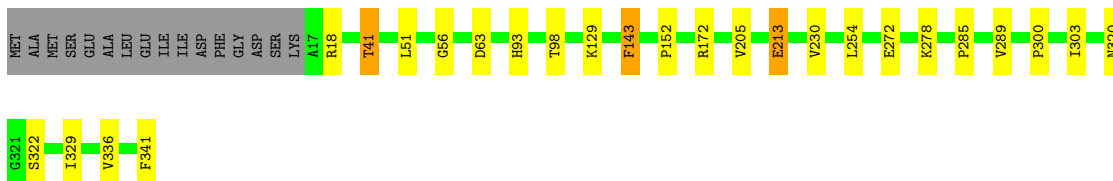
- Molecule 1: Hydroquinone dioxygenase small subunit

Chain G:  82% 14% ..



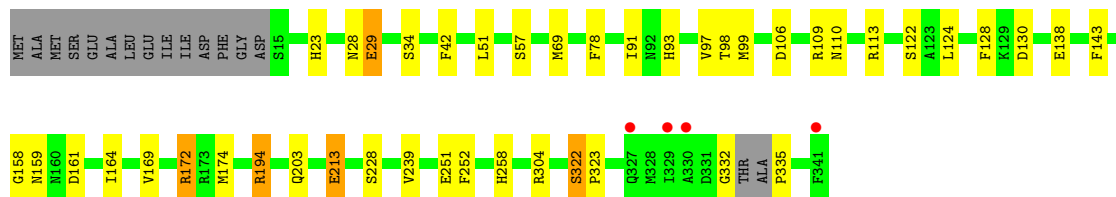
- Molecule 2: Hydroquinone dioxygenase large subunit

Chain B:  88% 7% 5% ..



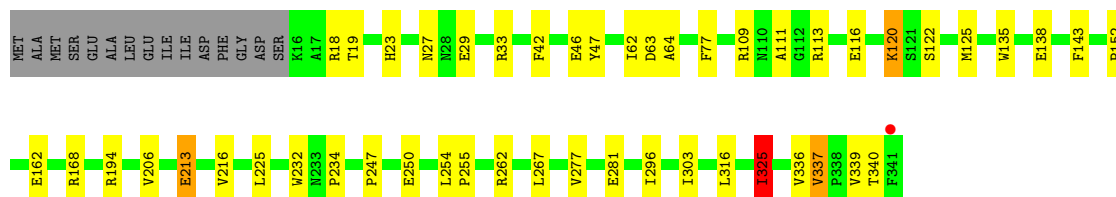
- Molecule 2: Hydroquinone dioxygenase large subunit

Chain D:  82% 11% 5%



- Molecule 2: Hydroquinone dioxygenase large subunit

Chain F:  81% 13% 2%



- Molecule 2: Hydroquinone dioxygenase large subunit

Chain H:  81% 14% 2%



4 Data and refinement statistics

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 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-2.40) 97.4 (30.00-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.69%)	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)	0.34 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.78	0/1298	1.02	2/1761 (0.1%)
1	C	0.84	0/1309	1.09	7/1775 (0.4%)
1	E	0.83	0/1302	1.01	3/1768 (0.2%)
1	G	0.78	0/1275	0.95	2/1730 (0.1%)
2	B	0.85	0/2631	1.03	7/3578 (0.2%)
2	D	0.82	0/2607	1.02	5/3546 (0.1%)
2	F	0.82	1/2633 (0.0%)	1.03	4/3580 (0.1%)
2	H	0.84	0/2649	1.03	3/3602 (0.1%)
All	All	0.83	1/15704 (0.0%)	1.02	33/21340 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	325	ILE	CA-CB	5.11	1.57	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	99	ASP	CA-C-N	-9.02	111.59	120.52
1	C	99	ASP	C-N-CA	-9.02	111.59	120.52
1	E	151	SER	N-CA-C	7.33	117.65	108.19
1	C	161	TRP	N-CA-C	6.85	118.44	110.97
1	E	161	TRP	N-CA-C	6.71	118.28	110.97
2	B	322	SER	CA-C-N	6.70	126.39	119.56
2	B	322	SER	C-N-CA	6.70	126.39	119.56
1	C	4	VAL	N-CA-C	6.61	118.29	109.37
2	B	272	GLU	N-CA-C	6.20	118.50	109.07
1	C	22	ILE	N-CA-C	-6.13	105.72	111.48
1	C	18	GLY	N-CA-C	5.99	119.19	110.63
1	E	18	GLY	N-CA-C	5.95	119.68	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	325	ILE	CB-CA-C	-5.94	106.22	114.00
2	H	272	GLU	N-CA-C	5.75	118.02	108.99
2	F	337	VAL	CA-C-N	-5.68	114.39	120.47
2	F	337	VAL	C-N-CA	-5.68	114.39	120.47
1	G	151	SER	N-CA-C	5.68	115.35	107.73
1	G	115	GLY	N-CA-C	5.56	119.11	110.88
2	D	239	VAL	N-CA-C	5.52	116.07	108.12
2	B	56	GLY	N-CA-C	5.51	121.35	110.83
1	A	49	VAL	N-CA-C	-5.51	107.91	113.47
1	C	57	ILE	N-CA-C	-5.48	100.59	108.53
2	D	28	ASN	N-CA-C	5.47	117.32	111.36
2	D	169	VAL	CB-CA-C	5.47	117.80	110.42
2	F	325	ILE	N-CA-CB	5.41	114.67	110.45
2	H	277	VAL	N-CA-C	5.22	115.29	107.51
2	D	322	SER	CA-C-N	5.15	124.76	119.56
2	D	322	SER	C-N-CA	5.15	124.76	119.56
1	A	18	GLY	N-CA-C	5.07	117.44	110.69
2	H	325	ILE	N-CA-C	5.05	119.78	108.88
2	B	254	LEU	CA-C-N	-5.03	115.70	120.83
2	B	254	LEU	C-N-CA	-5.03	115.70	120.83
2	B	289	VAL	N-CA-C	5.01	114.78	107.37

