



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:33 AM GMT

PDB ID : 2X53
Title : STRUCTURE OF THE PHAGE P2 BASEPLATE IN ITS ACTIVATED CONFORMATION WITH SR
Authors : Sciara, G.; Bebeacua, C.; Bron, P.; Tremblay, D.; Ortiz-Lombardia, M.; Lichiere, J.; Vanheel, M.; Campanacci, V.; Moineau, S.; Cambillau, C.
Deposited on : 2010-02-05
Resolution : 3.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : trunk26765
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

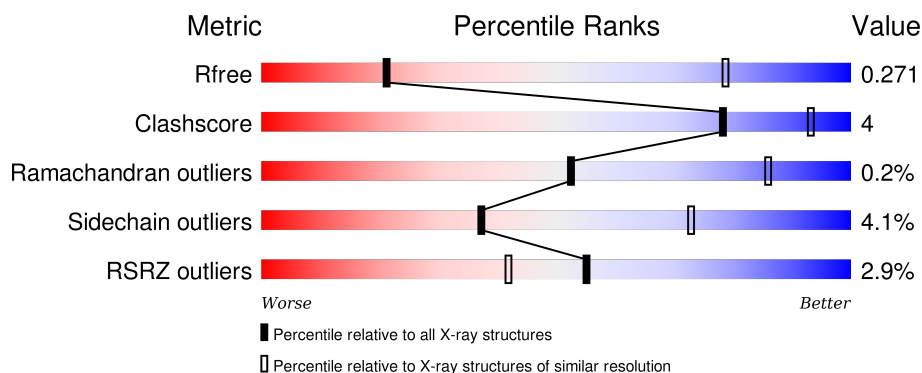
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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	1	375	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>
1	Y	375	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>..</div> </div> </div>
1	Z	375	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>..</div> </div> </div>
2	A	263	<div> <div></div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
2	B	263	<div> <div></div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	C	263	
2	D	263	
2	E	263	
2	F	263	
2	G	263	
2	H	263	
2	I	263	
2	J	263	
2	K	263	
2	L	263	
2	M	263	
2	N	263	
2	O	263	
2	P	263	
2	Q	263	
2	R	263	
3	S	298	
3	T	298	
3	U	298	
3	V	298	
3	W	298	
3	X	298	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SR	V	1299	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 59742 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 ORF16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	Y	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	Z	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			

- Molecule 2 is a protein called PUTATIVE RECEPTOR BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	B	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	C	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	D	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	E	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	F	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	G	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	H	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	I	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	J	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	K	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	M	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	N	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	O	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	P	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	Q	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	R	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0

- Molecule 3 is a protein called ORF15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	T	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	U	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	V	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	W	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	X	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0

- Molecule 4 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	V	1	Total 1	Sr 1	0	0
4	W	1	Total 1	Sr 1	0	0
4	T	1	Total 1	Sr 1	0	0
4	U	1	Total 1	Sr 1	0	0

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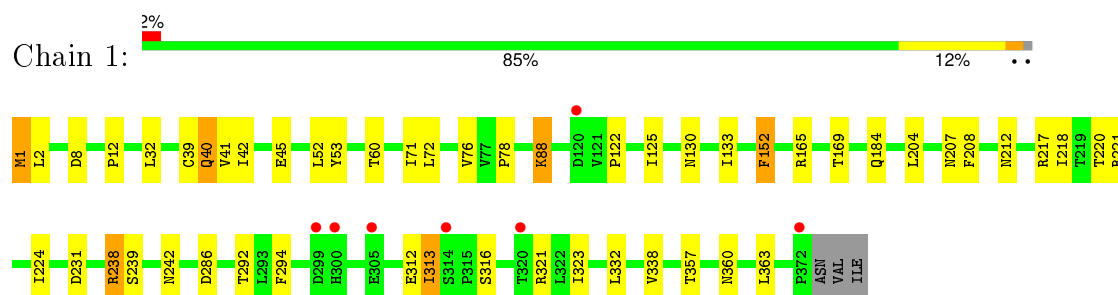
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	1	Total 1	Sr 1	0	0
4	S	1	Total 1	Sr 1	0	0

