



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:03 AM GMT

PDB ID : 2VRC
Title : CRYSTAL STRUCTURE OF THE CITROBACTER SP. TRIPHENYL-
METHANE REDUCTASE COMPLEXED WITH NADP(H)
Authors : Kim, Y.; Park, H.J.; Kwak, S.N.; Lee, J.S.; Oh, T.K.; Kim, M.H.
Deposited on : 2008-03-31
Resolution : 2.50 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

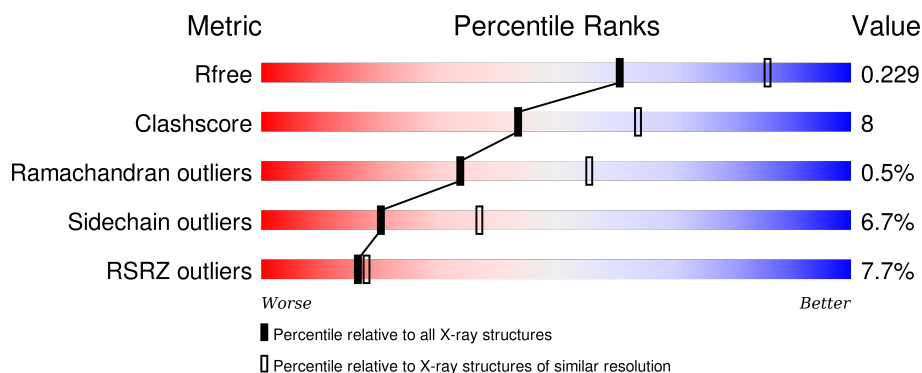
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	287	 3% 85% 11% ..
1	B	287	 3% 82% 16% ..
1	C	287	 14% 74% 21% ..
2	D	287	 10% 81% 16% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8912 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 TRIPHENYLMETHANE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	Se	0	1	0
			2170	1379	367	422	2			
1	B	285	Total	C	N	O	Se	0	1	0
			2168	1376	367	423	2			
1	C	285	Total	C	N	O	Se	0	0	0
			2162	1373	366	421	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PHE	MET	CONFLICT	UNP Q2TNI4
A	21	MSE	LEU	ENGINEERED MUTATION	UNP Q2TNI4
A	22	ALA	LYS	ENGINEERED MUTATION	UNP Q2TNI4
A	23	ALA	LYS	ENGINEERED MUTATION	UNP Q2TNI4
A	156	THR	ILE	CONFLICT	UNP Q2TNI4
A	235	MSE	LEU	ENGINEERED MUTATION	UNP Q2TNI4
B	1	PHE	MET	CONFLICT	UNP Q2TNI4
B	21	MSE	LEU	ENGINEERED MUTATION	UNP Q2TNI4
B	22	ALA	LYS	ENGINEERED MUTATION	UNP Q2TNI4
B	23	ALA	LYS	ENGINEERED MUTATION	UNP Q2TNI4
B	156	THR	ILE	CONFLICT	UNP Q2TNI4
B	235	MSE	LEU	ENGINEERED MUTATION	UNP Q2TNI4
C	1	PHE	MET	CONFLICT	UNP Q2TNI4
C	21	MSE	LEU	ENGINEERED MUTATION	UNP Q2TNI4
C	22	ALA	LYS	ENGINEERED MUTATION	UNP Q2TNI4
C	23	ALA	LYS	ENGINEERED MUTATION	UNP Q2TNI4
C	156	THR	ILE	CONFLICT	UNP Q2TNI4
C	235	MSE	LEU	ENGINEERED MUTATION	UNP Q2TNI4

- Molecule 2 is a protein called TRIPHENYLMETHANE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	285	Total 2170	C 1376	N 368	O 424	Se 2	0	1	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	PHE	MET	CONFLICT	UNP Q2TNI4
D	21	MSE	LEU	ENGINEERED MUTATION	UNP Q2TNI4
D	22	ALA	LYS	ENGINEERED MUTATION	UNP Q2TNI4
D	23	ALA	LYS	ENGINEERED MUTATION	UNP Q2TNI4
D	128	THR	ILE	CONFLICT	UNP Q2TNI4
D	156	THR	ILE	CONFLICT	UNP Q2TNI4
D	235	MSE	LEU	ENGINEERED MUTATION	UNP Q2TNI4

