



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2025 – 04:41 pm BST

PDB ID : 9QZK / pdb_00009qzk
Title : SadB of Pseudomonas aeruginosa
Authors : Opatowsky, Y.; Sporny, M.
Deposited on : 2025-04-23
Resolution : 3.16 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 Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

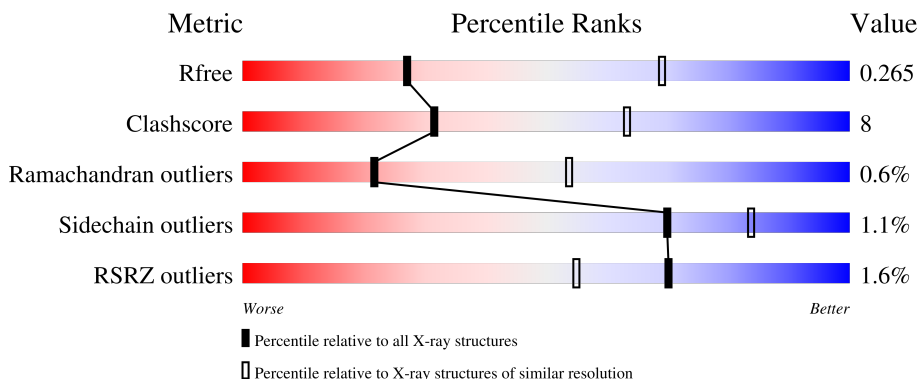
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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}	164625	2168 (3.20-3.12)
Clashscore	180529	2333 (3.20-3.12)
Ramachandran outliers	177936	2266 (3.20-3.12)
Sidechain outliers	177891	2265 (3.20-3.12)
RSRZ outliers	164620	2169 (3.20-3.12)

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	457	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 83% 16% </div> </div>
1	B	457	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 2% </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 82% 16% </div> </div>
1	C	457	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 3% </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 82% 17% </div> </div>
1	D	457	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 79% 20% </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14188 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.

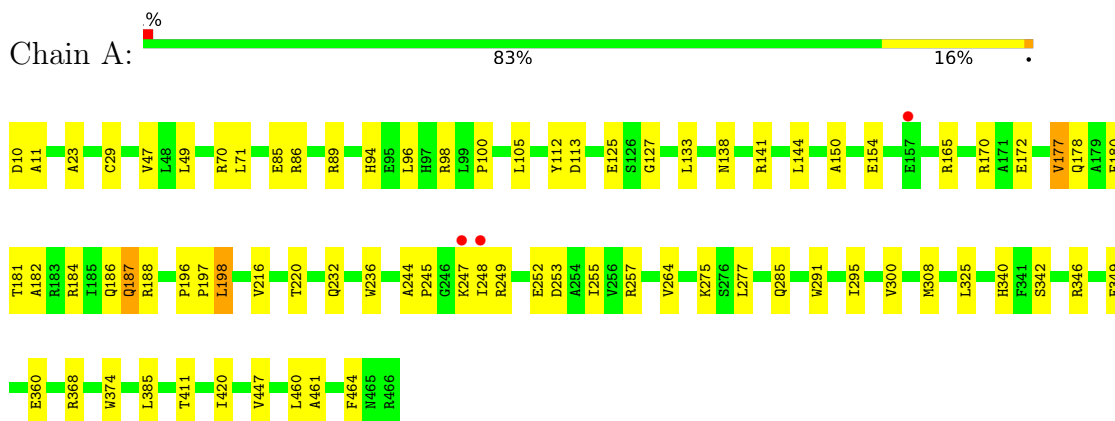
- Molecule 1 is a protein called HDOD domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3547	2258	630	650	9			
1	B	457	Total	C	N	O	S	0	0	0
			3547	2258	630	650	9			
1	C	457	Total	C	N	O	S	0	0	0
			3547	2258	630	650	9			
1	D	457	Total	C	N	O	S	0	0	0
			3547	2258	630	650	9			

