



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 10:48 AM EDT

PDB ID : 3EE1
Title : Novel fold of VirA, a type III secretion system effector protein from *Shigella flexneri*
Authors : Davis, J.S.
Deposited on : unknown
Resolution : 3.01 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

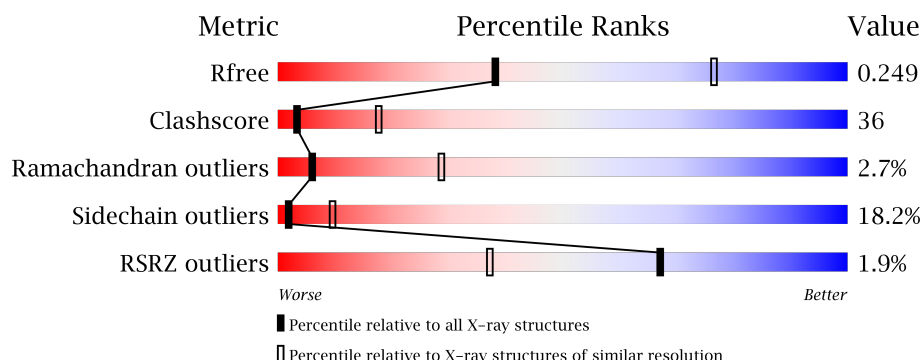
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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}	100719	1924 (3.04-3.00)
Clashscore	112137	2279 (3.04-3.00)
Ramachandran outliers	110173	2207 (3.04-3.00)
Sidechain outliers	110143	2210 (3.04-3.00)
RSRZ outliers	101464	1948 (3.04-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	400	<div> <div>2%</div> <div> <div></div> <div>41%</div> <div>36%</div> <div>8%</div> <div>15%</div> </div> </div>
1	B	400	<div> <div>2%</div> <div> <div></div> <div>40%</div> <div>36%</div> <div>9%</div> <div>15%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5244 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 Effector protein virA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	Se	0	0	0
			2622	1660	439	511	7	5			
1	B	341	Total	C	N	O	S	Se	0	0	0
			2622	1660	439	511	7	5			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	-	EXPRESSION TAG	UNP Q7BU69
A	2	VAL	-	EXPRESSION TAG	UNP Q7BU69
A	3	ALA	-	EXPRESSION TAG	UNP Q7BU69
A	4	SER	-	EXPRESSION TAG	UNP Q7BU69
A	5	TYR	-	EXPRESSION TAG	UNP Q7BU69
A	6	CYS	-	EXPRESSION TAG	UNP Q7BU69
A	7	ASP	-	EXPRESSION TAG	UNP Q7BU69
A	8	ARG	-	EXPRESSION TAG	UNP Q7BU69
A	9	VAL	-	EXPRESSION TAG	UNP Q7BU69
A	10	VAL	-	EXPRESSION TAG	UNP Q7BU69
A	11	ALA	-	EXPRESSION TAG	UNP Q7BU69
A	12	ALA	-	EXPRESSION TAG	UNP Q7BU69
A	13	VAL	-	EXPRESSION TAG	UNP Q7BU69
A	36	VAL	ILE	VARIANT	UNP Q7BU69
A	56	TYR	HIS	VARIANT	UNP Q7BU69
A	173	PRO	HIS	VARIANT	UNP Q7BU69
A	239	LEU	VAL	VARIANT	UNP Q7BU69
B	1	GLU	-	EXPRESSION TAG	UNP Q7BU69
B	2	VAL	-	EXPRESSION TAG	UNP Q7BU69
B	3	ALA	-	EXPRESSION TAG	UNP Q7BU69
B	4	SER	-	EXPRESSION TAG	UNP Q7BU69
B	5	TYR	-	EXPRESSION TAG	UNP Q7BU69
B	6	CYS	-	EXPRESSION TAG	UNP Q7BU69
B	7	ASP	-	EXPRESSION TAG	UNP Q7BU69
B	8	ARG	-	EXPRESSION TAG	UNP Q7BU69

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	VAL	-	EXPRESSION TAG	UNP Q7BU69
B	10	VAL	-	EXPRESSION TAG	UNP Q7BU69
B	11	ALA	-	EXPRESSION TAG	UNP Q7BU69
B	12	ALA	-	EXPRESSION TAG	UNP Q7BU69
B	13	VAL	-	EXPRESSION TAG	UNP Q7BU69
B	36	VAL	ILE	VARIANT	UNP Q7BU69
B	56	TYR	HIS	VARIANT	UNP Q7BU69
B	173	PRO	HIS	VARIANT	UNP Q7BU69
B	239	LEU	VAL	VARIANT	UNP Q7BU69

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

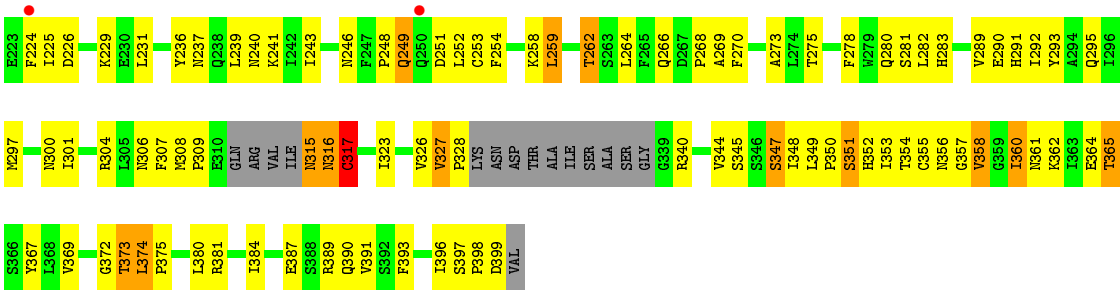
Chain A:

2% 41% 36% 8% 15%

E1 S68 L69 S4 S70 Q71 D72 K73 P74 D75 F78 SER TRP MSE SER THR VAL LYS SER THR THR GLU VAL SER TRP ASN LYS LEU SER PHE CYS ASP VAL LEU LEU LYS ILE ILE THR PHE GLY ILE TVR SER SER PRO HIS GLU THR LEU ALA GLU LYS TVR SER E53 E58 L61 M62 D63 S64 S65 P65

T138 V141 S142 G143 H144 F145 A151 P152 E153 V154 A158 C161 S164 I165 Q166 P167 N168 D169 I170 Y171 K175 D176 T177 D178 F179 N180 S181 V182 I186 Q187 R188 R191 T198 F202 N203 P208 L209 K210 L211 I212 L215 N217 I221 N222 E223 F224 L225 D226 K229 Y236 N237 Q238 L239 N240 K241 L242 I243 N246 F247 P248 Q249 Q250 P251 L252 C253 F254 K258 L259 T262 S263 L264 F265 Q266 F270 A273 L274 T275 F278 Q279 Q280 S281 L282 H283 T284 V289 E290 H291 L292 V293 Q294 Q295 T296 N297 V299 I301 R304 L305 N306 F307 P308 E310 GLN ARG VAL ILE N315 N316 C317 I323 V326 V327 P328 LYS ASN ASP THR ALA ILE SER ALA SER GLY G339 R340 V344 S346 S347 L348 L349 P350 S351 H352 T353 T354 C355 N356 G357 G359 G359 I360 N361 N362 I363 E364 T365 S366 V367 I368

[illegible]



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.25Å 170.91Å 46.16Å 90.00° 104.89° 90.00°	Depositor
Resolution (Å)	28.63 – 3.01 28.63 – 3.01	Depositor EDS
% Data completeness (in resolution range)	96.2 (28.63-3.01) 96.3 (28.63-3.01)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.77 (at 3.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.256 0.204 , 0.249	Depositor DCC
R_{free} test set	1096 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	98.9	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 85.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.032 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5244	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.56	0/2670	0.74	2/3618 (0.1%)
1	B	0.53	0/2670	0.72	2/3618 (0.1%)
All	All	0.54	0/5340	0.73	4/7236 (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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	104	GLY	N-CA-C	-6.59	96.63	113.10
1	B	104	GLY	N-CA-C	-6.23	97.52	113.10
1	A	102	LEU	CA-CB-CG	5.45	127.83	115.30
1	B	102	LEU	CA-CB-CG	5.19	127.23	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ASP	Peptide
1	B	103	ASP	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	2622	0	2537	190	0
1	B	2622	0	2537	187	0
All	All	5244	0	5074	369	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 36.

