



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:22 AM UTC

PDB ID : 2JAA / pdb_00002jaa
Title : SeMet substituted Shigella Flexneri Ipad
Authors : Johnson, S.; Roversi, P.; Espina, M.; Olive, A.; Deane, J.E.; Birket, S.; Field, T.; Picking, W.D.; Blocker, A.J.; Galyov, E.E.; Picking, W.L.; Lea, S.M.
Deposited on : 2006-11-24
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

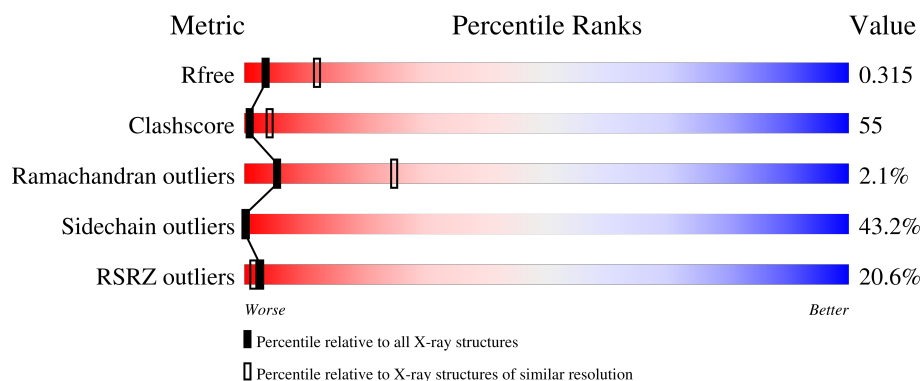
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	212	
1	B	212	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2767 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 INVASIN IPAD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	Se	0	0	0
			1322	837	220	260	5			
1	B	182	Total	C	N	O	Se	0	0	0
			1437	908	239	285	5			

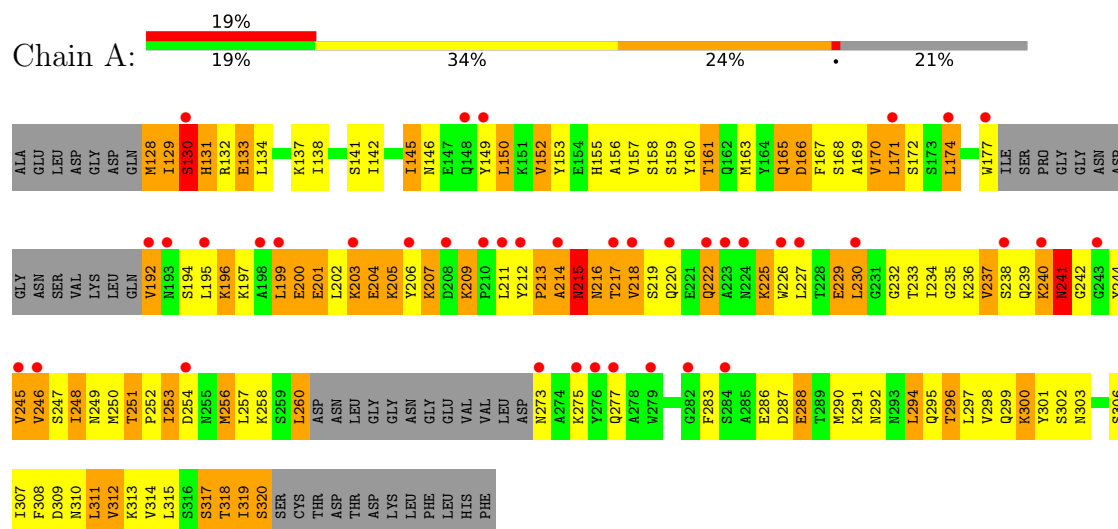
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	B	5	Total	O	0	0
			5	5		

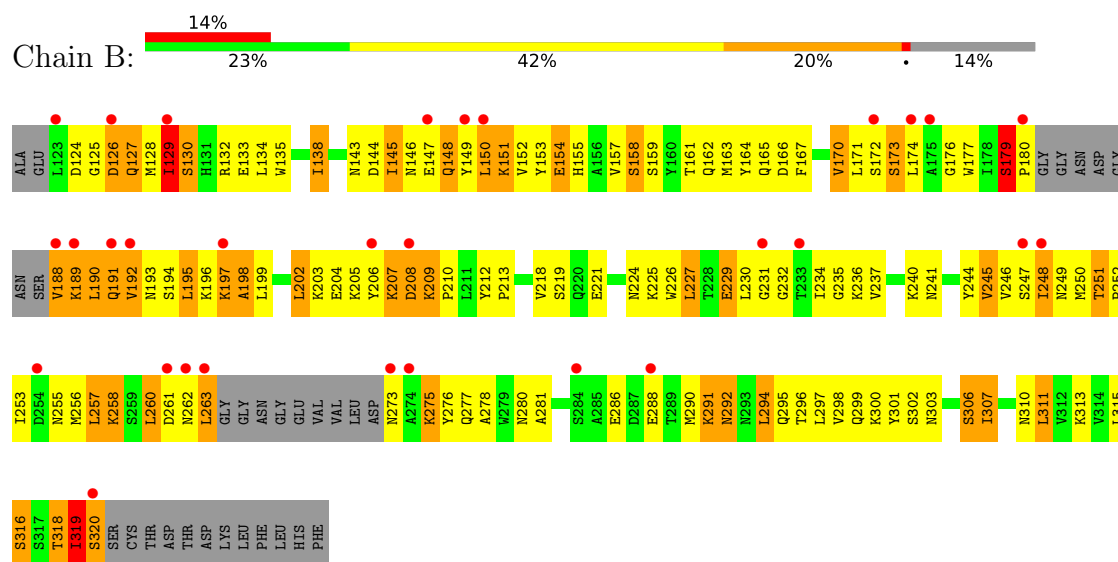
3 Residue-property plots [i](#)