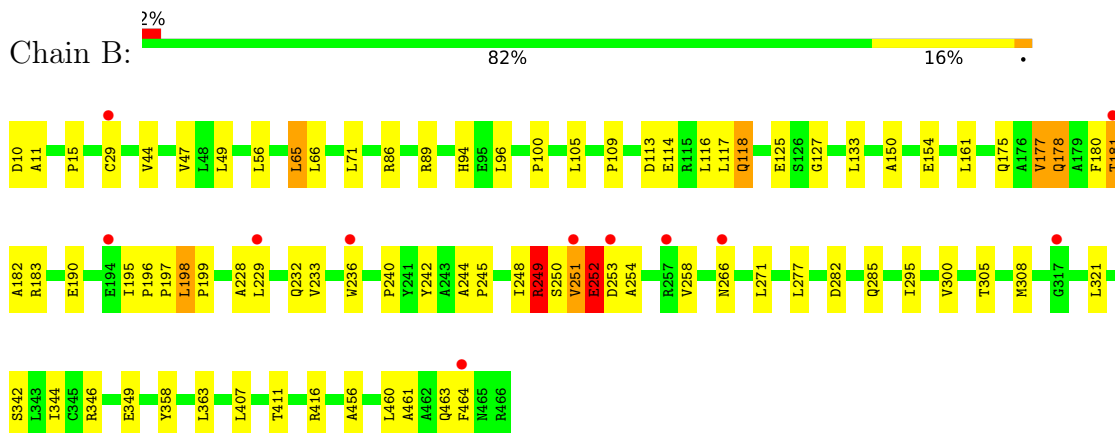
3 Residue-property plots [i](#)

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.

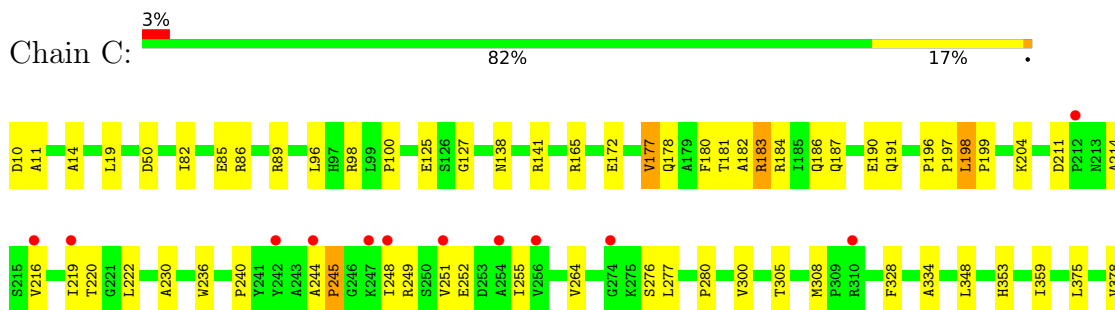
• Molecule 1: HDOD domain-containing protein



• Molecule 1: HDOD domain-containing protein



• Molecule 1: HDOD domain-containing protein





- Molecule 1: HDOD domain-containing protein

Chain D: 79% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.73Å 162.28Å 238.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 3.16 49.25 – 3.16	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.25-3.16) 98.4 (49.25-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.222 , 0.265 0.224 , 0.265	Depositor DCC
R_{free} test set	3271 reflections (2.81%)	wwPDB-VP
Wilson B-factor (Å ²)	128.7	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 92.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14188	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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

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	0.30	0/3619	0.54	0/4930
1	B	0.34	0/3619	0.62	1/4930 (0.0%)
1	C	0.32	0/3619	0.57	0/4930
1	D	0.29	0/3619	0.55	1/4930 (0.0%)
All	All	0.31	0/14476	0.57	2/19720 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	C	0	2
1	D	0	2
All	All	0	7

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	181	THR	CB-CA-C	-7.92	97.39	110.85
1	D	245	PRO	N-CA-CB	-5.44	97.54	103.25

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	183	ARG	Sidechain
1	B	245	PRO	Mainchain
1	B	249	ARG	Sidechain
1	C	183	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	184	ARG	Sidechain
1	D	183	ARG	Sidechain
1	D	184	ARG	Sidechain

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	3547	0	3626	58	0
1	B	3547	0	3626	56	0
1	C	3547	0	3626	54	0
1	D	3547	0	3626	62	0
All	All	14188	0	14504	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 8.