All (369) 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:102:LEU:HA	1:A:108:GLN:HA	1.24	1.13
1:B:102:LEU:HA	1:B:108:GLN:HA	1.28	1.12
1:A:102:LEU:HD13	1:A:103:ASP:OD1	1.59	1.00
1:B:102:LEU:HD13	1:B:103:ASP:OD1	1.61	0.98
1:A:102:LEU:HB2	1:A:108:GLN:HG3	1.54	0.90
1:A:209:LEU:HA	1:A:212:ILE:HD11	1.56	0.88
1:B:158:ALA:O	1:B:362:LYS:HE3	1.74	0.87
1:B:349:LEU:HB3	1:B:360:ILE:CD1	2.05	0.87
1:B:209:LEU:HA	1:B:212:ILE:HD11	1.57	0.86
1:A:349:LEU:HB3	1:A:360:ILE:CD1	2.05	0.86
1:B:104:GLY:HA3	1:B:107:ILE:HD12	1.56	0.86
1:B:143:GLY:HA3	1:B:356:ASN:O	1.76	0.85
1:B:102:LEU:HB2	1:B:108:GLN:HG3	1.58	0.85
1:B:326:VAL:HG22	1:B:327:VAL:H	1.39	0.85
1:A:344:VAL:HG11	1:A:367:TYR:CE2	2.11	0.85
1:A:104:GLY:HA3	1:A:107:ILE:HD12	1.57	0.84
1:A:143:GLY:HA3	1:A:356:ASN:O	1.78	0.83
1:A:326:VAL:HG22	1:A:327:VAL:H	1.43	0.83
1:B:344:VAL:HG11	1:B:367:TYR:CE2	2.14	0.82
1:A:349:LEU:HB3	1:A:360:ILE:HD12	1.63	0.80
1:A:102:LEU:HA	1:A:108:GLN:CA	2.11	0.80
1:A:158:ALA:O	1:A:362:LYS:HE3	1.82	0.80
1:A:226:ASP:HB3	1:A:229:LYS:HG2	1.64	0.79
1:A:350:PRO:HD2	1:A:361:ASN:O	1.83	0.79
1:A:100:PHE:O	1:A:102:LEU:HD12	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:PHE:CD2	1:A:81:ALA:HB2	2.19	0.78
1:A:297:MSE:O	1:A:301:ILE:HD13	1.85	0.76
1:B:226:ASP:HB3	1:B:229:LYS:HG2	1.65	0.76
1:A:216:ILE:HB	1:A:221:ILE:HG12	1.67	0.76
1:A:221:ILE:O	1:A:221:ILE:HG13	1.86	0.76
1:B:239:LEU:HD11	1:B:262:THR:HA	1.67	0.76
1:B:350:PRO:HD2	1:B:361:ASN:O	1.87	0.75
1:B:297:MSE:O	1:B:301:ILE:HD13	1.86	0.75
1:B:348:ILE:HG23	1:B:350:PRO:HD3	1.68	0.75
1:A:239:LEU:HD11	1:A:262:THR:HA	1.67	0.75
1:B:349:LEU:HB3	1:B:360:ILE:HD11	1.69	0.74
1:B:349:LEU:HB3	1:B:360:ILE:HD12	1.69	0.74
1:A:102:LEU:HD22	1:A:103:ASP:OD2	1.87	0.74
1:B:65:PHE:CD2	1:B:81:ALA:HB2	2.23	0.73
1:B:216:ILE:HB	1:B:221:ILE:HG12	1.71	0.73
1:A:208:PRO:O	1:A:212:ILE:HD13	1.89	0.72
1:B:100:PHE:O	1:B:102:LEU:HD12	1.89	0.72
1:B:317:CYS:HB3	1:B:349:LEU:O	1.90	0.72
1:A:317:CYS:HB3	1:A:349:LEU:O	1.90	0.72
1:B:326:VAL:HG22	1:B:327:VAL:N	2.05	0.72
1:A:348:ILE:HG23	1:A:350:PRO:HD3	1.70	0.71
1:A:306:ASN:HD21	1:B:188:ARG:NE	1.88	0.71
1:B:208:PRO:O	1:B:212:ILE:HD13	1.91	0.70
1:B:315:ASN:N	1:B:351:SER:HG	1.90	0.70
1:B:221:ILE:O	1:B:221:ILE:HG13	1.92	0.69
1:B:102:LEU:HA	1:B:108:GLN:CA	2.17	0.69
1:A:304:ARG:HA	1:A:353:ILE:HD12	1.75	0.69
1:A:349:LEU:HD22	1:A:360:ILE:HD11	1.73	0.69
1:A:326:VAL:HG22	1:A:327:VAL:N	2.08	0.68
1:A:237:ASN:O	1:A:241:LYS:HG2	1.94	0.67
1:A:349:LEU:HB3	1:A:360:ILE:HD11	1.76	0.67
1:B:102:LEU:HD22	1:B:103:ASP:OD2	1.95	0.66
1:A:101:TYR:O	1:A:103:ASP:N	2.28	0.66
1:B:237:ASN:O	1:B:241:LYS:HG2	1.94	0.66
1:A:100:PHE:C	1:A:102:LEU:HD12	2.15	0.66
1:B:300:ASN:ND2	1:B:353:ILE:H	1.93	0.66
1:B:349:LEU:HD22	1:B:360:ILE:HD11	1.76	0.66
1:A:101:TYR:O	1:A:103:ASP:OD1	2.14	0.66
1:A:306:ASN:HD21	1:B:188:ARG:HE	1.44	0.66
1:A:102:LEU:C	1:A:103:ASP:OD1	2.34	0.65
1:B:153:GLU:H	1:B:153:GLU:CD	2.00	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:PHE:CE2	1:A:81:ALA:HB2	2.32	0.65
1:A:68:SER:HB2	1:A:73:LYS:HE2	1.78	0.65
1:B:62:MSE:HG3	1:B:123:SER:O	1.95	0.65
1:B:101:TYR:O	1:B:103:ASP:N	2.30	0.64
1:B:304:ARG:HA	1:B:353:ILE:HD12	1.79	0.64
1:A:68:SER:CB	1:A:73:LYS:HE2	2.28	0.63
1:B:209:LEU:HD23	1:B:212:ILE:HD11	1.80	0.63
