



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2018 – 03:53 PM EST

PDB ID : 3CDX  
Title : Crystal structure of succinylglutamatedesuccinylase/aspartoacylase from Rhodobacter sphaeroides  
Authors : Bonanno, J.B.; Rutter, M.; Bain, K.T.; Iizuka, M.; Patterson, K.; Smith, D.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2008-02-27  
Resolution : 2.10 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](mailto: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
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031633
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

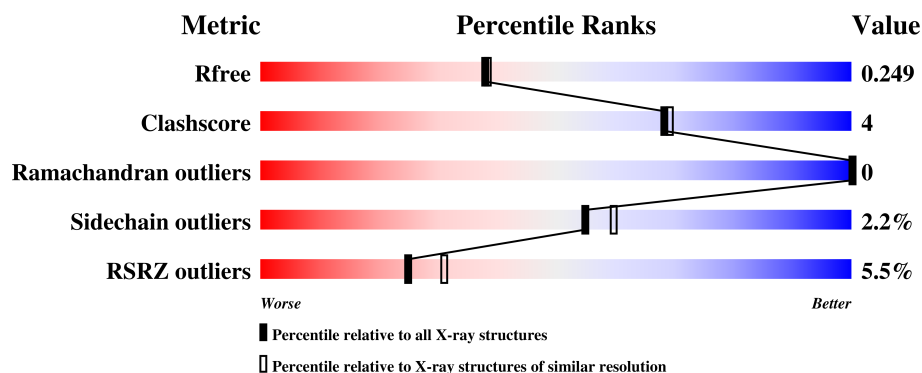
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (2.10-2.10)