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: INVASIN IPAD



• Molecule 1: INVASIN IPAD



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.84Å 44.48Å 100.31Å 90.00° 107.96° 90.00°	Depositor
Resolution (Å)	34.00 – 3.10 34.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (34.00-3.10) 99.4 (34.00-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 3.12Å)	Xtriage
Refinement program	TNT 5.6.1	Depositor
R, R_{free}	0.262 , 0.276 0.294 , 0.315	Depositor DCC
R_{free} test set	545 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	74.4	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 76.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	2767	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.49% 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	0.32	0/1340	0.74	2/1803 (0.1%)
1	B	0.26	0/1455	0.74	3/1958 (0.2%)
All	All	0.29	0/2795	0.74	5/3761 (0.1%)

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	A	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	215	ASN	N-CA-C	-8.78	92.11	110.80
1	B	151	LYS	N-CA-C	-7.42	103.69	112.89
1	B	198	ALA	N-CA-C	-5.56	107.14	114.04
1	A	218	VAL	N-CA-C	5.41	120.58	109.34
1	B	179	SER	N-CA-C	5.23	112.93	108.22

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	PRO	Peptide
1	A	214	ALA	Peptide

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	1322	0	1310	185	0
1	B	1437	0	1425	136	0
2	A	3	0	0	1	0
2	B	5	0	0	0	0
All	All	2767	0	2735	303	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 55.

