



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:40 PM UTC

PDB ID : 4FFA / pdb_00004ffa
Title : Sulfatase from Mycobacterium tuberculosis
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Deposited on : 2012-05-31
Resolution : 2.50 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

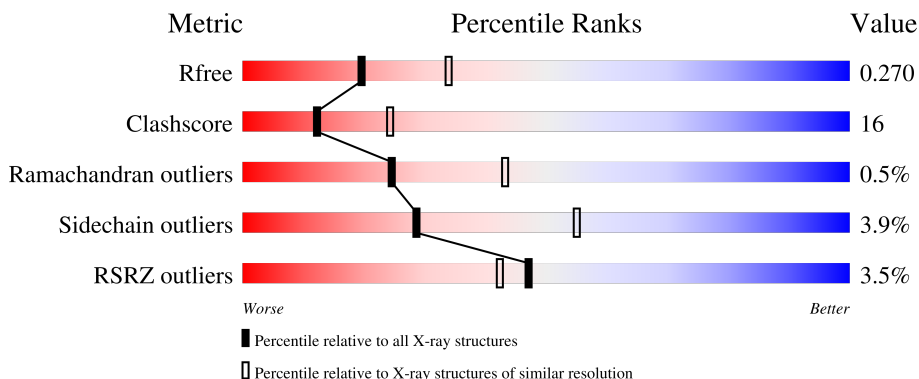
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	298	 0% 59% 20% 19% 2%
1	B	298	 0% 58% 18% 19% 2%
1	C	298	 5% 51% 26% 21% 1%
1	D	298	 3% 50% 26% 23%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7490 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 Rv3406 alkyl sulfatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	242	Total 1900	C 1199	N 349	O 347	S 5	0	0	0
1	B	240	Total 1880	C 1186	N 347	O 343	S 4	0	0	0
1	C	234	Total 1840	C 1164	N 338	O 334	S 4	0	0	0
1	D	230	Total 1809	C 1141	N 334	O 330	S 4	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P65075
A	-2	SER	-	expression tag	UNP P65075
A	-1	HIS	-	expression tag	UNP P65075
B	-3	GLY	-	expression tag	UNP P65075
B	-2	SER	-	expression tag	UNP P65075
B	-1	HIS	-	expression tag	UNP P65075
C	-3	GLY	-	expression tag	UNP P65075
C	-2	SER	-	expression tag	UNP P65075
C	-1	HIS	-	expression tag	UNP P65075
D	-3	GLY	-	expression tag	UNP P65075
D	-2	SER	-	expression tag	UNP P65075
D	-1	HIS	-	expression tag	UNP P65075

- Molecule 2 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	N O	0	0
			4	1 3		

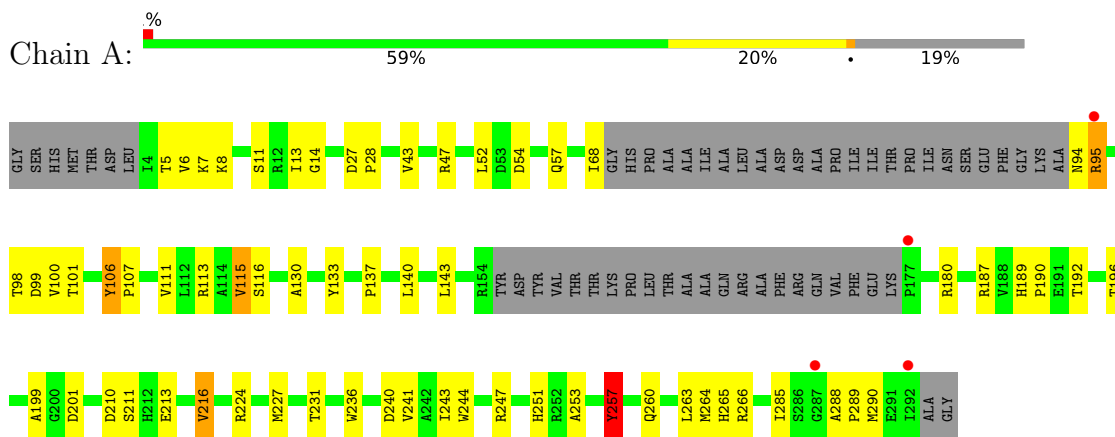
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	18	Total	O	0	0
			18	18		
3	C	9	Total	O	0	0
			9	9		
3	D	15	Total	O	0	0
			15	15		

