



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 09:41 PM EDT

PDB ID : 1RH5
Title : The structure of a protein conducting channel
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Deposited on : 2003-11-13
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

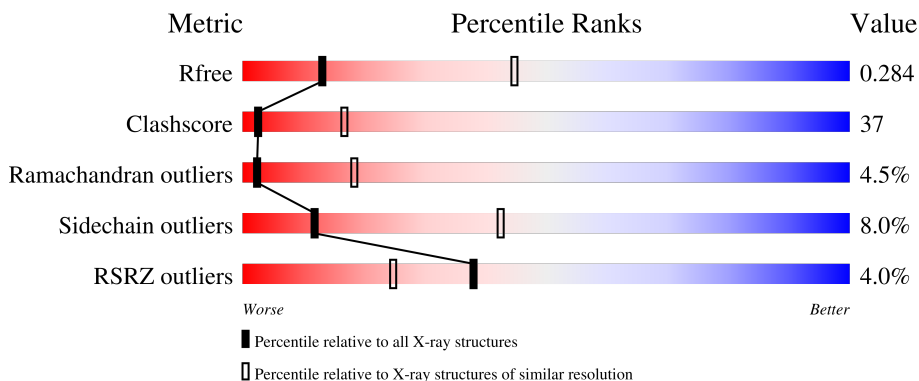
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	436	
2	B	74	
3	C	53	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3852 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 Preprotein translocase secY subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	410	3149	2104	493	534	18	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	ARG	LYS	engineered mutation	UNP Q60175
A	423	THR	VAL	engineered mutation	UNP Q60175

- Molecule 2 is a protein called Preprotein translocase secE subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	56	446	300	72	73	1	0	0	0

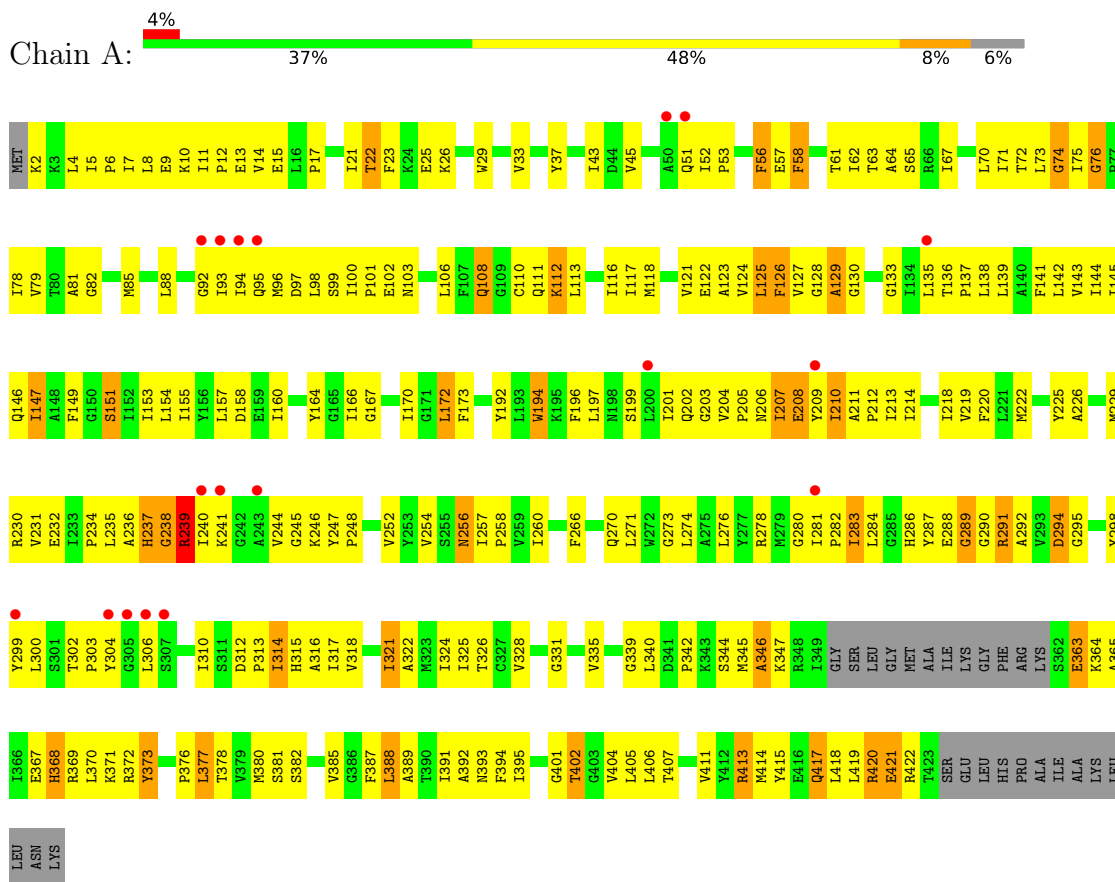
- Molecule 3 is a protein called SecBeta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	32	257	172	42	43	0	0	0