All (303) 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:B:195:LEU:HD13	1:B:260:LEU:HD21	1.32	1.07
1:A:318:THR:HG22	1:A:319:ILE:HG13	1.35	1.07
1:A:319:ILE:HG22	1:A:320:SER:HB2	1.47	0.95
1:A:219:SER:HB2	1:A:222:GLN:HB2	1.50	0.94
1:A:163:MSE:HA	1:A:206:TYR:CE2	2.03	0.94
1:A:206:TYR:HA	1:A:209:LYS:HG3	1.50	0.94
1:A:129:ILE:HG23	1:B:129:ILE:HD13	1.50	0.92
1:A:153:TYR:HB3	1:A:301:TYR:HD2	1.39	0.87
1:B:190:LEU:HD21	1:B:192:VAL:HG12	1.59	0.85
1:B:124:ASP:N	1:B:125:GLY:HA2	1.91	0.84
1:B:190:LEU:CD2	1:B:192:VAL:HG12	2.07	0.84
1:B:294:LEU:HD22	1:B:298:VAL:HG23	1.61	0.83
1:A:220:GLN:HG3	1:A:244:TYR:CD2	2.13	0.83
1:A:153:TYR:HB3	1:A:301:TYR:CD2	2.15	0.82
1:A:129:ILE:HG23	1:B:129:ILE:CD1	2.10	0.81
1:A:203:LYS:HG3	1:A:253:ILE:HG21	1.61	0.80
1:A:311:LEU:HD11	1:B:310:ASN:CB	2.11	0.80
1:B:177:TRP:HB3	1:B:191:GLN:HG2	1.63	0.80
1:A:152:VAL:HG11	1:A:226:TRP:CZ2	2.18	0.79
1:B:251:THR:HG22	1:B:252:PRO:HD3	1.63	0.78
1:B:236:LYS:HD3	1:B:249:ASN:HA	1.64	0.78
1:A:146:ASN:HA	1:A:150:LEU:HB2	1.67	0.77
1:A:227:LEU:CD2	1:A:232:GLY:HA2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HD12	1:A:195:LEU:CD1	2.15	0.76
1:A:131:HIS:HB2	1:B:128:MSE:H	1.51	0.76
1:B:177:TRP:HB3	1:B:191:GLN:CG	2.16	0.76
1:A:174:LEU:HA	1:A:177:TRP:CE3	2.21	0.75
1:B:256:MSE:O	1:B:260:LEU:HB2	1.87	0.74
1:A:227:LEU:HD23	1:A:232:GLY:HA2	1.69	0.74
1:A:318:THR:HG22	1:A:319:ILE:CG1	2.14	0.74
1:A:163:MSE:HE1	1:A:290:MSE:HE2	1.69	0.73
1:A:309:ASP:O	1:A:313:LYS:HG3	1.87	0.73
1:B:315:LEU:O	1:B:318:THR:HG22	1.89	0.72
1:A:159:SER:HB2	1:A:211:LEU:HD23	1.72	0.72
1:B:196:LYS:HB3	1:B:260:LEU:HD23	1.70	0.71
1:A:311:LEU:HD11	1:B:310:ASN:HB2	1.71	0.71
1:A:319:ILE:HG22	1:A:320:SER:CB	2.20	0.71
1:B:292:ASN:O	1:B:296:THR:HG23	1.90	0.71
1:A:195:LEU:HD22	1:A:260:LEU:HD21	1.73	0.71
1:B:195:LEU:HD13	1:B:260:LEU:CD2	2.14	0.71
1:B:227:LEU:HD22	1:B:232:GLY:HA2	1.74	0.70
1:B:129:ILE:HD12	1:B:129:ILE:H	1.56	0.69
1:A:310:ASN:O	1:A:314:VAL:HG23	1.93	0.69
1:B:126:ASP:HA	1:B:127:GLN:NE2	2.07	0.69
1:A:256:MSE:HE2	1:A:283:PHE:HD2	1.58	0.69
1:A:129:ILE:CG2	1:B:129:ILE:HD13	2.22	0.68
1:A:192:VAL:O	1:A:196:LYS:HB3	1.93	0.68
1:A:310:ASN:HB2	1:B:307:ILE:HD12	1.74	0.68
1:A:128:MSE:HA	1:B:130:SER:HA	1.75	0.68
1:A:307:ILE:HD13	1:B:306:SER:HB2	1.75	0.68
1:A:149:TYR:CE1	1:A:153:TYR:HE2	2.11	0.68
1:A:236:LYS:HD3	1:A:249:ASN:HA	1.76	0.68
1:B:213:PRO:HG3	1:B:218:VAL:HG13	1.74	0.67
1:B:205:LYS:HD3	1:B:206:TYR:CE2	2.30	0.67
1:B:227:LEU:HD21	1:B:235:GLY:O	1.95	0.67
1:B:164:TYR:OH	1:B:291:LYS:HD2	1.95	0.66
1:A:252:PRO:HG2	1:A:290:MSE:HE3	1.77	0.66
1:B:129:ILE:O	1:B:130:SER:HB2	1.95	0.66
1:A:227:LEU:HD12	1:A:237:VAL:HG12	1.78	0.65
1:A:174:LEU:HD12	1:A:195:LEU:HD11	1.78	0.65
1:A:227:LEU:HD23	1:A:227:LEU:O	1.96	0.65
1:A:313:LYS:NZ	2:A:2003:HOH:O	2.30	0.65
1:A:318:THR:CG2	1:A:319:ILE:HG13	2.20	0.65
1:A:319:ILE:CG2	1:A:320:SER:HB2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:HD11	1:A:206:TYR:HE2	1.61	0.64
1:A:163:MSE:CE	1:A:290:MSE:HE2	2.27	0.64
1:B:149:TYR:O	1:B:152:VAL:HB	1.98	0.64
1:B:199:LEU:HB2	1:B:257:LEU:HD11	1.80	0.63
1:A:157:VAL:HG22	1:A:297:LEU:HG	1.79	0.63
1:A:166:ASP:HB3	1:A:202:LEU:HD11	1.80	0.63
1:A:251:THR:N	1:A:252:PRO:HD2	2.14	0.63
1:A:252:PRO:HA	1:A:286:GLU:OE1	1.98	0.63
1:A:252:PRO:O	1:A:256:MSE:HG2	1.98	0.63
1:A:236:LYS:CD	1:A:249:ASN:HA	2.28	0.63
1:A:256:MSE:HE2	1:A:283:PHE:CD2	2.34	0.63
1:A:215:ASN:O	1:A:216:ASN:HB2	1.99	0.62