1:A:293:TYR:OH	1:A:297:MSE:HE3	1.99	0.63
1:A:61:LEU:O	1:A:64:SER:OG	2.17	0.63
1:B:273:ALA:HA	1:B:369:VAL:HG21	1.82	0.62
1:A:209:LEU:HD23	1:A:212:ILE:HD11	1.80	0.62
1:A:216:ILE:HD12	1:A:221:ILE:HD11	1.80	0.62
1:B:365:THR:HB	1:B:391:VAL:HG22	1.81	0.62
1:A:365:THR:HB	1:A:391:VAL:HG22	1.80	0.62
1:A:68:SER:CA	1:A:73:LYS:HE2	2.31	0.61
1:B:100:PHE:C	1:B:102:LEU:HD12	2.20	0.61
1:A:13:VAL:H	1:A:119:ASN:HD22	1.50	0.60
1:B:216:ILE:HD12	1:B:221:ILE:HD11	1.81	0.60
1:A:226:ASP:HB3	1:A:229:LYS:CG	2.31	0.60
1:A:300:ASN:ND2	1:A:353:ILE:H	1.99	0.60
1:B:300:ASN:HB2	1:B:352:HIS:CD2	2.37	0.60
1:B:68:SER:HB2	1:B:73:LYS:HE2	1.84	0.60
1:B:293:TYR:OH	1:B:297:MSE:HE3	2.02	0.59
1:B:353:ILE:HG22	1:B:354:THR:O	2.02	0.59
1:A:315:ASN:N	1:A:351:SER:HG	2.00	0.59
1:B:239:LEU:CD1	1:B:262:THR:HA	2.33	0.59
1:B:13:VAL:H	1:B:119:ASN:HD22	1.51	0.58
1:B:326:VAL:CG2	1:B:327:VAL:H	2.11	0.58
1:A:83:ILE:O	1:A:86:ILE:HB	2.02	0.58
1:B:68:SER:CB	1:B:73:LYS:HE2	2.33	0.58
1:A:100:PHE:HB3	1:A:102:LEU:HD12	1.84	0.58
1:A:153:GLU:H	1:A:153:GLU:CD	2.07	0.58
1:B:65:PHE:CE2	1:B:81:ALA:HB2	2.37	0.58
1:A:344:VAL:HG11	1:A:367:TYR:CD2	2.39	0.57
1:A:84:ASP:C	1:A:86:ILE:H	2.08	0.57
1:B:68:SER:HB2	1:B:73:LYS:HG3	1.85	0.57
1:B:101:TYR:O	1:B:103:ASP:OD1	2.22	0.57
1:B:300:ASN:HD22	1:B:353:ILE:H	1.51	0.57
1:A:62:MSE:HG3	1:A:123:SER:O	2.04	0.57
1:B:68:SER:CA	1:B:73:LYS:HE2	2.34	0.57
1:A:326:VAL:CG2	1:A:327:VAL:H	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ASP:HB3	1:B:229:LYS:CG	2.33	0.57
1:B:83:ILE:O	1:B:86:ILE:HB	2.04	0.57
1:A:102:LEU:C	1:A:103:ASP:CG	2.63	0.57
1:A:239:LEU:CD1	1:A:262:THR:HA	2.34	0.57
1:A:273:ALA:HA	1:A:369:VAL:HG21	1.86	0.57
1:A:209:LEU:HA	1:A:212:ILE:CD1	2.33	0.56
1:B:111:GLN:HG3	1:B:112:LEU:H	1.69	0.56
1:A:121:LEU:HA	1:A:124:LEU:HD23	1.87	0.56
1:A:300:ASN:HB2	1:A:352:HIS:CD2	2.41	0.56
1:B:168:ASN:HD21	1:B:289:VAL:HG23	1.70	0.56
1:B:254:PHE:O	1:B:258:LYS:HG3	2.05	0.56
1:A:315:ASN:O	1:A:317:CYS:N	2.39	0.56
1:B:316:ASN:O	1:B:317:CYS:O	2.23	0.56
1:B:61:LEU:O	1:B:64:SER:OG	2.21	0.55
1:B:100:PHE:HB3	1:B:102:LEU:HD12	1.88	0.55
1:A:316:ASN:O	1:A:317:CYS:O	2.25	0.55
1:B:90:LEU:HD13	1:B:120:LEU:HD21	1.88	0.55
1:A:291:HIS:CD2	1:B:290:GLU:OE1	2.60	0.55
1:B:243:ILE:HD12	1:B:258:LYS:HB3	1.89	0.55
1:B:300:ASN:HB2	1:B:352:HIS:HD2	1.72	0.55
1:A:254:PHE:O	1:A:258:LYS:HG3	2.06	0.55
1:A:104:GLY:O	1:A:105:ASP:HB2	2.06	0.54
1:B:151:ALA:O	1:B:154:VAL:HB	2.07	0.54
1:A:209:LEU:O	1:A:212:ILE:HG12	2.07	0.54
1:A:171:TYR:CD1	1:A:387:GLU:HA	2.43	0.54
1:A:151:ALA:O	1:A:154:VAL:HB	2.06	0.54
1:A:101:TYR:HB3	1:A:109:SER:HB2	1.90	0.54
1:B:121:LEU:HA	1:B:124:LEU:HD23	1.89	0.54
1:B:315:ASN:O	1:B:317:CYS:N	2.41	0.54
1:A:315:ASN:N	1:A:315:ASN:HD22	2.04	0.53
1:A:243:ILE:HD12	1:A:258:LYS:HB3	1.90	0.53
1:A:68:SER:HB2	1:A:73:LYS:HG3	1.88	0.53
1:B:304:ARG:CA	1:B:353:ILE:HD12	2.38	0.53
1:A:300:ASN:HD22	1:A:353:ILE:H	1.57	0.53
1:B:84:ASP:C	1:B:86:ILE:H	2.12	0.53
1:A:186:ILE:HD13	1:A:275:THR:HG22	1.90	0.53
1:A:353:ILE:HG22	1:A:354:THR:O	2.08	0.53
1:B:111:GLN:HG3	1:B:112:LEU:N	2.22	0.53
1:A:225:ILE:HG12	1:A:226:ASP:N	2.24	0.53
1:B:101:TYR:HB3	1:B:109:SER:HB2	1.91	0.52
1:B:225:ILE:HG12	1:B:226:ASP:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:GLY:O	1:B:105:ASP:HB2	2.08	0.52
