Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 07:22 am BST

PDB ID	:	2G9D
Title	:	Crystal Structure of Succinylglutamate desuccinylase from Vibrio cholerae, Northeast Structural Genomics Target VcR20
Authors	:	Zhou, W.; Jayaraman, S.; Forouhar, F.; Conover, K.; Rong, X.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2006-03-06
Resolution	:	3.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

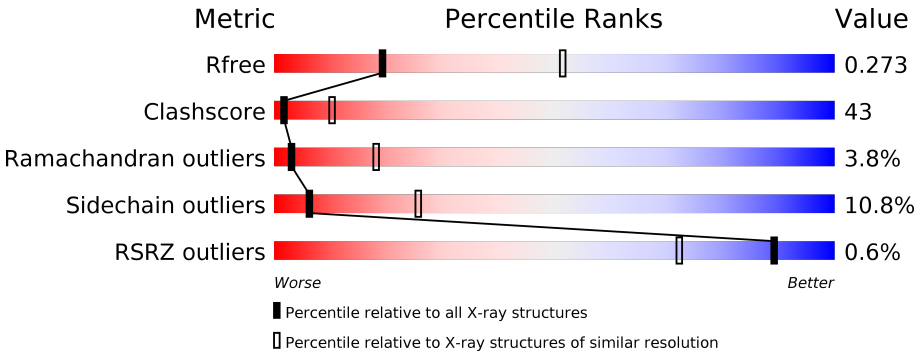
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	350	% 36% 51% 10% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2752 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 Succinylglutamate desuccinylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	Se	0	0	0
			2735	1728	494	498	4	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9KSL4
A	21	MSE	MET	MODIFIED RESIDUE	UNP Q9KSL4
A	56	MSE	MET	MODIFIED RESIDUE	UNP Q9KSL4
A	70	MSE	MET	MODIFIED RESIDUE	UNP Q9KSL4
A	95	MSE	MET	MODIFIED RESIDUE	UNP Q9KSL4
A	182	MSE	MET	MODIFIED RESIDUE	UNP Q9KSL4
A	194	MSE	MET	MODIFIED RESIDUE	UNP Q9KSL4
A	241	MSE	MET	MODIFIED RESIDUE	UNP Q9KSL4
A	259	MSE	MET	MODIFIED RESIDUE	UNP Q9KSL4
A	288	MSE	MET	MODIFIED RESIDUE	UNP Q9KSL4
A	302	MSE	MET	MODIFIED RESIDUE	UNP Q9KSL4
A	326	MSE	MET	MODIFIED RESIDUE	UNP Q9KSL4
A	343	LEU	-	EXPRESSION TAG	UNP Q9KSL4
A	344	GLU	-	EXPRESSION TAG	UNP Q9KSL4
A	345	HIS	-	EXPRESSION TAG	UNP Q9KSL4
A	346	HIS	-	EXPRESSION TAG	UNP Q9KSL4
A	347	HIS	-	EXPRESSION TAG	UNP Q9KSL4
A	348	HIS	-	EXPRESSION TAG	UNP Q9KSL4
A	349	HIS	-	EXPRESSION TAG	UNP Q9KSL4
A	350	HIS	-	EXPRESSION TAG	UNP Q9KSL4

