



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:59 pm BST

PDB ID : 3EQ2
Title : Structure of Hexagonal Crystal form of Pseudomonas aeruginosa RssB
Authors : Levchenko, I.; Grant, R.A.; Sauer, R.T.; Baker, T.A.
Deposited on : 2008-09-30
Resolution : 3.40 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

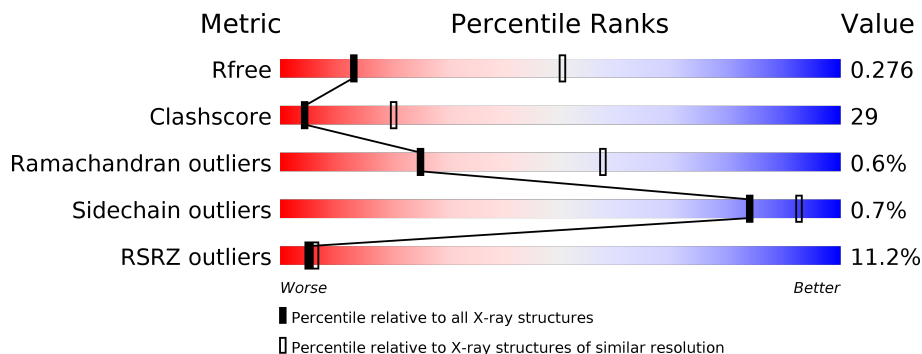
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 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	394	 10% 53% 39% • 7%
1	B	394	 11% 54% 40% • 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5536 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.

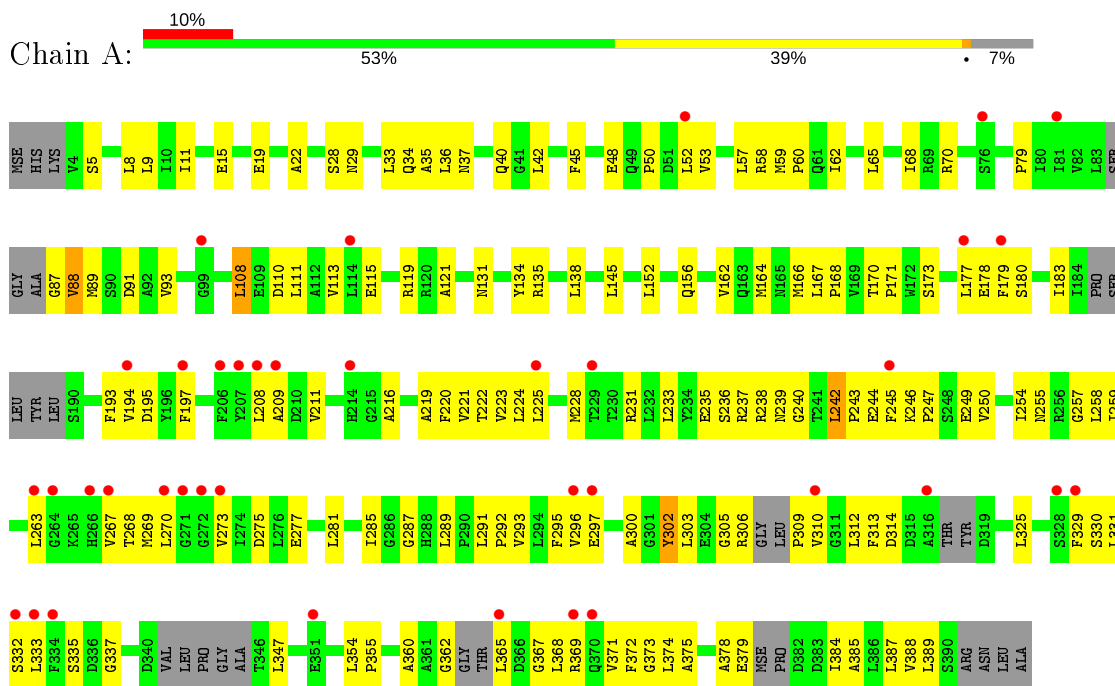
- Molecule 1 is a protein called Probable two-component response regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	366	2777	1767	477	525	1	7	0	0	0
1	B	372	2759	1762	454	535	1	7	0	0	0