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  $\geq 3$ , 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	354	<div> <div>3%</div> <div>85% 8% 7%</div> </div>
1	B	354	<div> <div>3%</div> <div>84% 8% 7%</div> </div>
1	C	354	<div> <div>3%</div> <div>83% 8% • 8%</div> </div>
1	D	354	<div> <div>12%</div> <div>78% 13% • 9%</div> </div>
1	E	354	<div> <div>7%</div> <div>84% 8% • 8%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	354	<div><div></div><div>3%</div><div>82%</div><div>10%</div><div>7%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16156 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 Succinylglutamatedesuccinylase/aspartoacylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	2	0
			2493	1557	451	471	14			
1	B	328	Total	C	N	O	S	0	4	0
			2503	1559	456	474	14			
1	C	325	Total	C	N	O	S	0	4	0
			2476	1547	449	466	14			
1	D	322	Total	C	N	O	S	0	1	0
			2432	1515	443	460	14			
1	E	326	Total	C	N	O	S	0	1	0
			2472	1544	447	467	14			
1	F	328	Total	C	N	O	S	0	4	0
			2518	1573	457	474	14			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP Q3HKK3
A	1	SER	-	EXPRESSION TAG	UNP Q3HKK3
A	2	LEU	-	EXPRESSION TAG	UNP Q3HKK3
A	346	GLU	-	EXPRESSION TAG	UNP Q3HKK3
A	347	GLY	-	EXPRESSION TAG	UNP Q3HKK3
A	348	HIS	-	EXPRESSION TAG	UNP Q3HKK3
A	349	HIS	-	EXPRESSION TAG	UNP Q3HKK3
A	350	HIS	-	EXPRESSION TAG	UNP Q3HKK3
A	351	HIS	-	EXPRESSION TAG	UNP Q3HKK3
A	352	HIS	-	EXPRESSION TAG	UNP Q3HKK3
A	353	HIS	-	EXPRESSION TAG	UNP Q3HKK3
B	0	MET	-	EXPRESSION TAG	UNP Q3HKK3
B	1	SER	-	EXPRESSION TAG	UNP Q3HKK3
B	2	LEU	-	EXPRESSION TAG	UNP Q3HKK3
B	346	GLU	-	EXPRESSION TAG	UNP Q3HKK3
B	347	GLY	-	EXPRESSION TAG	UNP Q3HKK3
B	348	HIS	-	EXPRESSION TAG	UNP Q3HKK3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	349	HIS	-	EXPRESSION TAG	UNP Q3HKK3
B	350	HIS	-	EXPRESSION TAG	UNP Q3HKK3
B	351	HIS	-	EXPRESSION TAG	UNP Q3HKK3
B	352	HIS	-	EXPRESSION TAG	UNP Q3HKK3
B	353	HIS	-	EXPRESSION TAG	UNP Q3HKK3
C	0	MET	-	EXPRESSION TAG	UNP Q3HKK3
