Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2017 – 11:20 AM EDT

PDB ID	:	5I84
Title	:	Structure of the Xanthomonas citri phosphate-binding protein PhoX
Authors	:	Pegos, V.R.; Medrano, F.J.; Balan, A.
Deposited on	:	unknown
Resolution	:	2.98 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 (i) symbol.

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

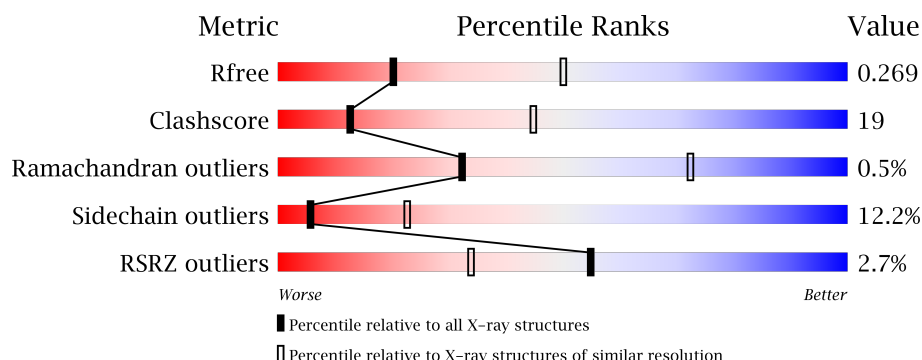|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.98 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	Percentile Ranks	Value
Rfree		0.269
Clashscore		19
Ramachandran outliers		0.5%
Sidechain outliers		12.2%
RSRZ outliers		2.7%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2168 (3.00-2.96)
Clashscore	112137	2535 (3.00-2.96)
Ramachandran outliers	110173	2451 (3.00-2.96)
Sidechain outliers	110143	2454 (3.00-2.96)
RSRZ outliers	101464	2192 (3.00-2.96)

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 <=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	335	3% 62% 30% • 6%
1	B	335	3% 64% 25% • 6%
1	C	335	.% 60% 30% • 7%
1	D	335	.% 61% 28% • 6%
1	E	335	2% 56% 33% • 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	335	2% [bar: 56% / 35% / · / 6%]
1	G	335	4% [bar: 59% / 29% / 5% / 6%]
1	H	335	3% [bar: 59% / 27% / 6% / 7%]

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
2	PO4	C	402	-	-	X	-
2	PO4	D	401	-	-	X	-
2	PO4	E	402	-	-	X	-

2   Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18875 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 Phosphate-binding protein PstS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2341	1505	389	443	4			
1	B	314	Total	C	N	O	S	0	0	0
			2341	1505	389	443	4			
1	C	312	Total	C	N	O	S	0	0	0
			2323	1493	385	441	4			
1	D	314	Total	C	N	O	S	0	0	0
			2341	1505	389	443	4			
1	E	314	Total	C	N	O	S	0	0	0
			2341	1505	389	443	4			
1	F	314	Total	C	N	O	S	0	0	0
			2341	1505	389	443	4			
1	G	314	Total	C	N	O	S	0	0	0
			2341	1505	389	443	4			
1	H	310	Total	C	N	O	S	0	0	0
			2308	1484	382	438	4			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MET	-	initiating methionine	UNP Q8PM55
A	7	GLY	-	expression tag	UNP Q8PM55
A	8	SER	-	expression tag	UNP Q8PM55
A	9	SER	-	expression tag	UNP Q8PM55
A	10	HIS	-	expression tag	UNP Q8PM55
A	11	HIS	-	expression tag	UNP Q8PM55
A	12	HIS	-	expression tag	UNP Q8PM55
A	13	HIS	-	expression tag	UNP Q8PM55
A	14	HIS	-	expression tag	UNP Q8PM55
A	15	SER	-	expression tag	UNP Q8PM55
A	16	SER	-	expression tag	UNP Q8PM55
A	17	GLY	-	expression tag	UNP Q8PM55
A	18	LEU	-	expression tag	UNP Q8PM55

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	VAL	-	expression tag	UNP Q8PM55
A	20	PRO	-	expression tag	UNP Q8PM55
A	21	ARG	-	expression tag	UNP Q8PM55
A	22	GLY	-	expression tag	UNP Q8PM55
A	23	SER	-	expression tag	UNP Q8PM55
A	24	HIS	-	expression tag	UNP Q8PM55
A	25	MET	-	expression tag	UNP Q8PM55
B	6	MET	-	initiating methionine	UNP Q8PM55
B	7	GLY	-	expression tag	UNP Q8PM55
B	8	SER	-	expression tag	UNP Q8PM55
B	9	SER	-	expression tag	UNP Q8PM55
B	10	HIS	-	expression tag	UNP Q8PM55
B	11	HIS	-	expression tag	UNP Q8PM55
B	12	HIS	-	expression tag	UNP Q8PM55
B	13	HIS	-	expression tag	UNP Q8PM55
B	14	HIS	-	expression tag	UNP Q8PM55
B	15	SER	-	expression tag	UNP Q8PM55
B	16	SER	-	expression tag	UNP Q8PM55
B	17	GLY	-	expression tag	UNP Q8PM55
B	18	LEU	-	expression tag	UNP Q8PM55
B	19	VAL	-	expression tag	UNP Q8PM55
B	20	PRO	-	expression tag	UNP Q8PM55
B	21	ARG	-	expression tag	UNP Q8PM55
B	22	GLY	-	expression tag	UNP Q8PM55
B	23	SER	-	expression tag	UNP Q8PM55
B	24	HIS	-	expression tag	UNP Q8PM55
B	25	MET	-	expression tag	UNP Q8PM55
C	6	MET	-	initiating methionine	UNP Q8PM55
C	7	GLY	-	expression tag	UNP Q8PM55
C	8	SER	-	expression tag	UNP Q8PM55
C	9	SER	-	expression tag	UNP Q8PM55
C	10	HIS	-	expression tag	UNP Q8PM55
C	11	HIS	-	expression tag	UNP Q8PM55
C	12	HIS	-	expression tag	UNP Q8PM55
C	13	HIS	-	expression tag	UNP Q8PM55
C	14	HIS	-	expression tag	UNP Q8PM55
C	15	SER	-	expression tag	UNP Q8PM55
C	16	SER	-	expression tag	UNP Q8PM55
C	17	GLY	-	expression tag	UNP Q8PM55
C	18	LEU	-	expression tag	UNP Q8PM55
C	19	VAL	-	expression tag	UNP Q8PM55
C	20	PRO	-	expression tag	UNP Q8PM55