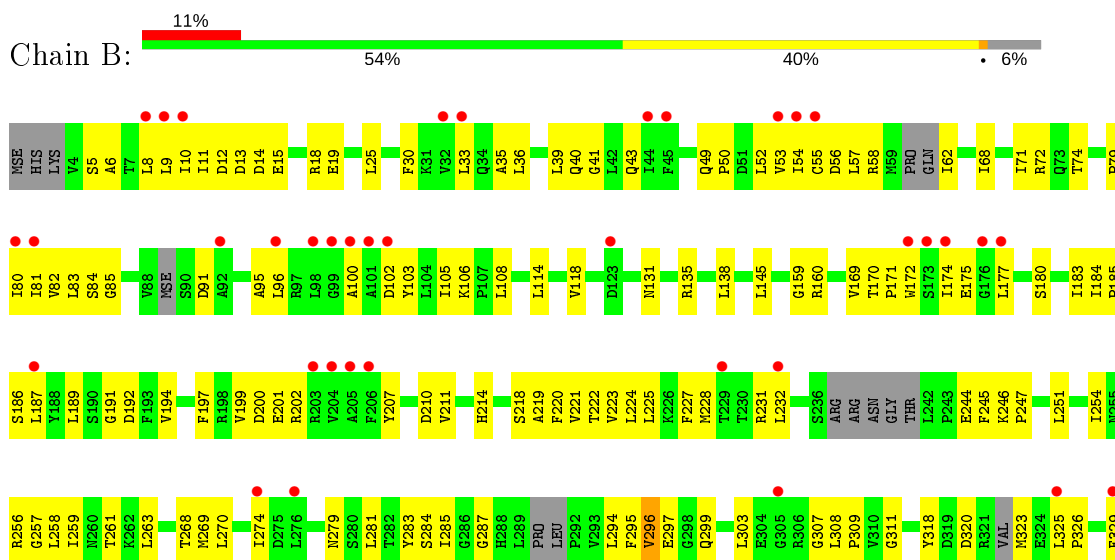
3 Residue-property plots i

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 ($RSRZ > 2$). 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: Probable two-component response regulator



- Molecule 1: Probable two-component response regulator





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	76.28Å 76.28Å 305.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.05 – 3.40 38.14 – 3.40	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.05-3.40) 98.7 (38.14-3.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.40Å)	Xtriage
Refinement program	REFMAC, PHENIX	Depositor
R, R_{free}	0.271 , 0.307 0.270 , 0.276	Depositor DCC
R_{free} test set	679 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	73.7	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.438 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.509 for k,h,-l	Depositor
Outliers	0 of 13579 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	5536	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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	0.22	0/2806	0.39	0/3789
1	B	0.21	0/2790	0.37	0/3780
All	All	0.21	0/5596	0.38	0/7569

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	2777	0	2759	166	1
1	B	2759	0	2690	160	1
All	All	5536	0	5449	319	1

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 29.

