



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:42 PM UTC

PDB ID : 5IOF / pdb_00005iof
Title : Structure of the transmembrane domain of the transporter SLC26Dg
Authors : Dutzler, R.; Geertsma, E.R.G.; Shaik, F.R.
Deposited on : 2016-03-08
Resolution : 4.20 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

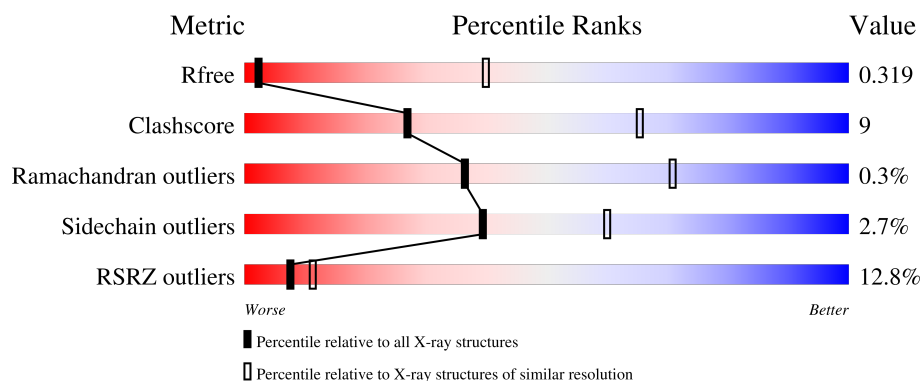
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	401	10% 72% 21% 7%
1	B	401	18% 73% 20% 7%
1	C	401	7% 73% 20% 7%
1	D	401	12% 72% 21% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11096 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.

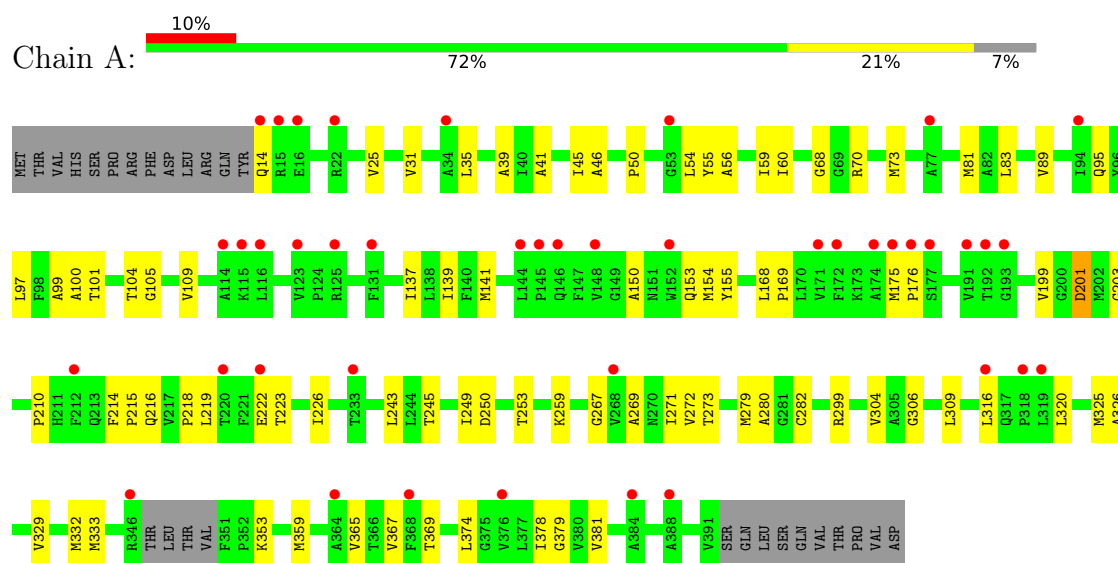
- Molecule 1 is a protein called Sulphate transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2774	1836	446	474	18			
1	B	374	Total	C	N	O	S	0	0	0
			2774	1836	446	474	18			
1	C	374	Total	C	N	O	S	0	0	0
			2774	1836	446	474	18			
1	D	374	Total	C	N	O	S	0	0	0
			2774	1836	446	474	18			