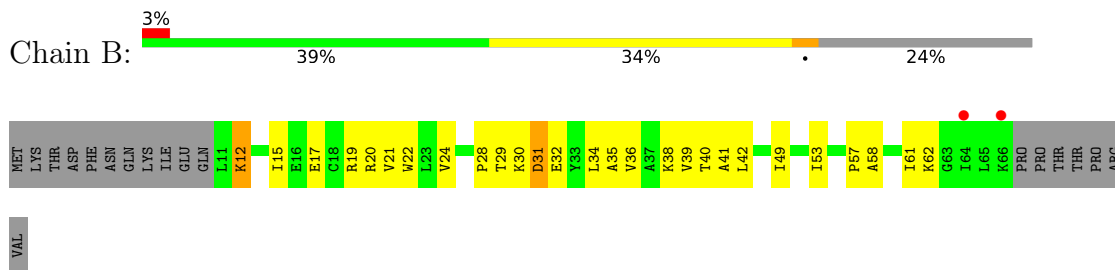
3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

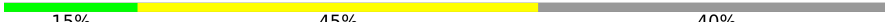
- Molecule 1: Preprotein translocase secY subunit



- Molecule 2: Preprotein translocase secE subunit



- Molecule 3: SecBeta

Chain C:  15% 45% 40%

MET	SER	LYS	ARG	GLU	THR	GLY	LEU	ALA	THR	SER	ALA	GLY	LEU	ILE	ARG	TYR	MET	ASP	E21	F22	F23	S24	K25	I26	R27	V28	K29	P30	E31	H32	V33	I34	G35	V36	T37	V38	A39	F40	V41	I42	I43	E44	A45	I46	Y49	G50	R51	F52	LEU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	102.93Å 156.65Å 69.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20 25.31 – 3.19	Depositor EDS
% Data completeness (in resolution range)	90.1 (10.00-3.20) 89.7 (25.31-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 3.17Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.288 0.239 , 0.284	Depositor DCC
R_{free} test set	1716 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å ²)	104.7	Xtrriage
Anisotropy	0.416	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3852	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% 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	0.44	0/3219	0.63	0/4374
2	B	0.43	0/454	0.56	0/613
3	C	0.50	0/262	0.60	0/354
All	All	0.44	0/3935	0.63	0/5341

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	3149	0	3341	260	0
2	B	446	0	495	31	0
3	C	257	0	272	23	0
All	All	3852	0	4108	294	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 37.