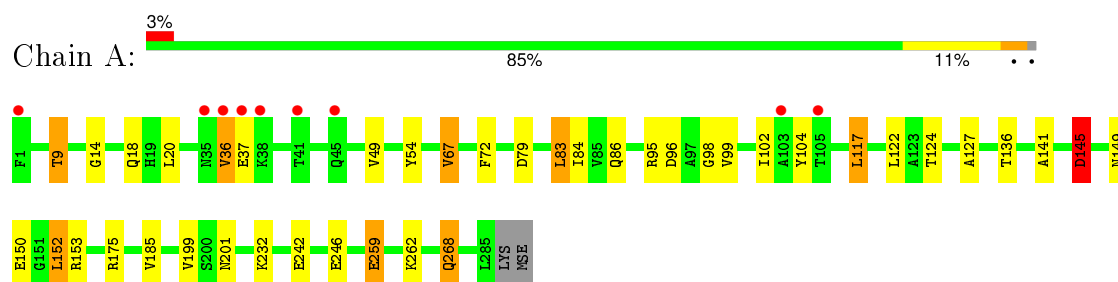
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	76	Total 76	O 76	0	0
3	B	80	Total 80	O 80	0	0
3	C	34	Total 34	O 34	0	0
3	D	52	Total 52	O 52	0	0

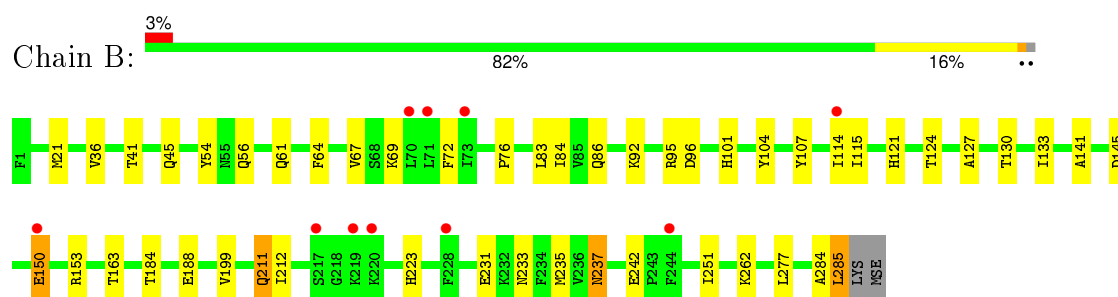
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

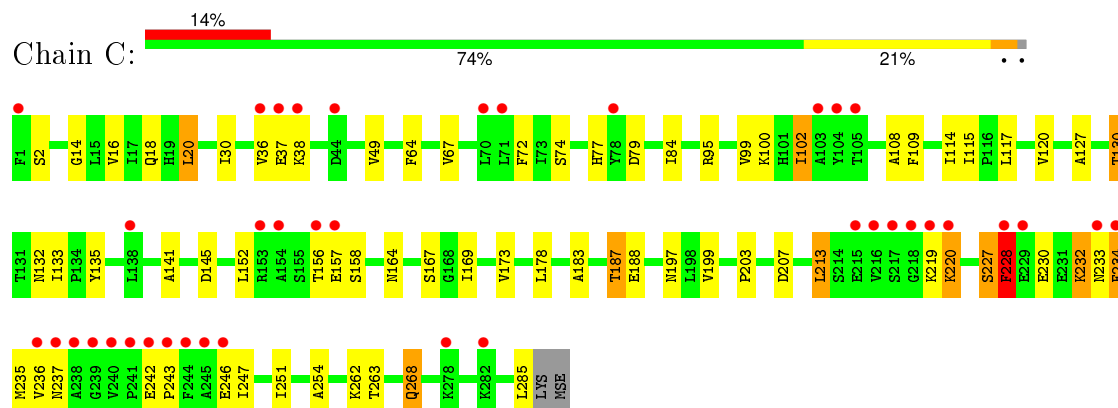
• Molecule 1: TRIPHENYLMETHANE REDUCTASE



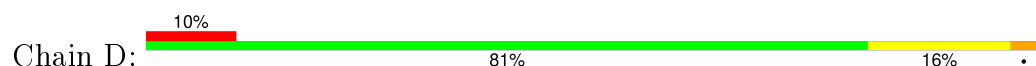
• Molecule 1: TRIPHENYLMETHANE REDUCTASE