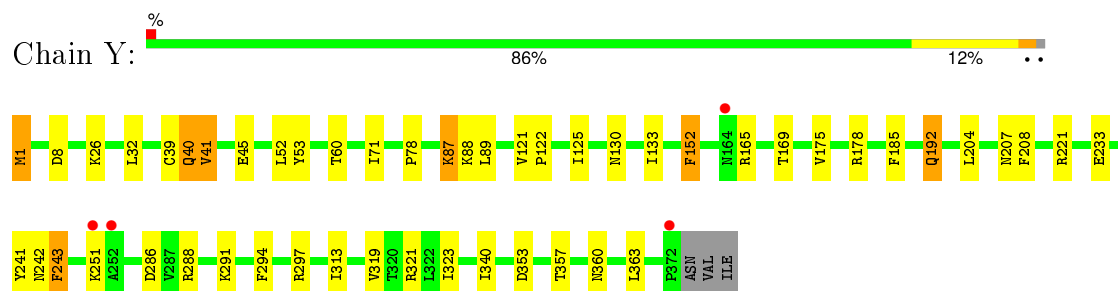
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

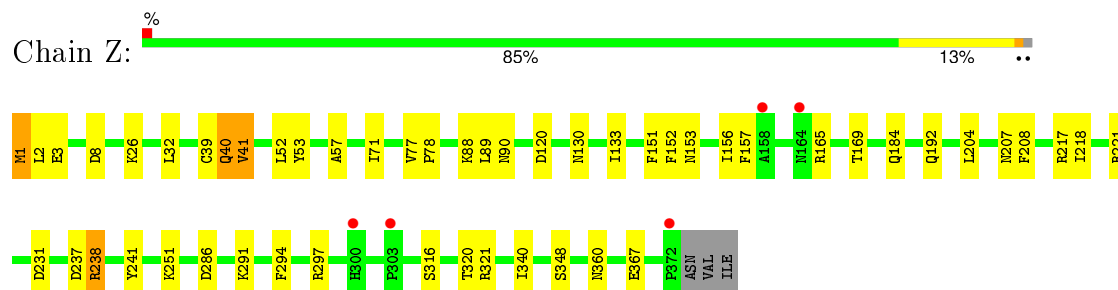
• Molecule 1: ORF16



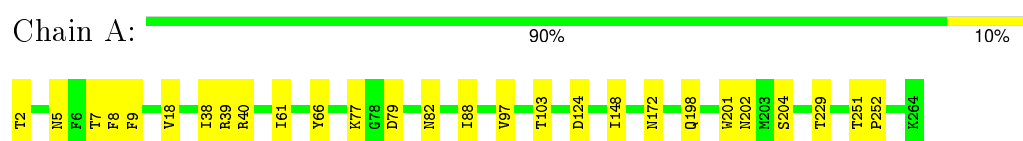
• Molecule 1: ORF16




• Molecule 1: ORF16



• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain B: 



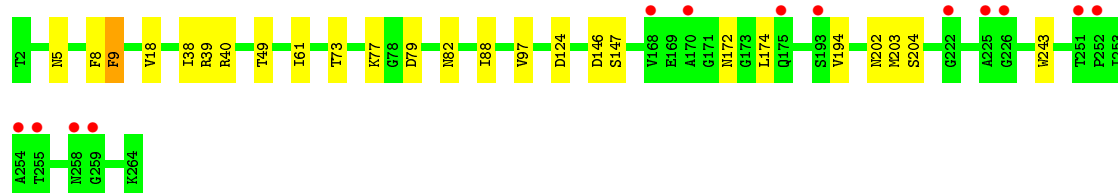
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain C: 



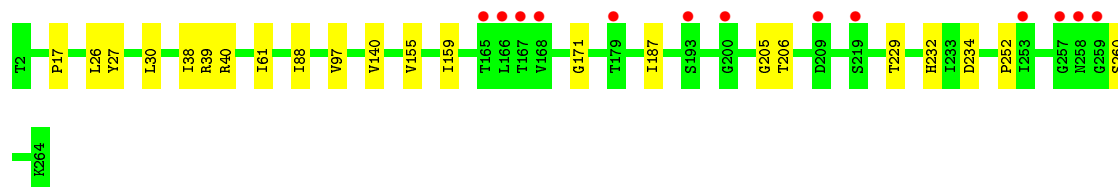
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain D: 



