



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:52 PM UTC

PDB ID : 3RG6 / pdb_00003rg6
Title : Crystal structure of a chaperone-bound assembly intermediate of form I Rubisco
Authors : Bracher, A.; Starling-Windhof, A.; Hartl, F.U.; Hayer-Hartl, M.
Deposited on : 2011-04-07
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 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

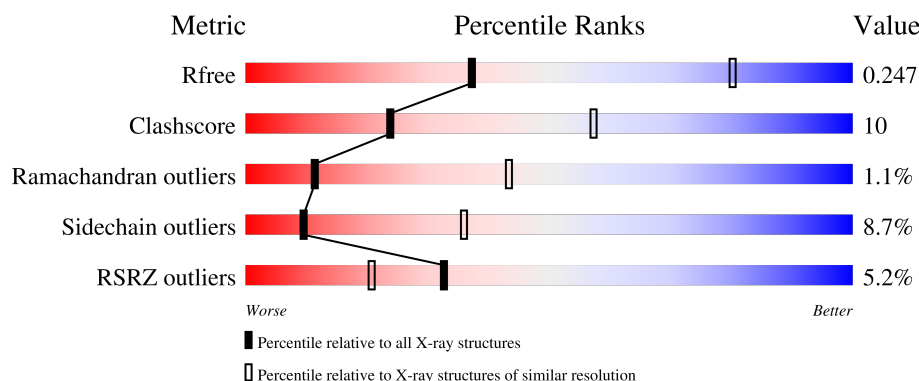
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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	472	2% 65% 24% • 6%
1	B	472	% 63% 27% • 7%
2	C	155	14% 63% 10% • 26%
2	D	155	6% 53% 15% • 31%
2	E	155	11% 66% 7% • 26%

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Mol	Chain	Length	Quality of chain
2	F	155	5% 57% 11% 32%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10078 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 Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3407	2164	596	629	18			
1	B	438	Total	C	N	O	S	0	0	0
			3356	2131	591	616	18			

- Molecule 2 is a protein called RbcX protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	115	Total	C	N	O	S	0	0	0
			867	551	150	161	5			
2	D	107	Total	C	N	O	S	0	0	0
			801	513	138	148	2			
2	E	114	Total	C	N	O	S	0	0	0
			855	543	149	159	4			
2	F	106	Total	C	N	O	S	0	0	0
			792	508	137	145	2			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	expression tag	UNP Q44212
C	-18	GLY	-	expression tag	UNP Q44212
C	-17	SER	-	expression tag	UNP Q44212
C	-16	SER	-	expression tag	UNP Q44212
C	-15	HIS	-	expression tag	UNP Q44212
C	-14	HIS	-	expression tag	UNP Q44212
C	-13	HIS	-	expression tag	UNP Q44212
C	-12	HIS	-	expression tag	UNP Q44212
C	-11	HIS	-	expression tag	UNP Q44212
C	-10	HIS	-	expression tag	UNP Q44212
C	-9	SER	-	expression tag	UNP Q44212
C	-8	SER	-	expression tag	UNP Q44212

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLY	-	expression tag	UNP Q44212
C	-6	LEU	-	expression tag	UNP Q44212
C	-5	VAL	-	expression tag	UNP Q44212
C	-4	PRO	-	expression tag	UNP Q44212
C	-3	ARG	-	expression tag	UNP Q44212
C	-2	GLY	-	expression tag	UNP Q44212
C	-1	SER	-	expression tag	UNP Q44212
C	0	HIS	-	expression tag	UNP Q44212
D	-19	MET	-	expression tag	UNP Q44212
D	-18	GLY	-	expression tag	UNP Q44212
D	-17	SER	-	expression tag	UNP Q44212
D	-16	SER	-	expression tag	UNP Q44212
D	-15	HIS	-	expression tag	UNP Q44212
D	-14	HIS	-	expression tag	UNP Q44212
D	-13	HIS	-	expression tag	UNP Q44212
D	-12	HIS	-	expression tag	UNP Q44212
D	-11	HIS	-	expression tag	UNP Q44212
D	-10	HIS	-	expression tag	UNP Q44212
D	-9	SER	-	expression tag	UNP Q44212
D	-8	SER	-	expression tag	UNP Q44212
D	-7	GLY	-	expression tag	UNP Q44212
D	-6	LEU	-	expression tag	UNP Q44212
D	-5	VAL	-	expression tag	UNP Q44212
D	-4	PRO	-	expression tag	UNP Q44212
D	-3	ARG	-	expression tag	UNP Q44212
D	-2	GLY	-	expression tag	UNP Q44212
D	-1	SER	-	expression tag	UNP Q44212
D	0	HIS	-	expression tag	UNP Q44212
E	-19	MET	-	expression tag	UNP Q44212
E	-18	GLY	-	expression tag	UNP Q44212
E	-17	SER	-	expression tag	UNP Q44212
E	-16	SER	-	expression tag	UNP Q44212
E	-15	HIS	-	expression tag	UNP Q44212
E	-14	HIS	-	expression tag	UNP Q44212
E	-13	HIS	-	expression tag	UNP Q44212
E	-12	HIS	-	expression tag	UNP Q44212
E	-11	HIS	-	expression tag	UNP Q44212
E	-10	HIS	-	expression tag	UNP Q44212
E	-9	SER	-	expression tag	UNP Q44212
E	-8	SER	-	expression tag	UNP Q44212
E	-7	GLY	-	expression tag	UNP Q44212
E	-6	LEU	-	expression tag	UNP Q44212