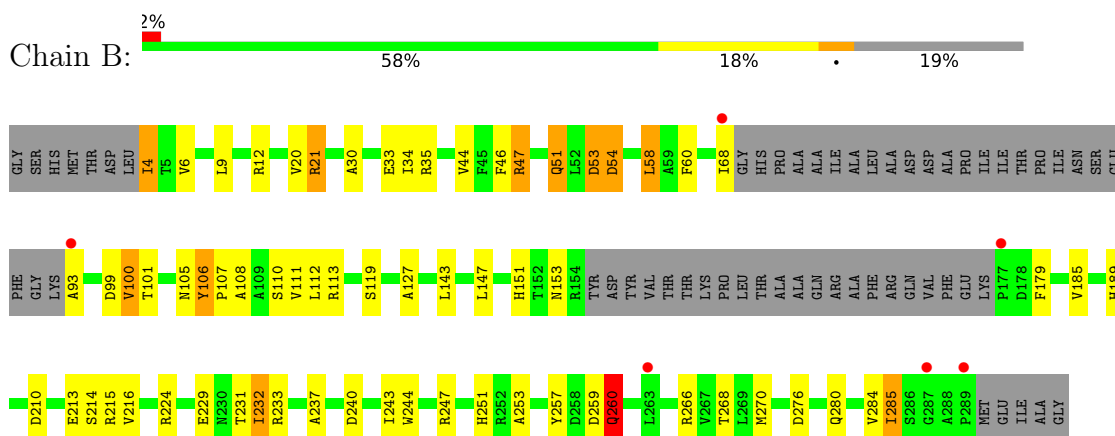
3 Residue-property plots i

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.