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:A:291:TRP:CE2	1:A:464:PHE:CE2	2.34	1.14
1:A:291:TRP:CZ2	1:A:464:PHE:CZ	2.40	1.09
1:A:291:TRP:CZ2	1:A:464:PHE:CE2	2.42	1.07
1:C:14:ALA:HB3	1:C:19:LEU:HD11	1.49	0.92
1:A:96:LEU:HD12	1:A:127:GLY:HA3	1.54	0.90
1:D:96:LEU:HD12	1:D:127:GLY:HA3	1.53	0.89
1:A:291:TRP:CE2	1:A:464:PHE:CZ	2.60	0.89
1:C:220:THR:HG21	1:C:252:GLU:HB2	1.58	0.82
1:B:244:ALA:HB2	1:B:258:VAL:HG22	1.63	0.80
1:B:96:LEU:HD12	1:B:127:GLY:HA3	1.64	0.78
1:C:96:LEU:HD12	1:C:127:GLY:HA3	1.66	0.76
1:C:14:ALA:CB	1:C:19:LEU:HD11	2.15	0.75
1:C:14:ALA:HB3	1:C:19:LEU:CD1	2.17	0.75
1:A:291:TRP:CD2	1:A:464:PHE:CE2	2.74	0.74
1:C:196:PRO:HG2	1:C:277:LEU:HD21	1.69	0.73
1:A:94:HIS:HB2	1:A:96:LEU:HD23	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:VAL:HG12	1:B:411:THR:HG22	1.74	0.69
1:A:248:ILE:HG13	1:A:249:ARG:H	1.57	0.69
1:D:300:VAL:HG12	1:D:411:THR:HG22	1.75	0.69
1:C:244:ALA:HB1	1:C:245:PRO:HD2	1.75	0.68
1:A:177:VAL:HA	1:A:181:THR:HG23	1.76	0.68
1:D:248:ILE:HG13	1:D:249:ARG:H	1.58	0.68
1:D:305:THR:HA	1:D:308:MET:HE3	1.75	0.67
1:A:29:CYS:HB2	1:A:133:LEU:HD12	1.76	0.67
1:A:291:TRP:CH2	1:A:464:PHE:CE2	2.82	0.66
1:C:308:MET:HE1	1:C:407:LEU:HD11	1.77	0.66
1:C:300:VAL:HG12	1:C:411:THR:HG22	1.77	0.66
1:C:204:LYS:HB3	1:C:222:LEU:HD11	1.79	0.65
1:A:291:TRP:CD2	1:A:464:PHE:CD2	2.85	0.65
1:B:44:VAL:HG13	1:B:116:LEU:HD11	1.80	0.64
1:D:344:ILE:HD13	1:D:363:LEU:HD12	1.78	0.64
1:D:184:ARG:O	1:D:192:THR:HG23	1.97	0.63
1:A:291:TRP:CH2	1:A:464:PHE:HE2	2.17	0.62
1:A:196:PRO:HG2	1:A:277:LEU:HD21	1.82	0.62
1:B:177:VAL:HG13	1:B:181:THR:HG21	1.80	0.62
1:A:300:VAL:HG12	1:A:411:THR:HG22	1.82	0.60
1:A:325:LEU:HD12	1:A:385:LEU:HD21	1.83	0.60
1:A:70:ARG:NH2	1:A:154:GLU:OE2	2.36	0.59
1:D:445:ASP:OD2	1:D:449:LYS:NZ	2.34	0.59
1:B:100:PRO:HG2	1:B:105:LEU:HD11	1.83	0.59
1:C:181:THR:O	1:C:182:ALA:HB3	2.03	0.59
1:A:23:ALA:HB1	1:C:180:PHE:O	2.01	0.59
1:C:406:ASN:OD1	1:C:435:ARG:NH1	2.36	0.58
1:B:29:CYS:HB2	1:B:133:LEU:HD12	1.84	0.58
1:B:250:SER:O	1:B:251:VAL:C	2.46	0.58
1:C:248:ILE:HG13	1:C:249:ARG:H	1.69	0.58
1:C:305:THR:HA	1:C:308:MET:HE3	1.84	0.58
1:C:50:ASP:HB3	1:C:82:ILE:HG22	1.85	0.58
1:B:181:THR:O	1:B:182:ALA:HB3	2.04	0.57
1:D:138:ASN:OD1	1:D:141:ARG:NH1	2.36	0.57
1:B:180:PHE:O	1:D:23:ALA:HB1	2.04	0.57
1:C:165:ARG:NH2	1:C:172:GLU:OE2	2.37	0.56
1:B:240:PRO:HG2	1:B:456:ALA:HB1	1.88	0.56
1:D:165:ARG:NH2	1:D:172:GLU:OE2	2.38	0.56
1:A:248:ILE:HG13	1:A:249:ARG:N	2.20	0.56
1:B:229:LEU:O	1:B:233:VAL:HG23	2.06	0.56
1:D:10:ASP:CG	1:D:11:ALA:H	2.14	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:VAL:O	1:B:252:GLU:C	2.48	0.56