C	1	SER	-	EXPRESSION TAG	UNP Q3HKK3
C	2	LEU	-	EXPRESSION TAG	UNP Q3HKK3
C	346	GLU	-	EXPRESSION TAG	UNP Q3HKK3
C	347	GLY	-	EXPRESSION TAG	UNP Q3HKK3
C	348	HIS	-	EXPRESSION TAG	UNP Q3HKK3
C	349	HIS	-	EXPRESSION TAG	UNP Q3HKK3
C	350	HIS	-	EXPRESSION TAG	UNP Q3HKK3
C	351	HIS	-	EXPRESSION TAG	UNP Q3HKK3
C	352	HIS	-	EXPRESSION TAG	UNP Q3HKK3
C	353	HIS	-	EXPRESSION TAG	UNP Q3HKK3
D	0	MET	-	EXPRESSION TAG	UNP Q3HKK3
D	1	SER	-	EXPRESSION TAG	UNP Q3HKK3
D	2	LEU	-	EXPRESSION TAG	UNP Q3HKK3
D	346	GLU	-	EXPRESSION TAG	UNP Q3HKK3
D	347	GLY	-	EXPRESSION TAG	UNP Q3HKK3
D	348	HIS	-	EXPRESSION TAG	UNP Q3HKK3
D	349	HIS	-	EXPRESSION TAG	UNP Q3HKK3
D	350	HIS	-	EXPRESSION TAG	UNP Q3HKK3
D	351	HIS	-	EXPRESSION TAG	UNP Q3HKK3
D	352	HIS	-	EXPRESSION TAG	UNP Q3HKK3
D	353	HIS	-	EXPRESSION TAG	UNP Q3HKK3
E	0	MET	-	EXPRESSION TAG	UNP Q3HKK3
E	1	SER	-	EXPRESSION TAG	UNP Q3HKK3
E	2	LEU	-	EXPRESSION TAG	UNP Q3HKK3
E	346	GLU	-	EXPRESSION TAG	UNP Q3HKK3
E	347	GLY	-	EXPRESSION TAG	UNP Q3HKK3
E	348	HIS	-	EXPRESSION TAG	UNP Q3HKK3
E	349	HIS	-	EXPRESSION TAG	UNP Q3HKK3
E	350	HIS	-	EXPRESSION TAG	UNP Q3HKK3
E	351	HIS	-	EXPRESSION TAG	UNP Q3HKK3
E	352	HIS	-	EXPRESSION TAG	UNP Q3HKK3
E	353	HIS	-	EXPRESSION TAG	UNP Q3HKK3
F	0	MET	-	EXPRESSION TAG	UNP Q3HKK3
F	1	SER	-	EXPRESSION TAG	UNP Q3HKK3
F	2	LEU	-	EXPRESSION TAG	UNP Q3HKK3
F	346	GLU	-	EXPRESSION TAG	UNP Q3HKK3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	347	GLY	-	EXPRESSION TAG	UNP Q3HKK3
F	348	HIS	-	EXPRESSION TAG	UNP Q3HKK3
F	349	HIS	-	EXPRESSION TAG	UNP Q3HKK3
F	350	HIS	-	EXPRESSION TAG	UNP Q3HKK3
F	351	HIS	-	EXPRESSION TAG	UNP Q3HKK3
F	352	HIS	-	EXPRESSION TAG	UNP Q3HKK3
F	353	HIS	-	EXPRESSION TAG	UNP Q3HKK3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

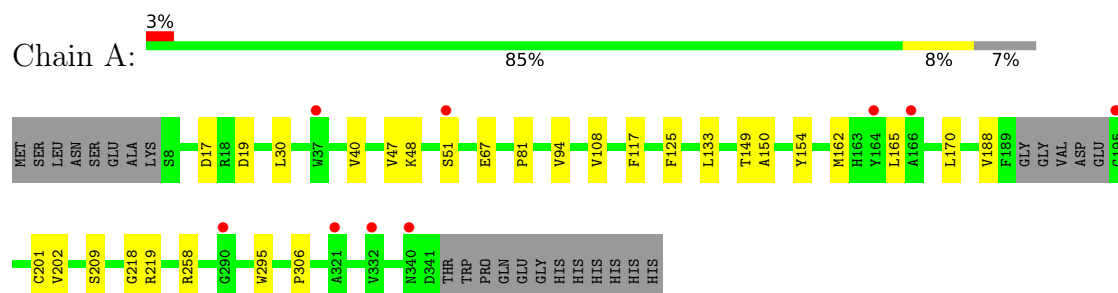
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	243	Total O 243 243	0	0
3	B	244	Total O 244 244	0	0
3	C	210	Total O 210 210	0	0
3	D	152	Total O 152 152	0	0
3	E	174	Total O 174 174	0	0
3	F	233	Total O 233 233	0	0