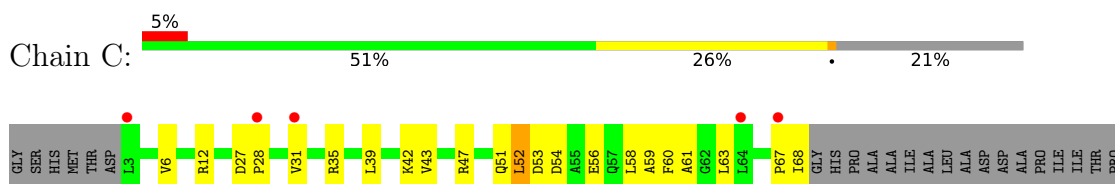
- Molecule 1: Rv3406 alkyl sulfatase

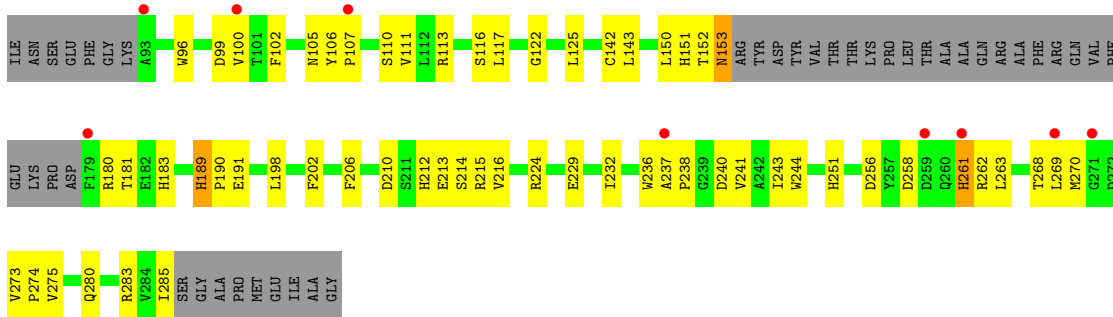


- Molecule 1: Rv3406 alkyl sulfatase

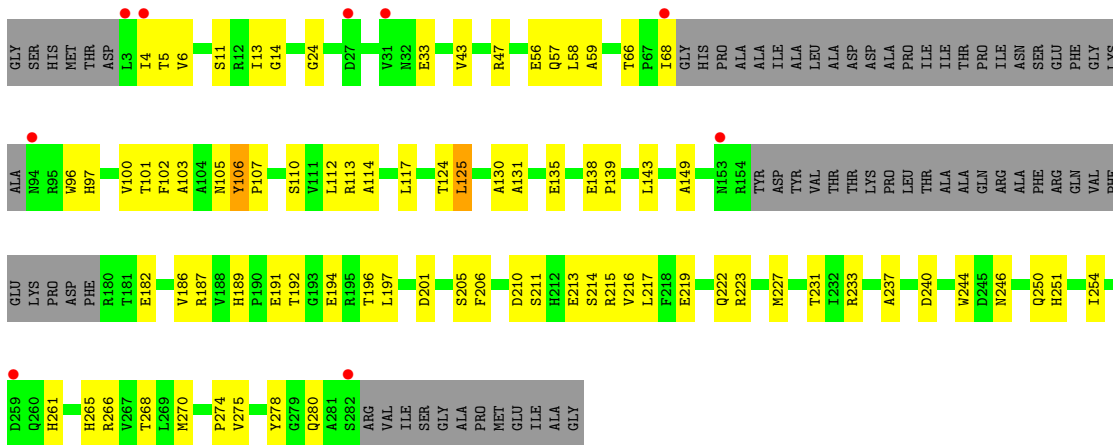


- Molecule 1: Rv3406 alkyl sulfatase





● Molecule 1: Rv3406 alkyl sulfatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.75Å 128.47Å 139.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.60 – 2.50 45.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (45.60-2.50) 98.4 (45.60-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.48Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.217 , 0.272 0.219 , 0.270	Depositor DCC
R_{free} test set	2040 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtrriage
Anisotropy	1.075	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7490	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: NO3

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	0.46	0/1945	0.85	4/2649 (0.2%)
1	B	0.49	0/1925	0.84	6/2623 (0.2%)
1	C	0.46	0/1883	0.83	3/2566 (0.1%)
1	D	0.47	0/1851	0.90	6/2522 (0.2%)
All	All	0.47	0/7604	0.86	19/10360 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	TYR	CA-C-N	7.17	127.20	119.89
1	A	106	TYR	C-N-CA	7.17	127.20	119.89
1	B	285	ILE	N-CA-C	-7.08	106.17	112.12
1	D	106	TYR	CA-C-N	6.87	126.91	119.90
1	D	106	TYR	C-N-CA	6.87	126.91	119.90
1	D	66	THR	CA-C-N	5.88	125.86	120.21
1	D	66	THR	C-N-CA	5.88	125.86	120.21
1	B	106	TYR	CA-C-N	5.73	125.74	119.90
1	B	106	TYR	C-N-CA	5.73	125.74	119.90
1	C	189	HIS	CA-C-N	5.71	126.10	119.47
1	C	189	HIS	C-N-CA	5.71	126.10	119.47
1	C	258	ASP	CB-CA-C	-5.47	110.28	116.63
1	B	189	HIS	CA-C-N	5.36	125.03	119.56
1	B	189	HIS	C-N-CA	5.36	125.03	119.56
1	A	257	TYR	N-CA-C	-5.30	105.26	112.26
1	D	237	ALA	CA-C-N	-5.18	114.44	119.78
1	D	237	ALA	C-N-CA	-5.18	114.44	119.78
1	B	257	TYR	N-CA-C	-5.05	106.42	112.59
1	A	95	ARG	N-CA-C	5.01	116.43	108.96

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	1900	0	1861	55	0
1	B	1880	0	1841	60	0
1	C	1840	0	1806	63	0
1	D	1809	0	1773	65	0
2	A	4	0	0	0	0
3	A	15	0	0	0	0
3	B	18	0	0	0	0
3	C	9	0	0	0	0
3	D	15	0	0	0	0
All	All	7490	0	7281	228	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 16.