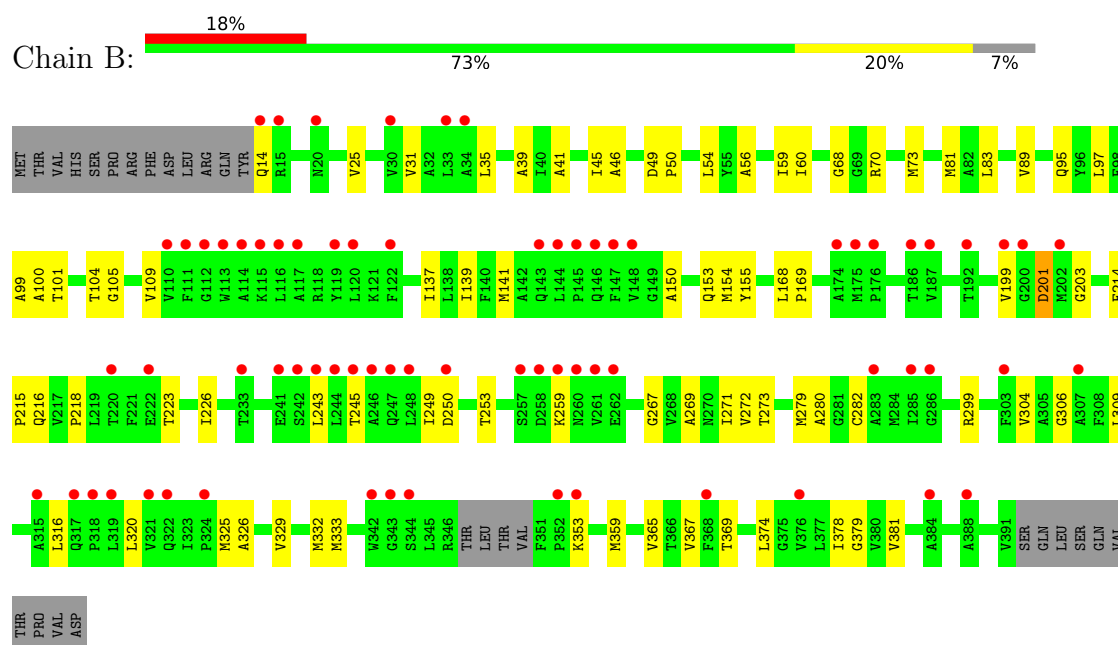
3 Residue-property plots [i](#)

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.

