Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2024 – 05:00 AM EST

PDB ID	:	3JV9
Title	:	The structure of a reduced form of OxyR from N. meningitidis
Authors	:	Sainsbury, S.; Ren, J.; Stuart, D.I.; Owens, R.J.; Oxford Protein Production Facility (OPPF)
Deposited on	:	2009-09-16
Resolution	:	2.39 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:

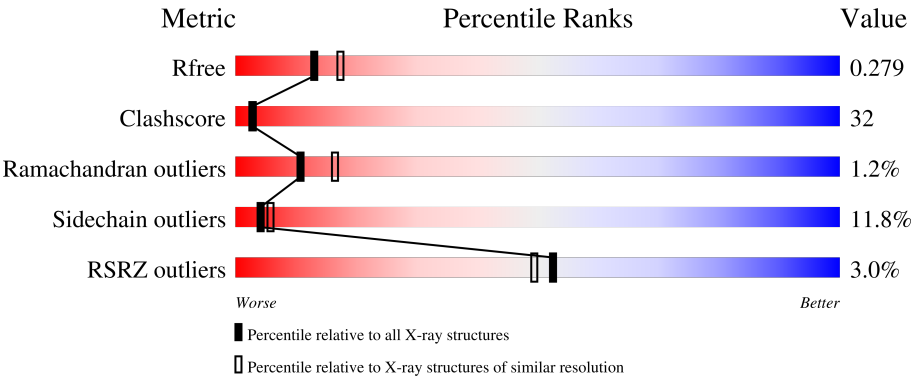
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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 <=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	219	2% 44% 46% 8%
1	B	219	4% 42% 45% 7% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3348 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 Transcriptional regulator, LysR family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	Se	0	0	0
			1671	1069	284	307	3	8			
1	B	204	Total	C	N	O	S	Se	0	0	0
			1580	1013	266	290	3	8			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

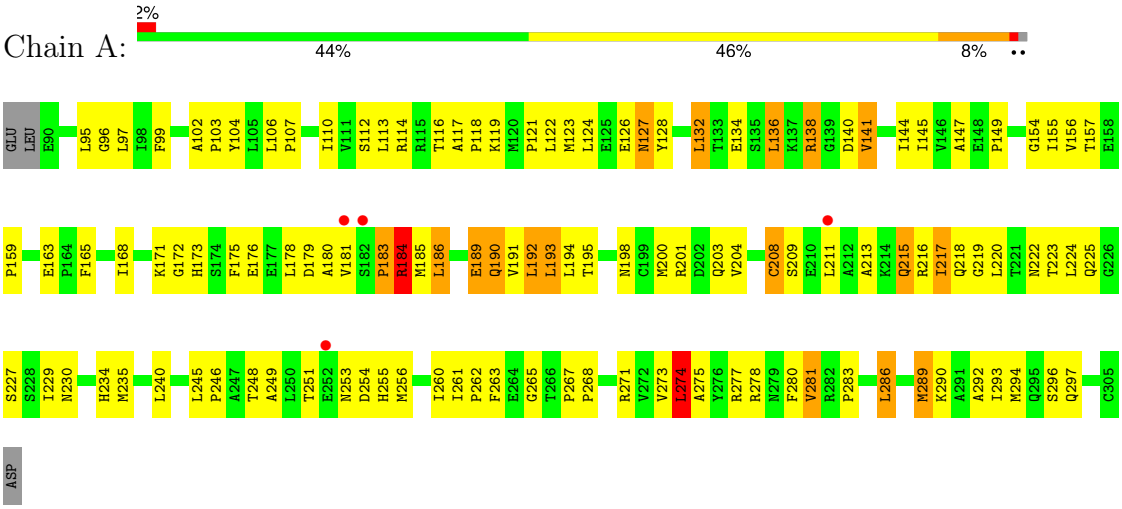
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		
3	B	49	Total	O	0	0
			49	49		

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.