All (294) 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:11:ILE:HD11	1:A:113:LEU:HD23	1.22	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ARG:HH11	1:A:413:ARG:HB2	1.30	0.96
1:A:63:THR:HG23	1:A:76:GLY:H	1.28	0.95
1:A:420:ARG:HB3	1:A:420:ARG:NH1	1.79	0.95
1:A:335:VAL:HG13	1:A:340:LEU:HB2	1.45	0.95
1:A:62:ILE:HD12	1:A:62:ILE:H	1.31	0.93
1:A:281:ILE:H	1:A:281:ILE:HD12	1.42	0.85
1:A:63:THR:HG23	1:A:76:GLY:N	1.92	0.84
1:A:170:ILE:H	1:A:170:ILE:HD12	1.42	0.83
1:A:56:PHE:HB3	1:A:58:PHE:CE2	2.14	0.83
1:A:129:ALA:HB1	1:A:274:LEU:HD12	1.61	0.82
1:A:246:LYS:O	1:A:248:PRO:HD3	1.80	0.82
1:A:239:ARG:HB3	1:A:240:ILE:HD12	1.61	0.81
1:A:43:ILE:HB	1:A:70:LEU:HD22	1.61	0.81
1:A:254:VAL:HG12	1:A:381:SER:HB3	1.64	0.80
1:A:230:ARG:HG3	1:A:230:ARG:HH11	1.47	0.79
1:A:11:ILE:CD1	1:A:113:LEU:HD23	2.11	0.78
1:A:22:THR:HG23	1:A:25:GLU:HG3	1.66	0.78
2:B:15:ILE:H	2:B:15:ILE:HD12	1.49	0.77
1:A:62:ILE:HD12	1:A:62:ILE:N	2.00	0.77
1:A:70:LEU:HD11	3:C:44:GLU:HG2	1.67	0.77
1:A:9:GLU:HB3	3:C:25:LYS:HG2	1.66	0.76
1:A:52:ILE:HD12	1:A:52:ILE:O	1.85	0.75
1:A:364:LYS:HA	1:A:367:GLU:HB3	1.68	0.75
1:A:420:ARG:HB3	1:A:420:ARG:HH11	1.49	0.74
1:A:75:ILE:HG22	1:A:79:VAL:HG23	1.69	0.73
1:A:63:THR:CG2	1:A:76:GLY:H	2.02	0.72
1:A:234:PRO:HA	1:A:246:LYS:HG2	1.71	0.72
1:A:62:ILE:H	1:A:62:ILE:CD1	2.02	0.72
1:A:331:GLY:O	1:A:335:VAL:HG23	1.89	0.72
1:A:56:PHE:N	1:A:56:PHE:CD2	2.57	0.71
1:A:21:ILE:HG22	1:A:25:GLU:HB2	1.74	0.70
3:C:38:VAL:O	3:C:42:ILE:HG12	1.91	0.70
2:B:12:LYS:HA	2:B:15:ILE:HD13	1.73	0.69
1:A:56:PHE:N	1:A:56:PHE:HD2	1.91	0.69
1:A:371:LYS:HB2	1:A:371:LYS:NZ	2.08	0.68
1:A:133:GLY:O	1:A:135:LEU:HD12	1.93	0.68
1:A:420:ARG:HH11	1:A:420:ARG:CB	2.05	0.68
1:A:232:GLU:HG2	1:A:248:PRO:HG3	1.75	0.67
1:A:276:LEU:HD13	1:A:283:ILE:HD12	1.76	0.67
1:A:274:LEU:HD13	1:A:274:LEU:O	1.94	0.66
3:C:32:HIS:O	3:C:36:VAL:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LYS:HA	1:A:164:TYR:O	1.96	0.66
1:A:141:PHE:O	1:A:145:ILE:HG12	1.97	0.65
1:A:11:ILE:HD11	1:A:113:LEU:CD2	2.14	0.65
2:B:57:PRO:O	2:B:61:ILE:HG13	1.95	0.65
1:A:2:LYS:HG2	1:A:106:LEU:HD11	1.78	0.65
1:A:5:ILE:O	1:A:9:GLU:HG3	1.97	0.65
1:A:202:GLN:O	1:A:204:VAL:HG23	1.97	0.64
1:A:413:ARG:HB2	1:A:413:ARG:NH1	2.09	0.64
1:A:85:MET:HG3	1:A:111:GLN:HG3	1.79	0.63
1:A:280:GLY:O	1:A:282:PRO:HD3	1.97	0.63
1:A:335:VAL:CG1	1:A:340:LEU:HB2	2.24	0.63
1:A:281:ILE:HD12	1:A:281:ILE:N	2.13	0.63
1:A:9:GLU:HB3	3:C:25:LYS:CG	2.29	0.62
1:A:99:SER:OG	1:A:100:ILE:HD12	1.99	0.62
1:A:313:PRO:O	1:A:317:ILE:HG13	1.97	0.62
1:A:373:TYR:O	1:A:376:PRO:HG2	2.00	0.61