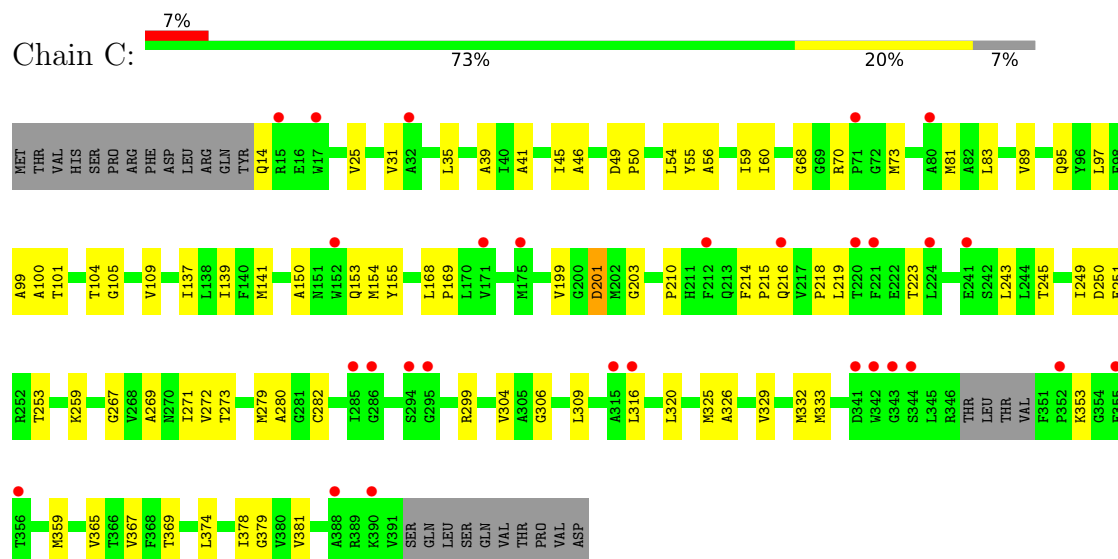
• Molecule 1: Sulphate transporter



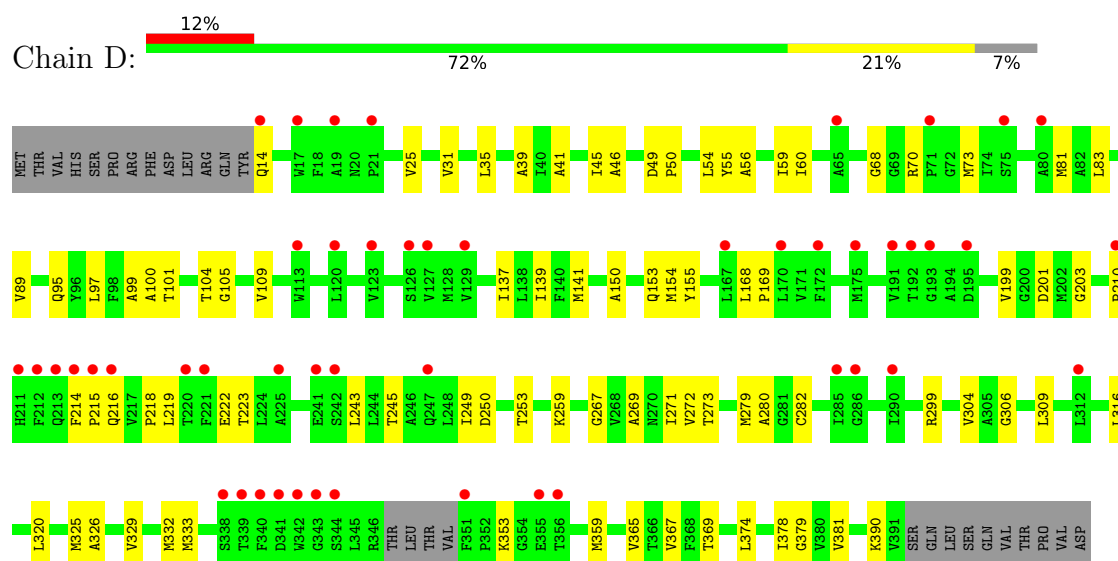
• Molecule 1: Sulphate transporter



● Molecule 1: Sulphate transporter



● Molecule 1: Sulphate transporter



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.59Å 82.49Å 166.37Å 96.33° 92.94° 119.23°	Depositor
Resolution (Å)	19.96 – 4.20 19.96 – 4.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (19.96-4.20) 84.0 (19.96-4.20)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 4.00Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.291 , 0.312 0.318 , 0.319	Depositor DCC
R_{free} test set	1527 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	185.7	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 590.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.048 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	11096	wwPDB-VP
Average B, all atoms (Å ²)	239.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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](#)

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	0.32	0/2828	0.78	0/3857
1	B	0.32	0/2828	0.78	0/3857
1	C	0.32	0/2828	0.78	0/3857
1	D	0.32	0/2828	0.78	0/3857
All	All	0.32	0/11312	0.78	0/15428

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	2774	0	2945	64	0
1	B	2774	0	2945	45	0
1	C	2774	0	2945	57	0
1	D	2774	0	2945	76	0
All	All	11096	0	11780	211	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 9.