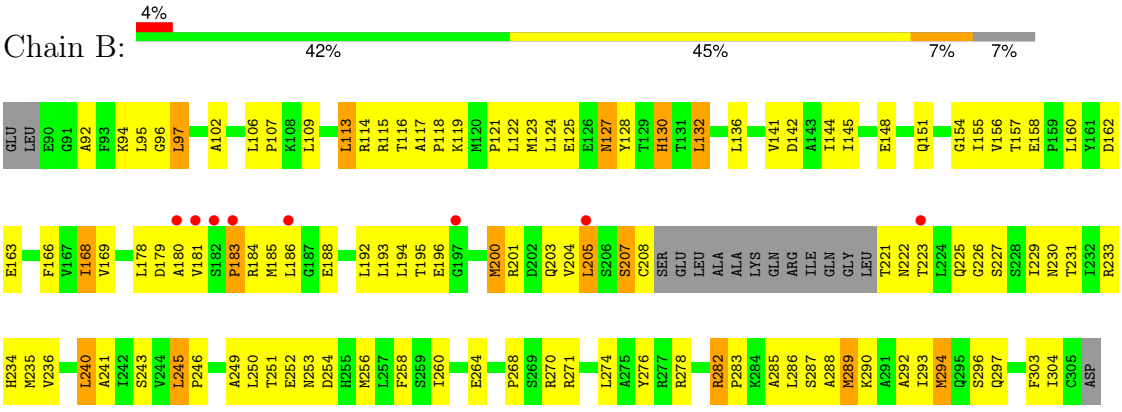
• Molecule 1: Transcriptional regulator, LysR family

Chain A:



• Molecule 1: Transcriptional regulator, LysR family

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.81Å 56.08Å 81.25Å 90.00° 104.91° 90.00°	Depositor
Resolution (Å)	29.80 – 2.39 29.80 – 2.39	Depositor EDS
% Data completeness (in resolution range)	95.5 (29.80-2.39) 95.9 (29.80-2.39)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_129)	Depositor
R, R_{free}	0.224 , 0.286 0.220 , 0.279	Depositor DCC
R_{free} test set	837 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.778	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3348	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.43	0/1696	0.66	1/2288 (0.0%)
1	B	0.43	0/1604	0.67	1/2164 (0.0%)
All	All	0.43	0/3300	0.66	2/4452 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	274	LEU	CA-CB-CG	5.27	127.42	115.30
1	B	245	LEU	CA-CB-CG	5.01	126.81	115.30

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	1671	0	1719	109	0
1	B	1580	0	1619	108	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	46	0	0	3	0
3	B	49	0	0	7	0
All	All	3348	0	3338	210	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 32.