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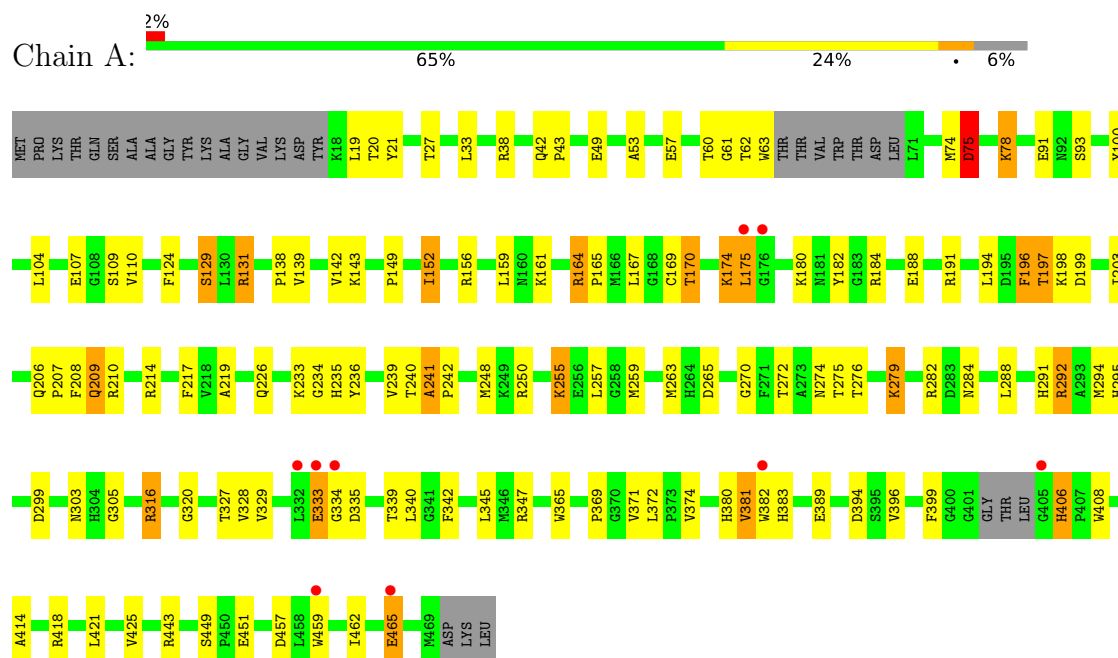
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	VAL	-	expression tag	UNP Q44212
E	-4	PRO	-	expression tag	UNP Q44212
E	-3	ARG	-	expression tag	UNP Q44212
E	-2	GLY	-	expression tag	UNP Q44212
E	-1	SER	-	expression tag	UNP Q44212
E	0	HIS	-	expression tag	UNP Q44212
F	-19	MET	-	expression tag	UNP Q44212
F	-18	GLY	-	expression tag	UNP Q44212
F	-17	SER	-	expression tag	UNP Q44212
F	-16	SER	-	expression tag	UNP Q44212
F	-15	HIS	-	expression tag	UNP Q44212
F	-14	HIS	-	expression tag	UNP Q44212
F	-13	HIS	-	expression tag	UNP Q44212
F	-12	HIS	-	expression tag	UNP Q44212
F	-11	HIS	-	expression tag	UNP Q44212
F	-10	HIS	-	expression tag	UNP Q44212
F	-9	SER	-	expression tag	UNP Q44212
F	-8	SER	-	expression tag	UNP Q44212
F	-7	GLY	-	expression tag	UNP Q44212
F	-6	LEU	-	expression tag	UNP Q44212
F	-5	VAL	-	expression tag	UNP Q44212
F	-4	PRO	-	expression tag	UNP Q44212
F	-3	ARG	-	expression tag	UNP Q44212
F	-2	GLY	-	expression tag	UNP Q44212
F	-1	SER	-	expression tag	UNP Q44212
F	0	HIS	-	expression tag	UNP Q44212