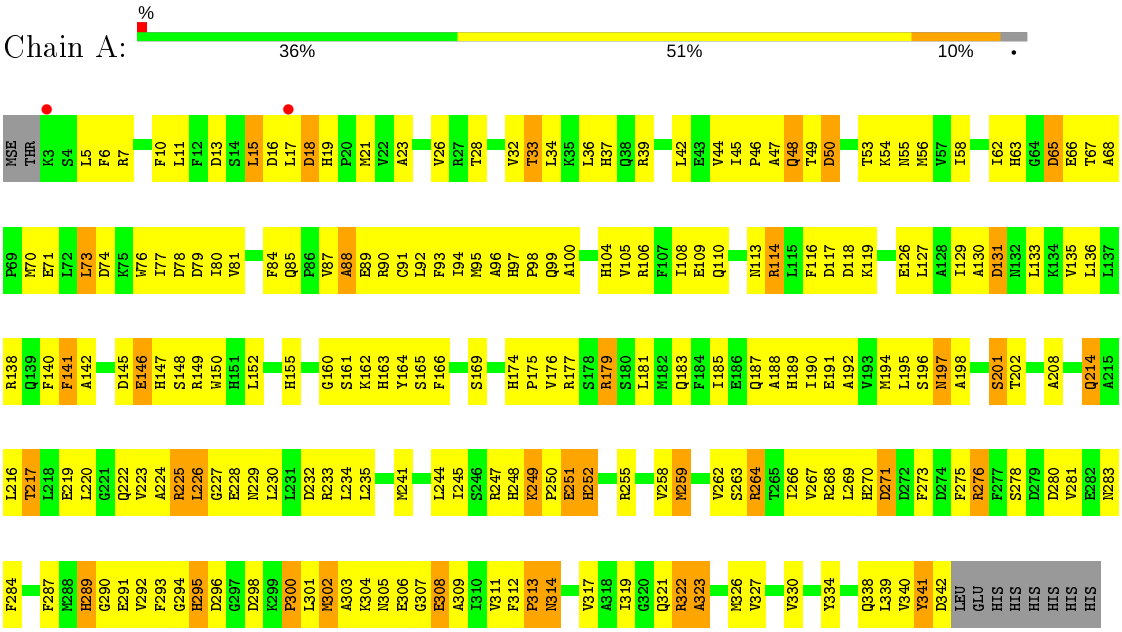
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	17	Total	O	0	0
			17	17		

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: Succinylglutamate desuccinylase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	82.93Å 82.93Å 116.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.94 – 3.00 23.94 – 2.81	Depositor EDS
% Data completeness (in resolution range)	96.6 (23.94-3.00) 99.1 (23.94-2.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.272 0.245 , 0.273	Depositor DCC
R_{free} test set	2074 reflections (9.56%)	wwPDB-VP
Wilson B-factor (Å^2)	75.9	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.177 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	2752	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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

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	0/2787	0.65	0/3753

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

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	2735	0	2691	236	0
2	A	17	0	0	3	0
All	All	2752	0	2691	236	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 43.