1:A:5:ILE:N	1:A:6:PRO:HD2	2.16	0.61
1:A:155:ILE:O	1:A:158:ASP:HB3	2.00	0.61
1:A:206:ASN:OD1	1:A:208:GLU:HB2	2.00	0.61
1:A:419:LEU:O	1:A:422:ARG:HB3	2.01	0.61
2:B:15:ILE:HD12	2:B:15:ILE:N	2.16	0.61
1:A:298:TYR:O	1:A:315:HIS:HE1	1.84	0.60
1:A:72:THR:HB	1:A:147:ILE:HD12	1.83	0.60
1:A:237:HIS:O	1:A:239:ARG:N	2.35	0.60
1:A:166:ILE:HG23	1:A:417:GLN:HE21	1.65	0.60
1:A:312:ASP:HB3	1:A:314:ILE:CD1	2.31	0.60
1:A:240:ILE:HD12	1:A:240:ILE:N	2.17	0.60
1:A:56:PHE:O	1:A:58:PHE:N	2.34	0.60
1:A:9:GLU:HA	3:C:24:SER:HA	1.84	0.59
1:A:75:ILE:HG21	1:A:170:ILE:HG23	1.82	0.59
1:A:192:TYR:HB3	1:A:209:TYR:O	2.01	0.59
1:A:117:ILE:O	1:A:121:VAL:HG23	2.02	0.59
1:A:125:LEU:HD23	1:A:271:LEU:HG	1.85	0.59
1:A:166:ILE:HG23	1:A:417:GLN:NE2	2.17	0.59
1:A:288:GLU:HG3	1:A:289:GLY:N	2.18	0.59
1:A:17:PRO:CG	1:A:21:ILE:HD11	2.33	0.59
1:A:29:TRP:CH2	3:C:30:PRO:HB2	2.38	0.59
1:A:273:GLY:HA3	1:A:287:TYR:OH	2.03	0.59
1:A:73:LEU:HD13	1:A:147:ILE:HG23	1.85	0.58
2:B:15:ILE:H	2:B:15:ILE:CD1	2.16	0.58
1:A:314:ILE:HD12	1:A:315:HIS:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ARG:HD2	1:A:373:TYR:CZ	2.38	0.58
2:B:38:LYS:O	2:B:42:LEU:HB2	2.04	0.58
1:A:196:PHE:CD1	1:A:210:ILE:HB	2.39	0.58
1:A:7:ILE:O	1:A:10:LYS:HB2	2.04	0.58
1:A:210:ILE:O	1:A:214:ILE:HG13	2.04	0.58
1:A:371:LYS:HB2	1:A:371:LYS:HZ2	1.68	0.58
1:A:128:GLY:C	1:A:130:GLY:H	2.06	0.58
1:A:287:TYR:HA	1:A:292:ALA:HA	1.86	0.57
1:A:287:TYR:CE2	1:A:292:ALA:HB2	2.39	0.57
1:A:231:VAL:O	1:A:248:PRO:HA	2.03	0.57
1:A:417:GLN:O	1:A:421:GLU:HB2	2.04	0.57
2:B:32:GLU:O	2:B:35:ALA:HB3	2.04	0.57
1:A:364:LYS:O	1:A:368:HIS:HB2	2.04	0.57
1:A:369:ARG:O	1:A:372:ARG:HB3	2.04	0.57
1:A:230:ARG:HG3	1:A:230:ARG:NH1	2.13	0.57
1:A:166:ILE:HA	1:A:417:GLN:HE22	1.70	0.57
1:A:72:THR:HG22	1:A:73:LEU:HD12	1.86	0.56
1:A:237:HIS:C	1:A:239:ARG:H	2.09	0.56
2:B:58:ALA:O	2:B:62:LYS:HG3	2.05	0.56
1:A:203:GLY:C	1:A:205:PRO:HD3	2.26	0.56
1:A:287:TYR:CD2	1:A:292:ALA:HB2	2.41	0.56
2:B:34:LEU:HB3	2:B:38:LYS:HE3	1.88	0.56
1:A:23:PHE:CZ	1:A:418:LEU:HG	2.40	0.56
1:A:199:SER:HB3	1:A:205:PRO:HA	1.87	0.56
1:A:2:LYS:O	1:A:5:ILE:HG13	2.05	0.56
1:A:151:SER:O	1:A:155:ILE:HG13	2.06	0.56
2:B:34:LEU:HB3	2:B:38:LYS:HZ2	1.71	0.56
1:A:4:LEU:C	1:A:6:PRO:HD2	2.27	0.55
1:A:316:ALA:HB1	1:A:394:PHE:CZ	2.41	0.55
1:A:387:PHE:O	1:A:391:ILE:HG22	2.07	0.55
3:C:31:GLU:CD	3:C:31:GLU:H	2.10	0.55
1:A:123:ALA:O	1:A:127:VAL:HG12	2.06	0.55
1:A:281:ILE:H	1:A:281:ILE:CD1	2.18	0.55
1:A:381:SER:O	1:A:385:VAL:HG22	2.06	0.55
1:A:411:VAL:O	1:A:414:MET:HB2	2.06	0.55
1:A:420:ARG:HB3	1:A:420:ARG:CZ	2.36	0.54