All (319) 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:291:LEU:HB2	1:A:302:TYR:CE1	1.20	1.65
1:A:291:LEU:CB	1:A:302:TYR:CE1	1.83	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LEU:CB	1:A:302:TYR:HE1	1.15	1.42
1:A:330:SER:OG	1:A:365:LEU:HD11	1.25	1.28
1:A:259:ILE:HD12	1:A:314:ASP:OD1	1.34	1.27
1:A:291:LEU:HB3	1:A:302:TYR:CD1	1.69	1.26
1:B:295:PHE:O	1:B:296:VAL:HG12	1.41	1.19
1:A:291:LEU:CB	1:A:302:TYR:CD1	2.26	1.11
1:A:291:LEU:HB3	1:A:302:TYR:CE1	1.76	1.10
1:A:295:PHE:HB3	1:A:330:SER:HB3	1.35	1.08
1:A:259:ILE:CD1	1:A:314:ASP:OD1	2.06	1.04
1:A:57:LEU:HD11	1:A:87:GLY:CA	1.89	1.03
1:B:351:GLU:O	1:B:355:PRO:HD3	1.59	1.02
1:B:295:PHE:O	1:B:296:VAL:CG1	2.11	0.99
1:A:246:LYS:HD3	1:A:249:GLU:HG3	1.47	0.96
1:B:6:ALA:HB3	1:B:30:PHE:HE1	1.32	0.94
1:B:346:THR:O	1:B:351:GLU:HG2	1.68	0.93
1:A:330:SER:OG	1:A:365:LEU:CD1	2.16	0.92
1:A:291:LEU:HB3	1:A:302:TYR:HD1	1.36	0.88
1:B:6:ALA:HB3	1:B:30:PHE:CE1	2.09	0.88
1:A:57:LEU:HD11	1:A:87:GLY:HA3	1.56	0.84
1:A:236:SER:HB2	1:A:240:GLY:HA2	1.59	0.84
1:B:57:LEU:HD23	1:B:57:LEU:O	1.78	0.84
1:A:37:ASN:H	1:A:40:GLN:HE21	1.25	0.84
1:A:57:LEU:HD11	1:A:87:GLY:HA2	1.60	0.82
1:B:295:PHE:CE1	1:B:360:ALA:HA	2.14	0.82
1:B:347:LEU:HD13	1:B:347:LEU:H	1.42	0.82
1:A:281:LEU:HB2	1:A:325:LEU:HD11	1.63	0.81
1:B:296:VAL:HG11	1:B:299:GLN:O	1.82	0.80
1:B:295:PHE:CE1	1:B:363:GLY:HA2	2.15	0.80
1:A:368:LEU:HD12	1:A:369:ARG:N	1.99	0.77
1:A:220:PHE:CE2	1:B:159:GLY:HA2	2.21	0.76
1:A:246:LYS:HD3	1:A:249:GLU:CG	2.14	0.76
1:A:88:VAL:HG12	1:A:89:MSE:H	1.48	0.76
1:B:284:SER:HB3	1:B:320:ASP:HB3	1.68	0.75
1:B:15:GLU:O	1:B:19:GLU:HG2	1.88	0.74
1:A:237:ARG:O	1:A:238:ARG:HG2	1.88	0.73
1:B:311:GLY:HA2	1:B:318:TYR:OH	1.88	0.73
1:B:303:LEU:CD2	1:B:323:MSE:SE	2.86	0.73
1:A:287:GLY:HA3	1:A:309:PRO:O	1.89	0.72
1:A:236:SER:HB2	1:A:240:GLY:CA	2.20	0.72
1:B:14:ASP:H	1:B:58:ARG:NH2	1.88	0.71
1:A:247:PRO:HG3	1:A:273:VAL:HG12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:PHE:C	1:B:296:VAL:HG12	2.11	0.71
1:B:36:LEU:H	1:B:40:GLN:HG2	1.56	0.71
1:A:332:SER:OG	1:A:369:ARG:NH2	2.23	0.70
1:B:191:GLY:HA3	1:B:211:VAL:HB	1.71	0.70
1:A:285:ILE:HG13	1:A:305:GLY:HA3	1.72	0.70
1:B:329:PHE:HB3	1:B:391:ARG:HB3	1.73	0.70
1:B:8:LEU:HD22	1:B:52:LEU:HB3	1.72	0.69
1:B:295:PHE:HD2	1:B:297:GLU:H	1.38	0.69
1:A:193:PHE:CE2	1:A:195:ASP:HB2	2.26	0.69
1:B:13:ASP:HB3	1:B:58:ARG:HH12	1.58	0.69
1:A:59:MSE:HE3	1:A:60:PRO:HA	1.76	0.68
1:B:172:TRP:CH2	1:B:174:ILE:HB	2.29	0.68
1:A:374:LEU:HG	1:A:375:ALA:H	1.58	0.68
1:A:373:GLY:O	1:A:374:LEU:HB3	1.94	0.67
1:A:335:SER:HB3	1:A:385:ALA:H	1.58	0.67
1:B:197:PHE:HE2	1:B:207:TYR:HE1	1.43	0.66
1:B:303:LEU:HD22	1:B:323:MSE:SE	2.46	0.66
1:A:378:ALA:O	1:A:379:GLU:HB2	1.96	0.66
1:B:13:ASP:HB3	1:B:58:ARG:HH22	1.61	0.65
1:A:291:LEU:CA	1:A:302:TYR:HE1	2.05	0.65