All (228) 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:D:222:GLN:HE22	1:D:250:GLN:HE22	1.09	0.90
1:A:94:ASN:HD22	1:A:253:ALA:H	1.21	0.87
1:D:215:ARG:O	1:D:219:GLU:HG2	1.76	0.86
1:D:114:ALA:HB1	1:D:117:LEU:HD21	1.59	0.84
1:B:210:ASP:OD1	1:B:213:GLU:HG3	1.82	0.79
1:B:216:VAL:CG1	1:D:216:VAL:HG13	2.11	0.79
1:C:261:HIS:CE1	1:C:263:LEU:HB2	2.18	0.79
1:C:53:ASP:H	1:C:56:GLU:HB2	1.50	0.75
1:C:261:HIS:HE1	1:C:263:LEU:HD22	1.51	0.73
1:A:216:VAL:HG13	1:C:216:VAL:CG1	2.19	0.72
1:B:100:VAL:O	1:B:100:VAL:HG23	1.90	0.72
1:C:106:TYR:HB2	1:C:107:PRO:HD2	1.72	0.72
1:C:116:SER:HB3	1:C:261:HIS:NE2	2.06	0.71
1:A:266:ARG:HG2	1:A:266:ARG:HH11	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:SER:H	1:B:260:GLN:NE2	1.90	0.69
1:C:61:ALA:HB1	1:C:269:LEU:HD21	1.75	0.69
1:D:114:ALA:CB	1:D:117:LEU:HD21	2.23	0.68
1:D:57:GLN:NE2	1:D:265:HIS:HD2	1.92	0.67
1:C:152:THR:HG22	1:C:180:ARG:HG2	1.76	0.67
1:C:39:LEU:O	1:C:42:LYS:HE3	1.95	0.66
1:A:115:VAL:HG22	1:A:263:LEU:O	1.95	0.66
1:A:210:ASP:OD1	1:A:213:GLU:HG3	1.97	0.65
1:B:47:ARG:HG3	1:B:240:ASP:OD1	1.97	0.65
1:B:216:VAL:HG13	1:D:216:VAL:HG13	1.79	0.65
1:B:119:SER:H	1:B:260:GLN:HE22	1.44	0.64
1:A:57:GLN:NE2	1:A:265:HIS:HD2	1.95	0.64
1:B:58:LEU:C	1:B:58:LEU:HD13	2.24	0.63
1:A:99:ASP:CG	1:A:251:HIS:HE1	2.05	0.63
1:B:127:ALA:HB2	1:B:231:THR:HG22	1.80	0.63
1:A:288:ALA:HB1	1:A:289:PRO:HD2	1.80	0.63
1:B:100:VAL:HG22	1:B:107:PRO:HD2	1.81	0.63
1:B:99:ASP:CG	1:B:251:HIS:HE1	2.07	0.62
1:C:106:TYR:HB2	1:C:107:PRO:CD	2.31	0.61
1:D:278:TYR:HB2	1:D:280:GLN:OE1	2.01	0.61
1:D:68:ILE:HD11	1:D:270:MET:SD	2.40	0.60
1:A:57:GLN:NE2	1:A:113:ARG:HE	1.99	0.60
1:B:68:ILE:HD12	1:B:68:ILE:C	2.27	0.60
1:A:227:MET:O	1:A:231:THR:HG23	2.01	0.59
1:D:112:LEU:CD1	1:D:266:ARG:HB2	2.33	0.59
1:C:51:GLN:HG2	1:C:52:LEU:N	2.18	0.58
1:B:53:ASP:HA	1:B:113:ARG:HH12	1.68	0.58
1:B:224:ARG:HD2	1:D:213:GLU:OE2	2.03	0.58
1:A:99:ASP:OD1	1:A:251:HIS:HE1	1.85	0.58
1:D:211:SER:O	1:D:215:ARG:HG2	2.03	0.58
1:B:216:VAL:CG1	1:D:216:VAL:CG1	2.80	0.57
1:C:256:ASP:O	1:D:11:SER:HB3	2.05	0.57
1:B:68:ILE:HG12	1:B:268:THR:HB	1.86	0.56
1:B:153:ASN:ND2	1:B:179:PHE:HD2	2.03	0.56
1:C:275:VAL:HA	1:C:280:GLN:O	2.05	0.56
1:B:53:ASP:O	1:B:54:ASP:C	2.47	0.56
1:C:100:VAL:O	1:C:106:TYR:HB3	2.06	0.56
1:C:273:VAL:HG13	1:C:274:PRO:HD2	1.88	0.55
1:D:47:ARG:NH1	1:D:240:ASP:OD2	2.39	0.55
1:B:12:ARG:HD3	1:B:229:GLU:O	2.06	0.55
1:B:237:ALA:O	1:B:240:ASP:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:VAL:HA	1:D:280:GLN:O	2.07	0.55
1:C:237:ALA:O	1:C:240:ASP:HB2	2.07	0.55
1:C:59:ALA:O	1:C:63:LEU:HD13	2.08	0.54
1:C:117:LEU:HD12	1:C:238:PRO:HD3	1.89	0.54
1:A:7:LYS:HD2	1:A:8:LYS:H	1.72	0.54
1:C:58:LEU:HD13	1:C:58:LEU:C	2.33	0.54
1:A:130:ALA:HB2	1:A:196:THR:HG22	1.89	0.54
1:C:151:HIS:ND1	1:C:183:HIS:HD2	2.06	0.54
1:A:54:ASP:OD1	1:A:113:ARG:NH2	2.41	0.53
1:C:212:HIS:O	1:C:216:VAL:HG23	2.08	0.53
1:A:6:VAL:HG13	1:A:6:VAL:O	2.09	0.53
1:C:60:PHE:O	1:C:63:LEU:HB2	2.08	0.53
1:D:223:ARG:O	1:D:227:MET:HE2	2.09	0.53
1:C:206:PHE:HD2	1:C:214:SER:HA	1.74	0.52
1:D:125:LEU:HD13	1:D:254:ILE:HD11	1.90	0.52
1:A:210:ASP:OD1	1:A:210:ASP:C	2.53	0.52
1:B:21:ARG:N	1:B:21:ARG:HD2	2.24	0.52
1:A:8:LYS:HE3	1:A:11:SER:HA	1.90	0.52
1:A:99:ASP:OD1	1:A:251:HIS:CE1	2.63	0.52
1:D:4:ILE:HG13	1:D:5:THR:N	2.23	0.52
1:C:99:ASP:CG	1:C:251:HIS:HE1	2.17	0.52
1:A:7:LYS:HD2	1:A:8:LYS:N	2.25	0.52
1:A:210:ASP:CG	1:A:213:GLU:HG3	2.35	0.52
1:A:236:TRP:CE3	1:A:264:MET:HE1	2.44	0.51