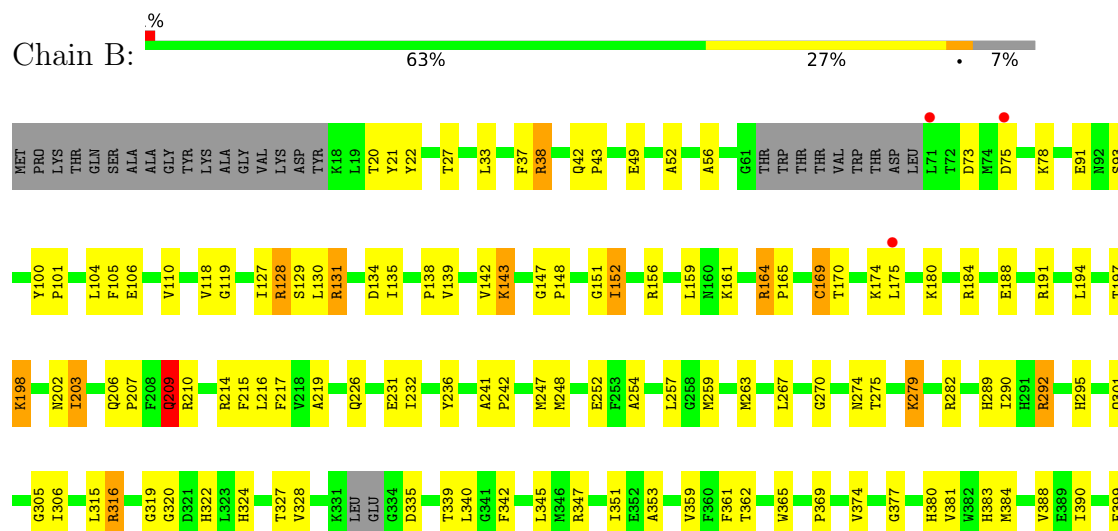
3 Residue-property plots

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

- Molecule 1: Ribulose biphosphate carboxylase large chain

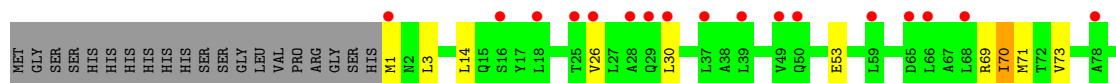


- Molecule 1: Ribulose biphosphate carboxylase large chain

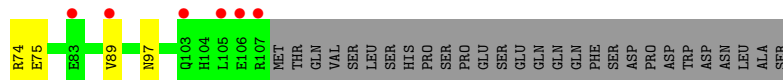
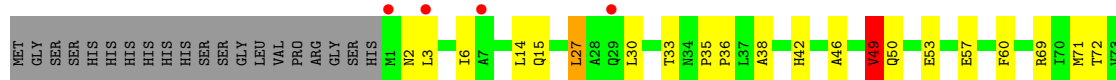




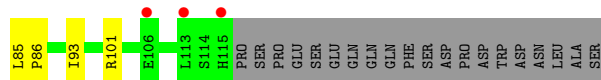
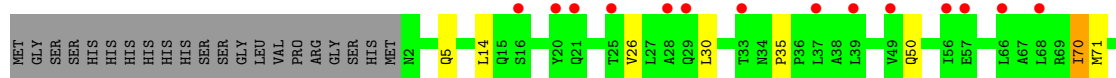
- Molecule 2: RbcX protein



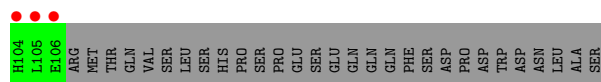
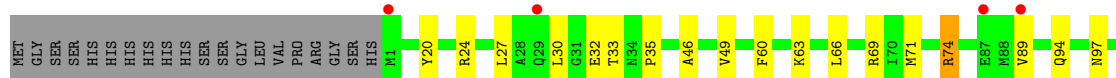
- Molecule 2: RbcX protein



- Molecule 2: RbcX protein



- Molecule 2: RbcX protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	244.75 Å 244.75 Å 99.67 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	84.5 (30.00-3.20) 84.4 (30.00-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 3.18 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.245 0.217 , 0.247	Depositor DCC
R_{free} test set	2067 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	72.3	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.053 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10078	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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	0.51	0/3492	0.92	7/4736 (0.1%)
1	B	0.52	0/3438	0.88	6/4662 (0.1%)
2	C	0.47	0/881	0.86	0/1200
2	D	0.46	0/815	0.90	0/1114
2	E	0.46	0/869	0.87	1/1186 (0.1%)
2	F	0.46	0/806	0.93	3/1102 (0.3%)
All	All	0.50	0/10301	0.89	17/14000 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	ASP	N-CA-C	-6.93	103.66	111.14
1	B	73	ASP	N-CA-C	-6.72	102.19	110.65
1	A	406	HIS	CA-C-N	6.42	126.11	119.82
1	A	406	HIS	C-N-CA	6.42	126.11	119.82
1	B	381	VAL	N-CA-C	6.08	116.86	110.72
1	B	335	ASP	N-CA-C	-6.07	104.35	110.97
1	A	381	VAL	N-CA-C	6.07	116.24	110.42
1	A	241	ALA	CA-C-N	6.03	125.51	119.24
1	A	241	ALA	C-N-CA	6.03	125.51	119.24
2	F	63	LYS	CA-C-N	5.77	127.06	119.84
2	F	63	LYS	C-N-CA	5.77	127.06	119.84
1	B	406	HIS	CA-C-N	5.61	126.86	119.84
1	B	406	HIS	C-N-CA	5.61	126.86	119.84
2	E	35	PRO	N-CA-C	5.42	117.31	110.70
2	F	35	PRO	N-CA-C	5.35	117.22	110.70
1	B	267	LEU	N-CA-C	5.27	116.88	111.03
1	A	196	PHE	N-CA-C	5.27	118.17	109.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3407	0	3251	90	0
1	B	3356	0	3202	80	0
2	C	867	0	838	14	0
2	D	801	0	763	19	0
2	E	855	0	817	10	0
2	F	792	0	757	11	0
All	All	10078	0	9628	199	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 10.