1:A:246:LYS:CD	1:A:249:GLU:HG3	2.23	0.64
1:A:8:LEU:HD22	1:A:52:LEU:HB3	1.78	0.64
1:A:367:GLY:O	1:A:371:VAL:HG23	1.97	0.64
1:B:169:VAL:HG23	1:B:172:TRP:HB2	1.79	0.64
1:B:220:PHE:O	1:B:223:VAL:HG22	1.97	0.64
1:A:310:VAL:HG23	1:A:312:LEU:H	1.62	0.64
1:A:79:PRO:HB3	1:A:121:ALA:HB1	1.80	0.64
1:A:365:LEU:HD13	1:A:388:VAL:HG13	1.80	0.64
1:B:177:LEU:HD21	1:B:391:ARG:HD2	1.81	0.63
1:B:12:ASP:HB3	1:B:18:ARG:HB2	1.80	0.63
1:B:192:ASP:HA	1:B:210:ASP:HA	1.80	0.63
1:A:365:LEU:CD1	1:A:388:VAL:HG13	2.29	0.63
1:A:295:PHE:HE1	1:A:360:ALA:HA	1.63	0.63
1:B:10:ILE:HD11	1:B:25:LEU:HD12	1.81	0.62
1:A:164:MSE:SE	1:A:183:ILE:HD11	2.49	0.62
1:B:270:LEU:HA	1:B:285:ILE:HG22	1.81	0.62
1:B:296:VAL:CG1	1:B:299:GLN:O	2.47	0.62
1:A:197:PHE:HE1	1:A:233:LEU:HD22	1.62	0.62
1:B:85:GLY:H	1:B:106:LYS:HE2	1.64	0.62
1:B:279:ASN:OD1	1:B:391:ARG:NH1	2.32	0.62
1:B:254:ILE:O	1:B:258:LEU:HG	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:LEU:O	1:B:371:VAL:HG22	2.00	0.62
1:A:231:ARG:HD3	1:A:231:ARG:O	1.99	0.61
1:A:242:LEU:O	1:A:242:LEU:HD12	2.00	0.61
1:A:197:PHE:CE1	1:A:233:LEU:HD22	2.36	0.60
1:B:10:ILE:HA	1:B:54:ILE:O	2.02	0.60
1:B:52:LEU:HD13	1:B:79:PRO:HB2	1.83	0.60
1:B:11:ILE:HG22	1:B:62:ILE:HD12	1.84	0.60
1:A:270:LEU:HD22	1:A:285:ILE:HD12	1.84	0.60
1:B:82:VAL:HG11	1:B:95:ALA:HB1	1.84	0.60
1:A:166:MSE:SE	1:A:223:VAL:HA	2.52	0.59
1:A:368:LEU:HD12	1:A:369:ARG:H	1.65	0.59
1:B:332:SER:HB3	1:B:369:ARG:NH2	2.17	0.59
1:A:115:GLU:HB3	1:A:119:ARG:HH12	1.67	0.59
1:A:5:SER:HB3	1:A:29:ASN:O	2.03	0.59
1:B:341:VAL:HA	1:B:354:LEU:HD13	1.83	0.59
1:B:364:THR:HA	1:B:369:ARG:NH2	2.17	0.59
1:B:39:LEU:HD11	1:B:43:GLN:HE21	1.66	0.59
1:A:168:PRO:HG3	1:A:195:ASP:OD2	2.03	0.59
1:A:291:LEU:CG	1:A:302:TYR:CD1	2.85	0.59
1:B:307:GLY:C	1:B:309:PRO:HD3	2.22	0.59
1:A:52:LEU:HD13	1:A:79:PRO:HB2	1.85	0.59
1:B:363:GLY:O	1:B:364:THR:HG22	2.03	0.59
1:A:108:LEU:HD13	1:A:108:LEU:H	1.68	0.59
1:A:292:PRO:HG2	1:A:303:LEU:HB2	1.85	0.58
1:A:224:LEU:O	1:A:228:MSE:HG2	2.03	0.58
1:A:152:LEU:O	1:A:156:GLN:HG2	2.03	0.58
1:B:244:GLU:HG3	1:B:245:PHE:CD2	2.39	0.58
1:A:57:LEU:HD22	1:A:91:ASP:HB3	1.85	0.58
1:B:224:LEU:HA	1:B:227:PHE:HB3	1.86	0.58
1:A:162:VAL:HG11	1:B:220:PHE:HD1	1.69	0.58
1:A:57:LEU:HD12	1:A:57:LEU:O	2.04	0.57
1:B:189:LEU:O	1:B:214:HIS:HB2	2.03	0.57
1:B:268:THR:HB	1:B:287:GLY:HA3	1.87	0.57
1:B:68:ILE:HG23	1:B:80:ILE:HD12	1.86	0.57
1:B:82:VAL:HG22	1:B:102:ASP:O	2.05	0.57
1:A:108:LEU:O	1:A:108:LEU:HD22	2.05	0.57
1:B:354:LEU:N	1:B:355:PRO:CD	2.67	0.57
1:A:110:ASP:O	1:A:113:VAL:HG22	2.05	0.56
1:A:115:GLU:HB3	1:A:119:ARG:NH1	2.20	0.56
1:A:89:MSE:O	1:A:93:VAL:HG22	2.04	0.56
1:B:295:PHE:HB3	1:B:330:SER:OG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLU:O	1:A:19:GLU:HB2	2.07	0.55
