



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:04 PM UTC

PDB ID : 1YDG / pdb_00001ydg
Title : Crystal Structure of Trp repressor binding protein WrbA
Authors : Gorman, J.; Shapiro, L.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2004-12-23
Resolution : 2.00 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

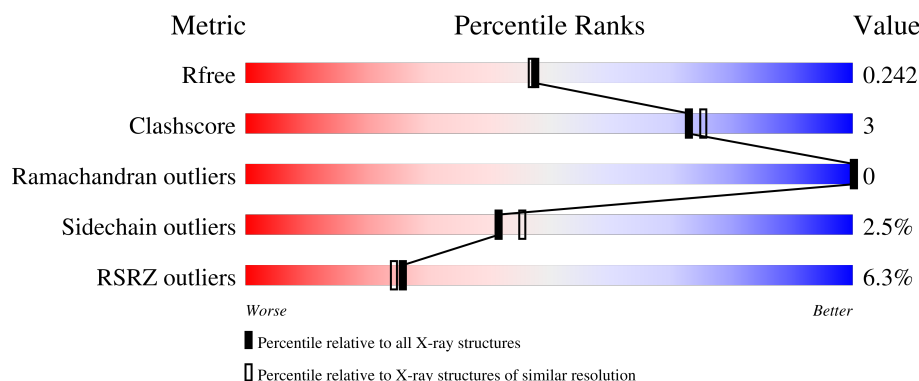
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	211	
1	B	211	
1	C	211	
1	D	211	
1	E	211	