All (236) 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:56:MSE:HE1	1:A:245:ILE:HG22	1.45	0.96
1:A:174:HIS:HB3	1:A:175:PRO:HD2	1.51	0.93
1:A:226:LEU:H	1:A:226:LEU:HD12	1.34	0.91
1:A:311:VAL:HG12	1:A:312:PHE:HD1	1.38	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:HA	1:A:136:LEU:HD12	1.55	0.89
1:A:196:SER:HA	1:A:262:VAL:HG21	1.56	0.88
1:A:108:ILE:HG22	1:A:109:GLU:HG3	1.56	0.85
1:A:152:LEU:HD23	1:A:241:MSE:HE1	1.63	0.78
1:A:311:VAL:HG12	1:A:312:PHE:CD1	2.19	0.77
1:A:91:CYS:HG	1:A:93:PHE:HE1	1.32	0.77
1:A:110:GLN:O	1:A:126:GLU:HG2	1.85	0.76
1:A:196:SER:HA	1:A:262:VAL:CG2	2.16	0.76
1:A:197:ASN:HD22	1:A:198:ALA:N	1.82	0.76
1:A:92:LEU:HB2	1:A:140:PHE:CE1	2.21	0.75
1:A:187:GLN:HG3	1:A:252:HIS:NE2	2.02	0.75
1:A:11:LEU:HD21	1:A:70:MSE:HB3	1.69	0.74
1:A:161:SER:HB2	1:A:283:ASN:HD22	1.52	0.74
1:A:126:GLU:OE2	1:A:126:GLU:N	2.21	0.74
1:A:5:LEU:HD12	1:A:26:VAL:HG12	1.70	0.74
1:A:304:LYS:HG2	1:A:305:ASN:ND2	2.02	0.73
1:A:62:ILE:HG21	1:A:113:ASN:HB2	1.71	0.72
1:A:78:ASP:O	1:A:81:VAL:HG22	1.90	0.72
1:A:127:LEU:O	1:A:127:LEU:HD23	1.90	0.72
1:A:87:VAL:HG12	1:A:88:ALA:N	2.04	0.71
1:A:295:HIS:CD2	1:A:295:HIS:H	2.06	0.70
1:A:217:THR:N	2:A:362:HOH:O	2.23	0.70
1:A:36:LEU:CD1	1:A:42:LEU:HD13	2.22	0.69
1:A:290:GLY:H	1:A:302:MSE:SE	2.26	0.69
1:A:42:LEU:HD23	1:A:77:ILE:HD12	1.75	0.69
1:A:330:VAL:HG21	1:A:341:TYR:HB2	1.74	0.68
1:A:21:MSE:HE3	1:A:36:LEU:HD21	1.75	0.68
1:A:267:VAL:HA	1:A:322:ARG:HA	1.75	0.68
1:A:287:PHE:HB2	1:A:303:ALA:HB2	1.76	0.68
1:A:146:GLU:HA	1:A:149:ARG:HD2	1.75	0.67
1:A:176:VAL:HG11	1:A:208:ALA:HB1	1.78	0.65
1:A:117:ASP:OD1	1:A:119:LYS:HD2	1.95	0.65
1:A:179:ARG:HG3	1:A:179:ARG:HH11	1.60	0.65
1:A:11:LEU:HD13	1:A:15:LEU:HD22	1.78	0.65
1:A:259:MSE:HE3	1:A:339:LEU:HD21	1.78	0.65
1:A:225:ARG:H	1:A:225:ARG:HD2	1.61	0.65
1:A:76:TRP:O	1:A:80:ILE:HG13	1.96	0.65
1:A:67:THR:HG21	1:A:226:LEU:HG	1.80	0.64
1:A:289:HIS:HB2	1:A:306:GLU:HG3	1.78	0.64
1:A:145:ASP:HB3	1:A:147:HIS:ND1	2.12	0.64
1:A:11:LEU:CD2	1:A:70:MSE:HB3	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:PHE:N	1:A:313:PRO:HD3	2.13	0.64
1:A:174:HIS:HB3	1:A:175:PRO:CD	2.27	0.63
1:A:36:LEU:HD12	1:A:42:LEU:HD13	1.80	0.63
1:A:268:ARG:NH2	1:A:271:ASP:HA	2.13	0.63
1:A:230:LEU:HG	1:A:232:ASP:HB2	1.81	0.63
1:A:163:HIS:CE1	1:A:258:VAL:HG21	2.34	0.62
1:A:62:ILE:HB	1:A:155:HIS:CE1	2.34	0.62
1:A:195:LEU:O	1:A:262:VAL:HG23	2.00	0.62
1:A:5:LEU:HD23	1:A:5:LEU:C	2.20	0.61
1:A:276:ARG:HB2	1:A:293:PHE:HA	1.81	0.61
1:A:187:GLN:CG	1:A:252:HIS:NE2	2.63	0.61
1:A:230:LEU:HD11	1:A:232:ASP:OD1	2.01	0.61