All (210) 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:235:MSE:HE2	1:B:124:LEU:H	1.23	0.99
1:A:178:LEU:HD23	1:A:181:VAL:HB	1.46	0.95
1:B:127:ASN:HD22	1:B:128:TYR:H	1.06	0.94
1:A:127:ASN:HD22	1:A:128:TYR:H	0.94	0.92
1:A:280:PHE:HD2	1:A:286:LEU:HD22	1.38	0.88
1:A:134:GLU:O	1:A:138:ARG:HG2	1.73	0.88
1:A:127:ASN:HD22	1:A:128:TYR:N	1.71	0.88
1:A:194:LEU:HB3	1:A:198:ASN:HD22	1.41	0.86
1:A:192:LEU:HD13	1:A:224:LEU:HG	1.59	0.85
1:A:200:MSE:O	1:A:204:VAL:HG23	1.78	0.84
1:A:235:MSE:HE2	1:B:124:LEU:N	1.94	0.82
1:A:251:THR:HG22	1:A:253:ASN:H	1.43	0.82
1:A:200:MSE:SE	1:A:246:PRO:HG3	2.32	0.79
1:A:201:ARG:HH12	1:A:225:GLN:NE2	1.81	0.78
1:B:294:MSE:HE2	1:B:303:PHE:CD2	2.19	0.78
1:A:95:LEU:HD11	1:A:145:ILE:CD1	2.14	0.77
1:B:229:ILE:O	1:B:233:ARG:HG2	1.85	0.76
1:B:183:PRO:HD2	1:B:185:MSE:H	1.50	0.75
1:A:219:GLY:HA2	1:A:223:THR:HG23	1.69	0.74
1:B:168:ILE:HD11	1:B:243:SER:HB3	1.71	0.72
1:B:289:MSE:HA	1:B:289:MSE:HE3	1.72	0.71
1:A:184:ARG:HH12	1:A:209:SER:HB2	1.56	0.71
1:B:168:ILE:HD12	1:B:245:LEU:HG	1.71	0.71
1:A:95:LEU:HD11	1:A:145:ILE:HD11	1.73	0.70
1:B:127:ASN:HD22	1:B:128:TYR:N	1.88	0.70
1:B:181:VAL:HG12	1:B:185:MSE:SE	2.41	0.70
1:B:158:GLU:OE2	1:B:290:LYS:HD2	1.91	0.70
1:B:283:PRO:HD2	3:B:313:HOH:O	1.93	0.69
1:B:178:LEU:HB3	1:B:181:VAL:HB	1.75	0.68
1:B:195:THR:HG23	1:B:227:SER:HA	1.76	0.68
1:A:190:GLN:HG3	1:A:224:LEU:HD22	1.75	0.67
1:B:236:VAL:HG22	1:B:241:ALA:O	1.95	0.67
1:B:294:MSE:HE2	1:B:303:PHE:HD2	1.60	0.66
1:A:280:PHE:CD2	1:A:286:LEU:HD22	2.27	0.66
1:B:109:LEU:O	1:B:113:LEU:HB2	1.96	0.65
1:B:282:ARG:HD2	1:B:285:ALA:HB2	1.78	0.65
1:A:201:ARG:HH21	1:A:215:GLN:HE21	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ARG:HH12	1:A:225:GLN:HE22	1.44	0.64
1:A:230:ASN:O	1:A:234:HIS:CD2	2.51	0.63
1:A:171:LYS:NZ	1:A:255:HIS:O	2.31	0.63
1:A:230:ASN:O	1:A:234:HIS:HD2	1.81	0.63
1:A:127:ASN:ND2	1:A:128:TYR:H	1.80	0.63
1:A:235:MSE:CE	1:B:124:LEU:H	2.05	0.62
1:B:276:TYR:CE2	1:B:286:LEU:HD21	2.33	0.62
1:B:127:ASN:ND2	1:B:128:TYR:H	1.89	0.61
1:A:175:PHE:HA	1:A:178:LEU:HD13	1.81	0.61
1:A:184:ARG:HB2	1:A:208:CYS:SG	2.41	0.60
1:B:183:PRO:HD3	1:B:185:MSE:SE	2.51	0.60
1:A:290:LYS:O	1:A:294:MSE:HG2	2.01	0.60
1:A:192:LEU:CD1	1:A:224:LEU:HG	2.32	0.59
1:B:188:GLU:HB3	3:B:41:HOH:O	2.02	0.59
1:B:254:ASP:HB3	3:B:73:HOH:O	2.02	0.59
1:A:157:THR:HA	1:A:274:LEU:O	2.02	0.59
1:A:180:ALA:HB1	1:A:262:PRO:HB2	1.83	0.59