1:A:213:PRO:HG2	1:A:218:VAL:HG13	1.81	0.62
1:B:203:LYS:HA	1:B:250:MSE:HE3	1.80	0.62
1:A:239:GLN:CD	1:A:239:GLN:H	2.08	0.62
1:A:313:LYS:O	1:A:317:SER:HB3	2.00	0.62
1:B:199:LEU:CD1	1:B:260:LEU:HD22	2.30	0.61
1:A:252:PRO:CG	1:A:290:MSE:HE3	2.30	0.61
1:A:195:LEU:CD2	1:A:260:LEU:HD21	2.30	0.61
1:B:195:LEU:CD1	1:B:260:LEU:HD21	2.21	0.61
1:A:157:VAL:O	1:A:161:THR:HB	2.00	0.61
1:A:319:ILE:HA	1:A:320:SER:CB	2.31	0.61
1:B:196:LYS:NZ	1:B:261:ASP:OD1	2.30	0.60
1:A:196:LYS:HG3	1:A:196:LYS:O	2.01	0.60
1:A:202:LEU:HD11	1:A:206:TYR:CE2	2.37	0.60
1:A:163:MSE:SE	1:A:290:MSE:HE2	2.52	0.60
1:B:129:ILE:HD12	1:B:129:ILE:N	2.16	0.60
1:B:234:ILE:HD12	1:B:234:ILE:H	1.65	0.60
1:A:203:LYS:HG3	1:A:253:ILE:CG2	2.31	0.59
1:A:236:LYS:HD3	1:A:249:ASN:OD1	2.02	0.59
1:A:318:THR:C	1:A:319:ILE:HG13	2.26	0.59
1:A:257:LEU:HD12	1:A:258:LYS:N	2.17	0.59
1:A:174:LEU:HD12	1:A:195:LEU:HD12	1.84	0.59
1:A:166:ASP:HB3	1:A:202:LEU:CD1	2.32	0.59
1:A:234:ILE:HD12	1:A:234:ILE:N	2.17	0.59
1:B:152:VAL:HG11	1:B:226:TRP:CZ2	2.38	0.59
1:B:231:GLY:HA3	1:B:234:ILE:CD1	2.33	0.59
1:A:300:LYS:HB2	1:A:300:LYS:NZ	2.17	0.59
1:A:236:LYS:HG2	1:A:249:ASN:HA	1.84	0.59
1:B:218:VAL:O	1:B:244:TYR:HB2	2.03	0.58
1:B:234:ILE:HD12	1:B:234:ILE:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ILE:HG22	1:B:133:GLU:HB3	1.86	0.57
1:B:177:TRP:O	1:B:190:LEU:HA	2.05	0.57
1:A:310:ASN:HB2	1:B:307:ILE:CD1	2.34	0.57
1:B:277:GLN:O	1:B:281:ALA:HB2	2.04	0.57
1:A:196:LYS:HA	1:A:260:LEU:HD23	1.87	0.56
1:A:203:LYS:O	1:A:207:LYS:HB3	2.05	0.56
1:A:233:THR:HG23	1:A:234:ILE:HD12	1.86	0.56
1:A:163:MSE:HA	1:A:206:TYR:CD2	2.40	0.56
1:A:196:LYS:HE2	1:A:260:LEU:O	2.05	0.56
1:A:254:ASP:HA	1:A:257:LEU:CD2	2.36	0.56
1:B:179:SER:O	1:B:189:LYS:N	2.37	0.56
1:A:218:VAL:HG23	1:A:244:TYR:O	2.06	0.56
1:B:127:GLN:O	1:B:128:MSE:HB2	2.05	0.56
1:A:195:LEU:C	1:A:195:LEU:HD23	2.30	0.56
1:A:303:ASN:O	1:A:307:ILE:HG13	2.05	0.55
1:B:213:PRO:HD2	1:B:245:VAL:HB	1.88	0.55
1:A:288:GLU:OE1	1:A:288:GLU:HA	2.06	0.55
1:B:154:GLU:HG3	1:B:155:HIS:N	2.20	0.55
1:A:253:ILE:HA	1:A:256:MSE:HG3	1.88	0.55
1:B:199:LEU:HD12	1:B:260:LEU:HD22	1.89	0.55
1:A:149:TYR:CZ	1:A:153:TYR:HE2	2.25	0.54
1:A:153:TYR:CE1	1:A:300:LYS:HG3	2.43	0.54
1:A:226:TRP:CZ3	1:A:229:GLU:HG2	2.42	0.54
1:A:254:ASP:HA	1:A:257:LEU:HD21	1.89	0.54
1:A:254:ASP:O	1:A:257:LEU:HG	2.08	0.54
1:A:132:ARG:NH1	1:B:126:ASP:HB2	2.23	0.53
1:A:257:LEU:HD12	1:A:257:LEU:C	2.33	0.53
1:A:156:ALA:HA	1:A:211:LEU:HD22	1.89	0.53
1:A:163:MSE:CE	1:A:248:ILE:HD11	2.38	0.53
1:A:220:GLN:CD	1:A:220:GLN:H	2.16	0.53
1:A:219:SER:CB	1:A:222:GLN:HB2	2.33	0.53
1:A:250:MSE:C	1:A:252:PRO:HD2	2.34	0.53
1:A:152:VAL:HG11	1:A:226:TRP:CE2	2.44	0.52
1:A:236:LYS:CG	1:A:249:ASN:HA	2.40	0.52
1:B:263:LEU:HG	1:B:275:LYS:NZ	2.25	0.52
1:A:145:ILE:HG21	1:A:308:PHE:CD1	2.44	0.52
1:B:212:TYR:O	1:B:246:VAL:N	2.39	0.52
1:B:206:TYR:HA	1:B:209:LYS:HG3	1.92	0.52
1:B:244:TYR:C	1:B:245:VAL:HG12	2.35	0.51
1:A:311:LEU:HD11	1:B:310:ASN:HB3	1.88	0.51
1:B:199:LEU:HD13	1:B:257:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:GLU:O	1:B:225:LYS:HG2	2.10	0.51
1:B:231:GLY:HA3	1:B:234:ILE:HD11	1.93	0.51
1:A:142:ILE:HG12	1:A:312:VAL:HG23	1.91	0.51
1:A:167:PHE:HA	1:A:170:VAL:HG23	1.91	0.51
1:B:195:LEU:O	1:B:198:ALA:HB3	2.11	0.51
1:A:196:LYS:HB2	1:A:260:LEU:HD23	1.91	0.51
1:B:235:GLY:HA2	1:B:249:ASN:H	1.75	0.51
1:A:170:VAL:HG11	1:A:199:LEU:HD23	1.93	0.51
1:A:213:PRO:CG	1:A:218:VAL:HG13	2.40	0.51