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Mol	Chain	Length	Quality of chain
1	F	211	7% 85% 10% 5%
1	G	211	15% 88% 8% •
1	H	211	% 88% 7% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13399 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 trp repressor binding protein WrbA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1500	938	261	295	6			
1	B	202	Total	C	N	O	S	0	0	0
			1507	942	262	297	6			
1	C	202	Total	C	N	O	S	0	0	0
			1507	942	262	297	6			
1	D	202	Total	C	N	O	S	0	0	0
			1507	942	262	297	6			
1	E	204	Total	C	N	O	S	0	0	0
			1521	951	264	300	6			
1	F	201	Total	C	N	O	S	0	0	0
			1500	938	261	295	6			
1	G	202	Total	C	N	O	S	0	0	0
			1507	942	262	297	6			
1	H	202	Total	C	N	O	S	0	0	0
			1507	942	262	297	6			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	cloning artifact	UNP Q9RYU4
A	0	SER	-	cloning artifact	UNP Q9RYU4
A	1	LEU	-	cloning artifact	UNP Q9RYU4
A	200	GLU	-	cloning artifact	UNP Q9RYU4
A	202	GLY	-	cloning artifact	UNP Q9RYU4
A	203	SER	-	cloning artifact	UNP Q9RYU4
A	204	HIS	-	expression tag	UNP Q9RYU4
A	205	HIS	-	expression tag	UNP Q9RYU4
A	206	HIS	-	expression tag	UNP Q9RYU4
A	207	HIS	-	expression tag	UNP Q9RYU4
A	208	HIS	-	expression tag	UNP Q9RYU4
A	209	HIS	-	expression tag	UNP Q9RYU4
B	-1	MET	-	cloning artifact	UNP Q9RYU4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	cloning artifact	UNP Q9RYU4
B	1	LEU	-	cloning artifact	UNP Q9RYU4
B	200	GLU	-	cloning artifact	UNP Q9RYU4
B	202	GLY	-	cloning artifact	UNP Q9RYU4
B	203	SER	-	cloning artifact	UNP Q9RYU4
B	204	HIS	-	expression tag	UNP Q9RYU4
B	205	HIS	-	expression tag	UNP Q9RYU4
B	206	HIS	-	expression tag	UNP Q9RYU4
B	207	HIS	-	expression tag	UNP Q9RYU4
B	208	HIS	-	expression tag	UNP Q9RYU4
B	209	HIS	-	expression tag	UNP Q9RYU4
C	-1	MET	-	cloning artifact	UNP Q9RYU4
C	0	SER	-	cloning artifact	UNP Q9RYU4
C	1	LEU	-	cloning artifact	UNP Q9RYU4
C	200	GLU	-	cloning artifact	UNP Q9RYU4
C	202	GLY	-	cloning artifact	UNP Q9RYU4
C	203	SER	-	cloning artifact	UNP Q9RYU4
C	204	HIS	-	expression tag	UNP Q9RYU4
C	205	HIS	-	expression tag	UNP Q9RYU4
C	206	HIS	-	expression tag	UNP Q9RYU4
C	207	HIS	-	expression tag	UNP Q9RYU4
C	208	HIS	-	expression tag	UNP Q9RYU4
C	209	HIS	-	expression tag	UNP Q9RYU4
D	-1	MET	-	cloning artifact	UNP Q9RYU4
D	0	SER	-	cloning artifact	UNP Q9RYU4
D	1	LEU	-	cloning artifact	UNP Q9RYU4
D	200	GLU	-	cloning artifact	UNP Q9RYU4
D	202	GLY	-	cloning artifact	UNP Q9RYU4
D	203	SER	-	cloning artifact	UNP Q9RYU4
D	204	HIS	-	expression tag	UNP Q9RYU4
D	205	HIS	-	expression tag	UNP Q9RYU4
D	206	HIS	-	expression tag	UNP Q9RYU4
D	207	HIS	-	expression tag	UNP Q9RYU4
D	208	HIS	-	expression tag	UNP Q9RYU4
D	209	HIS	-	expression tag	UNP Q9RYU4
E	-1	MET	-	cloning artifact	UNP Q9RYU4
E	0	SER	-	cloning artifact	UNP Q9RYU4
E	1	LEU	-	cloning artifact	UNP Q9RYU4
E	200	GLU	-	cloning artifact	UNP Q9RYU4
E	202	GLY	-	cloning artifact	UNP Q9RYU4
E	203	SER	-	cloning artifact	UNP Q9RYU4
E	204	HIS	-	expression tag	UNP Q9RYU4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	205	HIS	-	expression tag	UNP Q9RYU4
E	206	HIS	-	expression tag	UNP Q9RYU4
E	207	HIS	-	expression tag	UNP Q9RYU4
E	208	HIS	-	expression tag	UNP Q9RYU4
E	209	HIS	-	expression tag	UNP Q9RYU4
F	-1	MET	-	cloning artifact	UNP Q9RYU4
F	0	SER	-	cloning artifact	UNP Q9RYU4
F	1	LEU	-	cloning artifact	UNP Q9RYU4
F	200	GLU	-	cloning artifact	UNP Q9RYU4
F	202	GLY	-	cloning artifact	UNP Q9RYU4
F	203	SER	-	cloning artifact	UNP Q9RYU4
F	204	HIS	-	expression tag	UNP Q9RYU4
F	205	HIS	-	expression tag	UNP Q9RYU4
F	206	HIS	-	expression tag	UNP Q9RYU4
F	207	HIS	-	expression tag	UNP Q9RYU4
F	208	HIS	-	expression tag	UNP Q9RYU4
F	209	HIS	-	expression tag	UNP Q9RYU4
G	-1	MET	-	cloning artifact	UNP Q9RYU4
G	0	SER	-	cloning artifact	UNP Q9RYU4
G	1	LEU	-	cloning artifact	UNP Q9RYU4
G	200	GLU	-	cloning artifact	UNP Q9RYU4
G	202	GLY	-	cloning artifact	UNP Q9RYU4
G	203	SER	-	cloning artifact	UNP Q9RYU4
G	204	HIS	-	expression tag	UNP Q9RYU4
G	205	HIS	-	expression tag	UNP Q9RYU4
G	206	HIS	-	expression tag	UNP Q9RYU4
G	207	HIS	-	expression tag	UNP Q9RYU4
G	208	HIS	-	expression tag	UNP Q9RYU4
G	209	HIS	-	expression tag	UNP Q9RYU4
H	-1	MET	-	cloning artifact	UNP Q9RYU4
H	0	SER	-	cloning artifact	UNP Q9RYU4
H	1	LEU	-	cloning artifact	UNP Q9RYU4
H	200	GLU	-	cloning artifact	UNP Q9RYU4
H	202	GLY	-	cloning artifact	UNP Q9RYU4
H	203	SER	-	cloning artifact	UNP Q9RYU4
H	204	HIS	-	expression tag	UNP Q9RYU4
H	205	HIS	-	expression tag	UNP Q9RYU4
H	206	HIS	-	expression tag	UNP Q9RYU4
H	207	HIS	-	expression tag	UNP Q9RYU4
H	208	HIS	-	expression tag	UNP Q9RYU4
H	209	HIS	-	expression tag	UNP Q9RYU4