1:A:178:LEU:HD21	1:A:185:MSE:HE1	1.85	0.59
1:A:127:ASN:HB3	1:A:132:LEU:HD13	1.84	0.58
1:B:252:GLU:HG3	1:B:253:ASN:N	2.17	0.58
1:B:195:THR:HG23	1:B:226:GLY:O	2.04	0.57
1:A:112:SER:OG	1:A:296:SER:HA	2.04	0.57
1:A:183:PRO:HD2	1:A:185:MSE:HG2	1.85	0.57
1:B:116:THR:HG21	1:B:288:ALA:O	2.05	0.57
1:B:184:ARG:HD2	1:B:208:CYS:HA	1.85	0.57
1:B:96:GLY:O	1:B:144:ILE:HA	2.05	0.57
1:A:99:PHE:CE2	1:A:127:ASN:HA	2.39	0.57
1:A:190:GLN:HG3	1:A:224:LEU:CD2	2.34	0.57
1:B:203:GLN:NE2	3:B:1:HOH:O	2.38	0.57
1:B:162:ASP:OD2	1:B:304:ILE:HD11	2.04	0.56
1:B:130:HIS:H	1:B:130:HIS:CD2	2.23	0.56
1:A:165:PHE:HE1	1:A:200:MSE:SE	2.39	0.56
1:B:95:LEU:HD11	1:B:145:ILE:HD12	1.88	0.56
1:A:194:LEU:HB3	1:A:198:ASN:ND2	2.18	0.56
1:B:207:SER:OG	1:B:268:PRO:HB3	2.06	0.56
1:B:180:ALA:O	1:B:264:GLU:HB3	2.06	0.56
1:B:294:MSE:HA	1:B:294:MSE:CE	2.36	0.56
1:B:293:ILE:HG22	1:B:294:MSE:HE3	1.87	0.55
1:A:136:LEU:HD13	1:A:155:ILE:HD12	1.88	0.55
1:A:255:HIS:CE1	1:A:256:MSE:SE	3.10	0.55
1:B:230:ASN:ND2	1:B:234:HIS:CD2	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LEU:HD12	1:B:223:THR:HG21	1.88	0.54
1:A:123:MSE:HE2	3:A:45:HOH:O	2.06	0.54
1:B:222:ASN:HD22	1:B:222:ASN:N	2.04	0.54
1:A:224:LEU:HA	3:A:6:HOH:O	2.07	0.54
1:A:213:ALA:HA	1:A:216:ARG:HD2	1.89	0.54
1:B:296:SER:O	1:B:297:GLN:HB2	2.08	0.54
1:B:116:THR:HG22	1:B:288:ALA:HB1	1.89	0.54
1:A:263:PHE:CD2	1:A:268:PRO:HD2	2.44	0.53
1:A:145:ILE:N	1:A:145:ILE:HD12	2.22	0.53
1:B:245:LEU:HD12	1:B:250:LEU:HD21	1.91	0.52
1:B:154:GLY:C	1:B:155:ILE:HD12	2.30	0.52
1:B:183:PRO:HG2	1:B:185:MSE:HG3	1.92	0.52
1:A:107:PRO:HB2	3:A:52:HOH:O	2.10	0.52
1:B:192:LEU:CD1	1:B:241:ALA:HB3	2.39	0.51
1:A:218:GLN:O	1:A:222:ASN:HB3	2.10	0.51
1:A:168:ILE:HG21	1:A:245:LEU:HD12	1.91	0.51
1:A:260:ILE:HD12	1:A:260:ILE:N	2.25	0.51
1:B:92:ALA:HB1	1:B:123:MSE:HG3	1.92	0.51
1:B:290:LYS:O	1:B:290:LYS:HG2	2.11	0.51
1:A:172:GLY:H	1:A:176:GLU:CD	2.14	0.51
1:A:213:ALA:O	1:A:217:ILE:HG12	2.11	0.50
1:A:235:MSE:HE2	1:B:124:LEU:CA	2.41	0.50
1:B:178:LEU:HD13	1:B:181:VAL:HB	1.93	0.50
1:B:95:LEU:HD22	1:B:289:MSE:SE	2.60	0.50
1:A:281:VAL:C	1:A:283:PRO:HD3	2.31	0.50
1:B:136:LEU:HD12	1:B:141:VAL:O	2.12	0.50
1:B:195:THR:HG22	1:B:225:GLN:NE2	2.26	0.50
1:B:203:GLN:NE2	1:B:270:ARG:HD3	2.27	0.50
1:A:229:ILE:HG23	1:A:245:LEU:CD2	2.41	0.49
1:A:229:ILE:HG23	1:A:245:LEU:HD21	1.95	0.49
1:A:114:ARG:O	1:A:118:PRO:HG3	2.12	0.49
1:B:193:LEU:HD12	1:B:223:THR:CG2	2.43	0.49