1:A:387:LEU:HD23	1:A:388:VAL:N	2.22	0.55
1:A:231:ARG:O	1:A:235:GLU:N	2.39	0.55
1:B:295:PHE:HB2	1:B:364:THR:HB	1.89	0.55
1:B:374:LEU:HD23	1:B:375:ALA:N	2.21	0.55
1:A:108:LEU:CD1	1:A:108:LEU:H	2.20	0.55
1:A:183:ILE:HG22	1:A:385:ALA:HB1	1.89	0.55
1:B:308:LEU:N	1:B:309:PRO:HD3	2.21	0.55
1:A:374:LEU:O	1:A:375:ALA:HB3	2.06	0.54
1:A:138:LEU:HD13	1:B:138:LEU:HA	1.88	0.54
1:B:295:PHE:HE1	1:B:360:ALA:HA	1.71	0.54
1:B:159:GLY:HA3	1:B:189:LEU:HD11	1.88	0.54
1:B:14:ASP:H	1:B:58:ARG:HH22	1.56	0.54
1:A:329:PHE:C	1:A:329:PHE:CD1	2.81	0.54
1:A:291:LEU:HB2	1:A:302:TYR:HE1	0.44	0.53
1:B:295:PHE:HD2	1:B:297:GLU:N	2.05	0.53
1:A:166:MSE:HE1	1:A:222:THR:HG23	1.90	0.53
1:A:291:LEU:HG	1:A:302:TYR:CD1	2.44	0.53
1:B:251:LEU:HA	1:B:254:ILE:HG22	1.91	0.53
1:B:330:SER:CB	1:B:364:THR:HG21	2.38	0.53
1:B:85:GLY:HA2	1:B:106:LYS:H	1.74	0.53
1:A:238:ARG:HG3	1:A:239:ASN:N	2.23	0.52
1:B:96:LEU:HD11	1:B:103:TYR:CD2	2.44	0.52
1:B:274:ILE:HG12	1:B:281:LEU:HD13	1.91	0.52
1:A:296:VAL:O	1:A:297:GLU:HG2	2.10	0.52
1:B:329:PHE:CE2	1:B:331:LEU:HB2	2.43	0.52
1:B:330:SER:HB2	1:B:364:THR:CB	2.39	0.52
1:A:368:LEU:O	1:A:372:PHE:HD2	1.93	0.52
1:B:296:VAL:O	1:B:296:VAL:HG22	2.10	0.51
1:A:354:LEU:N	1:A:355:PRO:CD	2.74	0.51
1:B:354:LEU:N	1:B:355:PRO:HD2	2.25	0.50
1:B:177:LEU:CD2	1:B:391:ARG:HD2	2.41	0.50
1:A:173:SER:HB3	1:A:178:GLU:HA	1.93	0.50
1:B:294:LEU:HD12	1:B:330:SER:O	2.11	0.50
1:B:71:ILE:O	1:B:74:THR:HG22	2.11	0.50
1:A:259:ILE:HG13	1:A:312:LEU:HD12	1.93	0.50
1:B:285:ILE:HG13	1:B:308:LEU:HD22	1.94	0.50
1:A:238:ARG:CG	1:A:239:ASN:N	2.74	0.50
1:A:245:PHE:CE2	1:A:250:VAL:HG21	2.46	0.50
1:B:303:LEU:HD21	1:B:323:MSE:SE	2.62	0.50
1:A:374:LEU:HG	1:A:375:ALA:N	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ASN:OD1	1:B:325:LEU:HB2	2.12	0.50
1:B:296:VAL:O	1:B:297:GLU:HB3	2.12	0.50
1:B:367:GLY:O	1:B:371:VAL:HG13	2.12	0.50
1:A:313:PHE:CD2	1:A:313:PHE:C	2.85	0.49
1:B:363:GLY:O	1:B:365:LEU:HG	2.11	0.49
1:A:178:GLU:OE2	1:A:180:SER:HB2	2.12	0.49
1:A:58:ARG:O	1:A:62:ILE:HB	2.12	0.49
1:B:261:THR:HB	1:B:263:LEU:HD13	1.94	0.49
1:A:242:LEU:C	1:A:242:LEU:HD12	2.33	0.49
1:B:13:ASP:HB3	1:B:58:ARG:NH1	2.26	0.49
1:B:330:SER:HB2	1:B:364:THR:HG21	1.94	0.49
1:A:238:ARG:CG	1:A:239:ASN:H	2.26	0.49
1:B:160:ARG:HH12	1:B:187:LEU:HA	1.77	0.49
1:B:36:LEU:N	1:B:40:GLN:HG2	2.25	0.49
1:A:378:ALA:O	1:A:379:GLU:CB	2.58	0.49
1:B:347:LEU:H	1:B:347:LEU:CD1	2.20	0.49
1:A:225:LEU:CD1	1:A:269:MSE:HE1	2.42	0.49
1:B:218:SER:O	1:B:222:THR:HG23	2.12	0.49
1:A:193:PHE:CZ	1:A:195:ASP:HB2	2.48	0.48
1:A:228:MSE:HE2	1:A:254:ILE:HA	1.95	0.48
1:B:160:ARG:NH1	1:B:185:PRO:HB2	2.27	0.48
1:A:228:MSE:HE1	1:A:257:GLY:HA3	1.94	0.48
1:A:242:LEU:CD2	1:A:246:LYS:HE3	2.43	0.48
1:B:367:GLY:O	1:B:370:GLN:HB3	2.14	0.48
1:B:54:ILE:HG12	1:B:81:ILE:HB	1.95	0.48