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	225	Total	O	0	0
			225	225		
3	B	198	Total	O	0	0
			198	198		

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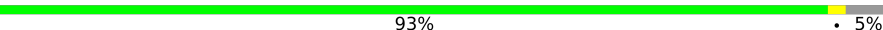
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	156	Total 156	O 156	0	0
3	D	195	Total 195	O 195	0	0
3	E	97	Total 97	O 97	0	0
3	F	143	Total 143	O 143	0	0
3	G	82	Total 82	O 82	0	0
3	H	197	Total 197	O 197	0	0

3 Residue-property plots

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.

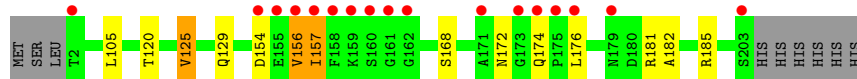
- Molecule 1: trp repressor binding protein WrbA

Chain A: 



- Molecule 1: trp repressor binding protein WrbA

Chain B: 



- Molecule 1: trp repressor binding protein WrbA

Chain C: 



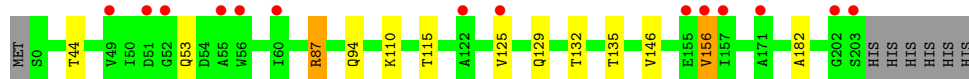
- Molecule 1: trp repressor binding protein WrbA

Chain D: 

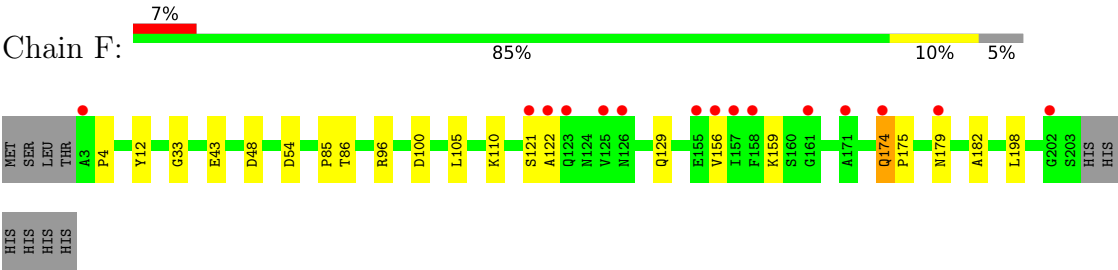


- Molecule 1: trp repressor binding protein WrbA

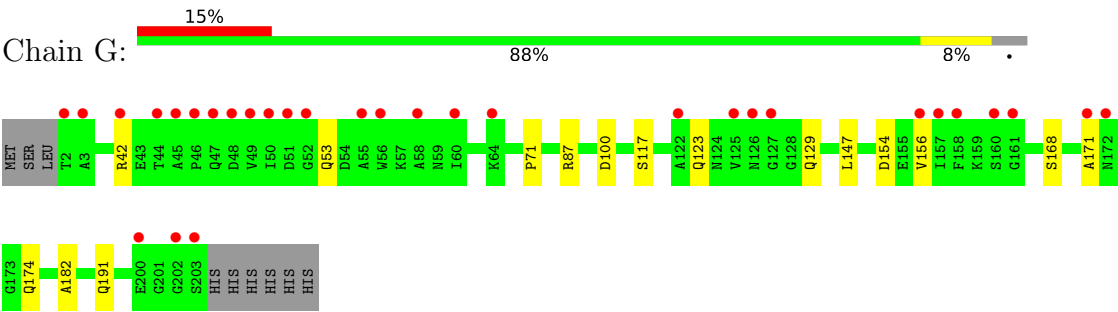
Chain E: 



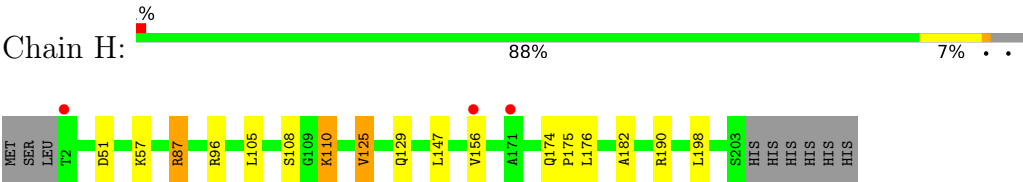
- Molecule 1: trp repressor binding protein WrbA