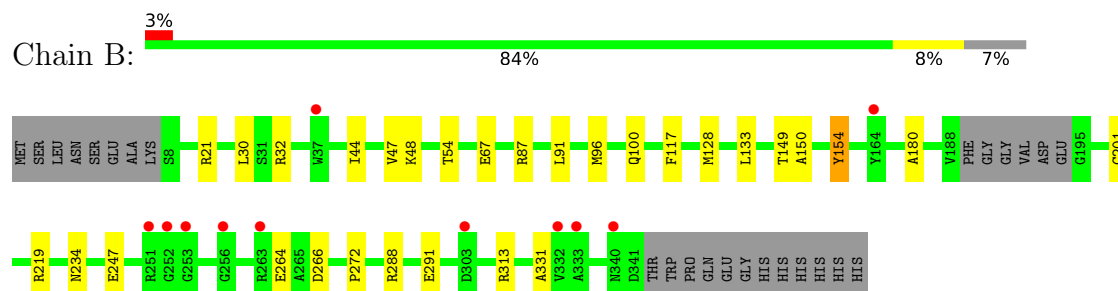
### 3 Residue-property plots [i](#)

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.

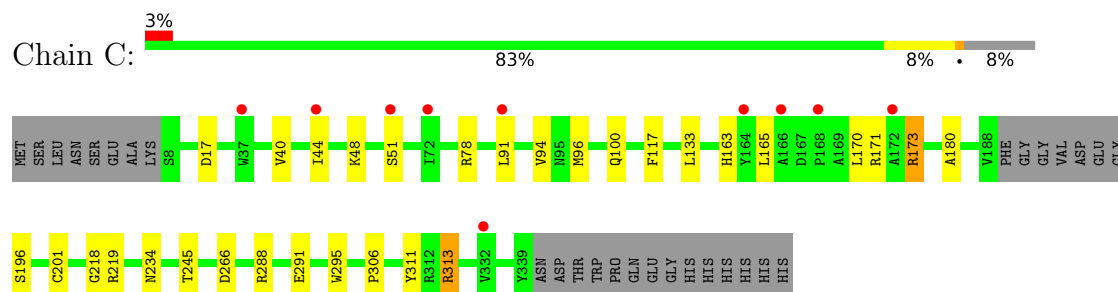
- Molecule 1: Succinylglutamatedesuccinylase/aspartoacylase



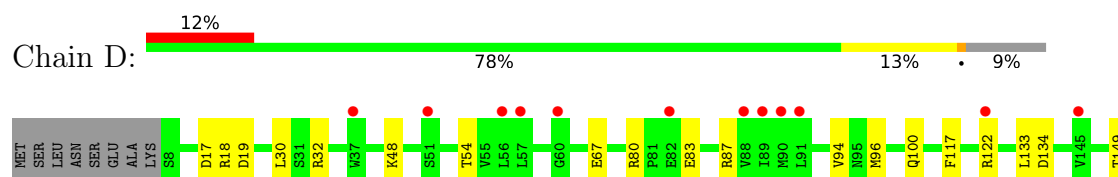
- Molecule 1: Succinylglutamatedesuccinylase/aspartoacylase