1:B:256:ARG:HA	1:B:259:ILE:HD11	1.96	0.48
1:B:323:MSE:O	1:B:323:MSE:HG3	2.13	0.48
1:A:145:LEU:HD13	1:B:145:LEU:HA	1.94	0.48
1:B:185:PRO:HA	1:B:383:ASP:CG	2.34	0.48
1:A:275:ASP:OD1	1:A:277:GLU:HG2	2.14	0.48
1:B:283:TYR:CZ	1:B:303:LEU:HB3	2.49	0.48
1:B:13:ASP:HB3	1:B:58:ARG:NH2	2.28	0.48
1:A:293:VAL:HG13	1:A:300:ALA:HB1	1.96	0.48
1:A:220:PHE:HE2	1:B:159:GLY:HA2	1.73	0.48
1:B:174:ILE:HG13	1:B:175:GLU:HG2	1.96	0.48
1:B:131:ASN:O	1:B:135:ARG:HG3	2.14	0.47
1:A:52:LEU:HD12	1:A:53:VAL:H	1.79	0.47
1:B:332:SER:HB3	1:B:369:ARG:CZ	2.44	0.47
1:A:242:LEU:HB2	1:A:243:PRO:HD2	1.95	0.47
1:A:270:LEU:HD12	1:A:333:LEU:HD22	1.95	0.47
1:B:201:GLU:O	1:B:201:GLU:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PHE:CZ	1:B:331:LEU:HB2	2.48	0.47
1:B:228:MSE:SE	1:B:231:ARG:HD3	2.64	0.47
1:B:221:VAL:HG22	1:B:263:LEU:HD23	1.97	0.47
1:A:220:PHE:HD1	1:B:220:PHE:CZ	2.33	0.47
1:A:362:GLY:HA3	1:A:368:LEU:CB	2.45	0.47
1:B:224:LEU:HD12	1:B:225:LEU:N	2.30	0.47
1:A:254:ILE:O	1:A:258:LEU:HG	2.15	0.46
1:A:221:VAL:HG13	1:A:263:LEU:HD23	1.98	0.46
1:A:255:ASN:HD21	1:A:313:PHE:H	1.63	0.46
1:B:9:LEU:HD12	1:B:33:LEU:O	2.15	0.46
1:A:216:ALA:O	1:A:220:PHE:HB2	2.15	0.46
1:A:246:LYS:O	1:A:250:VAL:HG23	2.15	0.46
1:A:168:PRO:CG	1:A:195:ASP:HA	2.46	0.46
1:A:179:PHE:CE1	1:A:389:LEU:HD13	2.50	0.46
1:A:65:LEU:O	1:A:68:ILE:HG22	2.16	0.46
1:B:186:SER:O	1:B:187:LEU:HB2	2.15	0.46
1:B:6:ALA:CB	1:B:30:PHE:HE1	2.16	0.46
1:B:231:ARG:HG3	1:B:232:LEU:HD12	1.97	0.46
1:A:347:LEU:O	1:A:347:LEU:HD12	2.16	0.46
1:B:325:LEU:HA	1:B:326:PRO:HD3	1.85	0.46
1:A:131:ASN:HA	1:A:134:TYR:HD2	1.81	0.45
1:B:171:PRO:HB3	1:B:180:SER:OG	2.16	0.45
1:B:183:ILE:O	1:B:185:PRO:HD3	2.16	0.45
1:A:293:VAL:CG1	1:A:300:ALA:HB1	2.47	0.45
1:B:68:ILE:O	1:B:72:ARG:HG2	2.15	0.45
1:A:228:MSE:CE	1:A:254:ILE:HA	2.46	0.45
1:A:331:LEU:HD12	1:A:332:SER:H	1.82	0.45
1:A:368:LEU:O	1:A:372:PHE:CD2	2.69	0.45
1:B:85:GLY:HA2	1:B:106:LYS:N	2.31	0.45
1:A:245:PHE:HE2	1:A:250:VAL:HG21	1.81	0.45
1:B:11:ILE:HG12	1:B:35:ALA:HB3	1.98	0.45
1:B:49:GLN:N	1:B:50:PRO:HD3	2.30	0.45
1:A:9:LEU:HD12	1:A:33:LEU:O	2.17	0.45
1:B:369:ARG:NH1	1:B:388:VAL:HG22	2.32	0.45
1:A:285:ILE:HG13	1:A:305:GLY:CA	2.42	0.45
1:A:374:LEU:CG	1:A:375:ALA:N	2.80	0.45
1:A:242:LEU:C	1:A:242:LEU:CD1	2.85	0.45
1:B:11:ILE:HB	1:B:55:CYS:HB2	1.99	0.45
1:A:362:GLY:HA3	1:A:368:LEU:HB3	1.99	0.45
1:B:106:LYS:HA	1:B:108:LEU:N	2.32	0.44
1:B:353:SER:C	1:B:355:PRO:HD2	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:SER:HB3	1:A:385:ALA:N	2.28	0.44
1:A:42:LEU:HD21	1:A:70:ARG:NE	2.31	0.44
1:B:285:ILE:HG13	1:B:308:LEU:CD2	2.48	0.44
1:A:48:GLU:O	1:A:50:PRO:HD3	2.17	0.44
1:A:219:ALA:HA	1:A:222:THR:HG22	1.99	0.44
1:B:184:ILE:N	1:B:184:ILE:HD12	2.33	0.44
1:B:194:VAL:HG21	1:B:387:LEU:HB2	1.99	0.44
1:B:56:ASP:HA	1:B:83:LEU:HB2	2.00	0.44