1:A:15:GLU:HG2	3:C:27:ARG:HB3	1.88	0.54
2:B:34:LEU:HB3	2:B:38:LYS:NZ	2.22	0.54
1:A:288:GLU:O	1:A:290:GLY:N	2.40	0.54
1:A:194:TRP:HE3	1:A:194:TRP:HA	1.72	0.54
1:A:274:LEU:O	1:A:278:ARG:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ILE:O	1:A:318:VAL:HG22	2.07	0.54
1:A:8:LEU:HD12	3:C:23:PHE:HD1	1.72	0.54
1:A:194:TRP:HA	1:A:194:TRP:CE3	2.42	0.54
1:A:420:ARG:NH1	1:A:420:ARG:CB	2.60	0.54
1:A:85:MET:CE	1:A:110:CYS:HB3	2.39	0.53
2:B:24:VAL:HG12	2:B:24:VAL:O	2.07	0.53
1:A:197:LEU:O	1:A:201:ILE:HG13	2.08	0.53
1:A:325:ILE:HG13	1:A:326:THR:H	1.74	0.53
3:C:34:ILE:O	3:C:38:VAL:HG23	2.09	0.53
1:A:85:MET:HE2	1:A:110:CYS:HB3	1.90	0.53
1:A:232:GLU:H	2:B:24:VAL:HG12	1.74	0.53
1:A:407:THR:O	1:A:411:VAL:HG23	2.08	0.53
1:A:325:ILE:HG13	1:A:326:THR:N	2.24	0.52
1:A:266:PHE:CZ	1:A:300:LEU:HD22	2.44	0.52
2:B:34:LEU:HB3	2:B:38:LYS:CE	2.39	0.52
3:C:42:ILE:O	3:C:46:ILE:HG13	2.09	0.52
1:A:78:ILE:O	1:A:81:ALA:HB3	2.09	0.52
1:A:72:THR:HG22	1:A:73:LEU:CD1	2.39	0.52
1:A:274:LEU:HD13	1:A:274:LEU:C	2.30	0.52
1:A:380:MET:HE1	2:B:21:VAL:HB	1.92	0.51
1:A:63:THR:HG22	1:A:63:THR:O	2.10	0.51
1:A:312:ASP:HB3	1:A:314:ILE:HD11	1.90	0.51
1:A:98:LEU:HD23	1:A:103:ASN:HB3	1.93	0.51
1:A:310:ILE:HG22	1:A:310:ILE:O	2.11	0.51
1:A:128:GLY:C	1:A:130:GLY:N	2.63	0.51
1:A:95:GLN:O	1:A:96:MET:HG3	2.11	0.51
1:A:97:ASP:O	1:A:98:LEU:HB2	2.11	0.51
1:A:78:ILE:HD11	1:A:155:ILE:HA	1.93	0.50
1:A:112:LYS:O	1:A:116:ILE:HG13	2.11	0.50
1:A:210:ILE:HD13	1:A:213:ILE:HB	1.92	0.50
2:B:49:ILE:O	2:B:53:ILE:HG13	2.11	0.50
1:A:239:ARG:HB3	1:A:240:ILE:CD1	2.37	0.50
1:A:302:THR:CG2	1:A:393:ASN:HB3	2.42	0.50
1:A:219:VAL:HG11	1:A:401:GLY:HA2	1.94	0.50
1:A:226:ALA:HA	1:A:229:MET:SD	2.51	0.50
1:A:75:ILE:O	1:A:76:GLY:C	2.50	0.50
1:A:128:GLY:O	1:A:130:GLY:N	2.44	0.50
1:A:240:ILE:HG22	1:A:241:LYS:N	2.26	0.50
1:A:298:TYR:O	1:A:315:HIS:CE1	2.64	0.50
1:A:33:VAL:HG13	1:A:157:LEU:HB3	1.93	0.49
1:A:364:LYS:O	1:A:368:HIS:N	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ALA:N	1:A:212:PRO:HD2	2.27	0.49
3:C:50:GLY:O	3:C:52:PHE:N	2.44	0.49
1:A:212:PRO:HD3	1:A:306:LEU:HD12	1.94	0.49
1:A:149:PHE:O	1:A:153:ILE:HG13	2.13	0.49
1:A:321:ILE:HG22	1:A:322:ALA:N	2.27	0.49
1:A:22:THR:O	1:A:25:GLU:N	2.46	0.48
1:A:51:GLN:O	1:A:52:ILE:HG23	2.13	0.48
1:A:100:ILE:HD12	1:A:100:ILE:N	2.27	0.48
1:A:124:VAL:HG22	1:A:144:ILE:HD13	1.95	0.48
1:A:401:GLY:O	1:A:405:LEU:HB2	2.14	0.48
1:A:402:THR:O	1:A:406:LEU:HG	2.14	0.48
1:A:79:VAL:O	1:A:82:GLY:N	2.46	0.48
1:A:122:GLU:O	1:A:126:PHE:HB2	2.13	0.48
1:A:139:LEU:O	1:A:143:VAL:HG23	2.14	0.48