All (211) 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:216:GLN:NE2	1:D:222:GLU:OE2	1.88	1.06
1:A:216:GLN:CD	1:D:222:GLU:CD	2.27	1.01
1:A:216:GLN:CD	1:D:222:GLU:OE2	2.11	0.94
1:C:251:GLU:CG	1:D:390:LYS:HA	2.02	0.90
1:C:251:GLU:HG3	1:D:390:LYS:HA	1.60	0.83
1:A:218:PRO:O	1:D:219:LEU:HD11	1.80	0.82
1:A:216:GLN:HG2	1:D:222:GLU:OE1	1.77	0.82
1:A:222:GLU:CD	1:D:216:GLN:CD	2.48	0.80
1:A:222:GLU:OE2	1:D:216:GLN:CD	2.32	0.72
1:A:222:GLU:OE1	1:D:216:GLN:HG2	1.89	0.72
1:C:251:GLU:HG2	1:D:390:LYS:HA	1.72	0.71
1:C:251:GLU:OE2	1:D:390:LYS:HG2	1.91	0.70
1:A:222:GLU:OE2	1:D:216:GLN:NE2	2.24	0.69
1:A:216:GLN:NE2	1:D:222:GLU:CD	2.43	0.69
1:C:251:GLU:CD	1:D:390:LYS:HB3	2.17	0.69
1:A:219:LEU:HD11	1:D:218:PRO:O	1.93	0.68
1:D:99:ALA:HB2	1:D:218:PRO:HG3	1.76	0.68
1:B:99:ALA:HB2	1:B:218:PRO:HG3	1.76	0.68
1:B:141:MET:HE1	1:B:367:VAL:HG13	1.76	0.68
1:C:141:MET:HE1	1:C:367:VAL:HG13	1.77	0.67
1:D:141:MET:HE1	1:D:367:VAL:HG13	1.77	0.67
1:A:141:MET:HE1	1:A:367:VAL:HG13	1.77	0.67
1:A:99:ALA:HB2	1:A:218:PRO:HG3	1.76	0.67
1:C:99:ALA:HB2	1:C:218:PRO:HG3	1.76	0.67
1:A:101:THR:HG22	1:A:280:ALA:HB2	1.78	0.66
1:B:101:THR:HG22	1:B:280:ALA:HB2	1.78	0.66
1:C:101:THR:HG22	1:C:280:ALA:HB2	1.78	0.64
1:D:101:THR:HG22	1:D:280:ALA:HB2	1.78	0.63
1:C:251:GLU:OE2	1:D:390:LYS:HB3	1.98	0.63
1:C:251:GLU:CG	1:D:390:LYS:CA	2.76	0.63
1:A:216:GLN:CG	1:D:222:GLU:CD	2.72	0.63
1:C:251:GLU:OE2	1:D:390:LYS:CG	2.48	0.62
1:C:251:GLU:HG3	1:D:390:LYS:CA	2.29	0.62
1:A:216:GLN:CG	1:D:222:GLU:OE1	2.48	0.62
1:A:70:ARG:HB3	1:A:73:MET:HE3	1.82	0.61
1:A:243:LEU:HD12	1:A:259:LYS:HG2	1.83	0.61
1:C:70:ARG:HB3	1:C:73:MET:HE3	1.82	0.61
1:C:243:LEU:HD12	1:C:259:LYS:HG2	1.83	0.61
1:B:70:ARG:HB3	1:B:73:MET:HE3	1.82	0.61
1:D:70:ARG:HB3	1:D:73:MET:HE3	1.82	0.61
1:B:243:LEU:HD12	1:B:259:LYS:HG2	1.83	0.60
1:D:243:LEU:HD12	1:D:259:LYS:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:LEU:O	1:B:320:LEU:N	2.34	0.60
1:A:316:LEU:O	1:A:320:LEU:N	2.35	0.59
1:C:100:ALA:O	1:C:104:THR:OG1	2.18	0.59
1:C:316:LEU:O	1:C:320:LEU:N	2.34	0.58
1:A:216:GLN:HG2	1:D:222:GLU:CD	2.27	0.58
1:D:316:LEU:O	1:D:320:LEU:N	2.35	0.57
1:D:81:MET:HE2	1:D:282:CYS:HB3	1.87	0.56
1:D:218:PRO:HB2	1:D:223:THR:HG21	1.88	0.56
1:C:218:PRO:HB2	1:C:223:THR:HG21	1.88	0.56
1:C:81:MET:HE2	1:C:282:CYS:HB3	1.86	0.56
1:A:218:PRO:HB2	1:A:223:THR:HG21	1.88	0.55
1:B:218:PRO:HB2	1:B:223:THR:HG21	1.88	0.55