1:A:291:TRP:CE2	1:A:464:PHE:CD2	2.91	0.56
1:C:14:ALA:CB	1:C:19:LEU:CD1	2.81	0.55
1:B:100:PRO:HG2	1:B:105:LEU:CD1	2.37	0.55
1:A:10:ASP:CG	1:A:11:ALA:H	2.15	0.55
1:C:248:ILE:HG13	1:C:249:ARG:N	2.22	0.55
1:B:248:ILE:O	1:B:249:ARG:C	2.47	0.55
1:C:98:ARG:HB2	1:C:127:GLY:HA2	1.89	0.55
1:C:236:TRP:CE2	1:C:460:LEU:HD21	2.42	0.55
1:B:308:MET:HE1	1:B:407:LEU:HD11	1.89	0.54
1:D:211:ASP:HB3	1:D:214:ALA:HB2	1.89	0.54
1:B:10:ASP:CG	1:B:11:ALA:H	2.15	0.54
1:D:94:HIS:HB2	1:D:96:LEU:HD23	1.90	0.54
1:B:65:LEU:HD23	1:B:154:GLU:HB3	1.90	0.54
1:C:190:GLU:OE1	1:C:190:GLU:N	2.38	0.53
1:C:181:THR:HB	1:C:183:ARG:HG2	1.89	0.53
1:A:100:PRO:HB3	1:A:125:GLU:O	2.07	0.53
1:A:187:GLN:HG2	1:A:188:ARG:HG3	1.90	0.53
1:D:29:CYS:HB2	1:D:133:LEU:HD12	1.91	0.53
1:D:216:VAL:O	1:D:220:THR:OG1	2.26	0.53
1:D:248:ILE:HG13	1:D:249:ARG:N	2.21	0.53
1:A:291:TRP:CZ2	1:A:464:PHE:HZ	2.19	0.52
1:B:271:LEU:HD23	1:B:464:PHE:CE2	2.44	0.52
1:C:255:ILE:HG12	1:C:264:VAL:HG21	1.90	0.52
1:B:175:GLN:HE22	1:B:178:GLN:HE22	1.56	0.52
1:C:138:ASN:OD1	1:C:141:ARG:NH1	2.43	0.52
1:D:244:ALA:HB1	1:D:245:PRO:HD2	1.92	0.52
1:A:285:GLN:HG2	1:A:349:GLU:HG2	1.92	0.52
1:C:177:VAL:HA	1:C:181:THR:HG23	1.92	0.52
1:C:177:VAL:HG13	1:C:181:THR:HG21	1.91	0.52
1:B:295:ILE:HD12	1:B:461:ALA:HB2	1.91	0.52
1:C:10:ASP:CG	1:C:11:ALA:H	2.18	0.51
1:C:211:ASP:HB3	1:C:214:ALA:HB2	1.91	0.51
1:D:100:PRO:HB3	1:D:125:GLU:O	2.10	0.51
1:D:275:LYS:O	1:D:275:LYS:HG2	2.11	0.51
1:B:228:ALA:O	1:B:232:GLN:HG3	2.11	0.51
1:C:86:ARG:HH11	1:C:89:ARG:NH1	2.08	0.51
1:C:204:LYS:HB2	1:C:222:LEU:HD21	1.93	0.51
1:D:190:GLU:OE1	1:D:190:GLU:N	2.41	0.51
1:D:253:ASP:OD1	1:D:257:ARG:HD2	2.10	0.51
1:B:177:VAL:HA	1:B:181:THR:HG23	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:ASN:HB3	1:C:432:LEU:HD11	1.92	0.50
1:C:454:GLU:OE1	1:C:458:ARG:NH2	2.42	0.50
1:D:295:ILE:HD12	1:D:461:ALA:HB2	1.93	0.50
1:B:56:LEU:HD12	1:B:109:PRO:O	2.12	0.50
1:A:112:TYR:CD1	1:A:144:LEU:HD13	2.46	0.50
1:B:285:GLN:HG2	1:B:349:GLU:HG2	1.94	0.50
1:D:186:GLN:OE1	1:D:191:GLN:HB3	2.11	0.50
1:B:100:PRO:HB3	1:B:125:GLU:O	2.11	0.50
1:C:197:PRO:O	1:C:198:LEU:HB3	2.12	0.49
1:A:138:ASN:OD1	1:A:141:ARG:NH1	2.45	0.49
1:A:112:TYR:CG	1:A:144:LEU:HD13	2.48	0.49
1:B:252:GLU:O	1:B:253:ASP:C	2.54	0.49
1:D:223:VAL:HG11	1:D:251:VAL:HG11	1.93	0.49
1:A:100:PRO:HG2	1:A:105:LEU:CD1	2.42	0.49
1:B:117:LEU:O	1:B:118:GLN:C	2.56	0.49
1:A:360:GLU:OE1	1:A:368:ARG:N	2.38	0.49
1:B:113:ASP:HA	1:B:150:ALA:O	2.13	0.49
1:D:183:ARG:HH11	1:D:184:ARG:HH22	1.60	0.49
1:D:183:ARG:HD3	1:D:184:ARG:HH22	1.77	0.49