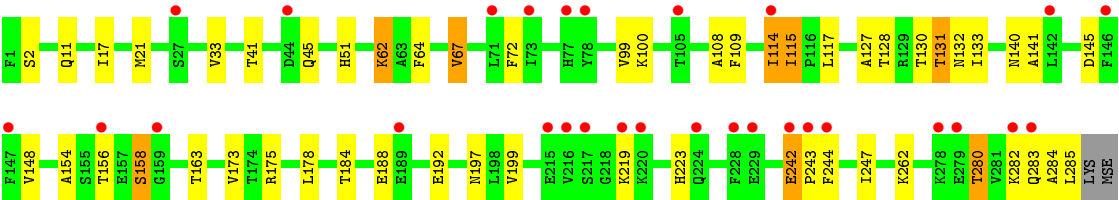


• Molecule 1: TRIPHENYLMETHANE REDUCTASE



• Molecule 2: TRIPHENYLMETHANE REDUCTASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.96Å 76.95Å 272.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.36 – 2.50 29.15 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.36-2.50) 95.9 (29.15-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	82.19 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.239 0.183 , 0.229	Depositor DCC
R_{free} test set	2747 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.9	EDS
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 53943 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8912	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.69	0/2208	0.77	4/3003 (0.1%)
1	B	0.65	0/2206	0.68	0/3000
1	C	0.58	1/2200 (0.0%)	0.68	1/2992 (0.0%)
2	D	0.60	0/2208	0.66	0/3003
All	All	0.63	1/8822 (0.0%)	0.70	5/11998 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	37	GLU	CB-CG	-7.27	1.38	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	228	PHE	CB-CA-C	-13.66	83.07	110.40
1	A	117[A]	LEU	CA-CB-CG	7.76	133.15	115.30
1	A	117[B]	LEU	CA-CB-CG	7.76	133.15	115.30
1	A	79	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	145	ASP	CB-CG-OD1	-5.34	113.49	118.30

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	2170	0	2171	25	0
1	B	2168	0	2165	41	0
1	C	2162	0	2161	47	0
2	D	2170	0	2164	41	0
3	A	76	0	0	2	0
3	B	80	0	0	4	0
3	C	34	0	0	1	0
3	D	52	0	0	2	0
All	All	8912	0	8661	141	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 8.