1:A:194:VAL:HB	1:A:208:LEU:HD13	2.00	0.43
1:A:168:PRO:HG3	1:A:195:ASP:HA	1.99	0.43
1:B:307:GLY:O	1:B:308:LEU:HD23	2.18	0.43
1:A:36:LEU:H	1:A:36:LEU:HD12	1.83	0.43
1:B:365:LEU:HB2	1:B:368:LEU:HD13	1.99	0.43
1:B:185:PRO:HA	1:B:383:ASP:HB3	1.99	0.43
1:A:291:LEU:CG	1:A:302:TYR:CE1	2.86	0.43
1:B:352:ALA:C	1:B:355:PRO:HD2	2.38	0.43
1:B:105:ILE:N	1:B:105:ILE:HD12	2.33	0.43
1:B:228:MSE:HA	1:B:231:ARG:HG2	2.01	0.43
1:A:22:ALA:CB	1:A:34:GLN:HE21	2.31	0.43
1:A:45:PHE:CD1	1:A:50:PRO:HD2	2.53	0.43
1:B:57:LEU:HD13	1:B:84:SER:HB3	2.01	0.43
1:B:325:LEU:HD22	1:B:329:PHE:CE1	2.54	0.43
1:A:173:SER:HA	1:A:177:LEU:O	2.18	0.43
1:A:36:LEU:HB2	1:A:40:GLN:NE2	2.33	0.43
1:A:131:ASN:O	1:A:135:ARG:HG3	2.19	0.42
1:A:162:VAL:HG11	1:B:220:PHE:CD1	2.49	0.42
1:B:221:VAL:O	1:B:224:LEU:HG	2.19	0.42
1:A:11:ILE:HG12	1:A:35:ALA:HB3	2.01	0.42
1:A:268:THR:C	1:A:289:LEU:HD21	2.40	0.42
1:A:330:SER:OG	1:A:365:LEU:HD21	2.20	0.42
1:A:57:LEU:HD13	1:A:91:ASP:OD2	2.20	0.42
1:B:257:GLY:O	1:B:261:THR:HG23	2.18	0.42
1:B:341:VAL:HA	1:B:354:LEU:CD1	2.49	0.42
1:A:8:LEU:CD2	1:A:52:LEU:HB3	2.49	0.42
1:A:291:LEU:HD12	1:A:303:LEU:O	2.19	0.42
1:A:167:LEU:HA	1:A:168:PRO:HD3	1.88	0.42
1:A:36:LEU:N	1:A:36:LEU:HD12	2.35	0.42
1:B:82:VAL:O	1:B:103:TYR:HA	2.20	0.42
1:B:96:LEU:HA	1:B:100:ALA:HB3	2.01	0.42
1:B:219:ALA:O	1:B:223:VAL:HG13	2.20	0.42
1:A:295:PHE:N	1:A:330:SER:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:GLY:HA3	1:A:384:ILE:HG22	2.02	0.41
1:A:108:LEU:HD23	1:A:110:ASP:O	2.21	0.41
1:B:246:LYS:HA	1:B:247:PRO:HD3	1.86	0.41
1:B:330:SER:HB3	1:B:364:THR:HG21	2.02	0.41
1:A:329:PHE:HD1	1:A:330:SER:N	2.17	0.41
1:A:183:ILE:HG22	1:A:385:ALA:CB	2.50	0.41
1:A:246:LYS:HG3	1:A:249:GLU:HB2	2.02	0.41
1:A:36:LEU:HB2	1:A:40:GLN:HE22	1.86	0.41
1:B:52:LEU:HD12	1:B:53:VAL:H	1.85	0.41
1:A:242:LEU:HD13	1:A:244:GLU:C	2.41	0.41
1:A:295:PHE:CB	1:A:330:SER:HB3	2.26	0.41
1:B:199:VAL:O	1:B:200:ASP:HB3	2.21	0.41
1:A:250:VAL:O	1:A:254:ILE:HD13	2.19	0.41
1:A:28:SER:O	1:A:29:ASN:HB2	2.21	0.41
1:B:11:ILE:HA	1:B:35:ALA:HB3	2.03	0.41
1:B:374:LEU:HD23	1:B:375:ALA:H	1.83	0.41
1:A:170:THR:HA	1:A:171:PRO:HA	1.79	0.41
1:B:11:ILE:CD1	1:B:41:GLY:HA3	2.51	0.41
1:B:114:LEU:O	1:B:118:VAL:HG23	2.21	0.40
1:B:170:THR:HG23	1:B:180:SER:HA	2.03	0.40
1:A:211:VAL:HA	1:A:267:VAL:HG22	2.03	0.40
1:A:374:LEU:O	1:A:375:ALA:CB	2.69	0.40
1:B:269:MSE:O	1:B:270:LEU:HD23	2.21	0.40
1:B:57:LEU:CD2	1:B:91:ASP:OD2	2.69	0.40
1:A:111:LEU:HD12	1:A:111:LEU:N	2.37	0.40
1:A:209:ALA:HB2	1:A:225:LEU:HD21	2.02	0.40
1:B:174:ILE:C	1:B:175:GLU:HG2	2.42	0.40
1:B:200:ASP:C	1:B:202:ARG:H	2.25	0.40
1:B:374:LEU:O	1:B:375:ALA:HB3	2.21	0.40
1:B:57:LEU:HD21	1:B:91:ASP:OD2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ARG:NH2	1:B:5:SER:OG[1_455]	1.78	0.42