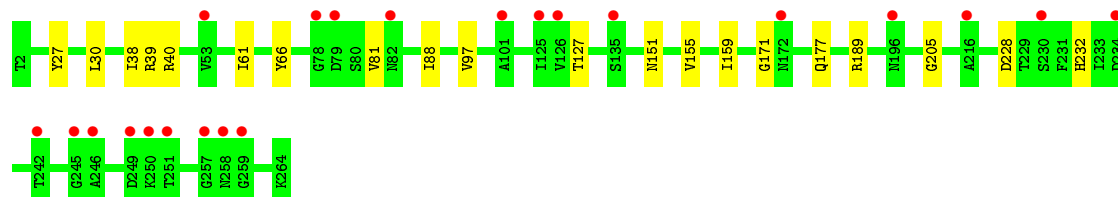
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain E: 




- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain F: 



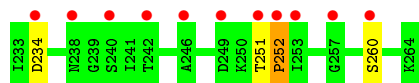
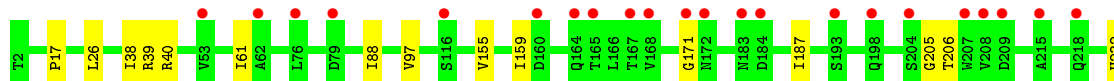
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain G: 

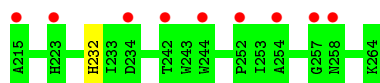




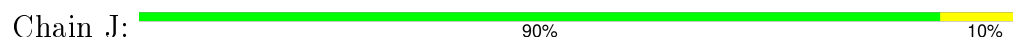
● Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



● Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



● Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



● Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



● Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



● Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN





- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain N: 92% 8%



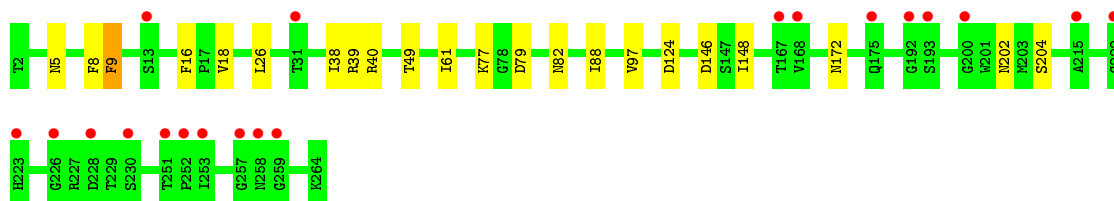
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain O: 92% 8%



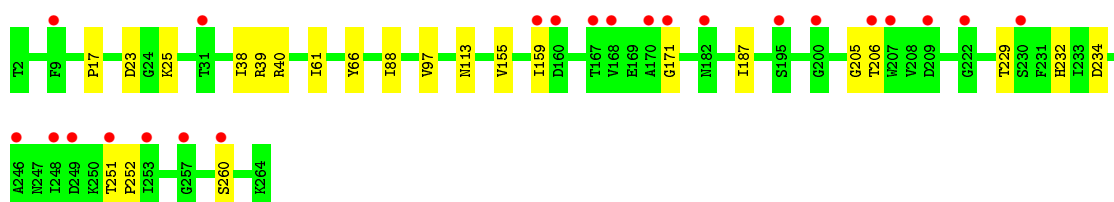
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain P: 8% 92% 8%



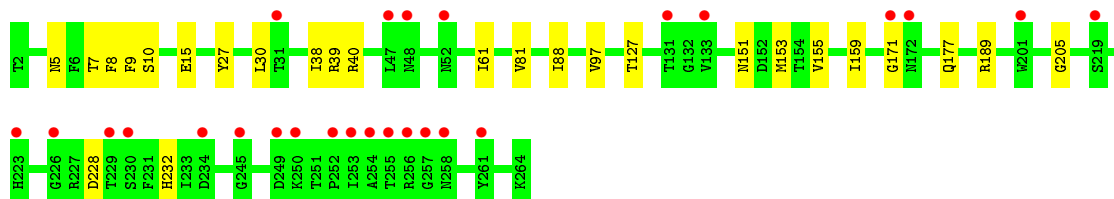
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain Q: 9% 91% 9%




- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain R: 10% 90% 10%



- Molecule 3: ORF15


R206	R215	V228	E232	Q233	V234	L239	T240	V241	T242	Q250	V251	L258	V263	V269	R270	T271	T272	T273	T274	L281	L282	N283	L284	S285	L291	R292	R293	V298
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------


Chain T:  79% 18%

I196	F199	L202	L203	K206	A212	R215	A226	K230	V234	Q235	D236	Y237	L238	L239	T240	N241	T242	D243	Y249	L258	V263	F266	E267	R268	Y269	R272	L282	N283	L284	S285	L291	K292	A295	V298
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