1:A:335:VAL:HG21	1:A:378:THR:HG23	1.94	0.48
1:A:373:TYR:O	1:A:376:PRO:HD2	2.13	0.48
1:A:380:MET:CE	2:B:21:VAL:HB	2.43	0.48
1:A:286:HIS:HD2	1:A:294:ASP:OD2	1.96	0.47
1:A:142:LEU:O	1:A:146:GLN:HG3	2.13	0.47
1:A:154:LEU:HG	1:A:173:PHE:CE1	2.49	0.47
1:A:160:ILE:HD11	3:C:33:VAL:HB	1.96	0.47
1:A:266:PHE:CE2	1:A:300:LEU:HD22	2.50	0.47
1:A:170:ILE:H	1:A:170:ILE:CD1	2.18	0.47
1:A:321:ILE:O	1:A:325:ILE:HG12	2.14	0.47
2:B:17:GLU:O	2:B:20:ARG:HB2	2.13	0.47
1:A:8:LEU:HD12	3:C:23:PHE:CD1	2.50	0.47
1:A:232:GLU:HA	1:A:248:PRO:HA	1.97	0.46
1:A:254:VAL:HG12	1:A:381:SER:CB	2.40	0.46
1:A:291:ARG:HG2	1:A:291:ARG:HH11	1.78	0.46
1:A:72:THR:HB	1:A:147:ILE:CD1	2.43	0.46
1:A:93:ILE:HG22	1:A:93:ILE:O	2.16	0.46
2:B:31:ASP:OD1	2:B:31:ASP:N	2.45	0.46
1:A:113:LEU:CD1	1:A:117:ILE:HD11	2.46	0.46
1:A:236:ALA:O	1:A:238:GLY:N	2.48	0.46
1:A:164:TYR:CZ	3:C:30:PRO:HG2	2.50	0.46
1:A:125:LEU:HD23	1:A:271:LEU:CD2	2.45	0.46
1:A:11:ILE:O	3:C:24:SER:HB2	2.14	0.46
1:A:274:LEU:N	1:A:287:TYR:CZ	2.83	0.46
1:A:73:LEU:O	1:A:74:GLY:C	2.55	0.46
1:A:295:GLY:O	1:A:298:TYR:HB3	2.15	0.46
1:A:225:TYR:OH	2:B:28:PRO:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:TYR:OH	1:A:64:ALA:O	2.29	0.45
1:A:118:MET:O	1:A:122:GLU:HG3	2.17	0.45
1:A:136:THR:O	1:A:138:LEU:N	2.50	0.45
1:A:129:ALA:CB	1:A:274:LEU:HD12	2.41	0.45
1:A:373:TYR:O	1:A:376:PRO:CG	2.65	0.45
1:A:391:ILE:O	1:A:395:ILE:HG13	2.16	0.45
1:A:15:GLU:HA	3:C:27:ARG:HH11	1.81	0.45
1:A:204:VAL:N	1:A:205:PRO:HD3	2.31	0.45
1:A:118:MET:HA	1:A:121:VAL:HB	1.99	0.45
1:A:222:MET:HG2	1:A:388:LEU:HD21	1.98	0.45
3:C:36:VAL:O	3:C:39:ALA:HB3	2.17	0.45
1:A:220:PHE:CZ	2:B:41:ALA:HB2	2.50	0.45
1:A:235:LEU:HD11	1:A:247:TYR:HB2	1.98	0.45
1:A:291:ARG:H	1:A:291:ARG:HD3	1.82	0.45
1:A:75:ILE:CG2	1:A:79:VAL:HG23	2.42	0.45
1:A:415:TYR:CD2	2:B:39:VAL:HG21	2.51	0.45
1:A:102:GLU:O	1:A:106:LEU:HG	2.18	0.44
1:A:370:LEU:O	1:A:373:TYR:N	2.49	0.44
2:B:17:GLU:OE2	2:B:17:GLU:HA	2.17	0.44
2:B:19:ARG:HA	2:B:22:TRP:HB3	2.00	0.44
1:A:67:ILE:HG23	1:A:72:THR:HG23	1.99	0.44
1:A:370:LEU:C	1:A:372:ARG:N	2.68	0.44
2:B:61:ILE:O	2:B:62:LYS:C	2.55	0.44
1:A:71:ILE:HG13	1:A:71:ILE:O	2.18	0.44
1:A:324:ILE:O	1:A:328:VAL:HG23	2.17	0.44
2:B:36:VAL:O	2:B:40:THR:HG23	2.18	0.44
1:A:370:LEU:O	1:A:372:ARG:N	2.51	0.43
1:A:97:ASP:HB3	1:A:103:ASN:OD1	2.19	0.43
1:A:52:ILE:HA	1:A:53:PRO:HD3	1.88	0.43
1:A:346:ALA:O	1:A:347:LYS:C	2.56	0.43
1:A:389:ALA:O	1:A:392:ALA:HB3	2.18	0.43
2:B:29:THR:OG1	2:B:32:GLU:HB3	2.18	0.43
1:A:11:ILE:HA	1:A:12:PRO:HD3	1.88	0.43
1:A:92:GLY:C	1:A:94:ILE:H	2.21	0.43