• Molecule 1: trp repressor binding protein WrbA



• Molecule 1: trp repressor binding protein WrbA



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.61Å 121.61Å 207.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.9 (20.00-2.00) 96.7 (20.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.49 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.186 , 0.236 0.196 , 0.242	Depositor DCC
R_{free} test set	5845 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13399	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.72	0/1529	0.82	0/2077
1	B	0.69	0/1536	0.85	0/2087
1	C	0.68	0/1536	0.81	0/2087
1	D	0.73	0/1536	0.83	0/2087
1	E	0.60	0/1550	0.78	0/2106
1	F	0.63	0/1529	0.80	0/2077
1	G	0.62	0/1536	0.80	0/2087
1	H	0.70	0/1536	0.82	0/2087
All	All	0.67	0/12288	0.81	0/16695

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 [i](#)

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	1500	0	1470	2	0
1	B	1507	0	1477	9	0
1	C	1507	0	1477	7	0
1	D	1507	0	1477	19	0
1	E	1521	0	1496	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1500	0	1470	14	0
1	G	1507	0	1477	12	0
1	H	1507	0	1477	12	1
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	10	0	0	0	0
3	A	225	0	0	1	0
3	B	198	0	0	2	0
3	C	156	0	0	2	0
3	D	195	0	0	3	0
3	E	97	0	0	2	0
3	F	143	0	0	2	0
3	G	82	0	0	3	0
3	H	197	0	0	4	0
All	All	13399	0	11821	77	1

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 3.