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ARG	-	expression tag	UNP Q8PM55
C	22	GLY	-	expression tag	UNP Q8PM55
C	23	SER	-	expression tag	UNP Q8PM55
C	24	HIS	-	expression tag	UNP Q8PM55
C	25	MET	-	expression tag	UNP Q8PM55
D	6	MET	-	initiating methionine	UNP Q8PM55
D	7	GLY	-	expression tag	UNP Q8PM55
D	8	SER	-	expression tag	UNP Q8PM55
D	9	SER	-	expression tag	UNP Q8PM55
D	10	HIS	-	expression tag	UNP Q8PM55
D	11	HIS	-	expression tag	UNP Q8PM55
D	12	HIS	-	expression tag	UNP Q8PM55
D	13	HIS	-	expression tag	UNP Q8PM55
D	14	HIS	-	expression tag	UNP Q8PM55
D	15	SER	-	expression tag	UNP Q8PM55
D	16	SER	-	expression tag	UNP Q8PM55
D	17	GLY	-	expression tag	UNP Q8PM55
D	18	LEU	-	expression tag	UNP Q8PM55
D	19	VAL	-	expression tag	UNP Q8PM55
D	20	PRO	-	expression tag	UNP Q8PM55
D	21	ARG	-	expression tag	UNP Q8PM55
D	22	GLY	-	expression tag	UNP Q8PM55
D	23	SER	-	expression tag	UNP Q8PM55
D	24	HIS	-	expression tag	UNP Q8PM55
D	25	MET	-	expression tag	UNP Q8PM55
E	6	MET	-	initiating methionine	UNP Q8PM55
E	7	GLY	-	expression tag	UNP Q8PM55
E	8	SER	-	expression tag	UNP Q8PM55
E	9	SER	-	expression tag	UNP Q8PM55
E	10	HIS	-	expression tag	UNP Q8PM55
E	11	HIS	-	expression tag	UNP Q8PM55
E	12	HIS	-	expression tag	UNP Q8PM55
E	13	HIS	-	expression tag	UNP Q8PM55
E	14	HIS	-	expression tag	UNP Q8PM55
E	15	SER	-	expression tag	UNP Q8PM55
E	16	SER	-	expression tag	UNP Q8PM55
E	17	GLY	-	expression tag	UNP Q8PM55
E	18	LEU	-	expression tag	UNP Q8PM55
E	19	VAL	-	expression tag	UNP Q8PM55
E	20	PRO	-	expression tag	UNP Q8PM55
E	21	ARG	-	expression tag	UNP Q8PM55
E	22	GLY	-	expression tag	UNP Q8PM55

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	23	SER	-	expression tag	UNP Q8PM55
E	24	HIS	-	expression tag	UNP Q8PM55
E	25	MET	-	expression tag	UNP Q8PM55
F	6	MET	-	initiating methionine	UNP Q8PM55
F	7	GLY	-	expression tag	UNP Q8PM55
F	8	SER	-	expression tag	UNP Q8PM55
F	9	SER	-	expression tag	UNP Q8PM55
F	10	HIS	-	expression tag	UNP Q8PM55
F	11	HIS	-	expression tag	UNP Q8PM55
F	12	HIS	-	expression tag	UNP Q8PM55
F	13	HIS	-	expression tag	UNP Q8PM55
F	14	HIS	-	expression tag	UNP Q8PM55
F	15	SER	-	expression tag	UNP Q8PM55
F	16	SER	-	expression tag	UNP Q8PM55
F	17	GLY	-	expression tag	UNP Q8PM55
F	18	LEU	-	expression tag	UNP Q8PM55
F	19	VAL	-	expression tag	UNP Q8PM55
F	20	PRO	-	expression tag	UNP Q8PM55
F	21	ARG	-	expression tag	UNP Q8PM55
F	22	GLY	-	expression tag	UNP Q8PM55
F	23	SER	-	expression tag	UNP Q8PM55
F	24	HIS	-	expression tag	UNP Q8PM55
F	25	MET	-	expression tag	UNP Q8PM55
G	6	MET	-	initiating methionine	UNP Q8PM55
G	7	GLY	-	expression tag	UNP Q8PM55
G	8	SER	-	expression tag	UNP Q8PM55
G	9	SER	-	expression tag	UNP Q8PM55
G	10	HIS	-	expression tag	UNP Q8PM55
G	11	HIS	-	expression tag	UNP Q8PM55
G	12	HIS	-	expression tag	UNP Q8PM55
G	13	HIS	-	expression tag	UNP Q8PM55
G	14	HIS	-	expression tag	UNP Q8PM55
G	15	SER	-	expression tag	UNP Q8PM55
G	16	SER	-	expression tag	UNP Q8PM55
G	17	GLY	-	expression tag	UNP Q8PM55
G	18	LEU	-	expression tag	UNP Q8PM55
G	19	VAL	-	expression tag	UNP Q8PM55
G	20	PRO	-	expression tag	UNP Q8PM55
G	21	ARG	-	expression tag	UNP Q8PM55
G	22	GLY	-	expression tag	UNP Q8PM55
G	23	SER	-	expression tag	UNP Q8PM55
G	24	HIS	-	expression tag	UNP Q8PM55