1:C:102:PHE:CD2	1:C:153:ASN:HB3	2.46	0.51
1:B:46:PHE:HE2	1:B:243:ILE:HD12	1.76	0.51
1:C:215:ARG:NH1	1:C:215:ARG:HG2	2.26	0.51
1:A:137:PRO:HD2	1:A:140:LEU:HD12	1.93	0.50
1:A:285:ILE:N	1:A:285:ILE:HD12	2.27	0.50
1:D:125:LEU:CD1	1:D:233:ARG:HG3	2.42	0.50
1:A:106:TYR:HB2	1:A:107:PRO:HD2	1.94	0.50
1:A:288:ALA:HB1	1:A:289:PRO:CD	2.41	0.50
1:D:106:TYR:HB2	1:D:107:PRO:HD2	1.94	0.49
1:B:51:GLN:CD	1:B:51:GLN:H	2.20	0.49
1:A:27:ASP:OD1	1:A:28:PRO:HD2	2.13	0.49
1:B:100:VAL:CG2	1:B:107:PRO:CD	2.90	0.49
1:C:105:ASN:HB3	1:C:273:VAL:HG23	1.95	0.49
1:D:189:HIS:CE1	1:D:191:GLU:HB2	2.47	0.49
1:D:125:LEU:CD1	1:D:254:ILE:HD11	2.43	0.49
1:B:106:TYR:HB2	1:B:107:PRO:HD2	1.95	0.48
1:D:47:ARG:HD2	1:D:240:ASP:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLN:HE21	1:A:113:ARG:HE	1.59	0.48
1:B:276:ASP:OD1	1:B:276:ASP:C	2.55	0.48
1:B:105:ASN:ND2	1:B:270:MET:HE3	2.28	0.48
1:D:131:ALA:O	1:D:135:GLU:HG2	2.14	0.48
1:A:111:VAL:HG22	1:A:243:ILE:HG12	1.94	0.48
1:A:213:GLU:OE2	1:C:224:ARG:HD2	2.14	0.48
1:C:67:PRO:C	1:C:68:ILE:HG13	2.39	0.48
1:C:96:TRP:CH2	1:C:125:LEU:HB3	2.49	0.47
1:C:6:VAL:HG23	1:C:6:VAL:O	2.13	0.47
1:C:215:ARG:HG2	1:C:215:ARG:HH11	1.79	0.47
1:A:187:ARG:NH1	1:A:247:ARG:HG2	2.29	0.47
1:C:181:THR:HG23	1:C:283:ARG:O	2.14	0.47
1:D:97:HIS:HE2	1:D:251:HIS:CE1	2.32	0.47
1:B:215:ARG:NE	1:B:215:ARG:HA	2.30	0.47
1:D:97:HIS:NE2	1:D:251:HIS:CE1	2.82	0.47
1:D:206:PHE:HD2	1:D:214:SER:HA	1.80	0.47
1:D:6:VAL:O	1:D:6:VAL:HG23	2.15	0.47
1:D:57:GLN:NE2	1:D:113:ARG:HE	2.13	0.47
1:A:68:ILE:HD13	1:A:290:MET:CE	2.45	0.47
1:C:110:SER:HB2	1:C:244:TRP:CZ2	2.50	0.47
1:A:47:ARG:NH1	1:A:240:ASP:OD2	2.48	0.46
1:D:57:GLN:HE21	1:D:113:ARG:HE	1.63	0.46
1:D:112:LEU:HD12	1:D:266:ARG:HB2	1.98	0.46
1:B:111:VAL:HG22	1:B:243:ILE:HG12	1.97	0.46
1:C:52:LEU:HD12	1:C:241:VAL:HG21	1.97	0.46
1:B:101:THR:OG1	1:B:151:HIS:HD2	1.99	0.46
1:B:216:VAL:HG11	1:D:216:VAL:HG13	1.95	0.46
1:B:284:VAL:O	1:B:285:ILE:HD13	2.16	0.46
1:C:68:ILE:HD11	1:C:270:MET:HA	1.97	0.46
1:C:99:ASP:OD1	1:C:251:HIS:HE1	1.98	0.46
1:B:232:ILE:HG13	1:B:233:ARG:N	2.31	0.46
1:C:122:GLY:O	1:C:236:TRP:HD1	1.99	0.46
1:C:180:ARG:HH11	1:C:285:ILE:HG22	1.80	0.46
1:D:24:GLY:HA3	1:D:59:ALA:HB1	1.97	0.46
1:A:43:VAL:HG23	1:A:244:TRP:HB3	1.97	0.46
1:A:216:VAL:HG13	1:C:216:VAL:HG11	1.96	0.45
1:C:102:PHE:CE2	1:C:153:ASN:HB3	2.51	0.45
1:A:68:ILE:HD13	1:A:290:MET:HE1	1.97	0.45
1:B:51:GLN:H	1:B:51:GLN:NE2	2.14	0.45
1:D:112:LEU:HD13	1:D:266:ARG:HB2	1.98	0.45
1:B:60:PHE:O	1:B:60:PHE:CG	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ASP:OD1	1:C:113:ARG:NH2	2.50	0.45
1:D:130:ALA:HB2	1:D:196:THR:HG22	1.97	0.45
1:A:266:ARG:HG2	1:A:266:ARG:NH1	2.25	0.45
1:C:12:ARG:NH1	1:C:229:GLU:HB3	2.32	0.45
1:D:58:LEU:O	1:D:59:ALA:C	2.59	0.45
1:D:105:ASN:CG	1:D:105:ASN:O	2.60	0.45
1:D:110:SER:HB2	1:D:244:TRP:CZ2	2.52	0.44
1:A:133:TYR:CD2	1:A:133:TYR:C	2.95	0.44
1:A:115:VAL:HG22	1:A:263:LEU:C	2.42	0.44
1:B:47:ARG:HD2	1:B:240:ASP:OD1	2.16	0.44
1:A:98:THR:HB	1:A:101:THR:HG21	1.98	0.44
1:B:99:ASP:OD1	1:B:251:HIS:HE1	2.00	0.44
1:C:263:LEU:HD12	1:C:263:LEU:HA	1.84	0.44
1:B:112:LEU:CD1	1:B:266:ARG:HB2	2.48	0.44
1:D:227:MET:O	1:D:231:THR:HG23	2.18	0.44
1:A:100:VAL:HG12	1:A:100:VAL:O	2.18	0.44
1:D:56:GLU:HA	1:D:56:GLU:OE1	2.18	0.44
1:D:96:TRP:O	1:D:201:ASP:HB2	2.18	0.44
1:B:4:ILE:HG12	1:B:33:GLU:OE1	2.18	0.43
1:C:210:ASP:OD1	1:C:213:GLU:HB2	2.18	0.43
1:D:57:GLN:CD	1:D:265:HIS:HD2	2.25	0.43