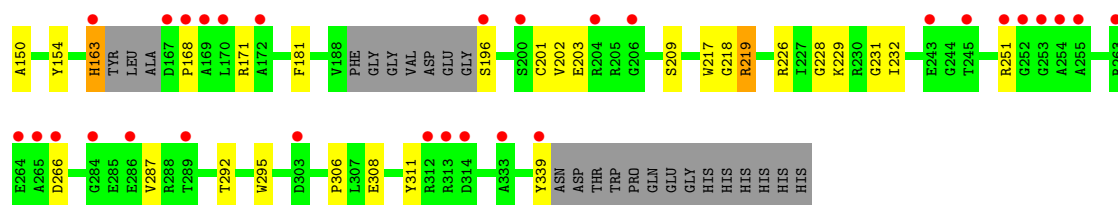


- Molecule 1: Succinylglutamatedesuccinylase/aspartoacylase

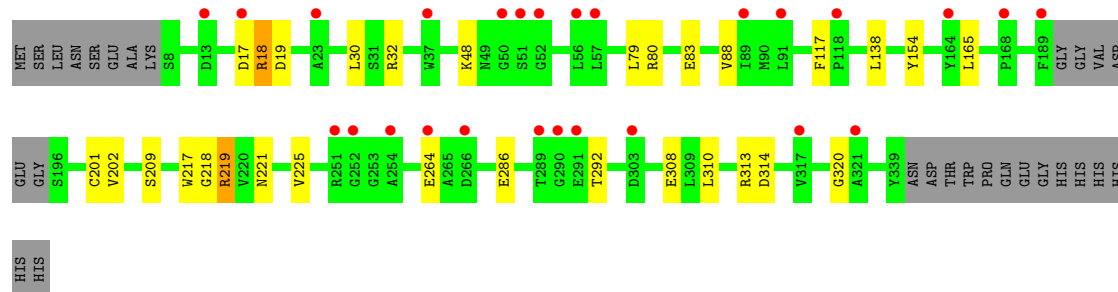
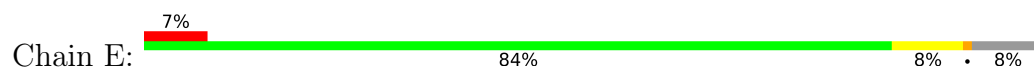


- Molecule 1: Succinylglutamatedesuccinylase/aspartoacylase

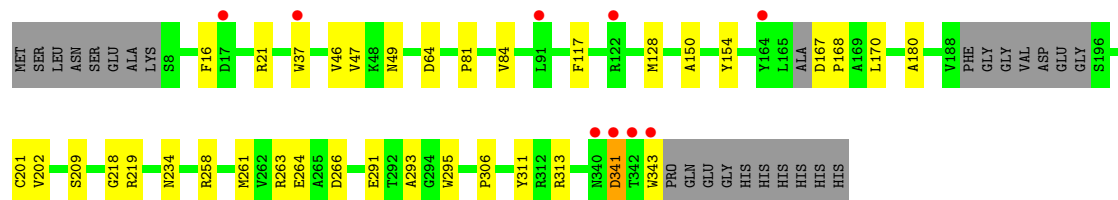
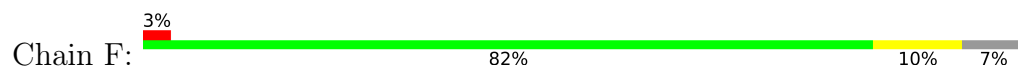




- Molecule 1: Succinylglutamatedesuccinylase/aspartoacylase



- Molecule 1: Succinylglutamatedesuccinylase/aspartoacylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.47Å 174.43Å 77.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 22.81 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.2 (20.00-2.10) 95.2 (22.81-2.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.09Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.181 , 0.244 0.186 , 0.249	Depositor DCC
$R_{free}$ test set	5820 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.2	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.78	0/2553	0.77	0/3471
1	B	0.73	0/2568	0.74	0/3489
1	C	0.73	0/2541	0.76	0/3454
1	D	0.60	0/2486	0.68	0/3378
1	E	0.66	0/2529	0.72	0/3438
1	F	0.73	0/2584	0.76	1/3511 (0.0%)
All	All	0.71	0/15261	0.74	1/20741 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	64	ASP	CB-CG-OD1	5.90	123.61	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	154	TYR	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2493	0	2420	18	0
1	B	2503	0	2445	15	0
1	C	2476	0	2417	17	0
1	D	2432	0	2361	30	0
1	E	2472	0	2400	19	0
1	F	2518	0	2461	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	243	0	0	2	0
3	B	244	0	0	2	0
3	C	210	0	0	2	0
3	D	152	0	0	5	0
3	E	174	0	0	2	0
3	F	233	0	0	3	0
All	All	16156	0	14504	121	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 4.