1:C:100:PRO:HB3	1:C:125:GLU:O	2.13	0.49
1:B:344:ILE:HD13	1:B:363:LEU:HD12	1.95	0.49
1:A:220:THR:HG21	1:A:252:GLU:HB2	1.96	0.48
1:C:456:ALA:O	1:C:459:GLU:HG2	2.13	0.48
1:C:328:PHE:HE2	1:C:375:LEU:HD23	1.78	0.48
1:D:314:PRO:HB2	1:D:404:TYR:CZ	2.49	0.48
1:D:416:ARG:HD2	1:D:416:ARG:HA	1.73	0.48
1:A:253:ASP:OD1	1:A:257:ARG:HD2	2.14	0.47
1:B:190:GLU:HA	1:B:195:ILE:HD11	1.97	0.47
1:B:305:THR:HA	1:B:308:MET:HE3	1.97	0.47
1:A:112:TYR:CE1	1:A:144:LEU:HB3	2.49	0.47
1:D:410:LEU:HB2	1:D:432:LEU:HD21	1.95	0.47
1:D:180:PHE:HB3	1:D:340:HIS:NE2	2.29	0.47
1:D:49:LEU:HD22	1:D:58:VAL:HG21	1.96	0.46
1:D:180:PHE:HB3	1:D:340:HIS:CD2	2.51	0.46
1:A:86:ARG:HH11	1:A:89:ARG:NH1	2.13	0.46
1:B:114:GLU:C	1:B:116:LEU:H	2.23	0.46
1:D:181:THR:O	1:D:183:ARG:NH2	2.49	0.46
1:A:255:ILE:HG12	1:A:264:VAL:HG21	1.96	0.46
1:D:198:LEU:HD12	1:D:199:PRO:HD2	1.97	0.46
1:D:406:ASN:HB3	1:D:432:LEU:HD11	1.98	0.46
1:C:230:ALA:HB1	1:C:251:VAL:HG21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:PHE:HB3	1:A:340:HIS:NE2	2.31	0.46
1:A:197:PRO:O	1:A:198:LEU:HB3	2.15	0.46
1:C:375:LEU:HA	1:C:378:VAL:HG22	1.98	0.46
1:B:198:LEU:HD12	1:B:199:PRO:HD2	1.97	0.45
1:C:353:HIS:HA	1:C:424:THR:HB	1.98	0.45
1:D:85:GLU:CD	1:D:85:GLU:H	2.23	0.45
1:D:229:LEU:O	1:D:233:VAL:HG23	2.15	0.45
1:A:216:VAL:O	1:A:220:THR:OG1	2.22	0.45
1:C:388:ALA:HA	1:C:405:ALA:HB2	1.99	0.45
1:D:228:ALA:O	1:D:232:GLN:HG3	2.17	0.45
1:D:102:LEU:HB2	1:D:105:LEU:HD12	1.99	0.45
1:A:342:SER:O	1:A:346:ARG:HG2	2.17	0.45
1:A:47:VAL:HG23	1:A:49:LEU:HD13	1.99	0.45
1:C:187:GLN:HE22	1:C:191:GLN:HG2	1.81	0.45
1:D:187:GLN:HG2	1:D:188:ARG:HG3	1.98	0.45
1:A:186:GLN:O	1:A:188:ARG:N	2.49	0.45
1:B:161:LEU:HD21	1:B:358:TYR:HA	1.99	0.45
1:A:170:ARG:NH1	1:A:374:TRP:HE1	2.15	0.44
1:A:181:THR:O	1:A:182:ALA:HB3	2.17	0.44
1:D:347:HIS:HA	1:D:350:VAL:HG22	1.99	0.44
1:A:236:TRP:CE2	1:A:460:LEU:HD21	2.52	0.44
1:D:308:MET:HE1	1:D:407:LEU:HD21	1.98	0.44
1:D:113:ASP:HA	1:D:150:ALA:O	2.17	0.44
1:A:165:ARG:NH2	1:A:172:GLU:OE2	2.51	0.44
1:A:464:PHE:O	1:A:464:PHE:CD1	2.71	0.43
1:A:98:ARG:HG2	1:A:98:ARG:HH11	1.83	0.43
1:B:236:TRP:CE2	1:B:460:LEU:HD21	2.53	0.43
1:C:196:PRO:HG2	1:C:277:LEU:CD2	2.42	0.43
1:D:236:TRP:CE2	1:D:460:LEU:HD21	2.53	0.43
1:D:204:LYS:HB3	1:D:222:LEU:HD11	2.00	0.43
1:D:308:MET:CE	1:D:407:LEU:HD21	2.48	0.43
1:A:71:LEU:HD12	1:A:71:LEU:HA	1.89	0.43
1:D:201:THR:O	1:D:205:ILE:HG13	2.18	0.43
1:A:180:PHE:HB3	1:A:340:HIS:CD2	2.53	0.43
1:A:295:ILE:HD12	1:A:461:ALA:HB2	2.01	0.43
1:B:86:ARG:HH11	1:B:89:ARG:NH1	2.17	0.43
1:C:348:LEU:HD23	1:C:359:ILE:HD12	2.00	0.43