1:A:248:ILE:HD13	1:A:248:ILE:O	2.11	0.51
1:A:174:LEU:O	1:A:174:LEU:HG	2.11	0.50
1:B:188:VAL:HG12	1:B:188:VAL:O	2.11	0.50
1:A:196:LYS:HE2	1:A:260:LEU:HB3	1.93	0.50
1:B:248:ILE:CD1	1:B:250:MSE:SE	3.10	0.50
1:B:179:SER:O	1:B:188:VAL:HA	2.12	0.50
1:B:196:LYS:C	1:B:198:ALA:H	2.18	0.50
1:A:152:VAL:HG22	1:A:212:TYR:CD2	2.46	0.50
1:A:310:ASN:CB	1:B:307:ILE:HD12	2.40	0.50
1:B:150:LEU:O	1:B:154:GLU:HB3	2.12	0.50
1:B:177:TRP:HB3	1:B:191:GLN:HG3	1.92	0.50
1:A:152:VAL:HG22	1:A:212:TYR:CE2	2.47	0.50
1:A:192:VAL:O	1:A:192:VAL:HG23	2.11	0.50
1:A:248:ILE:HD13	1:A:248:ILE:C	2.37	0.50
1:B:229:GLU:OE1	1:B:229:GLU:HA	2.11	0.50
1:A:160:TYR:HD2	1:A:294:LEU:HD23	1.76	0.50
1:B:288:GLU:OE1	1:B:288:GLU:HA	2.11	0.50
1:A:246:VAL:HG12	1:A:246:VAL:O	2.11	0.49
1:B:152:VAL:HG11	1:B:226:TRP:CE2	2.47	0.49
1:A:220:GLN:HG3	1:A:244:TYR:HD2	1.72	0.49
1:A:226:TRP:O	1:A:230:LEU:HD22	2.12	0.49
1:B:138:ILE:HB	1:B:315:LEU:HD13	1.94	0.49
1:A:245:VAL:HG23	1:A:246:VAL:N	2.26	0.49
1:B:192:VAL:O	1:B:196:LYS:HG2	2.12	0.49
1:A:239:GLN:HB3	1:A:244:TYR:CE1	2.46	0.49
1:B:248:ILE:C	1:B:248:ILE:HD13	2.37	0.49
1:A:233:THR:CG2	1:A:234:ILE:HD12	2.43	0.49
1:A:309:ASP:O	1:A:312:VAL:HG12	2.13	0.49
1:B:251:THR:O	1:B:255:ASN:OD1	2.31	0.49
1:B:316:SER:C	1:B:318:THR:H	2.21	0.49
1:A:166:ASP:O	1:A:169:ALA:HB3	2.13	0.48
1:A:205:LYS:HE3	1:A:206:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:C	1:A:174:LEU:HD23	2.39	0.48
1:B:230:LEU:O	1:B:234:ILE:HD13	2.13	0.48
1:A:134:LEU:O	1:A:137:LYS:HB2	2.13	0.48
1:B:197:LYS:HD2	1:B:197:LYS:HA	1.48	0.48
1:A:251:THR:N	1:A:252:PRO:CD	2.77	0.48
1:B:192:VAL:O	1:B:196:LYS:HE2	2.13	0.48
1:A:195:LEU:HD23	1:A:199:LEU:HG	1.95	0.48
1:B:255:ASN:ND2	1:B:286:GLU:OE2	2.47	0.48
1:A:130:SER:OG	1:A:133:GLU:HB2	2.13	0.47
1:A:253:ILE:HD13	1:A:290:MSE:HE1	1.96	0.47
1:A:152:VAL:HG12	1:A:153:TYR:N	2.29	0.47
1:A:292:ASN:O	1:A:296:THR:HG23	2.14	0.47
1:A:129:ILE:CG1	1:A:130:SER:N	2.77	0.47
1:B:143:ASN:O	1:B:147:GLU:HG2	2.14	0.47
1:A:294:LEU:O	1:A:298:VAL:HG23	2.15	0.47
1:B:170:VAL:HA	1:B:173:SER:OG	2.15	0.47
1:A:153:TYR:CB	1:A:301:TYR:HD2	2.20	0.47
1:A:277:GLN:HA	1:A:277:GLN:OE1	2.14	0.47
1:B:226:TRP:O	1:B:230:LEU:HG	2.14	0.47
1:B:303:ASN:O	1:B:307:ILE:HG12	2.15	0.47
1:B:319:ILE:HA	1:B:320:SER:HA	1.73	0.47
1:B:263:LEU:HG	1:B:275:LYS:HZ1	1.79	0.47
1:B:199:LEU:HD12	1:B:260:LEU:CD2	2.45	0.46
1:A:235:GLY:HA2	1:A:249:ASN:H	1.81	0.46
1:B:230:LEU:C	1:B:234:ILE:HD13	2.40	0.46
1:B:258:LYS:O	1:B:262:ASN:OD1	2.33	0.46
1:A:174:LEU:HA	1:A:177:TRP:CD2	2.49	0.46
1:B:144:ASP:O	1:B:148:GLN:HB2	2.14	0.46
1:A:253:ILE:CD1	1:A:290:MSE:HE1	2.46	0.45
1:B:210:PRO:HB3	1:B:245:VAL:CG2	2.46	0.45
1:B:234:ILE:O	1:B:249:ASN:HB3	2.17	0.45
1:B:318:THR:O	1:B:318:THR:HG23	2.15	0.45
1:B:202:LEU:HD23	1:B:202:LEU:HA	1.76	0.45
1:B:286:GLU:HA	1:B:286:GLU:OE1	2.16	0.45
1:A:227:LEU:CD1	1:A:237:VAL:HG12	2.44	0.45
1:A:236:LYS:HD3	1:A:249:ASN:CG	2.40	0.45
1:B:248:ILE:HD13	1:B:248:ILE:O	2.17	0.45
1:B:127:GLN:N	1:B:127:GLN:CD	2.73	0.45
1:B:294:LEU:HD22	1:B:298:VAL:CG2	2.39	0.45
1:A:132:ARG:HG3	1:B:126:ASP:CG	2.41	0.45
1:B:129:ILE:HB	1:B:130:SER:H	1.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LYS:O	1:A:241:ASN:OD1	2.35	0.45
1:A:312:VAL:CG1	1:A:313:LYS:N	2.80	0.45
1:B:166:ASP:CB	1:B:202:LEU:HD21	2.47	0.45
1:A:170:VAL:O	1:A:174:LEU:HB3	2.17	0.44
1:A:307:ILE:HA	1:B:307:ILE:HD11	1.99	0.44
1:B:157:VAL:HG22	1:B:297:LEU:HG	1.99	0.44
1:A:156:ALA:HA	1:A:211:LEU:CD2	2.47	0.44