1:C:58:LEU:HD13	1:C:58:LEU:O	2.17	0.43
1:C:102:PHE:HE2	1:C:202:PHE:CE1	2.36	0.43
1:B:68:ILE:C	1:B:68:ILE:CD1	2.92	0.43
1:B:147:LEU:HD23	1:B:185:VAL:HG21	2.01	0.43
1:D:124:THR:HG22	1:D:125:LEU:N	2.34	0.43
1:A:189:HIS:HB3	1:A:192:THR:OG1	2.17	0.43
1:C:43:VAL:HG23	1:C:244:TRP:HB3	2.00	0.43
1:D:275:VAL:HG23	1:D:280:GLN:O	2.18	0.43
1:A:143:LEU:HB2	1:C:143:LEU:HB2	2.00	0.43
1:A:189:HIS:HA	1:A:190:PRO:HD3	1.90	0.43
1:B:210:ASP:OD1	1:B:210:ASP:C	2.61	0.43
1:A:216:VAL:HG13	1:C:216:VAL:HG12	1.99	0.43
1:D:107:PRO:HB3	1:D:268:THR:CG2	2.48	0.43
1:C:183:HIS:HB3	1:C:198:LEU:HD23	2.01	0.43
1:C:47:ARG:HD3	1:C:240:ASP:OD1	2.19	0.43
1:B:100:VAL:O	1:B:100:VAL:CG2	2.63	0.42
1:C:107:PRO:HB3	1:C:268:THR:CG2	2.49	0.42
1:A:224:ARG:HD2	1:C:213:GLU:OE1	2.19	0.42
1:B:100:VAL:CG2	1:B:107:PRO:HD2	2.47	0.42
1:C:180:ARG:NH1	1:C:285:ILE:HG22	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:LEU:HD23	1:D:217:LEU:HA	1.85	0.42
1:D:222:GLN:NE2	1:D:250:GLN:HE22	1.94	0.42
1:D:107:PRO:O	1:D:246:ASN:HB3	2.19	0.42
1:A:227:MET:HE2	1:A:227:MET:HB2	1.90	0.42
1:B:216:VAL:HG13	1:D:216:VAL:CG1	2.45	0.42
1:C:31:VAL:HG21	1:C:63:LEU:HB3	2.00	0.42
1:D:58:LEU:C	1:D:58:LEU:HD23	2.45	0.42
1:A:13:ILE:HG12	1:A:14:GLY:N	2.35	0.42
1:A:130:ALA:CB	1:A:196:THR:HG22	2.50	0.42
1:B:58:LEU:C	1:B:58:LEU:CD1	2.93	0.42
1:D:13:ILE:HG12	1:D:14:GLY:N	2.35	0.42
1:B:110:SER:HB2	1:B:244:TRP:CZ2	2.55	0.42
1:D:100:VAL:HG12	1:D:102:PHE:CE2	2.54	0.42
1:B:53:ASP:OD1	1:B:54:ASP:N	2.53	0.41
1:B:100:VAL:HG22	1:B:107:PRO:CD	2.44	0.41
1:D:125:LEU:HD11	1:D:233:ARG:HD2	2.01	0.41
1:C:111:VAL:HG22	1:C:243:ILE:HG12	2.03	0.41
1:C:189:HIS:HA	1:C:190:PRO:HD3	1.86	0.41
1:D:187:ARG:NH1	1:D:274:PRO:HG3	2.35	0.41
1:A:99:ASP:CG	1:A:251:HIS:CE1	2.93	0.41
1:B:44:VAL:HG23	1:B:243:ILE:HB	2.01	0.41
1:D:97:HIS:NE2	1:D:251:HIS:NE2	2.68	0.41
1:A:57:GLN:HE22	1:A:113:ARG:HB3	1.86	0.41
1:D:101:THR:C	1:D:103:ALA:N	2.75	0.41
1:D:192:THR:C	1:D:194:GLU:H	2.28	0.41
1:A:95:ARG:HD3	1:A:201:ASP:OD1	2.20	0.41
1:B:107:PRO:HB3	1:B:268:THR:CG2	2.50	0.41
1:A:52:LEU:HD12	1:A:241:VAL:HG21	2.02	0.41
1:B:9:LEU:HD23	1:B:9:LEU:HA	1.94	0.41
1:B:108:ALA:HA	1:B:247:ARG:HG3	2.03	0.41
1:C:35:ARG:O	1:C:39:LEU:HG	2.20	0.41
1:C:189:HIS:HE1	1:C:191:GLU:HB2	1.86	0.41
1:D:149:ALA:O	1:D:182:GLU:HA	2.21	0.41
1:D:186:VAL:HG22	1:D:197:LEU:HD23	2.02	0.41
1:B:93:ALA:O	1:B:253:ALA:N	2.46	0.40
1:B:6:VAL:O	1:B:6:VAL:HG23	2.21	0.40
1:B:51:GLN:CD	1:B:51:GLN:N	2.80	0.40
1:B:101:THR:OG1	1:B:151:HIS:CD2	2.74	0.40
1:C:236:TRP:CD1	1:C:262:ARG:HH21	2.40	0.40
1:D:57:GLN:HE22	1:D:113:ARG:HG2	1.85	0.40
1:D:138:GLU:HB3	1:D:139:PRO:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:GLY:HA2	1:D:43:VAL:O	2.22	0.40
1:A:216:VAL:CG1	1:C:216:VAL:CG1	2.96	0.40
1:B:30:ALA:O	1:B:34:ILE:HG13	2.22	0.40
1:B:143:LEU:HB2	1:D:143:LEU:HB2	2.02	0.40
1:B:259:ASP:C	1:B:260:GLN:O	2.64	0.40
1:A:257:TYR:CD2	1:A:257:TYR:N	2.89	0.40
1:A:264:MET:HE3	1:A:264:MET:HB3	1.99	0.40
1:C:27:ASP:OD1	1:C:28:PRO:HD2	2.22	0.40
1:D:101:THR:C	1:D:103:ALA:H	2.28	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	236/298 (79%)	223 (94%)	11 (5%)	2 (1%)	16	31
1	B	234/298 (78%)	220 (94%)	12 (5%)	2 (1%)	14	27
1	C	228/298 (76%)	210 (92%)	17 (8%)	1 (0%)	30	49
1	D	224/298 (75%)	209 (93%)	15 (7%)	0	100	100
All	All	922/1192 (77%)	862 (94%)	55 (6%)	5 (0%)	24	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	B	54	ASP
1	A	199	ALA
1	B	260	GLN
1	C	52	LEU