All (141) 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:C:228:PHE:O	1:C:228:PHE:CD2	1.69	1.45
1:B:284:ALA:O	1:B:285:LEU:HD12	1.41	1.20
1:B:284:ALA:C	1:B:285:LEU:HD12	1.76	1.03
1:B:284:ALA:C	1:B:285:LEU:CD1	2.30	1.00
1:C:228:PHE:HD2	1:C:228:PHE:O	1.21	0.94
1:A:84:ILE:HD13	1:B:127:ALA:HA	1.52	0.91
1:C:228:PHE:CD2	1:C:228:PHE:C	2.46	0.89
1:A:150:GLU:HG2	1:A:153:ARG:HH22	1.38	0.88
1:B:231:GLU:HG3	1:B:235:MSE:HE2	1.60	0.83
1:C:232:LYS:HE2	1:C:246:GLU:HG2	1.63	0.79
1:C:109:PHE:H	1:C:197:ASN:ND2	1.80	0.79
2:D:148:VAL:HG11	2:D:280:THR:HG22	1.70	0.74
1:B:284:ALA:C	1:B:285:LEU:HD13	2.07	0.74
1:C:228:PHE:CG	1:C:228:PHE:O	2.31	0.72
1:B:21:MSE:HE1	1:B:45:GLN:HE21	1.55	0.71
1:A:98:GLY:HA3	2:D:62:LYS:HG3	1.72	0.71
1:B:233:ASN:O	1:B:237:ASN:HB2	1.91	0.71
1:B:76:PRO:HD2	3:B:2022:HOH:O	1.91	0.71
2:D:64:PHE:O	2:D:67:VAL:HG13	1.89	0.71
1:B:150:GLU:O	1:B:153:ARG:HG3	1.91	0.71
1:B:114:ILE:HA	3:B:2032:HOH:O	1.90	0.70
1:B:284:ALA:O	1:B:285:LEU:CD1	2.30	0.70
1:B:285:LEU:N	1:B:285:LEU:CD1	2.52	0.69
2:D:109:PHE:H	2:D:197:ASN:ND2	1.90	0.69
2:D:192:GLU:HG3	3:D:2039:HOH:O	1.92	0.69
1:C:183:ALA:O	1:C:187:THR:HB	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:GLU:HG2	1:C:243:PRO:HD3	1.76	0.67
2:D:131:THR:HG22	2:D:133:ILE:H	1.59	0.67
1:C:84:ILE:CD1	2:D:130:THR:HG21	2.26	0.65
1:C:227:SER:HB3	1:C:230:GLU:HB2	1.76	0.65
1:A:84:ILE:CD1	1:B:127:ALA:HA	2.24	0.65
1:C:84:ILE:HD13	2:D:127:ALA:HA	1.79	0.64
1:B:141:ALA:HB2	1:B:199:VAL:HG12	1.80	0.64
1:B:64:PHE:O	1:B:67:VAL:HG13	1.97	0.63
1:C:2:SER:HB2	1:C:30:ILE:CD1	2.29	0.63
2:D:51:HIS:ND1	2:D:62:LYS:NZ	2.46	0.63
1:B:92:LYS:NZ	1:B:96:ASP:OD2	2.32	0.62
2:D:128:THR:O	2:D:131:THR:HB	1.99	0.62
1:C:247:ILE:O	1:C:251:ILE:HG12	1.98	0.62
1:C:141:ALA:HB2	1:C:199:VAL:HG12	1.81	0.62
2:D:132:ASN:ND2	3:D:2028:HOH:O	2.31	0.61
1:A:145:ASP:OD1	1:A:175:ARG:HD2	2.00	0.61
1:C:173:VAL:HG22	1:C:178:LEU:HG	1.83	0.60
1:C:77:HIS:HD2	1:C:79:ASP:H	1.49	0.60
1:A:136:THR:HG21	1:A:185:VAL:HG11	1.83	0.60
1:C:227:SER:O	1:C:228:PHE:HB2	2.02	0.59
1:C:227:SER:O	1:C:228:PHE:CB	2.51	0.58
1:C:132:ASN:ND2	3:C:2022:HOH:O	2.36	0.58
1:A:67:VAL:HG22	1:A:99:VAL:HG22	1.85	0.58
1:B:285:LEU:N	1:B:285:LEU:HD13	2.18	0.58
2:D:131:THR:CG2	2:D:133:ILE:H	2.17	0.57
1:A:150:GLU:HG2	1:A:153:ARG:NH2	2.15	0.56
1:C:233:ASN:C	1:C:235:MSE:H	2.09	0.56
1:C:84:ILE:HD11	2:D:130:THR:HG21	1.86	0.56
2:D:67:VAL:HG22	2:D:99:VAL:HG22	1.88	0.56
1:C:14:GLY:O	1:C:18:GLN:HG2	2.05	0.56
1:C:228:PHE:HD2	1:C:228:PHE:C	1.97	0.56
1:A:36:VAL:HG22	3:A:2006:HOH:O	2.06	0.55
1:B:95:ARG:HD2	1:B:95:ARG:C	2.27	0.55
1:A:104:TYR:CE1	1:A:124:THR:HG21	2.42	0.54
2:D:148:VAL:HG11	2:D:280:THR:CG2	2.38	0.54
2:D:243:PRO:O	2:D:247:ILE:HG12	2.08	0.53
1:B:212:ILE:HD12	1:B:277:LEU:HD23	1.91	0.53
1:C:64:PHE:O	1:C:67:VAL:HG13	2.08	0.53
2:D:108:ALA:HA	2:D:197:ASN:HD22	1.73	0.52
1:C:219:LYS:HG2	1:C:220:LYS:HG2	1.92	0.52
1:C:84:ILE:HD12	2:D:130:THR:HG21	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:TYR:HB3	1:A:86:GLN:HB3	1.92	0.52
1:B:69:LYS:HG2	1:B:101:HIS:HB3	1.90	0.51
1:B:163:THR:OG1	1:B:223:HIS:HE1	1.93	0.51
1:A:84:ILE:HD11	1:B:130:THR:HG21	1.93	0.51
2:D:17:ILE:O	2:D:21:MSE:HG2	2.10	0.51
2:D:163:THR:OG1	2:D:223:HIS:HE1	1.92	0.51
1:C:16:VAL:HG12	1:C:20:LEU:HD22	1.92	0.51