[illegible]


S175	W190	E194	E195	I196	M200	L203	K206	G213	G214	R215	A226	V228	F229	E232	G233	V234	T238	L239	T240	M241	T242	L258	N259	L260	V263	M264	R268	T269	R270	R271	R272	T273	L274	L281	T282	N283	L284	S285	T291	R292	R293	V295
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

Chain V: 

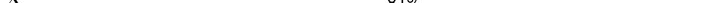


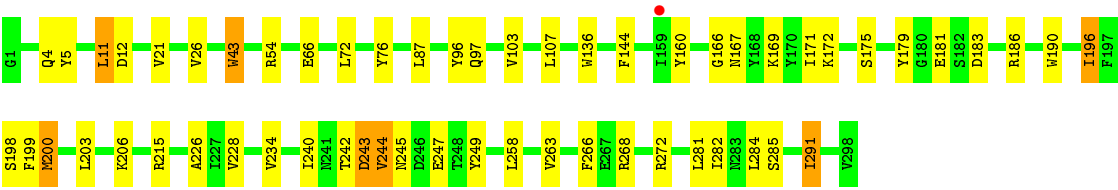
Label	Color
G1	Green
V2	Green
R3	Green
L11	Green
D12	Green
P31	Green
L36	Yellow
I48	Green
R54	Green
S55	Green
E66	Green
L72	Yellow
Y76	Green
L87	Green
Y96	Green
V103	Green
Y118	Green
G119	Green
K120	Green
M121	Green
G122	Green
W136	Green
L142	Green
T143	Green
F144	Green
Y160	Green
G166	Green
I171	Green
K172	Green
S175	Green
G180	Green
W190	Green
E194	Green
E195	Green
I196	Green
F197	Green
S198	Green
F199	Green

L203	F206	R215	A226	T227	E232	Q233	V234	T240	N241	T242	D243	V244	N245	D246	E247	T248	Y249	L258	F262	V263	F266	E267	R268	V269	I274	T282	S285	I291	R292	R293	F297	V298
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

Chain W:  83% 14%

Category	Count
A226	10
I227	10
V228	10
Q232	10
Q233	10
V234	10
T242	10
E247	10
T248	10
Y249	10
L258	10
V263	10
R268	10
Y269	10
R270	10
I274	10
L281	10
L282	10
S283	10
L284	10
S285	10
I291	10
R292	10
R293	10
V298	10

Chain X:  81% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	300.28Å 239.51Å 274.78Å 90.00° 124.36° 90.00°	Depositor
Resolution (Å)	39.31 – 3.90 39.15 – 3.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.31-3.90) 96.9 (39.15-3.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 3.87Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.229 , 0.242 0.258 , 0.271	Depositor DCC
R_{free} test set	4219 reflections (2.99%)	DCC
Wilson B-factor (Å ²)	83.1	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 85.7	EDS
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 141150 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	59742	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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](#)

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

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	1	0.38	0/3069	0.64	0/4175
1	Y	0.38	0/3069	0.65	0/4175
1	Z	0.38	0/3069	0.63	0/4175
2	A	0.32	0/2048	0.63	0/2791
2	B	0.36	0/2048	0.58	0/2791
2	C	0.35	0/2048	0.59	0/2791
2	D	0.32	0/2048	0.61	0/2791
2	E	0.36	0/2048	0.58	0/2791
2	F	0.36	0/2048	0.58	0/2791
2	G	0.32	0/2048	0.62	0/2791
2	H	0.37	0/2048	0.58	0/2791
2	I	0.37	0/2048	0.58	0/2791
2	J	0.34	0/2048	0.63	0/2791
2	K	0.36	0/2048	0.59	0/2791
2	L	0.36	0/2048	0.58	0/2791
2	M	0.34	0/2048	0.63	0/2791
2	N	0.36	0/2048	0.58	0/2791
2	O	0.36	0/2048	0.58	0/2791
2	P	0.34	0/2048	0.63	0/2791
2	Q	0.37	0/2048	0.58	0/2791
2	R	0.37	0/2048	0.59	0/2791
3	S	0.36	0/2485	0.69	0/3356
3	T	0.36	0/2485	0.69	0/3356
3	U	0.35	0/2485	0.67	0/3356
3	V	0.36	0/2485	0.67	0/3356
3	W	0.35	0/2485	0.66	0/3356
3	X	0.36	0/2485	0.67	0/3356
All	All	0.36	0/60981	0.62	0/82899