All (77) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:129:GLN:C	3:H:1453:HOH:O	2.30	0.74
1:D:123:GLN:NE2	1:D:171:ALA:O	2.25	0.70
1:E:129:GLN:C	3:E:1378:HOH:O	2.37	0.68
1:D:159:LYS:HB3	1:D:179:ASN:HD21	1.58	0.67
1:G:154:ASP:HB3	1:G:156:VAL:HG12	1.82	0.62
1:B:125:VAL:HG11	1:D:125:VAL:HG11	1.81	0.61
1:E:87:ARG:HG2	1:G:100:ASP:OD1	2.02	0.59
1:F:48:ASP:HB2	3:F:1448:HOH:O	2.02	0.59
1:G:123:GLN:HA	1:G:171:ALA:O	2.04	0.58
1:E:125:VAL:HG11	1:H:125:VAL:HG11	1.86	0.58
1:E:156:VAL:HG21	1:E:182:ALA:HB1	1.86	0.57
1:D:156:VAL:HG21	1:D:182:ALA:C	2.29	0.56
1:F:100:ASP:OD1	1:H:87:ARG:HG2	2.05	0.56
1:F:156:VAL:HG21	1:F:182:ALA:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:THR:HG21	1:D:122:ALA:HB2	1.89	0.54
1:G:42:ARG:HD3	3:G:1329:HOH:O	2.08	0.54
1:D:159:LYS:HB3	1:D:179:ASN:ND2	2.23	0.53
1:D:129:GLN:HG3	3:D:1457:HOH:O	2.09	0.53
1:H:174:GLN:HG3	1:H:175:PRO:HD2	1.91	0.52
1:H:190:ARG:HD2	3:H:1446:HOH:O	2.08	0.52
1:D:154:ASP:HB3	1:D:156:VAL:HG12	1.92	0.52
1:D:86:THR:CG2	1:D:122:ALA:HB2	2.41	0.51
1:F:96:ARG:HG3	1:H:96:ARG:HG3	1.92	0.51
1:C:2:THR:N	3:C:1447:HOH:O	2.43	0.51
1:D:157:ILE:HG22	1:D:162:GLY:HA2	1.93	0.51
1:G:117:SER:OG	1:G:191:GLN:NE2	2.44	0.50
1:H:156:VAL:HG21	1:H:182:ALA:CB	2.42	0.49
1:F:156:VAL:HG21	1:F:182:ALA:CB	2.42	0.49
1:E:156:VAL:HG21	1:E:182:ALA:CB	2.42	0.49
1:B:156:VAL:HG21	1:B:182:ALA:CB	2.42	0.49
1:C:132:THR:O	1:C:135:THR:HG22	2.12	0.48
1:B:157:ILE:HD13	1:B:157:ILE:N	2.28	0.48
1:D:174:GLN:HG3	1:D:175:PRO:HD2	1.96	0.48
1:H:125:VAL:HG23	3:H:1382:HOH:O	2.12	0.48
1:D:127:GLY:N	3:D:1457:HOH:O	2.46	0.48
1:C:202:GLY:O	1:C:203:SER:CB	2.62	0.47
1:D:129:GLN:NE2	1:D:168:SER:HB2	2.29	0.47
1:E:44:THR:OG1	1:E:94:GLN:HG3	2.13	0.47
1:G:71:PRO:HD3	3:G:1330:HOH:O	2.14	0.46
1:H:57:LYS:NZ	3:H:1479:HOH:O	2.31	0.46
1:D:129:GLN:NE2	3:D:1450:HOH:O	2.47	0.46
1:F:86:THR:HG22	1:F:122:ALA:HB2	1.98	0.45
1:F:12:TYR:O	1:F:85:PRO:HD3	2.16	0.45
1:C:72:ALA:HB1	1:F:54:ASP:HA	1.99	0.44
1:D:156:VAL:HG21	1:D:182:ALA:CB	2.47	0.44
1:B:154:ASP:O	1:B:157:ILE:HG12	2.17	0.44
1:F:159:LYS:HB2	1:F:179:ASN:HD21	1.83	0.44
1:E:115:THR:HA	1:E:146:VAL:O	2.18	0.43
1:G:156:VAL:HG21	1:G:182:ALA:C	2.43	0.43
1:B:129:GLN:NE2	3:B:1382:HOH:O	2.51	0.43
1:G:53:GLN:NE2	3:G:1377:HOH:O	2.51	0.43
1:G:147:LEU:HD12	1:H:147:LEU:HD12	2.01	0.43
1:H:156:VAL:HG21	1:H:182:ALA:HB1	2.00	0.43
1:F:129:GLN:C	3:F:1450:HOH:O	2.61	0.43
1:A:120:THR:O	1:A:168:SER:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:SER:OG	1:D:191:GLN:NE2	2.51	0.42
1:A:48:ASP:HB3	3:A:1527:HOH:O	2.17	0.42
1:C:77:ALA:O	1:C:114:LYS:NZ	2.52	0.42
1:F:4:PRO:HB3	1:F:33:GLY:O	2.19	0.42
1:F:174:GLN:HE21	1:F:174:GLN:HA	1.83	0.42
1:F:12:TYR:OH	1:F:43:GLU:OE2	2.37	0.42
1:B:181:ARG:O	1:B:185:ARG:HG3	2.20	0.42
1:H:108:SER:HB3	1:H:110:LYS:HE3	2.02	0.41
1:C:165:TYR:CE2	1:D:138:MET:HE3	2.56	0.41
1:B:176:LEU:HB2	1:B:181:ARG:NH2	2.36	0.41
1:F:174:GLN:HG3	1:F:175:PRO:HD2	2.01	0.41
1:D:120:THR:O	1:D:168:SER:HA	2.20	0.41
1:E:129:GLN:HG2	3:E:1402:HOH:O	2.19	0.41
1:B:157:ILE:HD12	3:B:1319:HOH:O	2.20	0.41
1:B:120:THR:O	1:B:168:SER:HA	2.21	0.41
1:C:135:THR:CG2	3:C:1373:HOH:O	2.67	0.41
1:G:129:GLN:HE21	1:G:168:SER:HB2	1.85	0.41
1:G:156:VAL:HG21	1:G:182:ALA:CB	2.51	0.41
1:E:125:VAL:HA	1:E:129:GLN:OE1	2.21	0.40
1:G:156:VAL:HG21	1:G:182:ALA:HB1	2.02	0.40
1:E:132:THR:O	1:E:135:THR:HG22	2.21	0.40
1:D:9:ILE:CD1	1:D:26:ALA:HA	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:ASP:OD2	1:H:51:ASP:OD2[6_555]	2.08	0.12