1:A:247:ARG:HG2	1:A:247:ARG:O	2.00	0.61
1:A:268:ARG:HH21	1:A:271:ASP:HA	1.66	0.60
1:A:304:LYS:C	1:A:305:ASN:HD22	2.04	0.60
1:A:33:THR:HG23	1:A:45:ILE:HB	1.84	0.60
1:A:117:ASP:HB3	1:A:201:SER:OG	2.01	0.60
1:A:314:ASN:HB3	1:A:317:VAL:HG22	1.84	0.60
1:A:177:ARG:CZ	1:A:195:LEU:HD22	2.32	0.59
1:A:92:LEU:HD22	1:A:140:PHE:CD1	2.38	0.59
1:A:263:SER:HB3	1:A:326:MSE:HB2	1.83	0.59
1:A:217:THR:HB	2:A:362:HOH:O	2.04	0.58
1:A:5:LEU:O	1:A:5:LEU:HD23	2.03	0.58
1:A:99:GLN:CD	1:A:108:ILE:HD11	2.24	0.57
1:A:275:PHE:HA	1:A:294:GLY:HA3	1.87	0.57
1:A:305:ASN:N	1:A:305:ASN:HD22	2.03	0.57
1:A:276:ARG:HD3	1:A:292:VAL:O	2.05	0.57
1:A:105:VAL:HG22	1:A:106:ARG:N	2.20	0.57
1:A:294:GLY:O	1:A:301:LEU:HB2	2.05	0.56
1:A:177:ARG:H	1:A:338:GLN:HE22	1.53	0.56
1:A:225:ARG:HD2	1:A:225:ARG:N	2.20	0.56
1:A:330:VAL:CG2	1:A:341:TYR:HB2	2.35	0.56
1:A:56:MSE:CE	1:A:245:ILE:HG22	2.28	0.56
1:A:113:ASN:ND2	1:A:202:THR:HG22	2.20	0.55
1:A:16:ASP:O	1:A:39:ARG:NH1	2.40	0.55
1:A:79:ASP:HB3	1:A:84:PHE:HB3	1.87	0.55
1:A:62:ILE:HB	1:A:155:HIS:HE1	1.72	0.55
1:A:230:LEU:HD23	1:A:233:ARG:NH1	2.22	0.55
1:A:268:ARG:O	1:A:319:ILE:O	2.25	0.55
1:A:73:LEU:HA	1:A:76:TRP:CE3	2.42	0.55
1:A:222:GLN:HG2	1:A:223:VAL:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ASN:ND2	1:A:198:ALA:N	2.55	0.55
1:A:62:ILE:CG2	1:A:113:ASN:HB2	2.36	0.54
1:A:44:VAL:O	1:A:90:ARG:HA	2.07	0.54
1:A:161:SER:OG	1:A:283:ASN:HB2	2.06	0.54
1:A:5:LEU:HD21	1:A:36:LEU:HD13	1.90	0.54
1:A:87:VAL:HG12	1:A:88:ALA:H	1.73	0.54
1:A:270:HIS:CG	1:A:271:ASP:H	2.27	0.53
1:A:87:VAL:CG1	1:A:88:ALA:N	2.71	0.52
1:A:11:LEU:HB2	1:A:74:ASP:CG	2.30	0.52
1:A:97:HIS:NE2	1:A:100:ALA:HB2	2.25	0.52
1:A:56:MSE:SE	1:A:244:LEU:HG	2.59	0.52
1:A:108:ILE:HG22	1:A:109:GLU:N	2.25	0.52
1:A:76:TRP:CH2	1:A:241:MSE:HG2	2.44	0.52
1:A:34:LEU:HD11	1:A:81:VAL:HG12	1.90	0.52
1:A:28:THR:CG2	1:A:32:VAL:HB	2.40	0.52
1:A:17:LEU:HD12	1:A:17:LEU:N	2.26	0.51
1:A:177:ARG:NE	1:A:195:LEU:HD22	2.25	0.51
1:A:267:VAL:HG23	1:A:269:LEU:HD21	1.92	0.51
1:A:6:PHE:O	1:A:7:ARG:HD2	2.10	0.51
1:A:225:ARG:O	1:A:226:LEU:C	2.49	0.51
1:A:270:HIS:CD2	1:A:271:ASP:H	2.29	0.51
1:A:187:GLN:HB2	2:A:360:HOH:O	2.09	0.51
1:A:269:LEU:O	1:A:319:ILE:HG23	2.12	0.50
1:A:116:PHE:HB2	1:A:201:SER:O	2.11	0.50
1:A:267:VAL:O	1:A:269:LEU:HD22	2.12	0.50
1:A:258:VAL:HG23	1:A:258:VAL:O	2.11	0.50
1:A:127:LEU:HD23	1:A:131:ASP:OD1	2.12	0.50
1:A:175:PRO:O	1:A:175:PRO:HG2	2.11	0.50
1:A:6:PHE:CZ	1:A:10:PHE:HB2	2.47	0.50
1:A:179:ARG:O	1:A:183:GLN:HG3	2.12	0.49
1:A:197:ASN:HB3	1:A:262:VAL:HB	1.92	0.49