1:B:4:SER:O	1:B:101:TYR:HE1	1.93	0.52
1:B:344:VAL:HG11	1:B:367:TYR:CD2	2.44	0.52
1:A:62:MSE:O	1:A:65:PHE:HB2	2.10	0.52
1:A:186:ILE:HG23	1:A:278:PHE:CD2	2.44	0.52
1:A:168:ASN:HD21	1:A:289:VAL:HG23	1.75	0.52
1:A:306:ASN:ND2	1:B:188:ARG:NE	2.57	0.52
1:A:158:ALA:HA	1:A:396:ILE:HG13	1.92	0.52
1:B:5:TYR:O	1:B:8:ARG:N	2.44	0.51
1:B:102:LEU:C	1:B:103:ASP:OD1	2.48	0.51
1:B:171:TYR:CD1	1:B:387:GLU:HA	2.45	0.51
1:B:304:ARG:HE	1:B:353:ILE:CD1	2.24	0.51
1:B:354:THR:HG22	1:B:357:GLY:O	2.10	0.51
1:B:153:GLU:OE2	1:B:153:GLU:N	2.43	0.51
1:B:349:LEU:CB	1:B:360:ILE:HD11	2.40	0.51
1:B:4:SER:HA	1:B:101:TYR:OH	2.10	0.51
1:A:304:ARG:CA	1:A:353:ILE:HD12	2.40	0.51
1:B:102:LEU:C	1:B:103:ASP:CG	2.69	0.51
1:B:304:ARG:HE	1:B:353:ILE:HD11	1.75	0.51
1:A:102:LEU:O	1:A:103:ASP:CG	2.49	0.51
1:B:209:LEU:O	1:B:212:ILE:HG12	2.11	0.51
1:B:4:SER:HA	1:B:101:TYR:CE1	2.45	0.51
1:A:103:ASP:N	1:A:103:ASP:OD1	2.44	0.50
1:A:297:MSE:O	1:A:301:ILE:CD1	2.57	0.50
1:B:186:ILE:HG23	1:B:278:PHE:CD2	2.46	0.50
1:A:168:ASN:HB2	1:A:171:TYR:CZ	2.47	0.50
1:A:4:SER:HA	1:A:101:TYR:CE1	2.46	0.50
1:B:158:ALA:HA	1:B:396:ILE:HG13	1.94	0.50
1:A:161:CYS:SG	1:A:396:ILE:HD11	2.52	0.50
1:B:178:ASP:O	1:B:179:PHE:HB2	2.12	0.50
1:A:69:LEU:H	1:A:73:LYS:HZ3	1.58	0.50
1:A:111:GLN:HG3	1:A:112:LEU:H	1.77	0.50
1:B:145:PHE:HZ	1:B:355:CYS:O	1.95	0.50
1:A:102:LEU:HD22	1:A:103:ASP:CG	2.32	0.49
1:A:102:LEU:C	1:A:107:ILE:O	2.50	0.49
1:A:300:ASN:HB2	1:A:352:HIS:HD2	1.74	0.49
1:A:178:ASP:O	1:A:179:PHE:HB2	2.13	0.49
1:A:202:PHE:CE2	1:A:264:LEU:HD11	2.48	0.49
1:B:153:GLU:CD	1:B:153:GLU:N	2.65	0.49
1:A:4:SER:HA	1:A:101:TYR:OH	2.13	0.49
1:B:161:CYS:SG	1:B:396:ILE:HD11	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LEU:C	1:B:107:ILE:O	2.51	0.48
1:B:168:ASN:HB2	1:B:171:TYR:CZ	2.48	0.48
1:B:138:THR:HA	1:B:397:SER:O	2.13	0.48
1:A:373:THR:C	1:A:374:LEU:HD23	2.33	0.48
1:B:354:THR:HG23	1:B:355:CYS:N	2.28	0.48
1:A:306:ASN:ND2	1:B:188:ARG:HE	2.10	0.48
1:B:113:SER:CB	1:B:116:GLU:HG3	2.44	0.48
1:A:166:ILE:HD12	1:A:292:ILE:HG13	1.96	0.48
1:A:354:THR:HG23	1:A:356:ASN:H	1.79	0.47
1:B:249:GLN:CD	1:B:249:GLN:H	2.17	0.47
1:A:4:SER:O	1:A:101:TYR:HE1	1.97	0.47
1:A:226:ASP:CB	1:A:229:LYS:HE2	2.45	0.47
1:A:13:VAL:N	1:A:119:ASN:HD22	2.11	0.47
1:B:102:LEU:CD1	1:B:103:ASP:OD1	2.49	0.47
1:A:111:GLN:HG3	1:A:112:LEU:N	2.29	0.47
1:A:153:GLU:N	1:A:153:GLU:OE2	2.46	0.47
1:A:5:TYR:O	1:A:8:ARG:N	2.47	0.47
1:B:70:SER:O	1:B:73:LYS:HD3	2.15	0.47
1:A:100:PHE:HB3	1:A:102:LEU:CD1	2.45	0.47
1:A:252:LEU:O	1:A:252:LEU:HD12	2.14	0.47
1:B:102:LEU:HD22	1:B:103:ASP:CG	2.35	0.47
1:B:354:THR:HG23	1:B:356:ASN:H	1.79	0.47
1:A:90:LEU:HD13	1:A:120:LEU:HD21	1.97	0.47
1:B:145:PHE:HD2	1:B:308:MSE:CG	2.28	0.47
1:B:209:LEU:HA	1:B:212:ILE:CD1	2.35	0.47
1:B:186:ILE:HD13	1:B:275:THR:HG22	1.96	0.47
1:A:249:GLN:CD	1:A:249:GLN:H	2.18	0.46
1:B:202:PHE:HA	1:B:323:ILE:O	2.15	0.46
1:A:100:PHE:CB	1:A:102:LEU:HD12	2.45	0.46
1:A:226:ASP:HB3	1:A:229:LYS:CE	2.44	0.46
1:A:188:ARG:HE	1:B:306:ASN:HD21	1.63	0.46
1:A:187:TYR:CE1	1:A:222:ASN:HA	2.50	0.46
1:B:187:TYR:CE1	1:B:222:ASN:HA	2.51	0.46
1:A:202:PHE:HA	1:A:323:ILE:O	2.15	0.46
1:A:304:ARG:HE	1:A:353:ILE:HD11	1.81	0.46