1:A:81:MET:HE2	1:A:282:CYS:HB3	1.86	0.55
1:D:378:ILE:HA	1:D:381:VAL:HG22	1.89	0.55
1:B:81:MET:HE2	1:B:282:CYS:HB3	1.87	0.55
1:C:378:ILE:HA	1:C:381:VAL:HG22	1.89	0.55
1:D:100:ALA:O	1:D:104:THR:OG1	2.18	0.54
1:D:56:ALA:HB2	1:D:279:MET:H	1.73	0.54
1:A:70:ARG:NH2	1:A:253:THR:OG1	2.41	0.53
1:B:70:ARG:NH2	1:B:253:THR:OG1	2.41	0.53
1:A:56:ALA:HB2	1:A:279:MET:H	1.73	0.53
1:C:70:ARG:NH2	1:C:253:THR:OG1	2.41	0.53
1:B:56:ALA:HB2	1:B:279:MET:H	1.73	0.53
1:C:56:ALA:HB2	1:C:279:MET:H	1.73	0.53
1:A:378:ILE:HA	1:A:381:VAL:HG22	1.89	0.53
1:B:378:ILE:HA	1:B:381:VAL:HG22	1.89	0.53
1:B:59:ILE:HD11	1:B:272:VAL:HG22	1.91	0.52
1:A:59:ILE:HD11	1:A:272:VAL:HG22	1.91	0.52
1:C:68:GLY:O	1:C:299:ARG:NH2	2.43	0.52
1:D:70:ARG:NH2	1:D:253:THR:OG1	2.42	0.52
1:B:68:GLY:O	1:B:299:ARG:NH2	2.43	0.52
1:D:68:GLY:O	1:D:299:ARG:NH2	2.43	0.51
1:C:59:ILE:HD11	1:C:272:VAL:HG22	1.91	0.51
1:C:251:GLU:OE2	1:D:390:LYS:CB	2.58	0.51
1:A:68:GLY:O	1:A:299:ARG:NH2	2.43	0.51
1:D:59:ILE:HD11	1:D:272:VAL:HG22	1.92	0.50
1:C:39:ALA:HB3	1:C:54:LEU:HD23	1.93	0.50
1:A:219:LEU:HA	1:D:219:LEU:HD11	1.93	0.50
1:B:365:VAL:HG21	1:B:378:ILE:HD13	1.93	0.50
1:D:25:VAL:HG22	1:D:304:VAL:HG21	1.94	0.50
1:D:46:ALA:O	1:D:89:VAL:HG21	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ALA:HB3	1:D:54:LEU:HD23	1.93	0.50
1:A:39:ALA:HB3	1:A:54:LEU:HD23	1.93	0.49
1:C:46:ALA:O	1:C:89:VAL:HG21	2.12	0.49
1:A:46:ALA:O	1:A:89:VAL:HG21	2.12	0.49
1:A:365:VAL:HG21	1:A:378:ILE:HD13	1.93	0.49
1:B:41:ALA:O	1:B:45:ILE:HG12	2.13	0.49
1:A:41:ALA:O	1:A:45:ILE:HG12	2.13	0.49
1:C:25:VAL:HG22	1:C:304:VAL:HG21	1.94	0.49
1:D:41:ALA:O	1:D:45:ILE:HG12	2.13	0.49
1:B:46:ALA:O	1:B:89:VAL:HG21	2.12	0.49
1:B:25:VAL:HG22	1:B:304:VAL:HG21	1.94	0.48
1:C:365:VAL:HG21	1:C:378:ILE:HD13	1.93	0.48
1:A:25:VAL:HG22	1:A:304:VAL:HG21	1.94	0.48
1:B:39:ALA:HB3	1:B:54:LEU:HD23	1.93	0.48
1:C:41:ALA:O	1:C:45:ILE:HG12	2.13	0.48
1:D:365:VAL:HG21	1:D:378:ILE:HD13	1.93	0.48
1:D:150:ALA:HB1	1:D:155:TYR:HE1	1.80	0.47
1:C:150:ALA:HB1	1:C:155:TYR:HE1	1.80	0.47
1:C:50:PRO:HD2	1:C:203:GLY:HA3	1.96	0.47
1:A:100:ALA:O	1:A:104:THR:OG1	2.18	0.47
1:B:150:ALA:HB1	1:B:155:TYR:HE1	1.79	0.47
1:A:150:ALA:HB1	1:A:155:TYR:HE1	1.79	0.47
1:B:100:ALA:O	1:B:104:THR:OG1	2.18	0.47
1:D:50:PRO:HD2	1:D:203:GLY:HA3	1.97	0.47
1:A:219:LEU:HD11	1:D:219:LEU:HA	1.96	0.47
1:C:139:ILE:HG23	1:C:332:MET:HE3	1.97	0.47