1:B:197:PRO:O	1:B:198:LEU:HB3	2.19	0.43
1:C:86:ARG:HH11	1:C:89:ARG:HH12	1.66	0.43
1:D:14:ALA:HB3	1:D:19:LEU:HD13	2.01	0.43
1:B:114:GLU:C	1:B:116:LEU:N	2.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:ARG:HA	1:C:416:ARG:HD2	1.88	0.43
1:D:346:ARG:HD3	1:D:349:GLU:OE1	2.18	0.42
1:B:177:VAL:HG13	1:B:181:THR:CG2	2.49	0.42
1:C:199:PRO:HD3	1:C:276:SER:HB3	2.01	0.42
1:D:220:THR:HG21	1:D:252:GLU:HB2	2.01	0.42
1:B:196:PRO:HG2	1:B:277:LEU:HD21	2.02	0.42
1:D:119:GLU:O	1:D:137:SER:HB2	2.19	0.42
1:A:420:ILE:HD12	1:A:420:ILE:H	1.84	0.42
1:A:300:VAL:HG13	1:A:447:VAL:HG22	2.01	0.42
1:B:308:MET:HE3	1:B:308:MET:HB2	1.87	0.42
1:D:183:ARG:HA	1:D:183:ARG:NH1	2.34	0.42
1:D:340:HIS:O	1:D:344:ILE:HG12	2.19	0.42
1:D:346:ARG:NH1	1:D:349:GLU:OE2	2.52	0.42
1:B:15:PRO:HG2	1:B:96:LEU:HD11	2.01	0.42
1:C:85:GLU:H	1:C:85:GLU:CD	2.28	0.42
1:B:342:SER:O	1:B:346:ARG:HG2	2.19	0.42
1:B:282:ASP:OD2	1:B:346:ARG:NH2	2.52	0.41
1:B:416:ARG:HA	1:B:416:ARG:HD2	1.82	0.41
1:D:237:ALA:O	1:D:243:ALA:HB3	2.20	0.41
1:A:244:ALA:HB3	1:A:247:LYS:NZ	2.35	0.41
1:B:86:ARG:HH11	1:B:89:ARG:HH12	1.67	0.41
1:C:216:VAL:HA	1:C:219:ILE:HG22	2.02	0.41
1:B:94:HIS:HB2	1:B:96:LEU:HD23	2.02	0.41
1:C:240:PRO:HG2	1:C:456:ALA:CB	2.51	0.41
1:D:183:ARG:HD3	1:D:184:ARG:NH2	2.36	0.41
1:A:232:GLN:OE1	1:A:275:LYS:NZ	2.52	0.41
1:B:47:VAL:HG23	1:B:49:LEU:HD13	2.02	0.41
1:D:460:LEU:O	1:D:463:GLN:HG2	2.21	0.41
1:B:463:GLN:HG3	1:B:464:PHE:N	2.36	0.41
1:D:255:ILE:HG12	1:D:264:VAL:HG21	2.01	0.41
1:B:66:LEU:HD11	1:B:71:LEU:HD22	2.02	0.41
1:B:181:THR:OG1	1:B:182:ALA:N	2.54	0.41
1:B:266:ASN:HB3	1:B:321:LEU:HB2	2.02	0.41
1:C:308:MET:HE2	1:C:407:LEU:HD21	2.02	0.41
1:A:85:GLU:CD	1:A:85:GLU:H	2.29	0.41
1:C:446:ALA:O	1:C:450:VAL:HG23	2.20	0.41
1:A:113:ASP:HA	1:A:150:ALA:O	2.21	0.40
1:B:251:VAL:O	1:B:254:ALA:N	2.54	0.40
1:B:177:VAL:O	1:B:181:THR:OG1	2.32	0.40
1:D:66:LEU:HD23	1:D:350:VAL:HB	2.03	0.40
1:D:333:LEU:HD23	1:D:333:LEU:HA	1.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:TRP:CZ3	1:A:464:PHE:HE2	2.38	0.40
1:A:308:MET:HE3	1:A:308:MET:HB2	1.92	0.40
1:B:346:ARG:HA	1:B:346:ARG:HD3	1.89	0.40
1:C:280:PRO:HB3	1:C:334:ALA:CB	2.52	0.40
1:D:198:LEU:HD13	1:D:379:TRP:CE3	2.57	0.40
1:C:240:PRO:HG2	1:C:456:ALA:HB1	2.03	0.40
1:D:197:PRO:O	1:D:198:LEU:HB3	2.20	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	455/457 (100%)	444 (98%)	8 (2%)	3 (1%)	19	51
1	B	455/457 (100%)	443 (97%)	8 (2%)	4 (1%)	14	45
1	C	455/457 (100%)	447 (98%)	6 (1%)	2 (0%)	30	61
1	D	455/457 (100%)	446 (98%)	7 (2%)	2 (0%)	30	61
All	All	1820/1828 (100%)	1780 (98%)	29 (2%)	11 (1%)	22	54