1:A:201:ARG:HE	1:A:215:GLN:NE2	2.11	0.49
1:B:160:LEU:HB3	1:B:294:MSE:HE1	1.95	0.49
1:B:178:LEU:HB3	1:B:181:VAL:CB	2.42	0.49
1:A:97:LEU:O	1:A:126:GLU:HA	2.13	0.49
1:A:200:MSE:HA	1:A:203:GLN:NE2	2.29	0.48
1:B:271:ARG:HH21	1:B:304:ILE:HD11	1.77	0.48
1:B:195:THR:CG2	1:B:227:SER:HA	2.42	0.48
1:B:117:ALA:N	1:B:118:PRO:HD3	2.27	0.48
1:B:178:LEU:HB3	1:B:181:VAL:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HD23	1:A:292:ALA:HB2	1.95	0.48
1:B:157:THR:HA	1:B:274:LEU:O	2.14	0.48
1:B:160:LEU:HD22	1:B:293:ILE:HG21	1.96	0.48
1:B:200:MSE:HA	1:B:203:GLN:HG2	1.96	0.48
1:A:97:LEU:HD12	1:A:97:LEU:N	2.29	0.47
1:A:106:LEU:HD23	1:A:106:LEU:HA	1.57	0.47
1:A:168:ILE:HD13	1:A:245:LEU:CD1	2.43	0.47
1:A:265:GLY:O	1:A:267:PRO:HD3	2.13	0.47
1:A:184:ARG:C	1:A:186:LEU:H	2.17	0.47
1:B:294:MSE:HE2	1:B:303:PHE:CE2	2.49	0.47
1:A:183:PRO:HD2	1:A:185:MSE:H	1.79	0.47
1:A:260:ILE:C	1:A:261:ILE:HD12	2.34	0.47
1:B:195:THR:HG22	1:B:225:GLN:HE21	1.79	0.47
1:A:154:GLY:HA2	1:A:278:ARG:NH1	2.29	0.47
1:B:179:ASP:HB2	3:B:307:HOH:O	2.14	0.47
1:A:136:LEU:HD22	1:A:277:ARG:HG3	1.97	0.46
1:A:178:LEU:HD21	1:A:185:MSE:CE	2.45	0.46
1:B:271:ARG:HH21	1:B:304:ILE:CD1	2.29	0.46
1:A:235:MSE:HG3	1:B:124:LEU:HD12	1.97	0.46
1:B:245:LEU:HD12	1:B:250:LEU:CD2	2.45	0.46
1:B:294:MSE:HA	1:B:294:MSE:HE3	1.98	0.46
1:A:201:ARG:HH21	1:A:215:GLN:NE2	2.11	0.46
1:B:94:LYS:O	1:B:142:ASP:HB2	2.16	0.46
1:A:159:PRO:HA	1:A:273:VAL:HG12	1.98	0.46
1:B:230:ASN:ND2	1:B:234:HIS:HD2	2.13	0.46
1:A:136:LEU:HA	1:A:141:VAL:HG12	1.98	0.45
1:B:282:ARG:HD2	1:B:285:ALA:CB	2.45	0.45
1:A:200:MSE:HG2	1:A:203:GLN:NE2	2.31	0.45
1:A:254:ASP:C	1:A:256:MSE:H	2.20	0.45
1:B:246:PRO:HD2	1:B:249:ALA:HB3	1.98	0.45
1:A:124:LEU:HD12	1:B:235:MSE:HG3	1.98	0.45
1:B:156:VAL:HB	1:B:276:TYR:CE1	2.50	0.45
1:A:168:ILE:HD13	1:A:245:LEU:HD12	1.99	0.45
1:B:293:ILE:HG22	1:B:294:MSE:CE	2.47	0.44
1:A:117:ALA:N	1:A:118:PRO:HD3	2.31	0.44
1:A:173:HIS:NE2	1:A:189:GLU:OE2	2.50	0.44
1:B:169:VAL:O	1:B:258:PHE:HB2	2.17	0.44
1:A:147:ALA:HA	1:A:271:ARG:O	2.18	0.44
1:B:222:ASN:N	1:B:222:ASN:ND2	2.65	0.44
1:A:195:THR:OG1	1:A:227:SER:HA	2.16	0.44
1:B:252:GLU:CG	1:B:253:ASN:N	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:MSE:CG	1:B:124:LEU:HD12	2.48	0.44
1:B:163:GLU:OE1	1:B:246:PRO:HB2	2.18	0.44
1:A:156:VAL:O	1:A:275:ALA:HA	2.18	0.43
1:B:204:VAL:HG23	1:B:205:LEU:N	2.33	0.43
1:B:122:LEU:HD23	1:B:122:LEU:HA	1.63	0.43