1:A:70:SER:O	1:A:73:LYS:HD3	2.15	0.46
1:B:349:LEU:CD2	1:B:360:ILE:HD11	2.45	0.46
1:A:358:VAL:HG22	1:A:358:VAL:O	2.15	0.46
1:B:78:PHE:CD2	1:B:92:LEU:HD12	2.51	0.46
1:A:182:VAL:O	1:A:186:ILE:HG13	2.16	0.46
1:A:354:THR:HG22	1:A:357:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ASP:HB3	1:B:229:LYS:HE2	1.97	0.46
1:B:259:LEU:HA	1:B:259:LEU:HD13	1.87	0.46
1:A:100:PHE:O	1:A:102:LEU:CD1	2.61	0.46
1:A:349:LEU:CD2	1:A:360:ILE:HD11	2.42	0.46
1:B:315:ASN:N	1:B:315:ASN:HD22	2.13	0.46
1:B:62:MSE:O	1:B:65:PHE:HB2	2.15	0.46
1:B:102:LEU:O	1:B:103:ASP:CG	2.54	0.46
1:B:13:VAL:N	1:B:119:ASN:HD22	2.12	0.46
1:B:104:GLY:H	1:B:107:ILE:HB	1.79	0.45
1:B:106:LYS:HB2	1:B:106:LYS:HE3	1.71	0.45
1:B:354:THR:HG23	1:B:356:ASN:N	2.31	0.45
1:A:372:GLY:O	1:A:373:THR:O	2.35	0.45
1:B:226:ASP:HB3	1:B:229:LYS:CE	2.46	0.45
1:A:138:THR:HA	1:A:397:SER:O	2.16	0.45
1:A:354:THR:HG23	1:A:355:CYS:N	2.32	0.45
1:A:124:LEU:HD12	1:A:125:PRO:CD	2.47	0.45
1:B:142:SER:HA	1:B:399:ASP:C	2.36	0.45
1:B:226:ASP:CB	1:B:229:LYS:HE2	2.46	0.45
1:B:297:MSE:O	1:B:300:ASN:HB3	2.17	0.45
1:B:373:THR:C	1:B:374:LEU:HD23	2.36	0.45
1:A:145:PHE:HD2	1:A:308:MSE:CG	2.29	0.45
1:A:304:ARG:HE	1:A:353:ILE:CD1	2.29	0.45
1:B:145:PHE:CE2	1:B:307:PHE:HB3	2.51	0.45
1:B:157:THR:O	1:B:161:CYS:HB3	2.16	0.45
1:A:248:PRO:HD2	1:A:249:GLN:OE1	2.16	0.45
1:B:248:PRO:HD2	1:B:249:GLN:OE1	2.17	0.45
1:A:226:ASP:HB3	1:A:229:LYS:HE2	1.97	0.45
1:A:367:TYR:CE2	1:A:384:ILE:HD13	2.52	0.45
1:A:209:LEU:HD23	1:A:209:LEU:HA	1.61	0.45
1:A:246:ASN:C	1:A:248:PRO:HD3	2.37	0.45
1:A:293:TYR:CZ	1:A:297:MSE:HE3	2.52	0.44
1:A:349:LEU:CB	1:A:360:ILE:HD11	2.46	0.44
1:A:104:GLY:H	1:A:107:ILE:HB	1.81	0.44
1:A:347:SER:HA	1:A:364:GLU:HA	1.98	0.44
1:A:133:LYS:HE3	1:A:135:HIS:CE1	2.52	0.44
1:A:264:LEU:HD22	1:A:270:PHE:CD1	2.51	0.44
1:A:145:PHE:HZ	1:A:355:CYS:O	1.99	0.44
1:B:374:LEU:HA	1:B:375:PRO:HD3	1.74	0.44
1:B:297:MSE:O	1:B:301:ILE:CD1	2.63	0.44
1:A:290:GLU:OE1	1:B:291:HIS:CD2	2.71	0.44
1:A:100:PHE:HB3	1:A:102:LEU:HG	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:HIS:HE1	1:A:295:GLN:OE1	2.00	0.44
1:A:354:THR:HG23	1:A:356:ASN:N	2.32	0.44
1:B:202:PHE:CE2	1:B:264:LEU:HD11	2.53	0.44
1:B:252:LEU:O	1:B:252:LEU:HD12	2.17	0.44
1:A:344:VAL:CG1	1:A:367:TYR:CD2	3.01	0.44
1:B:293:TYR:CZ	1:B:297:MSE:HE3	2.52	0.44
1:A:113:SER:CB	1:A:116:GLU:HG3	2.48	0.44
1:B:326:VAL:CG2	1:B:327:VAL:N	2.73	0.44
1:A:88:ILE:HD12	1:A:88:ILE:N	2.33	0.44
1:A:102:LEU:CD1	1:A:103:ASP:OD1	2.48	0.43
1:A:4:SER:HA	1:A:101:TYR:HE1	1.83	0.43
1:A:153:GLU:N	1:A:153:GLU:CD	2.71	0.43
1:A:384:ILE:O	1:A:389:ARG:NH1	2.51	0.43
1:A:100:PHE:HB3	1:A:102:LEU:CG	2.48	0.43
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.80	0.43
1:A:297:MSE:O	1:A:300:ASN:HB3	2.18	0.43
1:B:246:ASN:C	1:B:248:PRO:HD3	2.39	0.43
1:A:202:PHE:O	1:A:203:ASN:C	2.57	0.43
1:A:308:MSE:N	1:A:309:PRO:HD3	2.33	0.43
1:B:182:VAL:O	1:B:186:ILE:HG13	2.19	0.43
1:B:264:LEU:HD22	1:B:270:PHE:CD1	2.54	0.43
1:A:236:TYR:O	1:A:240:ASN:HB2	2.19	0.43
1:B:102:LEU:HD22	1:B:102:LEU:O	2.18	0.43
1:B:202:PHE:O	1:B:203:ASN:C	2.56	0.43
1:A:142:SER:HA	1:A:399:ASP:C	2.39	0.43
1:B:283:HIS:CD2	1:B:283:HIS:H	2.36	0.43
1:B:178:ASP:HB2	1:B:381:ARG:HB2	2.00	0.43
1:B:182:VAL:HG13	1:B:183:TRP:N	2.33	0.43