All (199) 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)
2:F:30:LEU:HA	2:F:33:THR:HG22	1.38	1.02
1:A:19:LEU:HD11	1:A:63:TRP:CH2	1.96	1.00
1:A:19:LEU:HD11	1:A:63:TRP:HH2	1.28	0.95
1:B:248:MET:HE2	1:B:248:MET:HA	1.49	0.94
1:B:209:GLN:HE22	1:B:214:ARG:HD3	1.34	0.92
1:A:49:GLU:HG2	2:D:33:THR:HG21	1.55	0.88
1:A:198:LYS:HB3	1:A:236:TYR:CD2	2.12	0.84
1:A:226:GLN:NE2	1:A:233:LYS:H	1.81	0.77
1:A:316:ARG:HG2	1:A:365:TRP:CZ3	2.19	0.77
2:C:14:LEU:HD23	2:D:89:VAL:HG21	1.68	0.76
1:A:198:LYS:HB3	1:A:236:TYR:HD2	1.46	0.76
1:A:169:CYS:HB2	1:A:399:PHE:O	1.89	0.73
1:A:380:HIS:H	1:A:383:HIS:HD2	1.34	0.73
1:A:255:LYS:HE2	1:A:284:ASN:HB3	1.71	0.73
1:B:138:PRO:O	1:B:142:VAL:HG23	1.92	0.69
1:A:270:GLY:HA3	1:B:270:GLY:HA3	1.73	0.69
1:A:19:LEU:CD1	1:A:63:TRP:CH2	2.76	0.68
1:A:294:MET:HG2	1:A:294:MET:O	1.92	0.68
1:B:164:ARG:HB2	1:B:425:VAL:HG21	1.74	0.68
1:A:250:ARG:NH2	1:B:106:GLU:OE2	2.26	0.68
1:A:184:ARG:O	1:A:188:GLU:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ALA:HB2	1:B:257:LEU:HD13	1.77	0.67
1:B:49:GLU:OE2	2:F:33:THR:HG21	1.96	0.65
1:B:198:LYS:HB2	1:B:236:TYR:HD2	1.61	0.65
1:B:259:MET:HA	1:B:259:MET:HE2	1.79	0.64
1:B:236:TYR:HB3	1:B:263:MET:HB3	1.77	0.64
1:A:380:HIS:H	1:A:383:HIS:CD2	2.15	0.64
1:A:49:GLU:CG	2:D:33:THR:HG21	2.28	0.64
1:B:247:MET:HE3	1:B:248:MET:HE3	1.77	0.64
1:A:174:LYS:HG2	1:A:203:ILE:HD11	1.80	0.63
1:A:174:LYS:HG2	1:A:175:LEU:N	2.13	0.63
1:A:209:GLN:OE1	1:A:214:ARG:HD3	1.98	0.63
1:B:215:PHE:HE2	1:B:254:ALA:HB2	1.65	0.61
1:A:199:ASP:OD1	1:A:235:HIS:HE1	1.83	0.61
1:B:241:ALA:HB1	1:B:242:PRO:HD2	1.83	0.61
1:A:208:PHE:O	1:A:209:GLN:HB2	2.01	0.60
1:A:342:PHE:HA	1:A:345:LEU:HB2	1.83	0.60
1:B:184:ARG:O	1:B:188:GLU:HG2	2.00	0.60
1:A:236:TYR:HB3	1:A:263:MET:HB3	1.82	0.60
1:A:169:CYS:HA	1:A:399:PHE:H	1.66	0.60
1:B:316:ARG:HG2	1:B:365:TRP:CZ3	2.37	0.60
2:C:1:MET:HG3	2:C:3:LEU:HD13	1.83	0.60
1:B:143:LYS:HE2	1:B:143:LYS:HA	1.85	0.59
1:A:197:THR:HB	1:A:235:HIS:HD2	1.67	0.59
1:A:164:ARG:HG2	1:A:165:PRO:O	2.02	0.59
1:A:259:MET:HA	1:A:259:MET:HE2	1.86	0.58
1:A:406:HIS:CE1	1:A:408:TRP:HB2	2.39	0.58
1:A:299:ASP:C	1:A:299:ASP:OD1	2.47	0.57
2:E:93:ILE:HG23	2:F:74:ARG:HD3	1.86	0.57
1:B:439:GLY:O	1:B:443:ARG:HD3	2.05	0.57
1:B:226:GLN:OE1	1:B:232:ILE:HA	2.05	0.57
1:A:333:GLU:HG2	1:A:334:GLY:N	2.20	0.57
1:A:197:THR:HB	1:A:235:HIS:CD2	2.40	0.56
2:E:14:LEU:HD23	2:F:89:VAL:HG21	1.88	0.56
1:B:289:HIS:HA	1:B:322:HIS:HB2	1.88	0.56
2:E:26:VAL:HG21	2:E:70:ILE:HD11	1.87	0.56
1:A:174:LYS:HG2	1:A:175:LEU:H	1.71	0.56
1:B:339:THR:HA	1:B:342:PHE:CE2	2.40	0.56
1:A:182:TYR:OH	1:A:199:ASP:HA	2.06	0.55
1:B:194:LEU:HG	1:B:414:ALA:HB1	1.87	0.55
1:A:49:GLU:HG2	2:D:33:THR:CG2	2.33	0.55
1:A:462:ILE:HG12	2:F:46:ALA:HA	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HB3	1:A:100:TYR:HB2	1.87	0.55
2:D:71:MET:HA	2:D:74:ARG:HD2	1.87	0.55
1:A:170:THR:HG23	1:A:198:LYS:HG3	1.89	0.55
1:B:248:MET:HA	1:B:248:MET:CE	2.31	0.55
1:B:118:VAL:HG11	1:B:306:ILE:HD11	1.89	0.55
1:A:382:TRP:HE1	1:A:459:TRP:HB2	1.72	0.54