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	198/240 (82%)	191 (96%)	7 (4%)	32	58
1	B	195/240 (81%)	182 (93%)	13 (7%)	15	31
1	C	191/240 (80%)	186 (97%)	5 (3%)	40	68
1	D	188/240 (78%)	183 (97%)	5 (3%)	39	67
All	All	772/960 (80%)	742 (96%)	30 (4%)	28	55

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	115	VAL
1	A	116	SER
1	A	180	ARG
1	A	211	SER
1	A	216	VAL
1	A	257	TYR
1	B	4	ILE
1	B	20	VAL
1	B	21	ARG
1	B	35	ARG
1	B	47	ARG
1	B	51	GLN
1	B	53	ASP
1	B	58	LEU
1	B	100	VAL
1	B	214	SER
1	B	232	ILE
1	B	260	GLN
1	B	280	GLN
1	C	142	CYS
1	C	150	LEU
1	C	153	ASN
1	C	232	ILE

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Mol	Chain	Res	Type
1	C	261	HIS
1	D	33	GLU
1	D	125	LEU
1	D	205	SER
1	D	210	ASP
1	D	261	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	94	ASN
1	A	235	ASN
1	A	251	HIS
1	A	265	HIS
1	B	151	HIS
1	B	235	ASN
1	B	251	HIS
1	B	260	GLN
1	C	16	GLN
1	C	57	GLN
1	C	151	HIS
1	C	212	HIS
1	C	261	HIS
1	C	265	HIS
1	C	280	GLN
1	D	57	GLN
1	D	146	ASN
1	D	222	GLN
1	D	265	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	NO3	A	301	-	1,3,3	3.20	1 (100%)	0,3,3	-	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NO3	O1-N	3.20	1.40	1.24