1:B:347:SER:HA	1:B:364:GLU:HA	1.99	0.43
1:A:239:LEU:CD2	1:A:266:GLN:HG3	2.49	0.43
1:A:78:PHE:CD2	1:A:92:LEU:HD12	2.54	0.43
1:B:308:MSE:N	1:B:309:PRO:HD3	2.34	0.43
1:B:367:TYR:CE2	1:B:384:ILE:HD13	2.54	0.42
1:A:210:LYS:HA	1:A:210:LYS:HD3	1.65	0.42
1:B:316:ASN:O	1:B:317:CYS:C	2.58	0.42
1:B:358:VAL:HG22	1:B:358:VAL:O	2.18	0.42
1:A:174:VAL:HG22	1:A:386:PRO:HD2	2.01	0.42
1:A:284:ILE:O	1:A:284:ILE:HG22	2.20	0.42
1:B:133:LYS:HE3	1:B:135:HIS:CE1	2.54	0.42
1:A:217:ASN:HA	1:A:217:ASN:HD22	1.70	0.42
1:A:84:ASP:C	1:A:86:ILE:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:VAL:HG11	1:B:367:TYR:CZ	2.54	0.42
1:A:116:GLU:H	1:A:116:GLU:HG2	1.53	0.42
1:B:100:PHE:CB	1:B:102:LEU:HD12	2.50	0.42
1:B:116:GLU:H	1:B:116:GLU:HG2	1.52	0.42
1:A:374:LEU:HD23	1:A:374:LEU:N	2.35	0.42
1:B:236:TYR:O	1:B:240:ASN:HB2	2.19	0.42
1:A:316:ASN:O	1:A:317:CYS:C	2.58	0.42
1:A:65:PHE:CE2	1:A:81:ALA:CB	3.02	0.42
1:A:145:PHE:CE2	1:A:307:PHE:HB3	2.55	0.42
1:B:209:LEU:HA	1:B:209:LEU:HD23	1.63	0.42
1:B:384:ILE:O	1:B:389:ARG:NH1	2.53	0.42
1:A:301:ILE:HD12	1:A:301:ILE:N	2.35	0.41
1:A:84:ASP:O	1:A:86:ILE:N	2.44	0.41
1:A:96:ILE:H	1:A:96:ILE:HG13	1.73	0.41
1:B:254:PHE:H	1:B:254:PHE:HD1	1.66	0.41
1:A:102:LEU:O	1:A:102:LEU:HD22	2.20	0.41
1:A:102:LEU:CB	1:A:108:GLN:HG3	2.37	0.41
1:A:124:LEU:HD12	1:A:125:PRO:HD3	2.01	0.41
1:A:168:ASN:CB	1:A:171:TYR:CZ	3.03	0.41
1:B:124:LEU:HD12	1:B:125:PRO:CD	2.50	0.41
1:B:209:LEU:CD2	1:B:212:ILE:HD11	2.50	0.41
1:B:241:LYS:HD3	1:B:241:LYS:N	2.35	0.41
1:B:268:PRO:O	1:B:269:ALA:C	2.58	0.41
1:B:291:HIS:HE1	1:B:295:GLN:OE1	2.02	0.41
1:A:131:LEU:HD13	1:A:131:LEU:N	2.35	0.41
1:A:326:VAL:O	1:A:328:PRO:HD3	2.20	0.41
1:B:213:ALA:O	1:B:216:ILE:HG12	2.20	0.41
1:B:304:ARG:CB	1:B:353:ILE:HD12	2.51	0.41
1:B:4:SER:HA	1:B:101:TYR:HE1	1.84	0.41
1:B:141:VAL:HG22	1:B:142:SER:O	2.21	0.41
1:B:168:ASN:CB	1:B:171:TYR:CZ	3.04	0.41
1:B:374:LEU:HD23	1:B:374:LEU:N	2.35	0.41
1:A:251:ASP:HB2	1:A:254:PHE:CD1	2.56	0.41
1:B:124:LEU:HA	1:B:125:PRO:HD3	1.85	0.41
1:B:134:VAL:CG2	1:B:393:PHE:HB2	2.51	0.41
1:B:372:GLY:O	1:B:373:THR:O	2.38	0.41
1:A:131:LEU:HB2	1:A:164:SER:HB2	2.01	0.41
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.69	0.41
1:B:251:ASP:HB2	1:B:254:PHE:CD1	2.55	0.41
1:A:295:GLN:HE21	1:A:295:GLN:HB3	1.70	0.41
1:A:384:ILE:HG22	1:A:389:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:PHE:HB3	1:B:102:LEU:CD1	2.51	0.41
1:B:114:SER:H	1:B:116:GLU:CG	2.34	0.41
1:A:216:ILE:HB	1:A:221:ILE:CG1	2.44	0.41
1:A:254:PHE:H	1:A:254:PHE:HD1	1.68	0.41
1:A:178:ASP:HB2	1:A:381:ARG:HB2	2.02	0.41
1:B:188:ARG:NH1	1:B:189:ASP:OD1	2.53	0.41
1:B:68:SER:HB2	1:B:73:LYS:CG	2.48	0.41
1:B:166:ILE:HD12	1:B:292:ILE:HG13	2.01	0.41
1:A:239:LEU:C	1:A:239:LEU:HD12	2.41	0.40
1:B:114:SER:H	1:B:116:GLU:HG3	1.86	0.40
1:B:326:VAL:O	1:B:328:PRO:HD3	2.21	0.40
1:A:188:ARG:NE	1:B:306:ASN:HD21	2.19	0.40
1:A:68:SER:HA	1:A:73:LYS:HE2	2.04	0.40
1:B:111:GLN:CG	1:B:112:LEU:H	2.34	0.40
1:B:239:LEU:CD2	1:B:266:GLN:HG3	2.51	0.40
1:B:295:GLN:HE21	1:B:295:GLN:HB3	1.71	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	333/400 (83%)	283 (85%)	41 (12%)	9 (3%)	6	29
1	B	333/400 (83%)	285 (86%)	39 (12%)	9 (3%)	6	29
All	All	666/800 (83%)	568 (85%)	80 (12%)	18 (3%)	6	29