2:F:20:TYR:OH	2:F:24:ARG:NH1	2.40	0.54
1:A:380:HIS:N	1:A:383:HIS:HD2	2.02	0.54
1:A:19:LEU:CD1	1:A:63:TRP:CZ3	2.91	0.54
1:B:324:HIS:HA	1:B:374:VAL:HB	1.90	0.53
2:D:46:ALA:HA	1:B:462:ILE:HG12	1.89	0.53
1:A:156:ARG:NH1	1:A:164:ARG:O	2.42	0.53
1:A:152:ILE:HG12	1:A:372:LEU:HG	1.91	0.52
1:B:353:ALA:HA	1:B:359:VAL:HG12	1.90	0.52
1:A:42:GLN:OE1	1:A:43:PRO:HD2	2.10	0.52
1:A:248:MET:CE	1:A:276:THR:HG22	2.39	0.52
1:A:62:THR:O	1:A:63:TRP:HB2	2.08	0.52
1:A:333:GLU:HB2	2:E:5:GLN:CD	2.34	0.52
1:A:198:LYS:CB	1:A:236:TYR:HD2	2.20	0.52
1:B:198:LYS:HB2	1:B:236:TYR:CD2	2.44	0.52
2:F:30:LEU:HA	2:F:33:THR:CG2	2.26	0.52
1:B:215:PHE:CE2	1:B:254:ALA:HB2	2.43	0.52
1:B:433:ASP:O	1:B:437:GLU:HB2	2.10	0.51
1:B:180:LYS:HD2	1:B:217:PHE:CE1	2.45	0.51
1:A:194:LEU:HG	1:A:414:ALA:HB1	1.91	0.51
1:B:33:LEU:HB3	1:B:100:TYR:HB2	1.91	0.51
2:C:71:MET:HE3	2:D:97:ASN:HA	1.91	0.51
1:B:131:ARG:HA	1:B:305:GLY:O	2.11	0.51
2:C:26:VAL:HG21	2:C:70:ILE:HD11	1.93	0.51
1:B:37:PHE:HB3	1:B:130:LEU:HD11	1.93	0.51
2:D:27:LEU:HD21	2:D:42:HIS:HD2	1.75	0.50
1:B:148:PRO:HD2	1:B:369:PRO:HD2	1.93	0.50
2:F:20:TYR:HD1	2:F:49:VAL:HG11	1.75	0.50
1:A:53:ALA:HB2	2:D:33:THR:HG23	1.92	0.50
1:B:275:THR:O	1:B:279:LYS:HG2	2.12	0.50
1:B:384:MET:O	1:B:388:VAL:HG23	2.12	0.50
1:A:316:ARG:NH1	1:A:369:PRO:O	2.44	0.50
1:B:248:MET:O	1:B:252:GLU:HG2	2.12	0.50
1:B:170:THR:HG23	1:B:198:LYS:HG2	1.93	0.50
1:B:263:MET:HA	1:B:289:HIS:O	2.12	0.49
2:E:26:VAL:O	2:E:30:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:100:LYS:HZ3	2:D:57:GLU:HG3	1.77	0.49
1:A:138:PRO:O	1:A:142:VAL:HG23	2.12	0.49
1:B:226:GLN:HG3	1:B:231:GLU:O	2.12	0.49
1:B:274:ASN:O	1:B:275:THR:C	2.55	0.49
1:A:333:GLU:HB2	2:E:5:GLN:NE2	2.28	0.49
2:D:49:VAL:HB	1:B:464:PHE:HD1	1.76	0.48
1:B:21:TYR:CE1	1:B:56:ALA:HA	2.47	0.48
1:B:134:ASP:OD2	1:B:135:ILE:N	2.46	0.48
1:A:374:VAL:HG22	1:A:396:VAL:HB	1.95	0.48
2:C:81:ILE:HD13	2:D:6:ILE:HG22	1.95	0.48
1:A:339:THR:HA	1:A:342:PHE:CE2	2.49	0.48
1:B:169:CYS:HA	1:B:399:PHE:H	1.79	0.48
2:D:74:ARG:HG2	2:D:75:GLU:N	2.28	0.47
2:C:97:ASN:ND2	2:D:71:MET:O	2.47	0.47
2:D:35:PRO:HB2	2:D:36:PRO:HD3	1.96	0.47
1:A:174:LYS:CG	1:A:175:LEU:H	2.25	0.47
1:B:38:ARG:O	1:B:38:ARG:HG3	2.15	0.47
1:B:131:ARG:NH2	1:B:301:GLN:O	2.47	0.47
1:B:209:GLN:NE2	1:B:214:ARG:HD3	2.17	0.47
1:B:342:PHE:HA	1:B:345:LEU:HB2	1.97	0.47
1:A:21:TYR:OH	1:A:60:THR:OG1	2.27	0.46
1:B:203:ILE:O	1:B:203:ILE:CG2	2.63	0.46
1:B:164:ARG:HG2	1:B:165:PRO:O	2.16	0.46
1:A:159:LEU:HB3	1:A:161:LYS:HD3	1.97	0.46
1:A:61:GLY:O	1:A:63:TRP:HD1	1.99	0.46
1:A:107:GLU:C	1:A:109:SER:H	2.24	0.46
1:A:288:LEU:HD23	1:A:320:GLY:HA2	1.98	0.46
1:A:292:ARG:HD3	1:A:295:HIS:CD2	2.51	0.46
1:A:19:LEU:HD12	1:A:19:LEU:HA	1.78	0.45
1:A:406:HIS:HE1	1:A:408:TRP:HB2	1.81	0.45
1:B:406:HIS:HA	1:B:407:PRO:HD2	1.78	0.45
2:C:100:LYS:NZ	2:D:57:GLU:HG3	2.31	0.45
1:A:57:GLU:HG3	1:A:124:PHE:CZ	2.51	0.45
1:A:265:ASP:OD1	1:A:291:HIS:HB3	2.17	0.45
2:C:26:VAL:O	2:C:30:LEU:HB2	2.17	0.45
1:B:159:LEU:HB3	1:B:161:LYS:HD3	1.99	0.45