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	15	0
1	C	1282	0	1226	22	0
1	E	1275	0	1209	16	0
1	G	1248	0	1186	22	0
2	B	2558	0	2419	15	0
2	D	2536	0	2358	44	0
2	F	2558	0	2408	29	0
2	H	2577	0	2396	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	8	0
All	All	15986	0	14418	187	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 (187) 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:G:76:PHE:CE1	2:H:174:MET:HE3	1.83	1.12
1:G:76:PHE:CD1	2:H:174:MET:HE3	1.94	1.03
2:H:70:MET:HE2	2:H:142:PRO:HG2	1.42	1.00
1:G:76:PHE:CD1	2:H:174:MET:CE	2.46	0.97
1:C:76:PHE:HD2	2:D:174:MET:HE2	1.27	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
1:C:76:PHE:CD2	2:D:174:MET:HE2	2.07	0.88
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	0.86
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
1:E:12:THR:HB	4:E:225:HOH:O	1.76	0.83
2:H:70:MET:HE1	2:H:164:ILE:HA	1.59	0.82
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:76:PHE:CE2	2:D:174:MET:HE3	2.20	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:HE21	1:E:161:TRP:NE1	1.81	0.76
1:E:159:GLN:NE2	1:E:161:TRP:HE1	1.81	0.75
2:D:99:MET:HE1	2:D:128:PHE:CE1	2.22	0.74
1:G:76:PHE:HE1	2:H:174:MET:HE3	1.45	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: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
1:C:130:LEU:N	2:D:174:MET:HE1	2.05	0.70
2:D:99:MET:HE2	2:D:128:PHE:HZ	1.55	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:76:PHE:CD2	2:D:174:MET:HE3	2.29	0.67
2:H:254:LEU:HD12	2:H:255:PRO:HD2	1.77	0.66
1:A:159:GLN:HE21	1:A:161:TRP:NE1	1.89	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:D:99:MET:HE1	2:D:128:PHE:HE1	1.63	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:CE	2:D:128:PHE:HZ	2.13	0.61
1:G:85:GLU:HG3	4:G:216:HOH:O	2.00	0.61
2:H:147:MET:HE1	4:H:621:HOH:O	2.00	0.61
1:A:58:GLU:OE2	1:A:157:THR:HB	2.00	0.61
1:A:153:GLU:HA	1:A:157:THR:HG21	1.83	0.60
1:C:76:PHE:HE2	2:D:174:MET:HE3	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:MET:HE3	2:D:124:LEU:HD21	1.86	0.57
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
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
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
2:F:77:PHE:CE2	2:F:125:MET:HE2	2.43	0.54
1:A:154:GLY:H	1:A:157:THR:HG23	1.70	0.53
2:B:129:LYS:CE	4:B:604:HOH:O	2.52	0.53
2:F:19:THR:HG22	2:F:120:LYS:HG3	1.91	0.51
2:D:99:MET:HE2	2:D:128:PHE:CZ	2.37	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:F:27:ASN:OD1	2:F:29:GLU:HG3	2.11	0.50
2:H:184:ARG:HG3	2:H:224:TYR:CE1	2.47	0.50
2:D:213:GLU:H	2:D:213:GLU:CD	2.20	0.50
2:H:113:ARG:NH2	2:H:113:ARG:CG	2.74	0.49
2:H:213:GLU:H	2:H:213:GLU:CD	2.19	0.49
2:D:110:ASN:CG	4:D:534:HOH:O	2.54	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
1:G:112:LEU:HD12	1:G:113:PRO:HD2	1.95	0.49
2:F:213:GLU:H	2:F:213:GLU:CD	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	2.30	0.47
1:C:71:CYS:SG	1:C:73:HIS:CE1	3.07	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:B:320:ASN:OD1	2:B:320:ASN:C	2.58	0.47
2:F:109:ARG:C	2:F:111:ALA:H	2.23	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:D:29:GLU:H	2:D:29:GLU:CD	2.24	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
2:H:70:MET:HE1	2:H:164:ILE:HG22	1.97	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:G:76:PHE:HD1	2:H:174:MET:HE1	1.71	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
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:H:303:ILE:HD12	2:H:303:ILE:C	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ALA:C	2:D:174:MET:HE1	2.42	0.44
1:G:150:GLN:HB2	2:H:245:PHE:CZ	2.53	0.43
1:C:159:GLN:HE21	1:C:161:TRP:NE1	2.13	0.43
2:H:120:LYS:O	2:H:121:SER:C	2.61	0.43
1:A:58:GLU:HB2	1:A:149:PHE:HB2	2.01	0.43
1:C:76:PHE:CE2	2:D:174:MET:CE	2.89	0.43
2:D:109:ARG:HD3	4:D:578:HOH:O	2.03	0.43
2:B:213:GLU:CD	2:B:213:GLU:H	2.27	0.43
1:C:130:LEU:CA	2:D:174:MET:HE1	2.48	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
1:C:29:TYR:O	1:C:30:VAL:C	2.63	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
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: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:F:303:ILE:HD12	2:F:303:ILE:C	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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%)	21	32
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%)	36	50
2	F	325/341 (95%)	306 (94%)	19 (6%)	0	100	100
2	H	327/341 (96%)	306 (94%)	19 (6%)	2 (1%)	21	32
All	All	1951/2044 (96%)	1833 (94%)	114 (6%)	4 (0%)	43	58