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	LEU
1	A	316	ASN

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Mol	Chain	Res	Type
1	A	317	CYS
1	A	373	THR
1	B	4	SER
1	B	102	LEU
1	B	316	ASN
1	B	317	CYS
1	B	373	THR
1	A	4	SER
1	A	70	SER
1	A	105	ASP
1	A	141	VAL
1	B	70	SER
1	B	105	ASP
1	B	141	VAL
1	A	398	PRO
1	B	398	PRO

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	294/357 (82%)	242 (82%)	52 (18%)	2	10
1	B	294/357 (82%)	239 (81%)	55 (19%)	2	9
All	All	588/714 (82%)	481 (82%)	107 (18%)	2	9

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	SER
1	A	73	LYS
1	A	75	ASP
1	A	92	LEU
1	A	96	ILE
1	A	98	SER
1	A	101	TYR

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Mol	Chain	Res	Type
1	A	102	LEU
1	A	103	ASP
1	A	106	LYS
1	A	110	THR
1	A	112	LEU
1	A	113	SER
1	A	116	GLU
1	A	118	ASN
1	A	122	SER
1	A	124	LEU
1	A	130	ASN
1	A	131	LEU
1	A	138	THR
1	A	153	GLU
1	A	169	ASP
1	A	170	ASP
1	A	176	ASP
1	A	177	THR
1	A	181	SER
1	A	186	ILE
1	A	191	ARG
1	A	198	THR
1	A	212	ILE
1	A	215	LEU
1	A	221	ILE
1	A	222	ASN
1	A	224	PHE
1	A	249	GLN
1	A	253	CYS
1	A	259	LEU
1	A	262	THR
1	A	280	GLN
1	A	281	SER
1	A	282	LEU
1	A	315	ASN
1	A	317	CYS
1	A	340	ARG
1	A	345	SER
1	A	347	SER
1	A	358	VAL
1	A	360	ILE
1	A	365	THR

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Mol	Chain	Res	Type
1	A	374	LEU
1	A	380	LEU
1	A	390	GLN
1	B	64	SER
1	B	73	LYS
1	B	75	ASP
1	B	92	LEU
1	B	96	ILE
1	B	98	SER
1	B	101	TYR
1	B	102	LEU
1	B	103	ASP
1	B	106	LYS
1	B	110	THR
1	B	112	LEU
1	B	113	SER
1	B	116	GLU
1	B	118	ASN
1	B	122	SER
1	B	124	LEU
1	B	130	ASN
1	B	131	LEU
1	B	138	THR
1	B	153	GLU
1	B	169	ASP
1	B	170	ASP
1	B	176	ASP
1	B	177	THR
1	B	186	ILE
1	B	191	ARG
1	B	194	ASP
1	B	198	THR
1	B	212	ILE
1	B	215	LEU
1	B	221	ILE
1	B	222	ASN
1	B	224	PHE
1	B	231	LEU
1	B	249	GLN
1	B	253	CYS
1	B	259	LEU
1	B	262	THR

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Mol	Chain	Res	Type
1	B	280	GLN
1	B	281	SER
1	B	282	LEU
1	B	315	ASN
1	B	317	CYS
1	B	327	VAL
1	B	340	ARG
1	B	345	SER
1	B	347	SER
1	B	351	SER
1	B	358	VAL
1	B	360	ILE
1	B	365	THR
1	B	374	LEU
1	B	380	LEU
1	B	390	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	135	HIS
1	A	168	ASN
1	A	180	ASN
1	A	217	ASN
1	A	283	HIS
1	A	291	HIS
1	A	295	GLN
1	A	300	ASN
1	A	306	ASN
1	A	352	HIS
1	B	111	GLN
1	B	119	ASN
1	B	168	ASN
1	B	180	ASN
1	B	217	ASN
1	B	283	HIS
1	B	291	HIS
1	B	295	GLN
1	B	300	ASN
1	B	306	ASN
1	B	352	HIS

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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	336/400 (84%)	-0.31	6 (1%) 69 39	68, 103, 171, 489	0
1	B	336/400 (84%)	-0.22	7 (2%) 64 34	71, 115, 212, 465	0
All	All	672/800 (84%)	-0.26	13 (1%) 67 37	68, 110, 192, 489	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	GLY	2.8
1	A	1	GLU	2.7
1	A	171	TYR	2.5
1	A	71	GLN	2.4
1	B	140	PRO	2.4
1	B	94	LYS	2.2
1	B	224	PHE	2.2
1	A	250	GLN	2.2
1	A	170	ASP	2.1
1	B	250	GLN	2.1
1	B	83	ILE	2.0
1	B	104	GLY	2.0
1	B	107	ILE	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 carbohydrates 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.