1:A:326:ALA:O	1:A:329:VAL:HG12	2.15	0.47
1:B:105:GLY:HA3	1:B:271:ILE:HG13	1.98	0.46
1:C:105:GLY:HA3	1:C:271:ILE:HG13	1.98	0.46
1:D:214:PHE:O	1:D:216:GLN:N	2.48	0.46
1:D:378:ILE:HG13	1:D:379:GLY:N	2.31	0.46
1:C:378:ILE:HG13	1:C:379:GLY:N	2.31	0.46
1:A:50:PRO:HD2	1:A:203:GLY:HA3	1.96	0.46
1:A:105:GLY:HA3	1:A:271:ILE:HG13	1.98	0.46
1:C:251:GLU:CD	1:D:390:LYS:CB	2.87	0.46
1:A:214:PHE:O	1:A:216:GLN:N	2.48	0.46
1:B:326:ALA:O	1:B:329:VAL:HG12	2.15	0.46
1:D:105:GLY:HA3	1:D:271:ILE:HG13	1.97	0.46
1:D:139:ILE:HG23	1:D:332:MET:HE3	1.97	0.46
1:D:326:ALA:O	1:D:329:VAL:HG12	2.15	0.46
1:C:326:ALA:O	1:C:329:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:PRO:HD2	1:B:203:GLY:HA3	1.97	0.46
1:A:139:ILE:HG23	1:A:332:MET:HE3	1.97	0.46
1:B:214:PHE:O	1:B:216:GLN:N	2.49	0.46
1:D:59:ILE:HD13	1:D:273:THR:HA	1.98	0.46
1:A:59:ILE:HD13	1:A:273:THR:HA	1.98	0.45
1:B:139:ILE:HG23	1:B:332:MET:HE3	1.97	0.45
1:D:369:THR:HG21	1:D:374:LEU:HD12	1.97	0.45
1:B:325:MET:HE2	1:B:325:MET:HA	1.98	0.45
1:A:378:ILE:HG13	1:A:379:GLY:N	2.31	0.45
1:B:369:THR:HG21	1:B:374:LEU:HD12	1.97	0.45
1:B:378:ILE:HG13	1:B:379:GLY:N	2.30	0.45
1:C:214:PHE:O	1:C:216:GLN:N	2.49	0.45
1:C:31:VAL:O	1:C:35:LEU:HB2	2.17	0.45
1:A:369:THR:HG21	1:A:374:LEU:HD12	1.97	0.45
1:B:59:ILE:HD13	1:B:273:THR:HA	1.98	0.45
1:B:109:VAL:HG13	1:B:267:GLY:HA3	1.99	0.45
1:C:369:THR:HG21	1:C:374:LEU:HD12	1.97	0.45
1:A:109:VAL:HG13	1:A:267:GLY:HA3	1.99	0.45
1:A:325:MET:HA	1:A:325:MET:HE2	1.98	0.45
1:A:250:ASP:OD2	1:A:259:LYS:NZ	2.48	0.45
1:D:31:VAL:O	1:D:35:LEU:HB2	2.17	0.45
1:C:59:ILE:HD13	1:C:273:THR:HA	1.98	0.45
1:D:325:MET:HE2	1:D:325:MET:HA	1.98	0.45
1:C:325:MET:HA	1:C:325:MET:HE2	1.98	0.44
1:D:60:ILE:HD13	1:D:269:ALA:HB1	2.00	0.44
1:A:60:ILE:HD13	1:A:269:ALA:HB1	2.00	0.44
1:B:31:VAL:O	1:B:35:LEU:HB2	2.17	0.44
1:B:154:MET:HE1	1:B:329:VAL:HG11	2.00	0.44
1:C:60:ILE:HD13	1:C:269:ALA:HB1	2.00	0.44
1:A:31:VAL:O	1:A:35:LEU:HB2	2.17	0.44
1:A:154:MET:HE1	1:A:329:VAL:HG11	2.00	0.44
1:B:60:ILE:HD13	1:B:269:ALA:HB1	2.00	0.44
1:C:245:THR:O	1:C:249:ILE:HG12	2.18	0.44
1:C:154:MET:HE1	1:C:329:VAL:HG11	2.00	0.44
1:D:109:VAL:HG13	1:D:267:GLY:HA3	1.99	0.44
1:D:154:MET:HE1	1:D:329:VAL:HG11	2.00	0.44
1:D:35:LEU:HB3	1:D:309:LEU:HD13	2.00	0.44
1:C:201:ASP:OD1	1:C:201:ASP:N	2.51	0.43
1:A:35:LEU:HB3	1:A:309:LEU:HD13	2.00	0.43
1:D:201:ASP:OD1	1:D:201:ASP:N	2.51	0.43