1:A:275:THR:O	1:A:279:LYS:HG2	2.16	0.44
2:C:85:LEU:HB2	2:C:86:PRO:HD3	1.99	0.44
1:A:131:ARG:HA	1:A:305:GLY:O	2.18	0.44
1:A:149:PRO:HD3	1:A:320:GLY:H	1.82	0.44
2:E:71:MET:HE3	2:F:97:ASN:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:TYR:CB	1:A:263:MET:HB3	2.47	0.44
1:A:316:ARG:HD3	1:A:371:VAL:HG23	2.00	0.44
1:B:156:ARG:NH1	1:B:164:ARG:O	2.49	0.44
1:B:406:HIS:CE1	1:B:408:TRP:HB2	2.52	0.44
1:B:417:ASN:HD22	1:B:417:ASN:N	2.15	0.44
1:A:196:PHE:HA	1:A:234:GLY:O	2.18	0.43
1:A:272:THR:HA	1:B:242:PRO:O	2.18	0.43
1:B:340:LEU:HD21	1:B:390:ILE:HG23	1.99	0.43
1:A:241:ALA:HB1	1:A:242:PRO:HD2	1.98	0.43
1:A:180:LYS:HD3	1:A:217:PHE:CE1	2.54	0.43
1:A:167:LEU:HG	1:A:421:LEU:HD22	2.00	0.43
1:B:169:CYS:HB2	1:B:399:PHE:O	2.19	0.43
2:E:85:LEU:HB2	2:E:86:PRO:HD3	2.00	0.43
1:A:206:GLN:HB3	1:A:207:PRO:HD2	2.01	0.43
1:B:292:ARG:HD3	1:B:295:HIS:CD2	2.53	0.43
2:E:101:ARG:HG3	2:F:71:MET:HE1	2.01	0.43
1:A:129:SER:HB2	1:A:303:ASN:O	2.19	0.42
1:A:274:ASN:O	1:A:275:THR:C	2.62	0.42
2:C:69:ARG:O	2:C:73:VAL:HG23	2.19	0.42
1:A:328:VAL:HG12	1:A:328:VAL:O	2.20	0.42
1:B:37:PHE:CD1	1:B:130:LEU:HD11	2.54	0.42
1:B:147:GLY:HA2	1:B:316:ARG:O	2.19	0.42
1:B:151:GLY:O	1:B:152:ILE:C	2.63	0.42
1:A:75:ASP:HA	1:A:78:LYS:HG2	2.02	0.42
2:C:100:LYS:NZ	2:D:53:GLU:O	2.53	0.42
1:B:290:ILE:HG21	1:B:315:LEU:HG	2.01	0.42
1:B:380:HIS:H	1:B:383:HIS:HD2	1.67	0.42
1:A:465:GLU:HA	2:E:50:GLN:HE22	1.84	0.42
1:B:101:PRO:HD2	1:B:104:LEU:HG	2.01	0.42
1:A:239:VAL:O	1:A:240:THR:C	2.62	0.41
1:A:156:ARG:NH2	1:A:394:ASP:OD1	2.54	0.41
1:A:197:THR:O	1:A:235:HIS:HA	2.20	0.41
1:A:174:LYS:CG	1:A:203:ILE:HD11	2.48	0.41
1:A:164:ARG:HB2	1:A:425:VAL:HG21	2.02	0.41
1:A:174:LYS:HB3	1:A:174:LYS:HE3	1.70	0.41
2:D:30:LEU:HB3	2:D:38:ALA:HB2	2.03	0.41
1:B:22:TYR:HB2	1:B:52:ALA:HB2	2.03	0.41
1:B:104:LEU:HB2	1:B:105:PHE:CE2	2.56	0.41
1:B:127:ILE:HG22	1:B:129:SER:H	1.86	0.41
1:B:147:GLY:O	1:B:319:GLY:HA2	2.20	0.41
1:A:164:ARG:HH21	1:A:418:ARG:CZ	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:82:ALA:HA	2:C:85:LEU:HD12	2.03	0.41
1:B:206:GLN:HB3	1:B:207:PRO:HD2	2.03	0.41
1:B:351:ILE:O	1:B:362:THR:HA	2.21	0.41
1:B:380:HIS:N	1:B:383:HIS:HD2	2.18	0.41
2:C:97:ASN:HB3	2:C:101:ARG:HH12	1.86	0.41
1:B:148:PRO:HA	1:B:320:GLY:H	1.86	0.41
1:B:128:ARG:HB3	1:B:128:ARG:HH11	1.85	0.40
2:F:30:LEU:CA	2:F:33:THR:HG22	2.28	0.40
2:D:71:MET:HA	2:D:74:ARG:CD	2.51	0.40
1:B:468:THR:O	1:B:469:MET:HB2	2.21	0.40
1:A:219:ALA:HB2	1:A:257:LEU:HD13	2.04	0.40
1:B:42:GLN:OE1	1:B:43:PRO:HD2	2.21	0.40
1:B:316:ARG:HG2	1:B:365:TRP:CH2	2.56	0.40
1:B:380:HIS:H	1:B:383:HIS:CD2	2.39	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	436/472 (92%)	404 (93%)	26 (6%)	6 (1%)	9	39
1	B	430/472 (91%)	389 (90%)	36 (8%)	5 (1%)	10	42
2	C	113/155 (73%)	108 (96%)	5 (4%)	0	100	100
2	D	105/155 (68%)	98 (93%)	4 (4%)	3 (3%)	3	24
2	E	112/155 (72%)	109 (97%)	3 (3%)	0	100	100
2	F	104/155 (67%)	101 (97%)	3 (3%)	0	100	100
All	All	1300/1564 (83%)	1209 (93%)	77 (6%)	14 (1%)	11	43