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	242/298 (81%)	0.39	4 (1%) 69 65	46, 63, 84, 102	0
1	B	240/298 (80%)	0.56	6 (2%) 58 54	46, 62, 87, 104	0
1	C	234/298 (78%)	0.74	14 (5%) 27 24	50, 70, 94, 111	0
1	D	230/298 (77%)	0.66	9 (3%) 43 38	51, 67, 86, 113	0
All	All	946/1192 (79%)	0.59	33 (3%) 47 42	46, 65, 90, 113	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	LEU	4.8
1	C	3	LEU	4.3
1	A	292	ILE	4.1
1	A	177	PRO	3.7
1	C	259	ASP	3.7
1	B	289	PRO	3.4
1	B	68	ILE	3.1
1	D	282	SER	3.1
1	C	93	ALA	3.0
1	B	177	PRO	3.0
1	A	287	GLY	2.9
1	C	107	PRO	2.8
1	C	28	PRO	2.7
1	D	4	ILE	2.7
1	D	94	ASN	2.7
1	C	237	ALA	2.7
1	C	271	GLY	2.5
1	C	179	PHE	2.5
1	D	68	ILE	2.5
1	C	261	HIS	2.5
1	C	64	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	95	ARG	2.3
1	C	31	VAL	2.3
1	C	269	LEU	2.2
1	D	259	ASP	2.2
1	C	67	PRO	2.2
1	D	153	ASN	2.1
1	B	263	LEU	2.1
1	D	27	ASP	2.1
1	C	100	VAL	2.1
1	D	31	VAL	2.1
1	B	287	GLY	2.1
1	B	93	ALA	2.1

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(Å ²)	Q<0.9
2	NO3	A	301	4/4	0.76	0.09	72,74,78,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.