1:A:167:GLY:H	1:A:417:GLN:NE2	2.17	0.43
1:A:101:PRO:O	1:A:102:GLU:C	2.57	0.43
2:B:15:ILE:O	2:B:19:ARG:HG3	2.18	0.43
1:A:211:ALA:O	1:A:214:ILE:HB	2.19	0.42
1:A:382:SER:O	1:A:385:VAL:HG23	2.19	0.42
1:A:291:ARG:N	1:A:291:ARG:CD	2.82	0.42
1:A:281:ILE:C	1:A:283:ILE:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ARG:O	1:A:372:ARG:CB	2.67	0.42
1:A:276:LEU:CD1	1:A:283:ILE:HD12	2.47	0.42
1:A:167:GLY:H	1:A:417:GLN:HE22	1.67	0.42
1:A:256:ASN:HD22	1:A:256:ASN:HA	1.54	0.42
1:A:244:VAL:HG12	1:A:245:GLY:N	2.35	0.42
1:A:257:ILE:N	1:A:258:PRO:CD	2.83	0.42
1:A:303:PRO:O	1:A:304:TYR:HB3	2.19	0.42
1:A:401:GLY:H	1:A:404:VAL:HG23	1.85	0.42
1:A:415:TYR:O	1:A:418:LEU:HB3	2.19	0.42
1:A:75:ILE:HD13	1:A:75:ILE:HA	1.78	0.42
1:A:218:ILE:HG22	1:A:219:VAL:N	2.35	0.42
1:A:364:LYS:O	1:A:365:ALA:C	2.58	0.42
3:C:49:TYR:CD1	3:C:49:TYR:N	2.88	0.42
1:A:413:ARG:HH11	1:A:413:ARG:CB	2.16	0.41
1:A:29:TRP:CH2	3:C:30:PRO:CB	3.02	0.41
1:A:43:ILE:HB	1:A:70:LEU:CD2	2.41	0.41
1:A:266:PHE:C	1:A:270:GLN:HE21	2.22	0.41
1:A:302:THR:HG21	1:A:393:ASN:HB3	2.01	0.41
1:A:342:PRO:HB3	1:A:370:LEU:HB2	2.02	0.41
1:A:33:VAL:CG1	1:A:157:LEU:HB3	2.50	0.41
1:A:206:ASN:O	1:A:207:ILE:C	2.58	0.41
1:A:260:ILE:HG12	1:A:406:LEU:HD22	2.02	0.41
3:C:37:THR:O	3:C:41:VAL:HG23	2.20	0.41
1:A:108:GLN:HA	1:A:108:GLN:NE2	2.36	0.41
1:A:232:GLU:HG2	1:A:248:PRO:CG	2.48	0.41
1:A:232:GLU:N	2:B:24:VAL:HG12	2.36	0.41
1:A:335:VAL:HG21	1:A:378:THR:CG2	2.51	0.41
1:A:2:LYS:C	1:A:4:LEU:H	2.24	0.41
1:A:103:ASN:N	1:A:103:ASN:HD22	2.18	0.41
2:B:20:ARG:O	2:B:24:VAL:HG23	2.21	0.41
1:A:63:THR:C	1:A:65:SER:N	2.74	0.41
3:C:35:GLY:O	3:C:36:VAL:C	2.58	0.41
1:A:370:LEU:C	1:A:372:ARG:H	2.25	0.41
2:B:36:VAL:HA	2:B:39:VAL:HG12	2.03	0.41
1:A:344:SER:O	1:A:345:MET:C	2.58	0.41
1:A:417:GLN:HE21	1:A:417:GLN:HB3	1.74	0.41
1:A:287:TYR:N	1:A:287:TYR:CD1	2.89	0.40
1:A:5:ILE:N	1:A:6:PRO:CD	2.84	0.40
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.87	0.40
1:A:33:VAL:HG13	1:A:157:LEU:HD13	2.04	0.40
1:A:257:ILE:HD13	1:A:257:ILE:HA	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:HD23	1:A:172:LEU:HA	1.88	0.40
1:A:13:GLU:O	1:A:14:VAL:C	2.60	0.40
1:A:142:LEU:O	1:A:145:ILE:HB	2.22	0.40
1:A:240:ILE:N	1:A:240:ILE:CD1	2.84	0.40
1:A:286:HIS:CD2	1:A:294:ASP:OD2	2.74	0.40
1:A:373:TYR:O	1:A:376:PRO:CD	2.70	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	406/436 (93%)	310 (76%)	75 (18%)	21 (5%)	2	15
2	B	54/74 (73%)	50 (93%)	4 (7%)	0	100	100
3	C	30/53 (57%)	25 (83%)	4 (13%)	1 (3%)	4	25
All	All	490/563 (87%)	385 (79%)	83 (17%)	22 (4%)	2	18