1:B:21:MSE:HE1	1:B:45:GLN:NE2	2.24	0.51
1:C:102:ILE:O	1:C:135:TYR:HA	2.11	0.51
2:D:114:ILE:HG13	2:D:114:ILE:O	2.11	0.51
2:D:282:LYS:C	2:D:284:ALA:H	2.14	0.50
1:A:141:ALA:HB2	1:A:199:VAL:HG12	1.94	0.49
1:A:36:VAL:HG12	1:A:49:VAL:HG12	1.93	0.49
2:D:141:ALA:HB2	2:D:199:VAL:HG12	1.94	0.49
1:B:184:THR:O	1:B:188:GLU:HG2	2.13	0.48
1:A:96:ASP:O	2:D:62:LYS:HD2	2.14	0.48
1:A:9:THR:HB	3:A:2001:HOH:O	2.13	0.48
1:A:127:ALA:HA	1:B:84:ILE:HD13	1.95	0.48
1:A:232:LYS:NZ	1:A:246:GLU:HG2	2.27	0.48
1:C:127:ALA:O	1:C:130:THR:HB	2.13	0.48
2:D:156:THR:O	2:D:219:LYS:HD2	2.14	0.48
1:B:233:ASN:HD22	2:D:11:GLN:NE2	2.12	0.47
2:D:115:ILE:HG22	2:D:117:LEU:H	1.79	0.47
2:D:21:MSE:HE1	2:D:45:GLN:NE2	2.30	0.47
1:B:237:ASN:ND2	2:D:175:ARG:HH22	2.13	0.47
2:D:184:THR:O	2:D:188:GLU:HG2	2.15	0.47
2:D:131:THR:HG23	2:D:133:ILE:HG13	1.96	0.46
1:C:227:SER:HB3	1:C:230:GLU:CB	2.44	0.46
1:B:104:TYR:CZ	1:B:124:THR:HG21	2.50	0.46
1:C:152:LEU:HD13	1:C:213:LEU:HD11	1.97	0.46
1:C:108:ALA:HA	1:C:197:ASN:HD22	1.81	0.46
1:B:211:GLN:HA	1:B:211:GLN:HE21	1.80	0.46
2:D:242:GLU:HG3	2:D:243:PRO:HD3	1.98	0.46
1:B:251:ILE:HA	1:B:251:ILE:HD13	1.81	0.45
2:D:140:ASN:HB3	2:D:178:LEU:HD13	1.99	0.45
1:B:107:TYR:HB2	1:B:121:HIS:CD2	2.51	0.45
2:D:284:ALA:O	2:D:285:LEU:HD12	2.15	0.45
1:C:115:ILE:HD11	1:C:254:ALA:HB2	1.98	0.45
1:C:173:VAL:CG2	1:C:178:LEU:HG	2.47	0.45
1:B:61:GLN:O	3:B:2017:HOH:O	2.20	0.45
1:C:95:ARG:HA	1:C:133:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ILE:HG23	1:C:203:PRO:HB2	1.99	0.44
1:B:54:TYR:HB3	1:B:86:GLN:HB3	2.00	0.44
2:D:244:PHE:N	2:D:244:PHE:CD1	2.85	0.44
1:A:259:GLU:O	1:A:259:GLU:HG3	2.17	0.44
1:B:114:ILE:C	1:B:115:ILE:HG12	2.36	0.44
2:D:131:THR:HG23	2:D:133:ILE:CG1	2.48	0.44
1:C:2:SER:HB2	1:C:30:ILE:HD12	2.00	0.43
1:A:95:ARG:HD2	1:A:95:ARG:C	2.39	0.43
1:B:104:TYR:CE1	1:B:124:THR:HG21	2.53	0.43
1:A:14:GLY:O	1:A:18:GLN:HG2	2.17	0.43
1:C:262:LYS:HG3	1:C:263:THR:N	2.32	0.43
1:C:114:ILE:HD11	1:C:254:ALA:HA	2.00	0.43
1:C:67:VAL:HG22	1:C:99:VAL:HG22	2.00	0.43
1:C:268:GLN:HB3	1:C:268:GLN:HE21	1.62	0.43
1:A:149:ASN:O	1:A:152:LEU:HB2	2.19	0.43
2:D:173:VAL:CG2	2:D:178:LEU:HG	2.49	0.42
1:B:262:LYS:HE2	1:B:262:LYS:HB3	1.90	0.42
1:C:102:ILE:O	1:C:102:ILE:CG2	2.68	0.42
1:A:84:ILE:HD13	1:B:127:ALA:CA	2.36	0.42
2:D:173:VAL:HG23	2:D:178:LEU:HG	2.00	0.42
1:B:83:LEU:HA	1:B:83:LEU:HD12	1.87	0.42
1:C:102:ILE:O	1:C:102:ILE:HG23	2.20	0.42
2:D:154:ALA:O	2:D:158:SER:HB3	2.20	0.42
1:A:268:GLN:HE21	1:A:268:GLN:HB3	1.52	0.41
1:C:109:PHE:H	1:C:197:ASN:HD22	1.62	0.41
1:B:61:GLN:CG	3:B:2027:HOH:O	2.68	0.41
1:C:36:VAL:HG23	1:C:49:VAL:HG12	2.02	0.41
1:C:117:LEU:O	1:C:120:VAL:HB	2.21	0.41
1:A:83:LEU:HA	1:A:83:LEU:HD12	1.89	0.41
2:D:41:THR:O	2:D:45:GLN:HG3	2.21	0.41
1:C:100:LYS:HA	1:C:100:LYS:HD3	1.96	0.41
1:B:95:ARG:HA	1:B:133:ILE:HD11	2.02	0.40
2:D:131:THR:O	2:D:132:ASN:HB2	2.21	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	284/287 (99%)	278 (98%)	6 (2%)	0	100	100
1	B	284/287 (99%)	277 (98%)	7 (2%)	0	100	100
1	C	283/287 (99%)	264 (93%)	14 (5%)	5 (2%)	11	18
2	D	284/287 (99%)	273 (96%)	10 (4%)	1 (0%)	39	61
All	All	1135/1148 (99%)	1092 (96%)	37 (3%)	6 (0%)	34	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	228	PHE
1	C	156	THR
1	C	220	LYS
1	C	234	PHE
1	C	38	LYS
2	D	283	GLN