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	1	3000	0	2956	35	0
1	Y	3000	0	2956	25	0
1	Z	3000	0	2956	32	0
2	A	2008	0	1971	13	0
2	B	2008	0	1971	10	0
2	C	2008	0	1971	10	0
2	D	2008	0	1971	14	0
2	E	2008	0	1971	10	0
2	F	2008	0	1971	10	0
2	G	2008	0	1971	16	0
2	H	2008	0	1971	7	0
2	I	2008	0	1971	9	0
2	J	2008	0	1971	13	0
2	K	2008	0	1971	9	0
2	L	2008	0	1971	11	0
2	M	2008	0	1971	13	0
2	N	2008	0	1971	11	0
2	O	2008	0	1971	11	0
2	P	2008	0	1971	14	0
2	Q	2008	0	1971	10	0
2	R	2008	0	1971	16	0
3	S	2432	0	2394	34	0
3	T	2432	0	2394	35	0
3	U	2432	0	2394	35	0
3	V	2432	0	2394	28	0
3	W	2432	0	2394	23	0
3	X	2432	0	2394	40	0
4	S	1	0	0	0	0
4	T	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
4	W	1	0	0	0	0
4	X	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	59742	0	58710	423	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.

The worst 5 of 423 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)
1:1:78:PRO:HG3	2:N:103:THR:HB	1.31	1.08
2:G:103:THR:HB	1:Z:78:PRO:HG3	1.41	1.00
3:S:242:THR:CG2	3:S:272:ARG:HG3	1.90	1.00
2:A:103:THR:HB	1:Y:78:PRO:HG3	1.48	0.94
1:1:42:ILE:HB	3:X:43:TRP:HZ2	1.33	0.94

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	1	370/375 (99%)	358 (97%)	12 (3%)	0	100	100
1	Y	370/375 (99%)	355 (96%)	15 (4%)	0	100	100
1	Z	370/375 (99%)	357 (96%)	13 (4%)	0	100	100
2	A	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	B	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	C	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	D	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	E	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	F	261/263 (99%)	246 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	H	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	I	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	J	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	K	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	L	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	M	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	N	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	O	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	P	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	Q	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	R	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
3	S	296/298 (99%)	278 (94%)	16 (5%)	2 (1%)	26	70
3	T	296/298 (99%)	273 (92%)	21 (7%)	2 (1%)	26	70
3	U	296/298 (99%)	274 (93%)	20 (7%)	2 (1%)	26	70
3	V	296/298 (99%)	275 (93%)	19 (6%)	2 (1%)	26	70
3	W	296/298 (99%)	280 (95%)	14 (5%)	2 (1%)	26	70
3	X	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	26	70
All	All	7584/7647 (99%)	7207 (95%)	365 (5%)	12 (0%)	52	86

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S	175	SER
3	T	175	SER
3	U	175	SER
3	V	175	SER
3	W	175	SER

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	1	337/340 (99%)	324 (96%)	13 (4%)	39	74
1	Y	337/340 (99%)	319 (95%)	18 (5%)	28	67
1	Z	337/340 (99%)	321 (95%)	16 (5%)	32	70
2	A	227/227 (100%)	218 (96%)	9 (4%)	38	73
2	B	227/227 (100%)	221 (97%)	6 (3%)	54	81
2	C	227/227 (100%)	223 (98%)	4 (2%)	66	87
2	D	227/227 (100%)	220 (97%)	7 (3%)	47	78
2	E	227/227 (100%)	221 (97%)	6 (3%)	54	81
2	F	227/227 (100%)	224 (99%)	3 (1%)	76	89
2	G	227/227 (100%)	219 (96%)	8 (4%)	43	76
2	H	227/227 (100%)	220 (97%)	7 (3%)	47	78
2	I	227/227 (100%)	223 (98%)	4 (2%)	66	87
2	J	227/227 (100%)	219 (96%)	8 (4%)	43	76
2	K	227/227 (100%)	221 (97%)	6 (3%)	54	81
2	L	227/227 (100%)	223 (98%)	4 (2%)	66	87
2	M	227/227 (100%)	219 (96%)	8 (4%)	43	76
2	N	227/227 (100%)	221 (97%)	6 (3%)	54	81
2	O	227/227 (100%)	224 (99%)	3 (1%)	76	89
2	P	227/227 (100%)	220 (97%)	7 (3%)	47	78
2	Q	227/227 (100%)	220 (97%)	7 (3%)	47	78
2	R	227/227 (100%)	223 (98%)	4 (2%)	66	87
3	S	264/264 (100%)	246 (93%)	18 (7%)	20	59
3	T	264/264 (100%)	247 (94%)	17 (6%)	22	61
3	U	264/264 (100%)	241 (91%)	23 (9%)	13	49
3	V	264/264 (100%)	241 (91%)	23 (9%)	13	49
3	W	264/264 (100%)	244 (92%)	20 (8%)	16	55
3	X	264/264 (100%)	247 (94%)	17 (6%)	22	61
All	All	6681/6690 (100%)	6409 (96%)	272 (4%)	37	73