1:A:119:LYS:O	1:A:121:PRO:HD3	2.18	0.43
1:B:96:GLY:HA2	1:B:125:GLU:O	2.19	0.43
1:A:261:ILE:HA	1:A:262:PRO:HD3	1.78	0.43
1:B:132:LEU:HD12	1:B:132:LEU:HA	1.82	0.43
1:B:168:ILE:HD13	1:B:243:SER:O	2.19	0.43
1:B:194:LEU:HD12	1:B:194:LEU:H	1.84	0.43
1:A:138:ARG:HD3	1:A:140:ASP:OD2	2.19	0.42
1:A:189:GLU:O	1:A:191:VAL:HG23	2.18	0.42
1:A:119:LYS:O	1:A:119:LYS:HG3	2.19	0.42
1:A:186:LEU:HD21	1:A:208:CYS:SG	2.59	0.42
1:A:254:ASP:C	1:A:256:MSE:N	2.72	0.42
1:A:289:MSE:O	1:A:293:ILE:HG13	2.19	0.42
1:B:119:LYS:O	1:B:121:PRO:HD3	2.20	0.42
1:B:200:MSE:O	1:B:204:VAL:HG13	2.19	0.42
1:B:201:ARG:O	1:B:205:LEU:HB3	2.20	0.42
1:A:102:ALA:N	1:A:103:PRO:CD	2.83	0.42
1:B:256:MSE:H	1:B:256:MSE:HG2	1.71	0.42
1:B:289:MSE:CE	1:B:292:ALA:HB3	2.50	0.42
1:B:97:LEU:HB2	1:B:102:ALA:HB2	2.01	0.42
1:A:296:SER:O	1:A:297:GLN:HB2	2.20	0.42
1:B:184:ARG:HB3	1:B:208:CYS:SG	2.60	0.42
1:A:209:SER:C	1:A:211:LEU:N	2.73	0.41
1:B:184:ARG:C	1:B:186:LEU:H	2.22	0.41
1:A:110:ILE:HD13	1:A:110:ILE:HA	1.90	0.41
1:A:186:LEU:H	1:A:186:LEU:CD2	2.32	0.41
1:A:203:GLN:HE21	1:A:203:GLN:HB2	1.64	0.41
1:A:99:PHE:CZ	1:A:127:ASN:HA	2.56	0.41
1:A:163:GLU:OE1	1:A:248:THR:HG23	2.20	0.41
1:B:223:THR:HG23	3:B:71:HOH:O	2.19	0.41
1:A:208:CYS:CB	1:A:211:LEU:HD12	2.50	0.41
1:B:294:MSE:HE3	1:B:294:MSE:CA	2.51	0.41
1:A:104:TYR:CE1	1:A:249:ALA:HA	2.55	0.41
1:B:106:LEU:O	1:B:107:PRO:C	2.57	0.41
1:B:231:THR:O	1:B:235:MSE:HG3	2.21	0.41
1:A:156:VAL:CG2	1:A:278:ARG:HG3	2.51	0.41
1:A:219:GLY:CA	1:A:223:THR:HG23	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LEU:HD12	1:B:97:LEU:N	2.35	0.41
1:B:114:ARG:HG3	3:B:80:HOH:O	2.20	0.41
1:B:240:LEU:O	1:B:241:ALA:HB2	2.21	0.41
1:B:109:LEU:HD12	1:B:109:LEU:HA	1.85	0.41
1:B:203:GLN:HE22	1:B:270:ARG:HD3	1.85	0.41
1:B:166:PHE:HB3	1:B:260:ILE:HG23	2.03	0.40
1:A:96:GLY:O	1:A:144:ILE:HA	2.22	0.40
1:A:281:VAL:O	1:A:283:PRO:HD3	2.21	0.40
1:A:193:LEU:N	1:A:193:LEU:CD2	2.83	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	214/219 (98%)	195 (91%)	15 (7%)	4 (2%)	6 8
1	B	200/219 (91%)	183 (92%)	16 (8%)	1 (0%)	25 38
All	All	414/438 (94%)	378 (91%)	31 (8%)	5 (1%)	11 16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	ASP
1	B	183	PRO
1	A	183	PRO
1	A	184	ARG
1	A	217	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	187/182 (103%)	165 (88%)	22 (12%)	4 6
1	B	178/182 (98%)	157 (88%)	21 (12%)	4 6
All	All	365/364 (100%)	322 (88%)	43 (12%)	4 6