1:C:35:LEU:HB3	1:C:309:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:VAL:HG13	1:C:267:GLY:HA3	1.99	0.43
1:D:245:THR:O	1:D:249:ILE:HG12	2.18	0.43
1:A:245:THR:O	1:A:249:ILE:HG12	2.18	0.43
1:A:97:LEU:HD21	1:A:279:MET:HA	2.01	0.43
1:B:97:LEU:HD21	1:B:279:MET:HA	2.01	0.43
1:C:97:LEU:HD21	1:C:279:MET:HA	2.01	0.43
1:B:35:LEU:HB3	1:B:309:LEU:HD13	2.00	0.42
1:B:245:THR:O	1:B:249:ILE:HG12	2.18	0.42
1:C:168:LEU:N	1:C:169:PRO:HD2	2.34	0.42
1:D:250:ASP:OD2	1:D:259:LYS:NZ	2.48	0.42
1:A:222:GLU:OE1	1:D:216:GLN:CG	2.61	0.42
1:B:49:ASP:HA	1:B:50:PRO:HD2	1.90	0.42
1:B:168:LEU:N	1:B:169:PRO:HD2	2.34	0.42
1:B:218:PRO:O	1:C:219:LEU:HD11	2.19	0.42
1:A:201:ASP:OD1	1:A:201:ASP:N	2.51	0.42
1:A:306:GLY:O	1:A:309:LEU:HB3	2.20	0.42
1:D:168:LEU:N	1:D:169:PRO:HD2	2.34	0.42
1:B:201:ASP:OD1	1:B:201:ASP:N	2.51	0.42
1:B:329:VAL:O	1:B:333:MET:HB2	2.20	0.42
1:A:168:LEU:N	1:A:169:PRO:HD2	2.34	0.42
1:A:329:VAL:O	1:A:333:MET:HB2	2.20	0.42
1:B:250:ASP:OD2	1:B:259:LYS:NZ	2.48	0.42
1:B:306:GLY:O	1:B:309:LEU:HB3	2.20	0.42
1:D:97:LEU:HD21	1:D:279:MET:HA	2.01	0.41
1:D:329:VAL:O	1:D:333:MET:HB2	2.20	0.41
1:C:49:ASP:HA	1:C:50:PRO:HD2	1.90	0.41
1:C:306:GLY:O	1:C:309:LEU:HB3	2.19	0.41
1:C:14:GLN:N	1:C:14:GLN:OE1	2.54	0.41
1:B:14:GLN:N	1:B:14:GLN:OE1	2.54	0.41
1:D:14:GLN:OE1	1:D:14:GLN:N	2.54	0.41
1:C:250:ASP:OD2	1:C:259:LYS:NZ	2.48	0.41
1:C:329:VAL:O	1:C:333:MET:HB2	2.20	0.41
1:D:306:GLY:O	1:D:309:LEU:HB3	2.20	0.41
1:D:55:TYR:O	1:D:59:ILE:HG22	2.21	0.41
1:D:97:LEU:O	1:D:101:THR:HG23	2.21	0.41
1:C:55:TYR:CD1	1:C:210:PRO:HG3	2.57	0.40
1:A:55:TYR:CD1	1:A:210:PRO:HG3	2.57	0.40
1:A:175:MET:HA	1:A:176:PRO:HD3	1.88	0.40
1:A:219:LEU:CA	1:D:219:LEU:HD11	2.51	0.40
1:A:223:THR:O	1:A:226:ILE:HG22	2.21	0.40
1:B:223:THR:O	1:B:226:ILE:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:ASP:HA	1:D:50:PRO:HD2	1.90	0.40
1:D:55:TYR:CD1	1:D:210:PRO:HG3	2.56	0.40
1:A:14:GLN:OE1	1:A:14:GLN:N	2.54	0.40
1:A:222:GLU:CD	1:D:216:GLN:NE2	2.74	0.40
1:C:55:TYR:O	1:C:59:ILE:HG22	2.21	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	370/401 (92%)	344 (93%)	25 (7%)	1 (0%)	36	71
1	B	370/401 (92%)	344 (93%)	25 (7%)	1 (0%)	36	71
1	C	370/401 (92%)	344 (93%)	25 (7%)	1 (0%)	36	71
1	D	370/401 (92%)	344 (93%)	25 (7%)	1 (0%)	36	71
All	All	1480/1604 (92%)	1376 (93%)	100 (7%)	4 (0%)	36	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	PRO
1	B	215	PRO
1	C	215	PRO
1	D	215	PRO