1:A:117:ASP:HB3	1:A:201:SER:HG	1.78	0.49
1:A:226:LEU:HD12	1:A:226:LEU:N	2.16	0.49
1:A:312:PHE:O	1:A:314:ASN:N	2.44	0.49
1:A:309:ALA:O	1:A:327:VAL:HG22	2.12	0.49
1:A:28:THR:HG22	1:A:32:VAL:HB	1.95	0.49
1:A:5:LEU:HD12	1:A:26:VAL:CG1	2.41	0.49
1:A:11:LEU:CD1	1:A:15:LEU:HD22	2.43	0.49
1:A:169:SER:HB3	1:A:195:LEU:HD23	1.95	0.49
1:A:162:LYS:O	1:A:162:LYS:HG2	2.13	0.48
1:A:264:ARG:NE	1:A:326:MSE:HG3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:HD23	1:A:136:LEU:CD1	2.44	0.48
1:A:224:ALA:HB1	1:A:228:GLU:HB2	1.96	0.48
1:A:225:ARG:HB2	1:A:228:GLU:OE1	2.13	0.48
1:A:89:GLU:OE1	1:A:247:ARG:HB2	2.14	0.48
1:A:281:VAL:O	1:A:281:VAL:HG13	2.13	0.48
1:A:36:LEU:HD13	1:A:42:LEU:HD13	1.95	0.47
1:A:58:ILE:N	1:A:58:ILE:HD12	2.29	0.47
1:A:252:HIS:CD2	1:A:252:HIS:H	2.33	0.47
1:A:73:LEU:HD11	1:A:93:PHE:HD2	1.79	0.47
1:A:70:MSE:O	1:A:74:ASP:HB2	2.14	0.47
1:A:94:ILE:HG22	1:A:96:ALA:H	1.80	0.47
1:A:296:ASP:C	1:A:298:ASP:H	2.17	0.47
1:A:185:ILE:HG23	1:A:190:ILE:HB	1.97	0.46
1:A:18:ASP:N	1:A:18:ASP:OD1	2.48	0.46
1:A:309:ALA:HB3	1:A:327:VAL:HG23	1.96	0.46
1:A:6:PHE:C	1:A:7:ARG:HD2	2.35	0.46
1:A:135:VAL:O	1:A:136:LEU:C	2.53	0.46
1:A:197:ASN:C	1:A:197:ASN:ND2	2.69	0.46
1:A:275:PHE:HA	1:A:293:PHE:O	2.15	0.46
1:A:11:LEU:HD13	1:A:11:LEU:C	2.35	0.46
1:A:181:LEU:HB2	1:A:214:GLN:HG2	1.97	0.46
1:A:91:CYS:SG	1:A:93:PHE:HE1	2.36	0.46
1:A:53:THR:HG22	1:A:54:LYS:N	2.31	0.46
1:A:49:THR:O	1:A:50:ASP:O	2.33	0.46
1:A:70:MSE:O	1:A:74:ASP:N	2.41	0.46
1:A:220:LEU:HB3	1:A:234:LEU:CD2	2.45	0.46
1:A:7:ARG:N	1:A:13:ASP:OD1	2.49	0.46
1:A:135:VAL:O	1:A:138:ARG:N	2.49	0.46
1:A:188:ALA:HB3	1:A:190:ILE:HG12	1.98	0.46
1:A:188:ALA:O	1:A:189:HIS:HB2	2.16	0.46
1:A:54:LYS:HB2	1:A:89:GLU:HG2	1.98	0.45
1:A:56:MSE:HG2	1:A:150:TRP:HB2	1.97	0.45
1:A:54:LYS:HA	1:A:148:SER:HB2	1.98	0.45
1:A:197:ASN:C	1:A:197:ASN:HD22	2.15	0.45
1:A:295:HIS:N	1:A:295:HIS:CD2	2.80	0.45
1:A:163:HIS:HD2	1:A:284:PHE:CG	2.35	0.45
1:A:307:GLY:O	1:A:309:ALA:N	2.50	0.45
1:A:296:ASP:O	1:A:298:ASP:N	2.46	0.44
1:A:266:ILE:O	1:A:323:ALA:HB3	2.17	0.44
1:A:65:ASP:O	1:A:67:THR:HG23	2.16	0.44
1:A:225:ARG:HG2	1:A:225:ARG:HH11	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:MSE:HB3	1:A:194:MSE:HE2	1.91	0.44
1:A:330:VAL:HG21	1:A:341:TYR:CB	2.44	0.44
1:A:292:VAL:HG12	1:A:302:MSE:CB	2.48	0.44
1:A:267:VAL:HG23	1:A:267:VAL:O	2.18	0.44
1:A:130:ALA:O	1:A:131:ASP:C	2.57	0.44
1:A:268:ARG:C	1:A:269:LEU:HD22	2.38	0.44
1:A:55:ASN:HA	1:A:90:ARG:O	2.18	0.44
1:A:291:GLU:O	1:A:302:MSE:HB2	2.17	0.43
1:A:166:PHE:HB3	1:A:192:ALA:HB3	1.98	0.43