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	THR
1	A	122	LEU
1	A	127	ASN
1	A	132	LEU
1	A	136	LEU
1	A	138	ARG
1	A	141	VAL
1	A	149	PRO
1	A	184	ARG
1	A	186	LEU
1	A	189	GLU
1	A	190	GLN
1	A	192	LEU
1	A	193	LEU
1	A	208	CYS
1	A	215	GLN
1	A	220	LEU
1	A	240	LEU
1	A	274	LEU
1	A	281	VAL
1	A	286	LEU
1	A	289	MSE
1	B	97	LEU
1	B	113	LEU
1	B	115	ARG
1	B	127	ASN
1	B	130	HIS

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Mol	Chain	Res	Type
1	B	132	LEU
1	B	148	GLU
1	B	151	GLN
1	B	168	ILE
1	B	196	GLU
1	B	200	MSE
1	B	205	LEU
1	B	207	SER
1	B	221	THR
1	B	240	LEU
1	B	251	THR
1	B	278	ARG
1	B	282	ARG
1	B	287	SER
1	B	289	MSE
1	B	294	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	190	GLN
1	A	198	ASN
1	A	203	GLN
1	A	215	GLN
1	A	222	ASN
1	A	225	GLN
1	A	234	HIS
1	B	127	ASN
1	B	203	GLN
1	B	222	ASN
1	B	230	ASN
1	B	234	HIS
1	B	255	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	208/219 (94%)	0.35	4 (1%) 66 62	30, 49, 86, 101	0
1	B	196/219 (89%)	0.39	8 (4%) 42 39	31, 48, 83, 120	0
All	All	404/438 (92%)	0.37	12 (2%) 52 49	30, 48, 85, 120	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	180	ALA	6.2
1	B	183	PRO	3.0
1	B	182	SER	2.9
1	A	182	SER	2.8
1	B	181	VAL	2.5
1	A	181	VAL	2.5
1	B	186	LEU	2.4
1	A	211	LEU	2.4
1	B	223	THR	2.3
1	A	252	GLU	2.2
1	B	197	GLY	2.1
1	B	205	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	A	307	1/1	0.78	0.16	68,68,68,68	0
2	CL	B	78	1/1	0.92	0.07	54,54,54,54	0

6.5 Other polymers

There are no such residues in this entry.