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	GLU
1	A	283	ILE
1	A	363	GLU
3	C	51	ARG
1	A	237	HIS
1	A	238	GLY
1	A	289	GLY
1	A	74	GLY
1	A	88	LEU
1	A	129	ALA
1	A	137	PRO

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Mol	Chain	Res	Type
1	A	208	GLU
1	A	58	PHE
1	A	239	ARG
1	A	284	LEU
1	A	299	TYR
1	A	346	ALA
1	A	76	GLY
1	A	207	ILE
1	A	339	GLY
1	A	252	VAL
1	A	147	ILE

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	335/355 (94%)	307 (92%)	28 (8%)	11	39
2	B	48/66 (73%)	45 (94%)	3 (6%)	18	52
3	C	28/45 (62%)	26 (93%)	2 (7%)	14	47
All	All	411/466 (88%)	378 (92%)	33 (8%)	12	42

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	45	VAL
1	A	56	PHE
1	A	61	THR
1	A	108	GLN
1	A	112	LYS
1	A	125	LEU
1	A	126	PHE
1	A	151	SER
1	A	172	LEU
1	A	194	TRP

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Mol	Chain	Res	Type
1	A	210	ILE
1	A	239	ARG
1	A	256	ASN
1	A	291	ARG
1	A	294	ASP
1	A	314	ILE
1	A	321	ILE
1	A	363	GLU
1	A	368	HIS
1	A	373	TYR
1	A	377	LEU
1	A	388	LEU
1	A	402	THR
1	A	413	ARG
1	A	417	GLN
1	A	420	ARG
1	A	421	GLU
2	B	12	LYS
2	B	30	LYS
2	B	31	ASP
3	C	26	ILE
3	C	28	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	202	GLN
1	A	256	ASN
1	A	270	GLN
1	A	286	HIS
1	A	315	HIS
1	A	417	GLN

5.3.3 RNA

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 monosaccharides 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	410/436 (94%)	-0.08	18 (4%) 34 21	49, 91, 141, 166	0
2	B	56/74 (75%)	0.03	2 (3%) 42 27	55, 100, 168, 176	0
3	C	32/53 (60%)	-0.40	0 100 100	54, 88, 132, 133	0
All	All	498/563 (88%)	-0.09	20 (4%) 38 25	49, 92, 146, 176	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	LEU	5.7
1	A	95	GLN	5.0
1	A	305	GLY	4.9
1	A	304	TYR	4.2
1	A	94	ILE	3.0
1	A	50	ALA	3.0
1	A	92	GLY	2.8
1	A	299	TYR	2.8
1	A	241	LYS	2.8
1	A	135	LEU	2.6
1	A	240	ILE	2.6
1	A	307	SER	2.5
1	A	200	LEU	2.5
1	A	281	ILE	2.4
2	B	64	ILE	2.3
1	A	243	ALA	2.3
1	A	93	ILE	2.2
1	A	51	GLN	2.2
1	A	209	TYR	2.1
2	B	66	LYS	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 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.