1:A:114:ARG:NH1	1:A:201:SER:HB2	2.33	0.43
1:A:280:ASP:N	1:A:280:ASP:OD2	2.51	0.43
1:A:268:ARG:HE	1:A:273:PHE:HB2	1.84	0.43
1:A:197:ASN:HD22	1:A:198:ALA:H	1.59	0.43
1:A:179:ARG:HG3	1:A:179:ARG:NH1	2.32	0.43
1:A:21:MSE:CE	1:A:36:LEU:HD21	2.46	0.43
1:A:185:ILE:HD11	1:A:216:LEU:CD1	2.50	0.42
1:A:71:GLU:OE1	1:A:227:GLY:N	2.52	0.42
1:A:174:HIS:CB	1:A:175:PRO:CD	2.97	0.42
1:A:249:LYS:HA	1:A:250:PRO:HD2	1.91	0.42
1:A:259:MSE:HE3	1:A:339:LEU:CD2	2.48	0.42
1:A:290:GLY:N	1:A:302:MSE:SE	2.97	0.42
1:A:36:LEU:HD12	1:A:42:LEU:CD1	2.47	0.42
1:A:232:ASP:O	1:A:235:LEU:HB2	2.20	0.42
1:A:341:TYR:N	1:A:341:TYR:CD1	2.88	0.42
1:A:63:HIS:ND1	1:A:66:GLU:CD	2.73	0.42
1:A:304:LYS:HG2	1:A:305:ASN:HD21	1.77	0.42
1:A:105:VAL:CG2	1:A:106:ARG:N	2.82	0.42
1:A:23:ALA:HB2	1:A:37:HIS:O	2.19	0.42
1:A:308:GLU:HG2	1:A:326:MSE:HE3	2.01	0.42
1:A:312:PHE:N	1:A:313:PRO:CD	2.82	0.42
1:A:46:PRO:C	1:A:48:GLN:H	2.23	0.42
1:A:185:ILE:HD11	1:A:216:LEU:HD11	2.01	0.42
1:A:334:TYR:HA	1:A:338:GLN:O	2.20	0.42
1:A:68:ALA:HB2	1:A:229:ASN:HB3	2.00	0.42
1:A:11:LEU:O	1:A:11:LEU:HD13	2.20	0.42
1:A:16:ASP:C	1:A:39:ARG:HH22	2.22	0.42
1:A:164:TYR:N	1:A:191:GLU:OE1	2.52	0.41
1:A:89:GLU:OE2	1:A:245:ILE:O	2.38	0.41
1:A:46:PRO:HG3	1:A:89:GLU:N	2.34	0.41
1:A:79:ASP:CG	1:A:84:PHE:HD1	2.24	0.41
1:A:165:SER:HA	1:A:219:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:VAL:O	1:A:26:VAL:HG13	2.20	0.41
1:A:249:LYS:HG3	1:A:251:GLU:HG3	2.03	0.41
1:A:161:SER:HA	1:A:283:ASN:H	1.84	0.41
1:A:79:ASP:C	1:A:85:GLN:HB3	2.41	0.41
1:A:55:ASN:OD1	1:A:90:ARG:HD3	2.20	0.41
1:A:160:GLY:O	1:A:161:SER:HB2	2.21	0.41
1:A:223:VAL:HG23	1:A:223:VAL:O	2.21	0.41
1:A:340:VAL:HG12	1:A:341:TYR:N	2.36	0.41
1:A:304:LYS:HZ2	1:A:305:ASN:ND2	2.18	0.41
1:A:305:ASN:N	1:A:305:ASN:ND2	2.67	0.41
1:A:87:VAL:CG1	1:A:88:ALA:H	2.32	0.41
1:A:295:HIS:HA	1:A:300:PRO:HA	2.02	0.41
1:A:42:LEU:HD23	1:A:77:ILE:CD1	2.49	0.41
1:A:113:ASN:O	1:A:114:ARG:HG2	2.20	0.40
1:A:141:PHE:CE1	1:A:149:ARG:HG2	2.56	0.40
1:A:165:SER:HB3	1:A:220:LEU:HA	2.02	0.40
1:A:48:GLN:HG2	1:A:49:THR:N	2.35	0.40
1:A:49:THR:HG22	1:A:49:THR:O	2.20	0.40
1:A:106:ARG:HG3	1:A:106:ARG:HH11	1.87	0.40
1:A:16:ASP:OD1	1:A:19:HIS:HB2	2.21	0.40
1:A:319:ILE:N	1:A:319:ILE:HD12	2.36	0.40
1:A:55:ASN:OD1	1:A:90:ARG:HB3	2.21	0.40
1:A:65:ASP:OD1	1:A:106:ARG:HB2	2.22	0.40
1:A:140:PHE:C	1:A:142:ALA:H	2.25	0.40
1:A:97:HIS:ND1	1:A:129:ILE:CD1	2.84	0.40
1:A:98:PRO:HG2	1:A:99:GLN:H	1.86	0.40
1:A:79:ASP:O	1:A:85:GLN:N	2.44	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	338/350 (97%)	254 (75%)	71 (21%)	13 (4%)	3 18