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	199/211 (94%)	198 (100%)	1 (0%)	0	100	100
1	B	200/211 (95%)	199 (100%)	1 (0%)	0	100	100
1	C	200/211 (95%)	198 (99%)	2 (1%)	0	100	100
1	D	200/211 (95%)	198 (99%)	2 (1%)	0	100	100
1	E	202/211 (96%)	201 (100%)	1 (0%)	0	100	100
1	F	199/211 (94%)	195 (98%)	4 (2%)	0	100	100
1	G	200/211 (95%)	195 (98%)	5 (2%)	0	100	100
1	H	200/211 (95%)	198 (99%)	2 (1%)	0	100	100
All	All	1600/1688 (95%)	1582 (99%)	18 (1%)	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	152/162 (94%)	150 (99%)	2 (1%)	61	68
1	B	153/162 (94%)	147 (96%)	6 (4%)	28	28
1	C	153/162 (94%)	150 (98%)	3 (2%)	48	54
1	D	153/162 (94%)	150 (98%)	3 (2%)	48	54
1	E	155/162 (96%)	151 (97%)	4 (3%)	40	44
1	F	152/162 (94%)	147 (97%)	5 (3%)	33	34
1	G	153/162 (94%)	151 (99%)	2 (1%)	61	68
1	H	153/162 (94%)	147 (96%)	6 (4%)	28	28
All	All	1224/1296 (94%)	1193 (98%)	31 (2%)	42	45

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LEU
1	A	176	LEU

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Mol	Chain	Res	Type
1	B	105	LEU
1	B	125	VAL
1	B	156	VAL
1	B	157	ILE
1	B	172	ASN
1	B	174	GLN
1	C	176	LEU
1	C	198	LEU
1	C	200	GLU
1	D	2	THR
1	D	87	ARG
1	D	125	VAL
1	E	53	GLN
1	E	87	ARG
1	E	110	LYS
1	E	156	VAL
1	F	105	LEU
1	F	110	LYS
1	F	121	SER
1	F	174	GLN
1	F	198	LEU
1	G	87	ARG
1	G	174	GLN
1	H	87	ARG
1	H	105	LEU
1	H	110	LYS
1	H	125	VAL
1	H	176	LEU
1	H	198	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	124	ASN
1	A	191	GLN
1	B	47	GLN
1	B	172	ASN
1	B	179	ASN
1	C	129	GLN
1	C	191	GLN
1	D	124	ASN

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Mol	Chain	Res	Type
1	D	191	GLN
1	E	129	GLN
1	E	191	GLN
1	F	53	GLN
1	F	113	ASN
1	F	123	GLN
1	F	126	ASN
1	F	174	GLN
1	F	191	GLN
1	G	129	GLN
1	G	174	GLN
1	G	191	GLN
1	H	124	ASN
1	H	129	GLN
1	H	191	GLN

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 ⓘ

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	F	1307	-	4,4,4	0.24	0	6,6,6	0.34	0
2	SO4	B	1303	-	4,4,4	0.22	0	6,6,6	0.34	0
2	SO4	D	1310	-	4,4,4	0.24	0	6,6,6	0.12	0
2	SO4	A	1302	-	4,4,4	0.25	0	6,6,6	0.24	0
2	SO4	H	1301	-	4,4,4	0.32	0	6,6,6	0.34	0
2	SO4	E	1306	-	4,4,4	0.25	0	6,6,6	0.40	0
2	SO4	C	1304	-	4,4,4	0.25	0	6,6,6	0.29	0
2	SO4	H	1309	-	4,4,4	0.21	0	6,6,6	0.19	0
2	SO4	G	1308	-	4,4,4	0.25	0	6,6,6	0.43	0
2	SO4	D	1305	-	4,4,4	0.22	0	6,6,6	0.34	0