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	231/229 (101%)	213 (92%)	18 (8%)	16	29
1	B	231/229 (101%)	221 (96%)	10 (4%)	35	61
1	C	230/229 (100%)	209 (91%)	21 (9%)	12	22
2	D	231/229 (101%)	217 (94%)	14 (6%)	23	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	923/916 (101%)	860 (93%)	63 (7%)	20	36

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	20	LEU
1	A	36	VAL
1	A	37	GLU
1	A	67	VAL
1	A	72	PHE
1	A	83	LEU
1	A	102	ILE
1	A	117[A]	LEU
1	A	117[B]	LEU
1	A	122	LEU
1	A	145	ASP
1	A	152	LEU
1	A	201	ASN
1	A	242	GLU
1	A	259	GLU
1	A	262	LYS
1	A	268	GLN
1	B	36	VAL
1	B	41	THR
1	B	56	GLN
1	B	72	PHE
1	B	145	ASP
1	B	150	GLU
1	B	211	GLN
1	B	237	ASN
1	B	242	GLU
1	B	285	LEU
1	C	20	LEU
1	C	72	PHE
1	C	74	SER
1	C	102	ILE
1	C	130	THR
1	C	145	ASP
1	C	157	GLU
1	C	158	SER
1	C	164	ASN

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Mol	Chain	Res	Type
1	C	167	SER
1	C	187	THR
1	C	188	GLU
1	C	207	ASP
1	C	213	LEU
1	C	227	SER
1	C	232	LYS
1	C	234	PHE
1	C	236	VAL
1	C	237	ASN
1	C	268	GLN
1	C	285	LEU
2	D	2	SER
2	D	33	VAL
2	D	62	LYS
2	D	67	VAL
2	D	72	PHE
2	D	100	LYS
2	D	114	ILE
2	D	115	ILE
2	D	131	THR
2	D	145	ASP
2	D	158	SER
2	D	242	GLU
2	D	262	LYS
2	D	280	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	86	GLN
1	A	101	HIS
1	A	176	ASN
1	A	268	GLN
1	A	283	GLN
1	B	18	GLN
1	B	28	GLN
1	B	45	GLN
1	B	55	ASN
1	B	86	GLN
1	B	211	GLN