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	25	MET	-	expression tag	UNP Q8PM55
H	6	MET	-	initiating methionine	UNP Q8PM55
H	7	GLY	-	expression tag	UNP Q8PM55
H	8	SER	-	expression tag	UNP Q8PM55
H	9	SER	-	expression tag	UNP Q8PM55
H	10	HIS	-	expression tag	UNP Q8PM55
H	11	HIS	-	expression tag	UNP Q8PM55
H	12	HIS	-	expression tag	UNP Q8PM55
H	13	HIS	-	expression tag	UNP Q8PM55
H	14	HIS	-	expression tag	UNP Q8PM55
H	15	SER	-	expression tag	UNP Q8PM55
H	16	SER	-	expression tag	UNP Q8PM55
H	17	GLY	-	expression tag	UNP Q8PM55
H	18	LEU	-	expression tag	UNP Q8PM55
H	19	VAL	-	expression tag	UNP Q8PM55
H	20	PRO	-	expression tag	UNP Q8PM55
H	21	ARG	-	expression tag	UNP Q8PM55
H	22	GLY	-	expression tag	UNP Q8PM55
H	23	SER	-	expression tag	UNP Q8PM55
H	24	HIS	-	expression tag	UNP Q8PM55
H	25	MET	-	expression tag	UNP Q8PM55