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	201/211 (95%)	-0.43	1 (0%) 87 87	10, 15, 27, 39	0
1	B	202/211 (95%)	0.05	17 (8%) 17 15	10, 18, 44, 53	0
1	C	202/211 (95%)	-0.18	3 (1%) 72 71	11, 19, 35, 42	0
1	D	202/211 (95%)	-0.02	18 (8%) 15 14	11, 17, 38, 47	0
1	E	204/211 (96%)	0.53	14 (6%) 23 21	21, 31, 47, 57	0
1	F	201/211 (95%)	0.33	15 (7%) 20 19	17, 28, 48, 53	0
1	G	202/211 (95%)	0.76	31 (15%) 5 4	19, 33, 54, 60	0
1	H	202/211 (95%)	-0.20	3 (1%) 72 71	14, 19, 38, 46	0
All	All	1616/1688 (95%)	0.11	102 (6%) 26 24	10, 23, 45, 60	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	156	VAL	7.7
1	B	160	SER	5.9
1	D	156	VAL	5.8
1	F	122	ALA	5.6
1	B	157	ILE	5.1
1	D	157	ILE	4.7
1	D	160	SER	4.6
1	B	2	THR	4.5
1	B	161	GLY	4.4
1	E	203	SER	4.4
1	F	125	VAL	4.3
1	D	158	PHE	4.3
1	D	203	SER	4.3
1	C	2	THR	4.2
1	B	173	GLY	4.1
1	G	125	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	174	GLN	3.9
1	G	156	VAL	3.8
1	A	203	SER	3.7
1	G	45	ALA	3.7
1	F	157	ILE	3.7
1	D	162	GLY	3.7
1	G	171	ALA	3.7
1	B	158	PHE	3.6
1	F	171	ALA	3.5
1	G	160	SER	3.5
1	G	52	GLY	3.4
1	G	158	PHE	3.4
1	B	162	GLY	3.4
1	D	171	ALA	3.3
1	G	157	ILE	3.2
1	G	60	ILE	3.1
1	F	202	GLY	3.1
1	E	125	VAL	3.1
1	F	161	GLY	3.0
1	B	155	GLU	3.0
1	G	56	TRP	3.0
1	E	55	ALA	2.9
1	D	124	ASN	2.9
1	B	159	LYS	2.9
1	D	155	GLU	2.9
1	D	122	ALA	2.9
1	F	126	ASN	2.8
1	F	156	VAL	2.7
1	F	174	GLN	2.7
1	C	203	SER	2.7
1	B	171	ALA	2.6
1	E	157	ILE	2.6
1	F	179	ASN	2.6
1	G	3	ALA	2.6
1	E	202	GLY	2.5
1	E	171	ALA	2.5
1	G	122	ALA	2.5
1	G	42	ARG	2.5
1	D	173	GLY	2.5
1	G	48	ASP	2.5
1	H	171	ALA	2.4
1	G	2	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	58	ALA	2.4
1	D	161	GLY	2.4
1	D	123	GLN	2.4
1	G	47	GLN	2.4
1	G	126	ASN	2.4
1	E	156	VAL	2.4
1	E	56	TRP	2.4
1	D	200	GLU	2.3
1	E	51	ASP	2.3
1	F	121	SER	2.3
1	G	50	ILE	2.3
1	G	49	VAL	2.3
1	G	161	GLY	2.3
1	C	155	GLU	2.3
1	B	154	ASP	2.3
1	G	200	GLU	2.3
1	B	176	LEU	2.3
1	G	44	THR	2.2
1	H	2	THR	2.2
1	D	2	THR	2.2
1	D	159	LYS	2.2
1	F	3	ALA	2.2
1	D	126	ASN	2.2
1	F	155	GLU	2.2
1	E	122	ALA	2.2
1	E	60	ILE	2.1
1	B	179	ASN	2.1
1	E	155	GLU	2.1
1	G	127	GLY	2.1
1	G	55	ALA	2.1
1	F	123	GLN	2.1
1	E	52	GLY	2.1
1	G	202	GLY	2.1
1	E	49	VAL	2.1
1	G	64	LYS	2.1
1	B	203	SER	2.1
1	G	46	PRO	2.1
1	F	158	PHE	2.1
1	H	156	VAL	2.1
1	D	179	ASN	2.0
1	G	203	SER	2.0
1	G	172	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	51	ASP	2.0
1	B	175	PRO	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
2	SO4	D	1310	5/5	0.83	0.13	72,72,73,73	0
2	SO4	H	1309	5/5	0.86	0.13	69,69,70,70	0
2	SO4	E	1306	5/5	0.94	0.08	29,31,32,33	0
2	SO4	G	1308	5/5	0.96	0.06	29,30,32,32	0
2	SO4	F	1307	5/5	0.98	0.05	16,18,19,20	0
2	SO4	B	1303	5/5	0.99	0.03	14,15,15,17	0
2	SO4	C	1304	5/5	0.99	0.04	18,20,21,24	0
2	SO4	D	1305	5/5	0.99	0.03	14,16,18,18	0
2	SO4	H	1301	5/5	0.99	0.04	15,17,18,18	0
2	SO4	A	1302	5/5	0.99	0.03	12,12,15,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.