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Mol	Chain	Res	Type
1	B	223	HIS
1	B	237	ASN
1	C	61	GLN
1	C	77	HIS
1	C	86	GLN
1	C	164	ASN
1	C	197	ASN
1	C	223	HIS
1	C	233	ASN
1	C	237	ASN
1	C	268	GLN
2	D	11	GLN
2	D	18	GLN
2	D	28	GLN
2	D	45	GLN
2	D	55	ASN
2	D	56	GLN
2	D	86	GLN
2	D	197	ASN
2	D	223	HIS

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 carbohydrates 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	283/287 (98%)	0.23	9 (3%) 51 56	23, 34, 50, 61	0
1	B	283/287 (98%)	0.21	10 (3%) 48 53	23, 35, 52, 60	0
1	C	283/287 (98%)	0.60	39 (13%) 4 4	35, 46, 77, 88	0
2	D	283/287 (98%)	0.39	29 (10%) 9 9	28, 41, 63, 67	0
All	All	1132/1148 (98%)	0.36	87 (7%) 16 18	23, 39, 63, 88	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	243	PRO	6.8
2	D	216	VAL	6.6
1	C	244	PHE	5.9
1	C	242	GLU	5.4
1	A	37	GLU	4.9
1	C	157	GLU	4.6
1	C	234	PHE	4.6
1	C	238	ALA	4.3
1	C	44	ASP	4.1
2	D	114	ILE	4.1
2	D	243	PRO	4.1
1	C	282	LYS	4.0
2	D	78	TYR	3.9
1	C	78	TYR	3.9
1	C	37	GLU	3.8
1	C	219	LYS	3.8
2	D	224	GLN	3.8
1	C	220	LYS	3.6
2	D	77	HIS	3.5
1	C	229	GLU	3.5
1	C	239	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	217	SER	3.4
1	A	35	ASN	3.3
2	D	220	LYS	3.2
1	C	240	VAL	3.2
1	A	38	LYS	3.1
1	C	216	VAL	3.1
1	C	38	LYS	3.1
2	D	229	GLU	3.1
1	C	246	GLU	3.1
1	C	228	PHE	3.0
2	D	244	PHE	3.0
1	A	36	VAL	2.9
1	B	114	ILE	2.9
1	C	153	ARG	2.9
1	C	218	GLY	2.8
1	C	237	ASN	2.8
1	B	244	PHE	2.8
1	B	220	LYS	2.7
2	D	219	LYS	2.7
1	C	233	ASN	2.6
2	D	159	GLY	2.6
1	C	236	VAL	2.6
2	D	215	GLU	2.5
1	C	241	PRO	2.5
1	A	1	PHE	2.5
1	C	104	TYR	2.5
2	D	44	ASP	2.5
1	C	138	LEU	2.5
1	C	1	PHE	2.4
2	D	242	GLU	2.4
1	B	73	ILE	2.4
1	B	71	LEU	2.4
2	D	283	GLN	2.4
1	B	219	LYS	2.3
1	C	245	ALA	2.3
2	D	278	LYS	2.3
1	C	105	THR	2.3
2	D	146	PHE	2.3
2	D	71	LEU	2.3
2	D	189	GLU	2.3
2	D	217	SER	2.3
1	C	154	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	147	PHE	2.2
2	D	142	LEU	2.2
1	B	228	PHE	2.2
2	D	73	ILE	2.2
1	A	45	GLN	2.2
2	D	279	GLU	2.2
2	D	228	PHE	2.2
1	C	71	LEU	2.2
2	D	282	LYS	2.2
1	C	278	LYS	2.2
2	D	105	THR	2.2
1	C	36	VAL	2.1
1	A	41	THR	2.1
2	D	27	SER	2.1
1	A	105	THR	2.1
1	C	103	ALA	2.1
2	D	156	THR	2.1
1	B	70	LEU	2.0
1	B	217	SER	2.0
1	C	156	THR	2.0
1	A	103	ALA	2.0
1	C	70	LEU	2.0
1	B	150	GLU	2.0
1	C	215	GLU	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.