All (121) 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:F:261:MET:HE3	1:F:343:TRP:CZ2	1.97	1.00
1:E:264:GLU:HG3	1:E:313:ARG:HH12	1.42	0.84
1:F:266:ASP:HB3	1:F:313:ARG:HG3	1.61	0.82
1:E:154:TYR:HE2	1:F:37[B]:TRP:CE3	1.99	0.80
1:F:261:MET:CE	1:F:343:TRP:CZ2	2.64	0.80
1:F:261:MET:HE2	1:F:263:ARG:HD3	1.66	0.77
1:F:261:MET:CE	1:F:263:ARG:HD3	2.21	0.69
1:D:32:ARG:NH2	3:D:426:HOH:O	2.25	0.69
1:E:264:GLU:HG3	1:E:313:ARG:NH1	2.08	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ARG:NH1	3:D:501:HOH:O	2.26	0.67
1:F:16:PHE:CE1	1:F:46:VAL:HG21	2.30	0.67
1:F:261:MET:CE	1:F:343:TRP:CE2	2.77	0.66
1:A:202:VAL:CG1	1:A:209:SER:HB2	2.29	0.61
1:F:128:MET:SD	3:F:570:HOH:O	2.55	0.60
1:C:165:LEU:HD23	1:C:171:ARG:HA	1.83	0.60
1:E:218:GLY:HA2	3:E:543:HOH:O	2.01	0.60
1:C:180:ALA:O	1:C:234:ASN:HB3	2.03	0.59
1:F:261:MET:HE3	1:F:343:TRP:CE2	2.38	0.58
1:F:16:PHE:CD1	1:F:46:VAL:HG21	2.38	0.58
1:E:154:TYR:CE2	1:F:37[B]:TRP:CE3	2.88	0.58
1:F:261:MET:HE1	1:F:343:TRP:CE2	2.38	0.57
1:F:202:VAL:CG1	1:F:209:SER:HB2	2.35	0.56
1:F:258:ARG:HD2	3:F:464:HOH:O	2.05	0.56
1:C:163:HIS:O	1:C:165:LEU:HD22	2.06	0.55
1:F:47:VAL:CG1	1:F:81:PRO:HA	2.37	0.55
1:A:165:LEU:HD13	1:A:170:LEU:HG	1.88	0.55
1:D:202:VAL:CG1	1:D:209:SER:HB2	2.37	0.54
1:C:96:MET:O	1:C:100:GLN:HG3	2.08	0.54
1:D:218:GLY:HA2	3:D:409:HOH:O	2.08	0.52
1:E:117:PHE:HB3	1:E:201:CYS:SG	2.49	0.52
1:D:94:VAL:CG1	1:D:133:LEU:HD11	2.40	0.52
1:B:266:ASP:HB3	1:B:313:ARG:HG3	1.91	0.51
1:F:295:TRP:HB3	1:F:306:PRO:HB2	1.92	0.51
1:B:96:MET:O	1:B:100:GLN:HG3	2.10	0.51
1:D:117:PHE:HB3	1:D:201:CYS:SG	2.51	0.51
1:F:180:ALA:O	1:F:234:ASN:HB3	2.11	0.51
1:D:163:HIS:HD2	1:D:203:GLU:OE2	1.93	0.50
1:E:292:THR:HG23	1:E:308:GLU:HG3	1.93	0.50
1:F:261:MET:HE3	1:F:343:TRP:HZ2	1.67	0.49
1:A:30:LEU:HD11	1:A:108:VAL:HG21	1.94	0.49
1:D:117:PHE:O	1:D:196:SER:HB2	2.12	0.49
1:C:295:TRP:HB3	1:C:306:PRO:HB2	1.95	0.49
1:F:117:PHE:HB3	1:F:201:CYS:SG	2.54	0.48
1:A:117:PHE:HB3	1:A:201:CYS:SG	2.53	0.48
1:A:202:VAL:HG11	1:A:209:SER:HB2	1.95	0.48
1:D:229:LYS:HG2	3:D:476:HOH:O	2.14	0.48
1:C:291:GLU:HG3	1:C:311:TYR:HD2	1.78	0.47
1:B:32:ARG:NH2	3:B:461:HOH:O	2.30	0.47
1:E:138:LEU:HD11	1:E:202:VAL:HG22	1.96	0.47
1:F:293:ALA:HA	1:F:311:TYR:CE2	2.49	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:ASN:HB3	1:F:84:VAL:O	2.15	0.47
1:D:134:ASP:OD1	1:D:201:CYS:HB3	2.15	0.47
1:D:228:GLY:O	1:D:232:ILE:HG12	2.13	0.47
1:B:288:ARG:O	1:B:291:GLU:HG2	2.15	0.47
1:A:94:VAL:CG1	1:A:133:LEU:HD11	2.44	0.47
1:A:47:VAL:CG1	1:A:81:PRO:HA	2.44	0.47
1:D:163:HIS:CD2	1:D:203:GLU:OE2	2.68	0.47
1:F:150:ALA:HB1	1:F:154:TYR:HB2	1.97	0.47
1:F:21:ARG:HB2	1:F:81:PRO:HG3	1.96	0.47
1:E:154:TYR:HB3	1:E:320:GLY:O	2.15	0.46
1:E:202:VAL:CG1	1:E:209:SER:HB2	2.45	0.46
1:A:150:ALA:HB1	1:A:154:TYR:HB2	1.96	0.46
1:C:170:LEU:HD13	1:C:173:ARG:NH2	2.31	0.46
1:E:221:ASN:O	1:E:225:VAL:HG23	2.15	0.46
1:B:150:ALA:HB1	1:B:154:TYR:HB2	1.97	0.46
1:E:32:ARG:NH2	3:E:538:HOH:O	2.47	0.46
1:A:17:ASP:O	1:A:48:LYS:HE2	2.16	0.45