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	292/319 (92%)	284 (97%)	8 (3%)	39	60
1	B	292/319 (92%)	284 (97%)	8 (3%)	39	60
1	C	292/319 (92%)	284 (97%)	8 (3%)	39	60
1	D	292/319 (92%)	285 (98%)	7 (2%)	43	63
All	All	1168/1276 (92%)	1137 (97%)	31 (3%)	39	60

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

Mol	Chain	Res	Type
1	A	83	LEU
1	A	95	GLN
1	A	137	ILE
1	A	153	GLN
1	A	199	VAL
1	A	201	ASP
1	A	353	LYS
1	A	359	MET
1	B	83	LEU
1	B	95	GLN
1	B	137	ILE
1	B	153	GLN
1	B	199	VAL
1	B	201	ASP
1	B	353	LYS
1	B	359	MET
1	C	83	LEU
1	C	95	GLN
1	C	137	ILE
1	C	153	GLN
1	C	199	VAL
1	C	201	ASP
1	C	353	LYS
1	C	359	MET
1	D	83	LEU
1	D	95	GLN
1	D	137	ILE
1	D	153	GLN
1	D	199	VAL
1	D	353	LYS

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Mol	Chain	Res	Type
1	D	359	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	287	GLN
1	B	20	ASN
1	B	216	GLN
1	B	287	GLN
1	C	20	ASN
1	C	216	GLN
1	D	20	ASN
1	D	287	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	374/401 (93%)	0.55	42 (11%)	10 14	160, 221, 298, 369	0
1	B	374/401 (93%)	0.98	71 (18%)	3 7	169, 231, 318, 394	0
1	C	374/401 (93%)	0.50	29 (7%)	19 21	174, 239, 314, 387	0
1	D	374/401 (93%)	0.78	49 (13%)	7 11	166, 236, 287, 343	0
All	All	1496/1604 (93%)	0.71	191 (12%)	7 11	160, 232, 307, 394	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	341	ASP	14.7
1	A	176	PRO	9.0
1	D	343	GLY	8.9
1	B	145	PRO	7.9
1	D	338	SER	7.4
1	D	211	HIS	7.2
1	C	341	ASP	7.0
1	D	286	GLY	6.9
1	D	344	SER	6.8
1	C	344	SER	6.7
1	B	112	GLY	6.5
1	B	176	PRO	5.9
1	D	342	TRP	5.8
1	A	145	PRO	5.7
1	B	220	THR	5.7
1	B	247	GLN	5.7
1	D	220	THR	5.6
1	B	245	THR	5.1
1	B	368	PHE	5.1
1	A	368	PHE	5.1
1	B	260	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	318	PRO	5.0
1	C	220	THR	5.0
1	B	192	THR	5.0
1	B	200	GLY	5.0
1	B	116	LEU	4.9
1	A	192	THR	4.9
1	D	210	PRO	4.8
1	C	286	GLY	4.6
1	B	342	TRP	4.5
1	C	342	TRP	4.5
1	A	220	THR	4.5
1	B	258	ASP	4.3
1	D	285	ILE	4.2
1	B	115	LYS	4.2
1	D	216	GLN	4.2
1	B	222	GLU	4.2
1	D	192	THR	4.2
1	C	315	ALA	4.1
1	D	193	GLY	4.0
1	B	114	ALA	3.9
1	D	340	PHE	3.9
1	A	116	LEU	3.9
1	D	113	TRP	3.8
1	C	343	GLY	3.8
1	B	352	PRO	3.8
1	B	388	ALA	3.8
1	D	247	GLN	3.7
1	D	339	THR	3.7
1	C	17	TRP	3.6
1	D	175	MET	3.6
1	B	113	TRP	3.6
1	A	174	ALA	3.6
1	B	344	SER	3.5
1	D	191	VAL	3.5
1	D	351	PHE	3.5
1	B	321	VAL	3.4
1	B	283	ALA	3.3
1	B	241	GLU	3.3
1	C	224	LEU	3.3
1	C	316	LEU	3.3
1	A	114	ALA	3.3
1	D	14	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	20	ASN	3.2
1	A	123	VAL	3.2
1	B	285	ILE	3.2
1	A	16	GLU	3.2
1	B	111	PHE	3.2
1	D	123	VAL	3.2
1	C	212	PHE	3.1
1	B	257	SER	3.1
1	B	199	VAL	3.1
1	D	170	LEU	3.1
1	C	216	GLN	3.1
1	A	14	GLN	3.0
1	B	119	TYR	3.0
1	A	388	ALA	3.0
1	B	384	ALA	3.0
1	B	14	GLN	3.0
1	D	214	PHE	3.0
1	A	125	ARG	3.0
1	C	171	VAL	3.0
1	D	241	GLU	3.0
1	B	146	GLN	3.0
1	A	376	VAL	3.0
1	B	250	ASP	3.0
1	A	384	ALA	3.0
1	D	215	PRO	3.0
1	B	322	GLN	2.9
1	D	212	PHE	2.9
1	A	364	ALA	2.9
1	D	242	SER	2.9
1	A	22	ARG	2.9
1	B	34	ALA	2.9
1	B	175	MET	2.9
1	C	80	ALA	2.9
1	B	233	THR	2.8
1	A	34	ALA	2.8
1	B	242	SER	2.8
1	A	191	VAL	2.8
1	D	225	ALA	2.8
1	B	353	LYS	2.8
1	A	318	PRO	2.8
1	B	319	LEU	2.8
1	D	126	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	152	TRP	2.7
1	B	148	VAL	2.7
1	B	286	GLY	2.7
1	B	117	ALA	2.7
1	B	376	VAL	2.7
1	D	120	LEU	2.7
1	C	294	SER	2.7
1	A	171	VAL	2.7
1	B	259	LYS	2.7
1	A	15	ARG	2.6
1	A	144	LEU	2.6
1	B	343	GLY	2.6
1	A	148	VAL	2.6
1	A	222	GLU	2.6
1	C	241	GLU	2.6
1	B	202	MET	2.6
1	B	30	VAL	2.6
1	A	115	LYS	2.5
1	C	152	TRP	2.5
1	C	221	PHE	2.5
1	B	174	ALA	2.5
1	C	32	ALA	2.5
1	B	143	GLN	2.5
1	A	212	PHE	2.5
1	B	187	VAL	2.5
1	B	315	ALA	2.5
1	B	144	LEU	2.4
1	A	146	GLN	2.4
1	A	346	ARG	2.4
1	B	244	LEU	2.4
1	D	80	ALA	2.4
1	D	167	LEU	2.4
1	C	71	PRO	2.4
1	B	317	GLN	2.4
1	A	177	SER	2.4
1	A	268	VAL	2.3
1	D	129	VAL	2.3
1	B	303	PHE	2.3
1	A	77	ALA	2.3
1	C	352	PRO	2.3
1	D	127	VAL	2.3
1	B	110	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	19	ALA	2.3
1	C	390	LYS	2.3
1	D	213	GLN	2.3
1	D	355	GLU	2.3
1	B	147	PHE	2.3
1	B	186	THR	2.3
1	D	221	PHE	2.3
1	A	175	MET	2.3
1	C	356	THR	2.2
1	D	172	PHE	2.2
1	B	246	ALA	2.2
1	B	33	LEU	2.2
1	A	53	GLY	2.2
1	B	324	PRO	2.2
1	D	65	ALA	2.2
1	B	122	PHE	2.2
1	B	15	ARG	2.2
1	C	295	GLY	2.2
1	C	388	ALA	2.2
1	D	356	THR	2.2
1	B	243	LEU	2.2
1	D	75	SER	2.2
1	D	71	PRO	2.1
1	A	316	LEU	2.1
1	C	285	ILE	2.1
1	B	261	VAL	2.1
1	C	355	GLU	2.1
1	A	319	LEU	2.1
1	B	120	LEU	2.1
1	D	312	LEU	2.1
1	D	21	PRO	2.1
1	D	17	TRP	2.1
1	A	193	GLY	2.0
1	B	262	GLU	2.0
1	C	15	ARG	2.0
1	A	94	ILE	2.0
1	A	172	PHE	2.0
1	D	290	ILE	2.0
1	B	307	ALA	2.0
1	D	195	ASP	2.0
1	A	233	THR	2.0
1	C	175	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	248	LEU	2.0
1	A	131	PHE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.