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ASP
1	A	174	LYS
1	A	209	GLN
1	A	333	GLU
1	B	152	ILE
1	A	74	MET
2	D	49	VAL
1	B	209	GLN
1	B	377	GLY
1	B	174	LYS
2	D	2	ASN
2	D	50	GLN
1	B	119	GLY
1	A	152	ILE

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	344/383 (90%)	309 (90%)	35 (10%)	7	29
1	B	337/383 (88%)	303 (90%)	34 (10%)	7	30
2	C	86/137 (63%)	84 (98%)	2 (2%)	44	70
2	D	76/137 (56%)	68 (90%)	8 (10%)	6	28
2	E	84/137 (61%)	83 (99%)	1 (1%)	63	79
2	F	75/137 (55%)	68 (91%)	7 (9%)	8	33
All	All	1002/1314 (76%)	915 (91%)	87 (9%)	9	36

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	27	THR
1	A	38	ARG
1	A	75	ASP
1	A	78	LYS

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Mol	Chain	Res	Type
1	A	91	GLU
1	A	93	SER
1	A	104	LEU
1	A	110	VAL
1	A	129	SER
1	A	131	ARG
1	A	139	VAL
1	A	143	LYS
1	A	164	ARG
1	A	170	THR
1	A	175	LEU
1	A	191	ARG
1	A	197	THR
1	A	210	ARG
1	A	255	LYS
1	A	279	LYS
1	A	282	ARG
1	A	292	ARG
1	A	316	ARG
1	A	327	THR
1	A	329	VAL
1	A	340	LEU
1	A	347	ARG
1	A	381	VAL
1	A	389	GLU
1	A	443	ARG
1	A	449	SER
1	A	451	GLU
1	A	457	ASP
1	A	465	GLU
2	C	53	GLU
2	C	70	ILE
2	D	3	LEU
2	D	14	LEU
2	D	15	GLN
2	D	27	LEU
2	D	49	VAL
2	D	60	PHE
2	D	69	ARG
2	D	72	THR
1	B	20	THR
1	B	27	THR