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	350/394 (89%)	327 (93%)	22 (6%)	1 (0%)	41	72
1	B	356/394 (90%)	334 (94%)	19 (5%)	3 (1%)	19	51
All	All	706/788 (90%)	661 (94%)	41 (6%)	4 (1%)	25	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	VAL
1	B	296	VAL
1	B	364	THR
1	B	330	SER

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	291/323 (90%)	288 (99%)	3 (1%)	76	88
1	B	285/323 (88%)	284 (100%)	1 (0%)	91	95
All	All	576/646 (89%)	572 (99%)	4 (1%)	84	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	242	LEU

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Mol	Chain	Res	Type
1	A	302	TYR
1	B	347	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	40	GLN
1	A	253	HIS
1	B	34	GLN
1	B	43	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no 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

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	359/394 (91%)	0.49	38 (10%) 6 7	34, 98, 190, 346	0
1	B	365/394 (92%)	0.68	43 (11%) 4 5	44, 106, 200, 299	0
All	All	724/788 (91%)	0.59	81 (11%) 5 6	34, 102, 198, 346	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	ALA	11.8
1	B	102	ASP	10.1
1	B	204	VAL	9.0
1	B	100	ALA	8.5
1	A	245	PHE	6.1
1	B	173	SER	5.7
1	B	32	VAL	5.5
1	B	229	THR	4.7
1	B	203	ARG	4.6
1	A	296	VAL	4.4
1	A	197	PHE	4.4
1	A	272	GLY	4.3
1	A	310	VAL	4.3
1	A	99	GLY	4.1
1	A	214	HIS	4.1
1	A	329	PHE	4.0
1	B	346	THR	4.0
1	B	187	LEU	4.0
1	A	271	GLY	3.9
1	B	54	ILE	3.8
1	A	209	ALA	3.7
1	A	177	LEU	3.7
1	A	334	PHE	3.7
1	A	225	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	9	LEU	3.5
1	A	333	LEU	3.3
1	B	331	LEU	3.3
1	B	345	ALA	3.3
1	B	99	GLY	3.2
1	B	205	ALA	3.1
1	B	344	GLY	3.1
1	A	267	VAL	3.1
1	B	174	ILE	3.1
1	B	55	CYS	3.1
1	A	76	SER	3.0
1	A	208	LEU	3.0
1	B	176	GLY	3.0
1	B	96	LEU	3.0
1	B	329	PHE	3.0
1	A	328	SER	3.0
1	B	305	GLY	2.9
1	B	81	ILE	2.9
1	B	80	ILE	2.9
1	B	177	LEU	2.9
1	A	206	PHE	2.8
1	A	52	LEU	2.7
1	A	365	LEU	2.7
1	B	232	LEU	2.7
1	A	332	SER	2.7
1	A	229	THR	2.6
1	A	370	GLN	2.6
1	A	179	PHE	2.6
1	A	351	GLU	2.6
1	B	387	LEU	2.6
1	B	381	PRO	2.6
1	B	325	LEU	2.6
1	A	273	VAL	2.5
1	A	266	HIS	2.5
1	A	194	VAL	2.5
1	B	92	ALA	2.5
1	A	207	TYR	2.5
1	B	44	ILE	2.4
1	B	53	VAL	2.4
1	B	206	PHE	2.4
1	B	98	LEU	2.4
1	B	33	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	276	LEU	2.3
1	B	123	ASP	2.3
1	A	297	GLU	2.3
1	A	316	ALA	2.3
1	B	8	LEU	2.3
1	B	274	ILE	2.3
1	B	45	PHE	2.2
1	B	10	ILE	2.2
1	A	81	ILE	2.1
1	A	263	LEU	2.1
1	A	369	ARG	2.1
1	B	172	TRP	2.1
1	A	264	GLY	2.1
1	A	114	LEU	2.1
1	A	270	LEU	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 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.