1:C:17:ASP:O	1:C:48:LYS:HE2	2.16	0.45
1:D:19:ASP:OD1	1:D:48:LYS:HE3	2.16	0.45
1:B:128:MET:HG3	3:B:624:HOH:O	2.15	0.45
1:A:40:VAL:HG11	1:A:125:PHE:CZ	2.52	0.45
1:D:295:TRP:HB3	1:D:306:PRO:HB2	1.97	0.45
1:D:339:TYR:C	3:D:427:HOH:O	2.55	0.45
1:C:288:ARG:O	1:C:291:GLU:HG2	2.17	0.45
1:C:266:ASP:HB3	1:C:313:ARG:HD2	1.99	0.45
1:B:44:ILE:HG12	1:B:91:LEU:HG	1.98	0.45
1:E:18:ARG:HG3	1:E:19:ASP:O	2.16	0.45
1:D:292:THR:HG23	1:D:308:GLU:HG3	1.99	0.45
1:E:17:ASP:O	1:E:48:LYS:HE2	2.17	0.45
1:F:218:GLY:HA2	3:F:590:HOH:O	2.16	0.45
1:A:94:VAL:HG13	1:A:133:LEU:HD11	1.99	0.44
1:B:67:GLU:N	1:B:67:GLU:OE1	2.51	0.44
1:F:341:ASP:N	1:F:341:ASP:OD2	2.33	0.44
1:B:21:ARG:HG3	1:B:47:VAL:HG22	1.99	0.44
1:C:94:VAL:CG1	1:C:133:LEU:HD11	2.47	0.44
1:A:218:GLY:HA2	3:A:404:HOH:O	2.18	0.44
1:E:79:LEU:HD21	1:E:88:VAL:HG21	1.99	0.44
1:D:94:VAL:HG11	1:D:133:LEU:HD11	1.99	0.44
1:D:96:MET:O	1:D:100:GLN:HG3	2.18	0.43
1:D:181:PHE:O	1:D:231:GLY:HA2	2.18	0.43
1:A:67:GLU:OE1	1:A:67:GLU:N	2.51	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:PHE:HB3	1:C:201:CYS:SG	2.58	0.43
1:D:287:VAL:HG21	1:D:311:TYR:CZ	2.53	0.43
1:A:162:MET:O	1:A:188:VAL:HA	2.18	0.43
1:A:19:ASP:OD1	1:A:48:LYS:HE3	2.19	0.43
1:D:217:TRP:CE2	1:E:219:ARG:HG2	2.54	0.43
1:B:67:GLU:OE1	1:B:149:THR:HG21	2.19	0.43
1:E:154:TYR:CE2	1:F:37[B]:TRP:HE3	2.34	0.43
1:E:80:ARG:HB2	1:E:83:GLU:HG3	2.00	0.43
1:C:165:LEU:O	1:C:171:ARG:HD3	2.18	0.42
1:D:150:ALA:HB1	1:D:154:TYR:HB2	2.02	0.42
1:D:67:GLU:OE1	1:D:149:THR:HG21	2.19	0.42
1:B:154:TYR:OH	1:B:331:ALA:HB3	2.19	0.42
1:D:17:ASP:O	1:D:48:LYS:HE2	2.19	0.42
1:D:202:VAL:HG12	1:D:209:SER:HB2	2.00	0.42
1:C:218:GLY:HA2	3:C:563:HOH:O	2.18	0.42
1:A:295:TRP:HB3	1:A:306:PRO:HB2	2.00	0.42
1:C:44:ILE:HG12	1:C:91:LEU:HG	2.01	0.42
1:D:219:ARG:HG2	1:E:217:TRP:CD2	2.55	0.42
1:B:180:ALA:O	1:B:234:ASN:HB3	2.20	0.41
1:B:54:THR:HA	1:B:87:ARG:O	2.20	0.41
1:C:78:ARG:NH1	3:C:501:HOH:O	2.53	0.41
1:D:168:PRO:HA	1:D:171:ARG:HB3	2.02	0.41
1:A:258:ARG:HD2	3:A:498:HOH:O	2.20	0.41
1:D:54:THR:HA	1:D:87:ARG:O	2.21	0.41
1:B:48:LYS:HD2	1:B:87:ARG:HD3	2.03	0.41
1:C:196:SER:HB3	1:D:122:ARG:NH2	2.36	0.40
1:B:117:PHE:HB3	1:B:201:CYS:SG	2.61	0.40
1:F:167:ASP:HA	1:F:168:PRO:HD2	1.99	0.40
1:A:67:GLU:OE1	1:A:149:THR:HG21	2.22	0.40
1:D:226:ARG:NE	1:D:251:ARG:HH21	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	327/354 (92%)	319 (98%)	8 (2%)	0	100	100
1	B	328/354 (93%)	320 (98%)	8 (2%)	0	100	100
1	C	325/354 (92%)	316 (97%)	9 (3%)	0	100	100
1	D	317/354 (90%)	305 (96%)	12 (4%)	0	100	100
1	E	323/354 (91%)	311 (96%)	12 (4%)	0	100	100
1	F	326/354 (92%)	318 (98%)	8 (2%)	0	100	100
All	All	1946/2124 (92%)	1889 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/281 (92%)	256 (99%)	2 (1%)	83	88
1	B	262/281 (93%)	256 (98%)	6 (2%)	53	58
1	C	257/281 (92%)	251 (98%)	6 (2%)	53	58
1	D	252/281 (90%)	245 (97%)	7 (3%)	47	50
1	E	256/281 (91%)	249 (97%)	7 (3%)	48	51
1	F	264/281 (94%)	259 (98%)	5 (2%)	60	66
All	All	1549/1686 (92%)	1516 (98%)	33 (2%)	55	62