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Mol	Chain	Res	Type
1	B	38	ARG
1	B	75	ASP
1	B	78	LYS
1	B	91	GLU
1	B	93	SER
1	B	110	VAL
1	B	128	ARG
1	B	131	ARG
1	B	139	VAL
1	B	143	LYS
1	B	164	ARG
1	B	169	CYS
1	B	175	LEU
1	B	191	ARG
1	B	197	THR
1	B	198	LYS
1	B	202	ASN
1	B	203	ILE
1	B	209	GLN
1	B	210	ARG
1	B	216	LEU
1	B	279	LYS
1	B	282	ARG
1	B	292	ARG
1	B	316	ARG
1	B	327	THR
1	B	328	VAL
1	B	347	ARG
1	B	361	PHE
1	B	418	ARG
1	B	449	SER
1	B	451	GLU
2	E	70	ILE
2	F	27	LEU
2	F	32	GLU
2	F	60	PHE
2	F	66	LEU
2	F	69	ARG
2	F	74	ARG
2	F	94	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	204	ASN
1	A	226	GLN
1	A	235	HIS
1	A	238	ASN
1	A	274	ASN
1	A	291	HIS
1	A	350	HIS
1	A	380	HIS
1	A	383	HIS
1	A	398	GLN
1	A	417	ASN
1	A	426	GLN
2	C	21	GLN
2	C	50	GLN
2	D	42	HIS
1	B	92	ASN
1	B	209	GLN
1	B	238	ASN
1	B	350	HIS
1	B	380	HIS
1	B	383	HIS
1	B	417	ASN
2	E	2	ASN
2	E	21	GLN
2	E	50	GLN
2	E	94	GLN
2	F	15	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	442/472 (93%)	-0.19	9 (2%) 65 45	36, 61, 94, 148	0
1	B	438/472 (92%)	-0.23	4 (0%) 81 64	36, 60, 94, 148	0
2	C	115/155 (74%)	1.22	22 (19%) 3 2	70, 162, 220, 229	2 (1%)
2	D	107/155 (69%)	0.49	10 (9%) 14 9	44, 111, 202, 252	2 (1%)
2	E	114/155 (73%)	1.11	17 (14%) 5 4	72, 160, 226, 236	2 (1%)
2	F	106/155 (68%)	0.44	7 (6%) 24 15	41, 102, 194, 249	2 (1%)
All	All	1322/1564 (84%)	0.14	69 (5%) 33 21	36, 75, 190, 252	8 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	29	GLN	9.4
2	E	29	GLN	9.3
2	C	16	SER	9.3
2	C	29	GLN	8.6
2	F	29	GLN	8.0
2	E	16	SER	6.8
2	D	89	VAL	4.7
2	C	49	VAL	4.1
2	F	1	MET	4.0
1	A	175	LEU	3.9
2	D	107	ARG	3.7
2	F	106	GLU	3.7
1	A	176	GLY	3.7
2	C	65	ASP	3.5
2	D	103	GLN	3.5
2	C	115	HIS	3.5
2	C	28	ALA	3.4
2	E	113	LEU	3.4
1	B	175	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	1	MET	3.3
2	F	105	LEU	3.1
2	E	106	GLU	3.1
2	E	28	ALA	3.1
2	E	39	LEU	3.1
2	F	89	VAL	3.1
2	D	1	MET	3.0
2	C	113	LEU	2.9
2	C	66	LEU	2.9
1	A	334	GLY	2.9
1	B	405	GLY	2.9
2	D	105	LEU	2.9
2	E	115	HIS	2.8
2	C	68	LEU	2.7
1	A	333	GLU	2.7
1	A	405	GLY	2.7
2	F	87	GLU	2.7
2	D	106	GLU	2.6
2	E	68	LEU	2.6
2	E	37	LEU	2.6
1	A	459	TRP	2.5
2	C	37	LEU	2.5
2	C	26	VAL	2.4
2	E	57	GLU	2.4
1	A	465	GLU	2.3
2	E	49	VAL	2.3
2	E	25	THR	2.3
2	C	83	GLU	2.3
2	C	25	THR	2.3
2	E	33	THR	2.3
2	D	3	LEU	2.2
1	A	382	TRP	2.1
2	E	20	TYR	2.1
2	C	111	VAL	2.1
2	F	104	HIS	2.1
2	C	30	LEU	2.1
2	C	82	ALA	2.1
1	B	71	LEU	2.1
1	B	75	ASP	2.1
2	C	59	LEU	2.1
2	E	21	GLN	2.1
2	E	56	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	39	LEU	2.0
2	D	7	ALA	2.0
2	C	50	GLN	2.0
2	D	83	GLU	2.0
1	A	332	LEU	2.0
2	E	66	LEU	2.0
2	C	78	ALA	2.0
2	C	18	LEU	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.