5 of 272 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	S	43	TRP
3	T	243	ASP
1	Y	286	ASP
3	S	66	GLU
3	T	12	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	175	GLN
2	M	175	GLN
3	X	250	GLN
2	J	196	ASN
2	M	71	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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, 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	1	372/375 (99%)	0.19	7 (1%) 70 59	63, 97, 170, 239	0
1	Y	372/375 (99%)	0.07	4 (1%) 82 74	62, 94, 151, 270	0
1	Z	372/375 (99%)	0.15	5 (1%) 79 70	63, 98, 166, 246	0
2	A	263/263 (100%)	-0.13	0 100 100	44, 76, 105, 140	0
2	B	263/263 (100%)	-0.01	1 (0%) 93 90	55, 88, 126, 147	0
2	C	263/263 (100%)	0.05	1 (0%) 93 90	55, 90, 137, 172	0
2	D	263/263 (100%)	0.27	13 (4%) 33 24	52, 106, 248, 290	0
2	E	263/263 (100%)	0.44	13 (4%) 33 24	64, 121, 259, 286	0
2	F	263/263 (100%)	0.51	22 (8%) 14 9	57, 144, 245, 291	0
2	G	263/263 (100%)	0.40	24 (9%) 11 8	60, 126, 249, 285	0
2	H	263/263 (100%)	0.80	33 (12%) 5 5	97, 155, 233, 282	0
2	I	263/263 (100%)	0.72	22 (8%) 14 9	75, 156, 262, 297	0
2	J	263/263 (100%)	0.07	1 (0%) 93 90	55, 102, 163, 246	0
2	K	263/263 (100%)	0.07	0 100 100	52, 84, 175, 233	0
2	L	263/263 (100%)	0.11	1 (0%) 93 90	62, 102, 162, 220	0
2	M	263/263 (100%)	0.21	2 (0%) 87 81	76, 126, 166, 208	0
2	N	263/263 (100%)	0.06	0 100 100	60, 95, 142, 163	0
2	O	263/263 (100%)	0.26	0 100 100	85, 128, 168, 184	0
2	P	263/263 (100%)	0.47	20 (7%) 17 11	65, 132, 296, 298	0
2	Q	263/263 (100%)	0.74	23 (8%) 13 9	96, 154, 288, 292	0
2	R	263/263 (100%)	0.75	26 (9%) 9 7	83, 160, 292, 300	0
3	S	298/298 (100%)	-0.24	0 100 100	41, 64, 106, 124	0
3	T	298/298 (100%)	-0.29	0 100 100	42, 65, 113, 145	0
3	U	298/298 (100%)	-0.19	0 100 100	43, 71, 129, 169	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
3	V	298/298 (100%)	-0.22	0	100 100	44, 66, 101, 127	0
3	W	298/298 (100%)	-0.18	1 (0%)	94 91	40, 67, 132, 161	0
3	X	298/298 (100%)	-0.17	1 (0%)	94 91	40, 67, 158, 202	0
All	All	7638/7647 (99%)	0.17	220 (2%)	55 42	40, 98, 207, 300	0

The worst 5 of 220 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	226	GLY	5.4
2	R	252	PRO	5.2
2	I	258	ASN	5.0
2	D	254	ALA	4.5
2	D	258	ASN	4.3

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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
4	SR	V	1299	1/1	0.96	0.26	2.89	80,80,80,80	0
4	SR	W	1299	1/1	0.98	0.29	1.96	80,80,80,80	0
4	SR	T	1299	1/1	0.98	0.27	1.76	80,80,80,80	0
4	SR	X	1299	1/1	0.97	0.25	0.38	83,83,83,83	0
4	SR	S	1299	1/1	0.94	0.25	0.14	87,87,87,87	0
4	SR	U	1299	1/1	0.93	0.26	-	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.