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	PRO
1	C	245	PRO
1	D	245	PRO
1	A	187	GLN
1	B	251	VAL
1	A	198	LEU
1	B	118	GLN
1	B	198	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	198	LEU
1	D	198	LEU
1	B	252	GLU

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	376/376 (100%)	373 (99%)	3 (1%)	79	89
1	B	376/376 (100%)	370 (98%)	6 (2%)	58	77
1	C	376/376 (100%)	373 (99%)	3 (1%)	79	89
1	D	376/376 (100%)	372 (99%)	4 (1%)	70	84
All	All	1504/1504 (100%)	1488 (99%)	16 (1%)	70	84

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	VAL
1	A	178	GLN
1	A	184	ARG
1	B	65	LEU
1	B	177	VAL
1	B	178	GLN
1	B	242	TYR
1	B	249	ARG
1	B	252	GLU
1	C	177	VAL
1	C	178	GLN
1	C	186	GLN
1	D	177	VAL
1	D	178	GLN
1	D	183	ARG
1	D	245	PRO

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	16	GLN
1	A	266	ASN
1	A	361	GLN
1	B	62	GLN
1	B	94	HIS
1	B	138	ASN
1	B	178	GLN
1	B	213	ASN
1	B	335	HIS
1	B	362	HIS
1	C	45	GLN
1	C	62	GLN
1	C	128	GLN
1	C	266	ASN
1	C	393	GLN
1	D	45	GLN
1	D	64	GLN
1	D	128	GLN
1	D	175	GLN
1	D	232	GLN