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	88	ALA
1	A	47	ALA
1	A	48	GLN
1	A	300	PRO
1	A	308	GLU
1	A	323	ALA
1	A	114	ARG
1	A	201	SER
1	A	249	LYS
1	A	313	PRO
1	A	141	PHE
1	A	214	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	297/295 (101%)	265 (89%)	32 (11%)	6 26

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	18	ASP
1	A	33	THR
1	A	65	ASP
1	A	73	LEU
1	A	95	MSE
1	A	104	HIS
1	A	118	ASP

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Mol	Chain	Res	Type
1	A	131	ASP
1	A	146	GLU
1	A	179	ARG
1	A	197	ASN
1	A	217	THR
1	A	225	ARG
1	A	226	LEU
1	A	248	HIS
1	A	251	GLU
1	A	252	HIS
1	A	255	ARG
1	A	259	MSE
1	A	264	ARG
1	A	271	ASP
1	A	276	ARG
1	A	278	SER
1	A	289	HIS
1	A	295	HIS
1	A	302	MSE
1	A	314	ASN
1	A	321	GLN
1	A	322	ARG
1	A	341	TYR
1	A	342	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	HIS
1	A	163	HIS
1	A	183	GLN
1	A	187	GLN
1	A	197	ASN
1	A	210	HIS
1	A	222	GLN
1	A	270	HIS
1	A	283	ASN
1	A	295	HIS
1	A	305	ASN
1	A	338	GLN

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, 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	329/350 (94%)	-0.03	2 (0%)	89	72	32, 62, 90, 98	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	LYS	3.0
1	A	17	LEU	2.4

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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.