1:A:165:GLN:OE1	1:A:165:GLN:HA	2.11	0.44
1:A:199:LEU:O	1:A:203:LYS:HB2	2.17	0.44
1:B:173:SER:HB2	1:B:177:TRP:CZ2	2.53	0.44
1:B:135:TRP:CZ2	1:B:319:ILE:CG2	3.00	0.44
1:A:207:LYS:HB2	1:A:207:LYS:HE2	1.56	0.44
1:B:225:LYS:HA	1:B:225:LYS:HD3	1.75	0.44
1:A:220:GLN:C	1:A:222:GLN:H	2.24	0.44
1:A:319:ILE:CA	1:A:320:SER:CB	2.96	0.44
1:B:166:ASP:HB3	1:B:202:LEU:HD21	2.00	0.44
1:A:227:LEU:HD23	1:A:227:LEU:C	2.43	0.44
1:A:145:ILE:HG21	1:A:308:PHE:HD1	1.83	0.44
1:B:205:LYS:HD3	1:B:206:TYR:HE2	1.80	0.44
1:B:202:LEU:HD22	1:B:206:TYR:CE2	2.53	0.43
1:A:256:MSE:CE	1:A:283:PHE:CD2	3.00	0.43
1:A:300:LYS:HB2	1:A:300:LYS:HZ2	1.83	0.43
1:B:240:LYS:HB3	1:B:245:VAL:CG1	2.49	0.43
1:A:300:LYS:NZ	1:A:300:LYS:CB	2.79	0.43
1:B:318:THR:CG2	1:B:319:ILE:HG12	2.48	0.43
1:B:174:LEU:C	1:B:176:GLY:H	2.27	0.43
1:A:256:MSE:HE3	1:A:286:GLU:HB2	2.01	0.43
1:B:191:GLN:C	1:B:193:ASN:H	2.27	0.43
1:A:200:GLU:O	1:A:204:GLU:OE2	2.36	0.43
1:A:273:ASN:O	1:A:277:GLN:N	2.41	0.43
1:B:252:PRO:O	1:B:256:MSE:HG3	2.19	0.43
1:A:152:VAL:CG2	1:A:212:TYR:CE2	3.01	0.43
1:A:217:THR:C	1:A:218:VAL:HG13	2.44	0.43
1:B:171:LEU:HD23	1:B:171:LEU:HA	1.90	0.42
1:B:278:ALA:O	1:B:281:ALA:HB3	2.19	0.42
1:A:219:SER:HB2	1:A:222:GLN:CB	2.36	0.42
1:A:234:ILE:N	1:A:234:ILE:CD1	2.80	0.42
1:B:166:ASP:OD2	1:B:205:LYS:HE2	2.19	0.42
1:A:171:LEU:HD23	1:A:172:SER:N	2.35	0.42
1:A:177:TRP:CZ3	1:A:195:LEU:HA	2.55	0.42
1:A:201:GLU:HA	1:A:201:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ILE:O	1:B:149:TYR:N	2.47	0.42
1:A:319:ILE:CA	1:A:320:SER:HB2	2.50	0.42
1:A:225:LYS:H	1:A:225:LYS:HG2	1.44	0.42
1:B:179:SER:HA	1:B:180:PRO:HD3	1.77	0.42
1:A:130:SER:O	1:A:131:HIS:HB2	2.20	0.42
1:B:124:ASP:N	1:B:125:GLY:CA	2.73	0.42
1:B:318:THR:HG22	1:B:319:ILE:CG1	2.50	0.42
1:A:149:TYR:CE1	1:A:153:TYR:CE2	3.01	0.41
1:B:263:LEU:HD23	1:B:263:LEU:HA	1.75	0.41
1:A:153:TYR:HE1	1:A:300:LYS:HG3	1.84	0.41
1:A:314:VAL:HG11	1:B:311:LEU:HD11	2.02	0.41
1:A:174:LEU:CD1	1:A:195:LEU:HD11	2.49	0.41
1:A:196:LYS:CA	1:A:260:LEU:HD23	2.50	0.41
1:A:163:MSE:HE1	1:A:290:MSE:CE	2.45	0.41
1:A:307:ILE:HD13	1:B:306:SER:CB	2.47	0.41
1:B:206:TYR:HB2	1:B:250:MSE:HE2	2.02	0.41
1:A:163:MSE:HG2	1:A:206:TYR:CD2	2.55	0.41
1:B:167:PHE:O	1:B:170:VAL:HG12	2.20	0.41
1:A:156:ALA:CA	1:A:211:LEU:HD22	2.48	0.41
1:A:174:LEU:CA	1:A:177:TRP:CE3	3.00	0.41
1:B:191:GLN:HG2	1:B:191:GLN:H	1.42	0.41
1:B:207:LYS:HD2	1:B:208:ASP:OD2	2.20	0.41
1:A:155:HIS:CD2	1:A:214:ALA:HB2	2.55	0.41
1:A:145:ILE:CG2	1:A:308:PHE:CD1	3.04	0.41
1:B:158:SER:O	1:B:162:GLN:HG3	2.21	0.41
1:B:163:MSE:SE	1:B:163:MSE:C	3.14	0.41
1:A:132:ARG:HG3	1:B:126:ASP:OD1	2.22	0.40
1:B:163:MSE:HE2	1:B:248:ILE:HD11	2.03	0.40
1:B:167:PHE:CE1	1:B:290:MSE:HE1	2.56	0.40
1:A:142:ILE:CD1	1:A:312:VAL:CG2	3.00	0.40
1:A:220:GLN:C	1:A:222:GLN:N	2.80	0.40
1:A:240:LYS:C	1:A:242:GLY:N	2.79	0.40
1:A:300:LYS:HB2	1:A:300:LYS:HZ3	1.85	0.40
1:B:153:TYR:HB3	1:B:301:TYR:CD2	2.57	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	161/212 (76%)	141 (88%)	16 (10%)	4 (2%)	4	21
1	B	176/212 (83%)	154 (88%)	19 (11%)	3 (2%)	7	30
All	All	337/424 (80%)	295 (88%)	35 (10%)	7 (2%)	5	25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	ASN
1	A	216	ASN
1	B	130	SER
1	B	319	ILE
1	A	130	SER
1	A	241	ASN
1	B	129	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	147/179 (82%)	81 (55%)	66 (45%)	0	0
1	B	161/179 (90%)	94 (58%)	67 (42%)	0	0
All	All	308/358 (86%)	175 (57%)	133 (43%)	0	0