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](#)

There are no ligands in this entry.

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	457/457 (100%)	-0.41	3 (0%) 84 72	82, 116, 161, 204	0
1	B	457/457 (100%)	-0.09	11 (2%) 59 44	85, 135, 183, 228	0
1	C	457/457 (100%)	-0.09	13 (2%) 55 39	93, 133, 194, 247	0
1	D	457/457 (100%)	-0.28	2 (0%) 89 80	97, 138, 188, 225	0
All	All	1828/1828 (100%)	-0.22	29 (1%) 70 55	82, 131, 185, 247	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	253	ASP	5.3
1	C	242	TYR	4.8
1	B	266	ASN	4.7
1	B	181	THR	3.9
1	C	464	PHE	3.8
1	B	464	PHE	3.6
1	C	254	ALA	3.4
1	C	247	LYS	3.2
1	B	236	TRP	3.2
1	A	248	ILE	3.2
1	D	248	ILE	2.8
1	C	310	ARG	2.7
1	C	251	VAL	2.7
1	C	216	VAL	2.6
1	C	274	GLY	2.5
1	C	248	ILE	2.5
1	D	247	LYS	2.4
1	B	251	VAL	2.4
1	C	244	ALA	2.4
1	C	256	VAL	2.3
1	B	229	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	219	ILE	2.2
1	C	212	PRO	2.2
1	B	317	GLY	2.2
1	B	194	GLU	2.2
1	B	257	ARG	2.1
1	A	247	LYS	2.0
1	A	157	GLU	2.0
1	B	29	CYS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.