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0
2	A	1	Total 5	O 4	P 1	0	0
2	A	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	C	1	Total 5	O 4	P 1	0	0
2	C	1	Total 5	O 4	P 1	0	0
2	C	1	Total 5	O 4	P 1	0	0
2	C	1	Total 5	O 4	P 1	0	0
2	D	1	Total 5	O 4	P 1	0	0
2	D	1	Total 5	O 4	P 1	0	0
2	D	1	Total 5	O 4	P 1	0	0
2	D	1	Total 5	O 4	P 1	0	0
2	D	1	Total 5	O 4	P 1	0	0
2	E	1	Total 5	O 4	P 1	0	0
2	E	1	Total 5	O 4	P 1	0	0
2	E	1	Total 5	O 4	P 1	0	0
2	E	1	Total 5	O 4	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total 5	O 4	P 1	0	0
2	F	1	Total 5	O 4	P 1	0	0
2	F	1	Total 5	O 4	P 1	0	0
2	F	1	Total 5	O 4	P 1	0	0
2	F	1	Total 5	O 4	P 1	0	0
2	F	1	Total 5	O 4	P 1	0	0
2	F	1	Total 5	O 4	P 1	0	0
2	G	1	Total 5	O 4	P 1	0	0
2	G	1	Total 5	O 4	P 1	0	0
2	H	1	Total 5	O 4	P 1	0	0
2	H	1	Total 5	O 4	P 1	0	0
2	H	1	Total 5	O 4	P 1	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total 7	O 7	0	0
3	B	4	Total 4	O 4	0	0
3	D	4	Total 4	O 4	0	0
3	E	1	Total 1	O 1	0	0
3	F	4	Total 4	O 4	0	0
3	G	4	Total 4	O 4	0	0
3	H	4	Total 4	O 4	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 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.
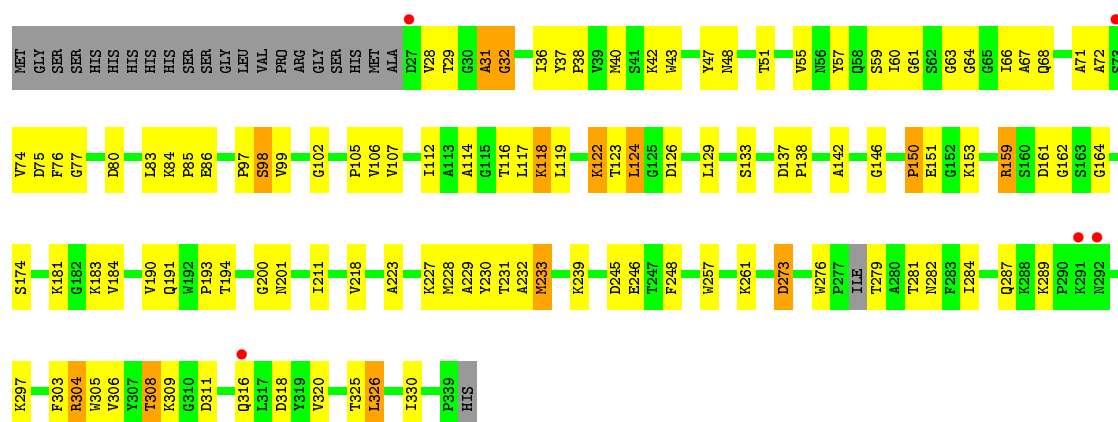
- Molecule 1: Phosphate-binding protein PstS
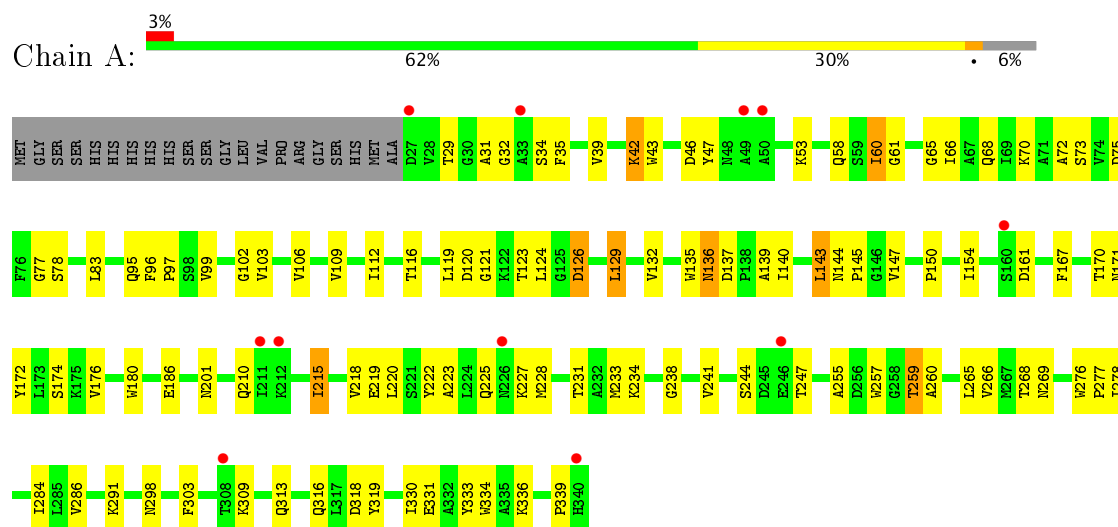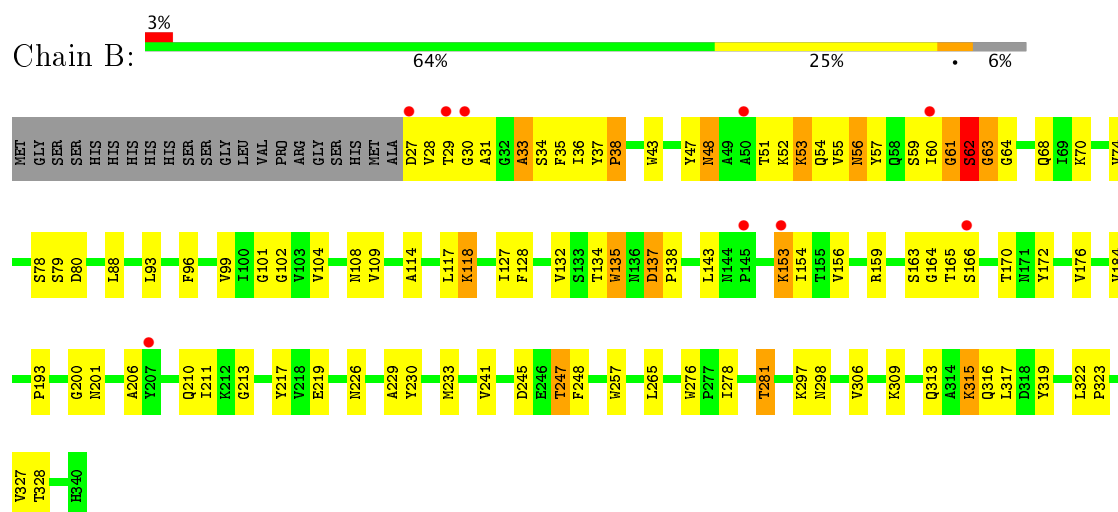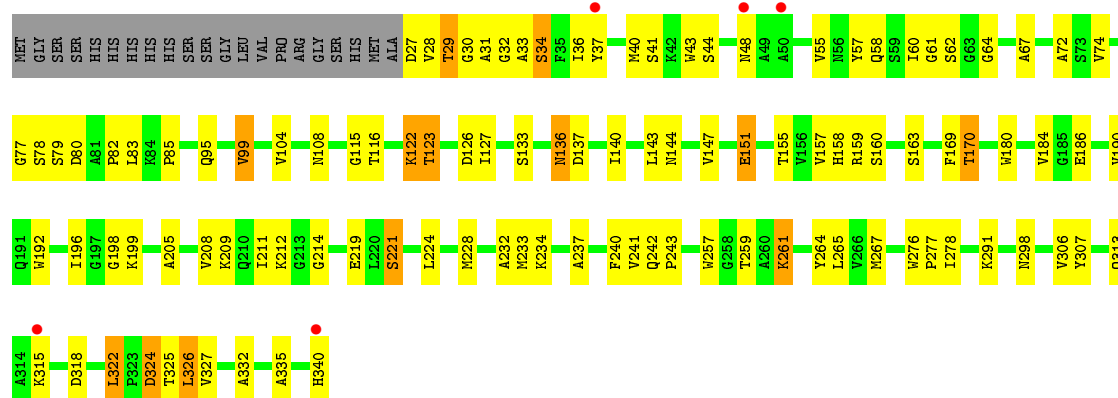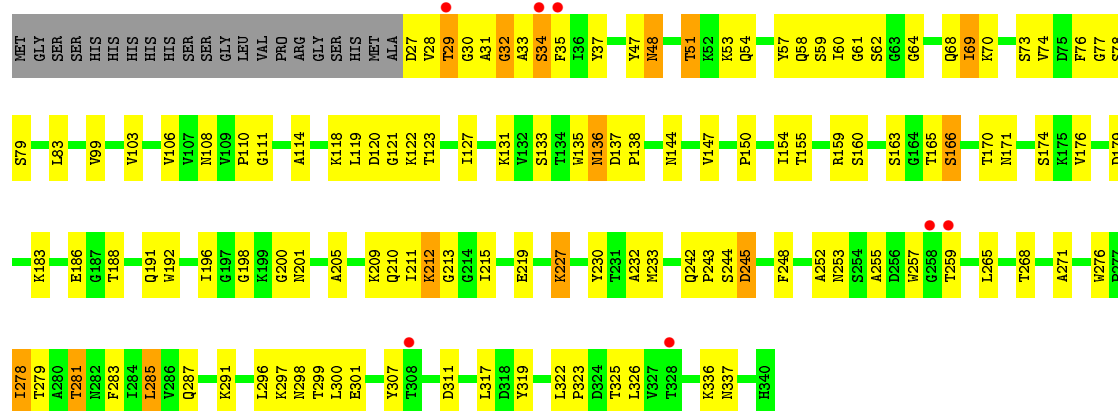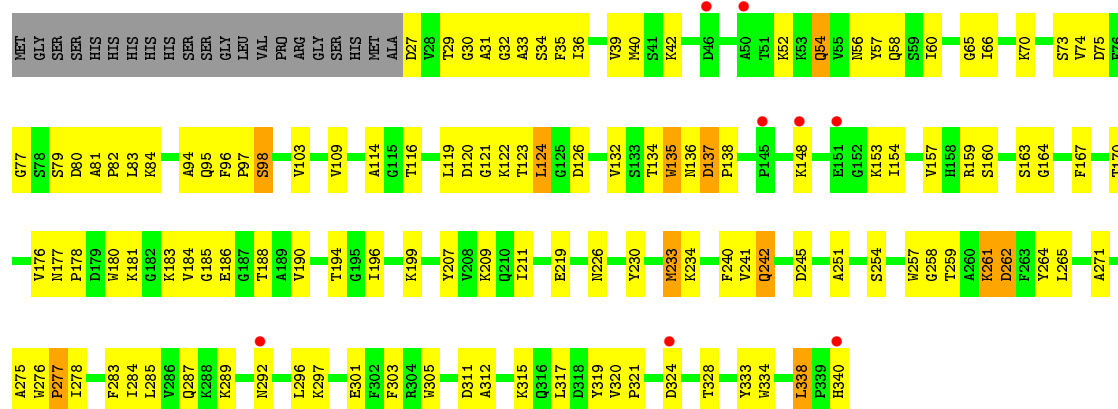