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	MSE
1	A	129	ILE
1	A	130	SER
1	A	131	HIS
1	A	133	GLU
1	A	138	ILE
1	A	141	SER
1	A	145	ILE
1	A	150	LEU
1	A	152	VAL
1	A	158	SER
1	A	161	THR
1	A	165	GLN
1	A	166	ASP
1	A	168	SER
1	A	170	VAL
1	A	171	LEU
1	A	174	LEU
1	A	192	VAL
1	A	194	SER
1	A	196	LYS
1	A	197	LYS
1	A	199	LEU
1	A	200	GLU
1	A	201	GLU
1	A	203	LYS
1	A	204	GLU
1	A	205	LYS
1	A	207	LYS
1	A	209	LYS
1	A	215	ASN
1	A	217	THR
1	A	222	GLN
1	A	225	LYS
1	A	229	GLU
1	A	230	LEU
1	A	237	VAL
1	A	238	SER
1	A	240	LYS
1	A	241	ASN
1	A	245	VAL
1	A	246	VAL
1	A	247	SER

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Mol	Chain	Res	Type
1	A	248	ILE
1	A	251	THR
1	A	253	ILE
1	A	256	MSE
1	A	260	LEU
1	A	275	LYS
1	A	287	ASP
1	A	288	GLU
1	A	291	LYS
1	A	294	LEU
1	A	295	GLN
1	A	296	THR
1	A	299	GLN
1	A	300	LYS
1	A	302	SER
1	A	306	SER
1	A	311	LEU
1	A	312	VAL
1	A	315	LEU
1	A	317	SER
1	A	318	THR
1	A	319	ILE
1	A	320	SER
1	B	126	ASP
1	B	127	GLN
1	B	129	ILE
1	B	132	ARG
1	B	134	LEU
1	B	138	ILE
1	B	145	ILE
1	B	146	ASN
1	B	148	GLN
1	B	150	LEU
1	B	151	LYS
1	B	154	GLU
1	B	158	SER
1	B	159	SER
1	B	161	THR
1	B	165	GLN
1	B	170	VAL
1	B	172	SER
1	B	173	SER