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 ⓘ

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%)	35	57
1	C	130/131 (99%)	128 (98%)	2 (2%)	57	77
1	E	127/131 (97%)	125 (98%)	2 (2%)	55	76
1	G	124/131 (95%)	118 (95%)	6 (5%)	23	40
2	B	266/284 (94%)	260 (98%)	6 (2%)	44	66
2	D	262/284 (92%)	252 (96%)	10 (4%)	29	49
2	F	266/284 (94%)	255 (96%)	11 (4%)	27	46
2	H	262/284 (92%)	253 (97%)	9 (3%)	32	54
All	All	1564/1660 (94%)	1514 (97%)	50 (3%)	34	56

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	12	THR
1	A	156	VAL
1	A	157	THR
2	B	41	THR
2	B	51	LEU
2	B	143	PHE
2	B	213	GLU
2	B	329	ILE
2	B	336	VAL
1	C	30	VAL
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	172	ARG
2	D	194	ARG

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Mol	Chain	Res	Type
2	D	203	GLN
2	D	213	GLU
2	D	228	SER
1	E	12	THR
1	E	138	ARG
2	F	18	ARG
2	F	46	GLU
2	F	120	LYS
2	F	122	SER
2	F	143	PHE
2	F	152	PRO
2	F	194	ARG
2	F	213	GLU
2	F	325	ILE
2	F	336	VAL
2	F	337	VAL
1	G	4	VAL
1	G	7	GLU
1	G	30	VAL
1	G	110	GLU
1	G	116	ARG
1	G	160	LYS
2	H	34	SER
2	H	54	PRO
2	H	113	ARG
2	H	143	PHE
2	H	169	VAL
2	H	184	ARG
2	H	194	ARG
2	H	213	GLU
2	H	250	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) 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	23	HIS
2	B	83	ASN
2	B	93	HIS

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Mol	Chain	Res	Type
1	C	28	ASN
1	C	40	ASN
1	C	83	GLN
1	C	143	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
2	F	23	HIS
2	F	83	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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	166/170 (97%)	-0.75	0 100 100	19, 28, 42, 58	0
1	C	166/170 (97%)	-0.63	0 100 100	20, 28, 56, 70	0
1	E	167/170 (98%)	-0.64	1 (0%) 85 83	19, 29, 49, 74	0
1	G	164/170 (96%)	-0.36	0 100 100	25, 39, 57, 79	0
2	B	325/341 (95%)	-0.85	0 100 100	15, 24, 37, 58	0
2	D	325/341 (95%)	-0.70	4 (1%) 76 73	17, 26, 55, 98	0
2	F	326/341 (95%)	-0.68	1 (0%) 90 88	16, 27, 53, 73	1 (0%)
2	H	331/341 (97%)	-0.64	5 (1%) 72 68	17, 28, 65, 95	0
All	All	1970/2044 (96%)	-0.68	11 (0%) 85 83	15, 27, 51, 98	1 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	341	PHE	3.8
2	H	331	ASP	3.1
2	D	329	ILE	3.0
2	H	335	PRO	2.9
2	F	341	PHE	2.6
2	H	336	VAL	2.5
2	H	334	ALA	2.4
2	D	330	ALA	2.3
1	E	169	ALA	2.2
2	D	327	GLN	2.1
2	H	14	ASP	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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
3	FE	B	401	1/1	1.00	0.03	24,24,24,24	0
3	FE	D	401	1/1	1.00	0.03	26,26,26,26	0
3	FE	F	401	1/1	1.00	0.02	24,24,24,24	0
3	FE	H	401	1/1	1.00	0.02	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.