- Molecule 1: Phosphate-binding protein PstS

- Molecule 1: Phosphate-binding protein PstS

• Molecule 1: Phosphate-binding protein PstS

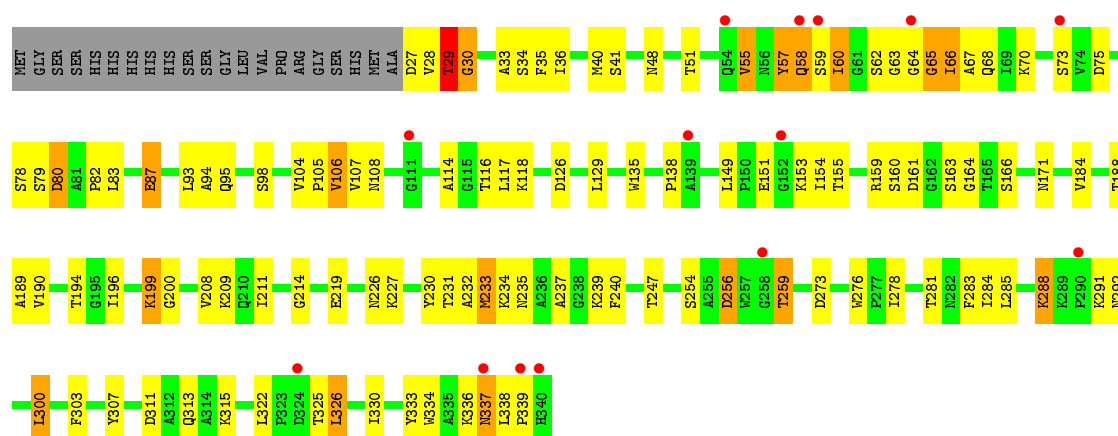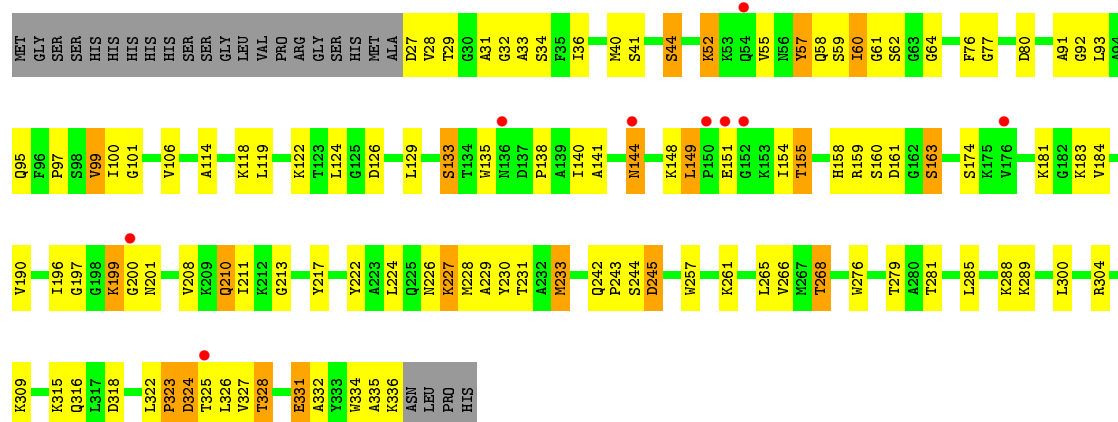Chain D:

• Molecule 1: Phosphate-binding protein PstS

Chain E:

• Molecule 1: Phosphate-binding protein PstS

Chain F:

• Molecule 1: Phosphate-binding protein PstS

Chain G:

• Molecule 1: Phosphate-binding protein PstS

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.56Å 115.64Å 133.32Å 90.00° 90.33° 90.00°	Depositor
Resolution (Å)	17.06 – 2.98 17.06 – 2.98	Depositor EDS
% Data completeness (in resolution range)	92.2 (17.06-2.98) 98.6 (17.06-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.97Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.174 , 0.249 0.195 , 0.269	Depositor DCC
R_{free} test set	2492 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	48.2	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
Reported twinning fraction	0.615 for H, K, L 0.385 for -h,-k,l	Depositor
Outliers	0 of 49511 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18875	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.80	0/2400	0.92	2/3269 (0.1%)
1	B	0.86	0/2400	0.96	3/3269 (0.1%)
1	C	0.99	1/2380 (0.0%)	1.07	5/3240 (0.2%)
1	D	0.95	0/2400	1.04	3/3269 (0.1%)
1	E	0.96	0/2400	1.03	4/3269 (0.1%)
1	F	1.04	1/2400 (0.0%)	1.06	3/3269 (0.1%)
1	G	0.89	0/2400	1.05	5/3269 (0.2%)
1	H	0.86	0/2365	0.97	1/3220 (0.0%)
All	All	0.92	2/19145 (0.0%)	1.02	26/26074 (0.1%)

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	2
1	C	0	2
1	D	0	1
1	F	0	1
1	G	0	3
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	305	TRP	CB-CG	-5.28	1.40	1.50
1	C	246	GLU	CG-CD	5.06	1.59	1.51

All (26) bond angle outliers are listed below:

Full wwPDB X-ray Structure Validation Report

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	29	THR	CB-CA-C	-9.35	86.35	111.60
1	C	32	GLY	N-CA-C	8.68	134.81	113.10
1	H	304	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	C	304	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	G	29	THR	N-CA-C	6.93	129.72	111.00
1	G	57	TYR	N-CA-C	6.54	128.65	111.00
1	B	245	ASP	CB-CG-OD1	6.24	123.92	118.30
1	E	27	ASP	CB-CG-OD1	6.20	123.88	118.30
1	E	186	GLU	OE1-CD-OE2	-5.92	116.19	123.30
1	B	33	ALA	N-CA-C	-5.88	95.12	111.00
1	D	126	ASP	CB-CG-OD1	5.83	123.55	118.30
1	D	267	MET	CB-CG-SD	-5.61	95.57	112.40
1	G	58	GLN	CB-CA-C	-5.58	99.24	110.40
1	C	233	MET	CG-SD-CE	-5.53	91.35	100.20
1	A	137	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	161	ASP	CB-CG-OD1	5.34	123.11	118.30
1	E	32	GLY	N-CA-C	5.31	126.37	113.10
1	F	124	LEU	CA-CB-CG	5.29	127.46	115.30
1	F	120	ASP	CB-CG-OD1	5.25	123.03	118.30
1	F	124	LEU	CB-CG-CD1	-5.21	102.15	111.00
1	B	62	SER	N-CA-C	-5.20	96.97	111.00
1	G	300	LEU	CB-CG-CD1	5.13	119.73	111.00
1	C	159	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	E	285	LEU	CA-CB-CG	5.11	127.05	115.30
1	D	326	LEU	CB-CG-CD2	-5.07	102.39	111.00
1	C	75	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	61	GLY	Peptide
1	B	63	GLY	Peptide
1	C	31	ALA	Peptide
1	C	59	SER	Peptide
1	D	198	GLY	Peptide
1	F	185	GLY	Peptide
1	G	29	THR	Peptide
1	G	30	GLY	Peptide
1	G	65	GLY	Peptide

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	2341	0	2324	73	0
1	B	2341	0	2324	118	1
1	C	2323	0	2305	64	0
1	D	2341	0	2324	81	0
1	E	2341	0	2324	105	0
1	F	2341	0	2324	77	0
1	G	2341	0	2324	118	0
1	H	2308	0	2293	78	0
2	A	20	0	0	0	0
2	B	25	0	0	1	0
2	C	20	0	0	2	0
2	D	25	0	0	4	0
2	E	25	0	0	2	0
2	F	30	0	0	1	0
2	G	10	0	0	0	0
2	H	15	0	0	0	1
3	A	7	0	0	1	0
3	B	4	0	0	0	0
3	D	4	0	0	0	0
3	E	1	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	0	0
All	All	18875	0	18542	697	1

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 19.