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Mol	Chain	Res	Type
1	B	179	SER
1	B	188	VAL
1	B	189	LYS
1	B	190	LEU
1	B	191	GLN
1	B	192	VAL
1	B	194	SER
1	B	195	LEU
1	B	197	LYS
1	B	202	LEU
1	B	204	GLU
1	B	207	LYS
1	B	208	ASP
1	B	209	LYS
1	B	219	SER
1	B	224	ASN
1	B	227	LEU
1	B	229	GLU
1	B	237	VAL
1	B	241	ASN
1	B	245	VAL
1	B	247	SER
1	B	248	ILE
1	B	251	THR
1	B	253	ILE
1	B	257	LEU
1	B	258	LYS
1	B	260	LEU
1	B	263	LEU
1	B	273	ASN
1	B	275	LYS
1	B	276	TYR
1	B	280	ASN
1	B	291	LYS
1	B	292	ASN
1	B	294	LEU
1	B	295	GLN
1	B	299	GLN
1	B	300	LYS
1	B	302	SER
1	B	306	SER
1	B	307	ILE

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Mol	Chain	Res	Type
1	B	311	LEU
1	B	313	LYS
1	B	316	SER
1	B	318	THR
1	B	319	ILE
1	B	320	SER

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	155	HIS
1	A	222	GLN
1	A	303	ASN
1	B	140	ASN
1	B	215	ASN
1	B	224	ASN
1	B	310	ASN

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	162/212 (76%)	1.32	40 (24%)	2 1	35, 80, 108, 118	0
1	B	177/212 (83%)	1.10	30 (16%)	4 2	28, 65, 101, 130	0
All	All	339/424 (79%)	1.20	70 (20%)	2 1	28, 69, 105, 130	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	LEU	4.9
1	B	180	PRO	4.5
1	A	211	LEU	4.5
1	A	192	VAL	4.4
1	A	238	SER	4.2
1	A	279	TRP	4.1
1	A	275	LYS	3.7
1	B	254	ASP	3.5
1	A	214	ALA	3.5
1	A	284	SER	3.4
1	A	254	ASP	3.4
1	A	246	VAL	3.4
1	B	126	ASP	3.4
1	B	188	VAL	3.3
1	A	217	THR	3.3
1	B	189	LYS	3.2
1	B	150	LEU	3.0
1	B	192	VAL	3.0
1	A	220	GLN	3.0
1	A	226	TRP	2.9
1	A	245	VAL	2.8
1	A	174	LEU	2.8
1	B	208	ASP	2.7
1	A	195	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	274	ALA	2.7
1	B	231	GLY	2.7
1	B	147	GLU	2.6
1	B	233	THR	2.6
1	B	123	LEU	2.6
1	A	212	TYR	2.6
1	B	197	LYS	2.6
1	A	210	PRO	2.6
1	B	149	TYR	2.5
1	A	218	VAL	2.5
1	A	206	TYR	2.5
1	B	273	ASN	2.5
1	A	198	ALA	2.5
1	B	284	SER	2.5
1	A	171	LEU	2.5
1	B	247	SER	2.4
1	B	288	GLU	2.4
1	A	224	ASN	2.4
1	B	320	SER	2.4
1	A	230	LEU	2.3
1	B	191	GLN	2.3
1	B	248	ILE	2.3
1	B	261	ASP	2.3
1	A	222	GLN	2.3
1	A	193	ASN	2.3
1	A	240	LYS	2.3
1	B	129	ILE	2.3
1	A	149	TYR	2.3
1	B	175	ALA	2.3
1	B	172	SER	2.3
1	A	282	GLY	2.2
1	A	227	LEU	2.2
1	A	130	SER	2.2
1	A	177	TRP	2.2
1	A	276	TYR	2.1
1	A	277	GLN	2.1
1	B	262	ASN	2.1
1	A	243	GLY	2.1
1	A	223	ALA	2.1
1	A	273	ASN	2.1
1	A	208	ASP	2.0
1	B	206	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	203	LYS	2.0
1	A	199	LEU	2.0
1	B	174	LEU	2.0
1	A	148	GLN	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.