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	A	219	ARG
1	B	30	LEU
1	B	133	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	219	ARG
1	B	247	GLU
1	B	264	GLU
1	B	272	PRO
1	C	40	VAL
1	C	51	SER
1	C	173	ARG
1	C	219	ARG
1	C	245	THR
1	C	313	ARG
1	D	18	ARG
1	D	30	LEU
1	D	80	ARG
1	D	83	GLU
1	D	163	HIS
1	D	219	ARG
1	D	266	ASP
1	E	18	ARG
1	E	30	LEU
1	E	165	LEU
1	E	219	ARG
1	E	286	GLU
1	E	310	LEU
1	E	314	ASP
1	F	170	LEU
1	F	219	ARG
1	F	264	GLU
1	F	291	GLU
1	F	341	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	100	GLN
1	C	281	HIS
1	D	163	HIS
1	E	100	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	329/354 (92%)	0.03	9 (2%) 54 61	19, 29, 44, 53	0
1	B	328/354 (92%)	0.13	11 (3%) 45 52	22, 32, 44, 53	0
1	C	325/354 (91%)	0.08	10 (3%) 49 56	22, 32, 46, 61	0
1	D	322/354 (90%)	0.70	42 (13%) 3 4	28, 44, 61, 74	0
1	E	326/354 (92%)	0.53	26 (7%) 12 16	26, 39, 57, 61	0
1	F	328/354 (92%)	0.03	9 (2%) 54 61	21, 31, 45, 59	0
All	All	1958/2124 (92%)	0.25	107 (5%) 25 31	19, 34, 53, 74	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	164	TYR	6.1
1	D	168	PRO	5.7
1	D	169	ALA	5.0
1	D	265	ALA	4.9
1	E	51	SER	4.6
1	D	243	GLU	4.5
1	D	252	GLY	4.4
1	C	164	TYR	4.4
1	A	166	ALA	4.2
1	A	290	GLY	4.2
1	D	339	TYR	4.2
1	C	166	ALA	4.2
1	D	91	LEU	4.1
1	F	343	TRP	4.0
1	E	290	GLY	4.0
1	D	206	GLY	4.0
1	D	57	LEU	4.0
1	E	252	GLY	3.8
1	E	91	LEU	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	164	TYR	3.6
1	B	164	TYR	3.5
1	D	163	HIS	3.5
1	A	340	ASN	3.4
1	D	312	ARG	3.4
1	F	17	ASP	3.4
1	D	266	ASP	3.3
1	E	37[A]	TRP	3.2
1	D	289	THR	3.2
1	D	314	ASP	3.1
1	E	251	ARG	3.1
1	D	145	VAL	3.1
1	E	264	GLU	3.1
1	F	37[A]	TRP	3.0
1	B	340	ASN	3.0
1	E	289	THR	3.0
1	E	317	VAL	2.9
1	E	56	LEU	2.9
1	D	264	GLU	2.9
1	E	321	ALA	2.9
1	F	91	LEU	2.9
1	C	168	PRO	2.8
1	A	195	GLY	2.8
1	A	51	SER	2.8
1	B	303	ASP	2.8
1	E	52	GLY	2.8
1	D	255	ALA	2.7
1	D	56	LEU	2.7
1	E	168	PRO	2.7
1	F	342	THR	2.7
1	D	89	ILE	2.7
1	F	341	ASP	2.7
1	B	251	ARG	2.6
1	E	189	PHE	2.6
1	D	253	GLY	2.6
1	E	50	GLY	2.6
1	A	332	VAL	2.6
1	C	91	LEU	2.6
1	D	170	LEU	2.6
1	D	245	THR	2.6
1	B	253	GLY	2.5
1	D	60	GLY	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	196	SER	2.5
1	D	313	ARG	2.5
1	D	254	ALA	2.5
1	D	303	ASP	2.5
1	E	17	ASP	2.4
1	D	263	ARG	2.4
1	D	284	GLY	2.4
1	C	37[A]	TRP	2.4
1	D	200	SER	2.4
1	E	89	ILE	2.4
1	D	82	GLU	2.4
1	A	37[A]	TRP	2.4
1	B	37[A]	TRP	2.4
1	E	291	GLU	2.3
1	D	88	VAL	2.3
1	B	332	VAL	2.3
1	D	167	ASP	2.3
1	D	333	ALA	2.3
1	E	266	ASP	2.3
1	B	256	GLY	2.3
1	C	51	SER	2.3
1	B	252	GLY	2.3
1	D	172	ALA	2.2
1	C	72	ILE	2.2
1	D	122	ARG	2.2
1	E	57	LEU	2.2
1	D	286	GLU	2.2
1	A	321	ALA	2.2
1	F	164	TYR	2.2
1	D	251	ARG	2.2
1	B	263	ARG	2.2
1	F	122	ARG	2.2
1	E	13	ASP	2.1
1	C	332	VAL	2.1
1	D	204	ARG	2.1
1	D	90	MET	2.1
1	C	172	ALA	2.1
1	E	118	PRO	2.1
1	D	51	SER	2.1
1	F	340	ASN	2.1
1	E	303	ASP	2.1
1	D	37[A]	TRP	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	44	ILE	2.0
1	E	23	ALA	2.0
1	B	333	ALA	2.0
1	E	254	ALA	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](#)

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	CA	E	401	1/1	0.94	0.10	52,52,52,52	0
2	CA	C	401	1/1	0.96	0.10	45,45,45,45	0
2	CA	D	401	1/1	0.96	0.12	65,65,65,65	0
2	CA	A	401	1/1	0.96	0.27	51,51,51,51	0
2	CA	F	401	1/1	0.98	0.10	48,48,48,48	0
2	CA	B	401	1/1	0.98	0.10	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.