All (697) 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:E:35:PHE:CE2	1:E:219:GLU:HB2	1.27	1.62
1:E:35:PHE:CE2	1:E:219:GLU:CB	2.20	1.23
1:G:30:GLY:O	1:G:57:TYR:HD1	1.17	1.22
1:G:30:GLY:O	1:G:57:TYR:CD1	1.92	1.22

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:PHE:CE2	1:B:219:GLU:OE1	1.95	1.19
1:B:62:SER:OG	1:B:79:SER:HA	1.40	1.18
1:G:33:ALA:HB2	1:G:57:TYR:OH	1.45	1.16
1:F:30:GLY:HA3	1:F:57:TYR:HA	1.31	1.07
1:E:31:ALA:HB3	1:E:77:GLY:HA2	1.33	1.07
1:E:31:ALA:CB	1:E:77:GLY:HA2	1.83	1.06
1:G:28:VAL:HG21	1:G:55:VAL:HG22	1.36	1.06
1:H:161:ASP:OD1	1:H:199:LYS:HB2	1.52	1.06
1:E:108:ASN:O	1:E:212:LYS:O	1.75	1.04
1:E:31:ALA:HB2	1:E:76:PHE:O	1.58	1.02
1:G:28:VAL:HG21	1:G:55:VAL:CG2	1.90	1.01
1:G:33:ALA:O	1:G:59:SER:OG	1.76	1.00
1:H:325:THR:O	1:H:328:THR:HG23	1.63	0.98
1:E:35:PHE:CD2	1:E:219:GLU:HB2	2.01	0.95
1:E:31:ALA:CB	1:E:76:PHE:O	2.14	0.95
1:G:60:ILE:HB	1:G:64:GLY:O	1.67	0.95
1:A:259:THR:HG23	1:A:259:THR:O	1.68	0.94
1:A:257:TRP:O	1:A:260:ALA:HB3	1.67	0.94
1:B:62:SER:OG	1:B:79:SER:CA	2.16	0.92
1:G:28:VAL:CG2	1:G:55:VAL:HG22	1.99	0.92
1:E:108:ASN:ND2	1:E:211:ILE:O	2.04	0.91
1:E:35:PHE:HE2	1:E:219:GLU:HB2	1.30	0.90
1:E:35:PHE:CZ	1:E:219:GLU:HB2	2.07	0.89
1:E:48:ASN:O	1:E:51:THR:O	1.91	0.89
1:G:33:ALA:CB	1:G:57:TYR:OH	2.19	0.89
1:H:324:ASP:O	1:H:328:THR:HG22	1.73	0.88
1:F:114:ALA:O	1:F:230:TYR:O	1.92	0.87
1:H:161:ASP:CG	1:H:199:LYS:HB2	1.94	0.87
1:E:37:TYR:CE2	1:E:57:TYR:HE1	1.92	0.87
1:D:219:GLU:OE1	1:D:221:SER:OG	1.93	0.86
1:C:112:ILE:HG23	1:C:116:THR:HB	1.57	0.86
1:E:136:ASN:OD1	1:E:150:PRO:O	1.93	0.85
1:F:157:VAL:HG22	1:F:196:ILE:HD11	1.58	0.84
1:A:259:THR:CG2	1:A:259:THR:O	2.27	0.83
1:B:35:PHE:CD2	1:B:219:GLU:HB2	2.13	0.83
1:B:31:ALA:HB3	1:B:57:TYR:CD1	2.14	0.83
1:B:51:THR:HB	1:B:53:LYS:HE3	1.62	0.82
1:F:96:PHE:CD2	1:F:334:TRP:HZ2	1.99	0.81
1:G:33:ALA:HB3	1:G:57:TYR:CE2	2.16	0.81
1:B:35:PHE:HE2	1:B:219:GLU:OE1	1.60	0.81
1:E:34:SER:O	1:E:201:ASN:ND2	2.14	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:PHE:CD1	1:G:219:GLU:HB2	2.16	0.80
1:H:325:THR:O	1:H:328:THR:CG2	2.29	0.80
1:B:109:VAL:HG12	1:B:135:TRP:CZ2	2.17	0.79
1:H:61:GLY:O	1:H:64:GLY:N	2.15	0.79
1:F:42:LYS:HD3	1:F:317:LEU:HD11	1.63	0.79
1:B:62:SER:O	1:B:164:GLY:N	2.17	0.77
1:E:31:ALA:HB3	1:E:77:GLY:CA	2.12	0.77
1:B:159:ARG:HH12	1:B:200:GLY:C	1.87	0.77
1:C:31:ALA:HB2	1:C:74:VAL:HG21	1.64	0.76
1:G:33:ALA:HB2	1:G:57:TYR:CZ	2.21	0.76
1:F:170:THR:HG22	1:F:186:GLU:HA	1.67	0.76
1:B:313:GLN:O	1:B:317:LEU:HD12	1.87	0.75
1:A:35:PHE:CE1	1:A:219:GLU:HG3	2.20	0.75
1:B:31:ALA:HB3	1:B:57:TYR:CE1	2.22	0.75
1:D:144:ASN:HB3	1:D:147:VAL:HG12	1.68	0.75
1:B:109:VAL:HG11	1:B:135:TRP:NE1	2.02	0.75
1:G:28:VAL:CG2	1:G:55:VAL:CG2	2.61	0.74
1:D:28:VAL:CG1	1:D:55:VAL:HG13	2.17	0.74
1:A:241:VAL:CG1	1:A:247:THR:HG21	2.18	0.74
1:F:135:TRP:CZ3	1:F:154:ILE:HA	2.24	0.73
1:G:30:GLY:O	1:G:57:TYR:CE1	2.41	0.73
1:H:257:TRP:CZ3	1:H:326:LEU:HB3	2.23	0.72
1:G:62:SER:HB2	1:G:79:SER:HA	1.72	0.72
1:B:35:PHE:HD2	1:B:219:GLU:HB2	1.52	0.72
1:B:135:TRP:HH2	1:B:213:GLY:HA3	1.53	0.72
1:B:47:TYR:CE2	1:B:53:LYS:HG3	2.24	0.72
1:E:37:TYR:CE2	1:E:57:TYR:CE1	2.76	0.72
1:E:73:SER:O	1:E:74:VAL:HG13	1.90	0.71
1:E:69:ILE:CD1	1:E:285:LEU:HB2	2.19	0.71
1:G:33:ALA:CB	1:G:57:TYR:CE2	2.74	0.70
1:E:31:ALA:HB1	1:E:77:GLY:HA2	1.72	0.70
1:G:33:ALA:HB3	1:G:57:TYR:HE2	1.56	0.70
1:B:52:LYS:N	1:B:53:LYS:HE2	2.07	0.69
1:A:39:VAL:HG22	1:A:319:TYR:CE2	2.28	0.69
1:D:205:ALA:O	1:D:209:LYS:HG3	1.92	0.69
1:D:208:VAL:HG11	1:D:228:MET:HE1	1.73	0.69
1:D:29:THR:HG23	1:D:30:GLY:N	2.07	0.69
1:B:135:TRP:CH2	1:B:213:GLY:HA3	2.28	0.69
1:E:30:GLY:HA3	1:E:57:TYR:HA	1.74	0.69
1:B:53:LYS:H	1:B:53:LYS:HE2	1.57	0.69
1:A:126:ASP:HB3	1:A:132:VAL:HG23	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:ALA:O	1:G:190:VAL:HG23	1.92	0.68
1:D:123:THR:HG21	1:D:143:LEU:HD11	1.75	0.68
1:H:31:ALA:HB2	1:H:76:PHE:O	1.94	0.68
1:F:297:LYS:O	1:F:301:GLU:HG3	1.93	0.68
1:D:60:ILE:HD12	1:D:64:GLY:HA3	1.75	0.67
1:G:108:ASN:ND2	1:G:208:VAL:O	2.20	0.67
1:D:180:TRP:CZ2	1:D:184:VAL:HG11	2.29	0.67
1:H:226:ASN:O	1:H:227:LYS:CG	2.42	0.67
1:F:209:LYS:NZ	1:F:226:ASN:O	2.28	0.67
1:G:33:ALA:CB	1:G:57:TYR:CZ	2.77	0.67
1:A:170:THR:HG22	1:A:186:GLU:HA	1.75	0.67
1:H:226:ASN:O	1:H:227:LYS:HG3	1.94	0.67
1:A:223:ALA:HA	1:A:228:MET:SD	2.36	0.67
1:B:135:TRP:HH2	1:B:213:GLY:CA	2.07	0.66
1:G:29:THR:OG1	1:G:30:GLY:HA3	1.94	0.66
1:B:35:PHE:CE2	1:B:219:GLU:CD	2.68	0.66
1:C:31:ALA:HB3	1:C:76:PHE:O	1.96	0.66
1:F:35:PHE:CE1	1:F:219:GLU:HG2	2.31	0.66
1:F:251:ALA:HB2	1:F:275:ALA:HB1	1.77	0.65
1:E:271:ALA:O	1:F:271:ALA:O	2.14	0.65
1:H:159:ARG:NE	1:H:200:GLY:O	2.29	0.65
1:D:67:ALA:HA	2:D:402:PO4:O2	1.97	0.65
1:B:51:THR:HB	1:B:53:LYS:CE	2.27	0.65
1:E:32:GLY:CA	1:E:58:GLN:O	2.45	0.65
1:G:307:TYR:CE1	1:G:322:LEU:HD12	2.31	0.65
1:B:241:VAL:HG13	1:B:247:THR:HG21	1.79	0.65
1:B:248:PHE:HE1	1:B:276:TRP:CD1	2.15	0.65
1:G:98:SER:CB	1:G:284:ILE:HD11	2.27	0.65
1:B:56:ASN:HD22	1:B:56:ASN:C	2.00	0.64
1:B:62:SER:OG	1:B:80:ASP:N	2.29	0.64
1:D:29:THR:CG2	1:D:30:GLY:N	2.60	0.64
1:E:35:PHE:HE2	1:E:219:GLU:CA	2.10	0.64
1:G:114:ALA:HB1	1:G:230:TYR:CZ	2.33	0.64
1:G:33:ALA:O	1:G:59:SER:CB	2.45	0.64
1:C:31:ALA:CB	1:C:74:VAL:HG21	2.28	0.64
1:E:31:ALA:CB	1:E:77:GLY:CA	2.71	0.64
1:F:30:GLY:N	1:F:56:ASN:O	2.31	0.64
1:B:109:VAL:CG1	1:B:135:TRP:CE2	2.81	0.64
1:E:144:ASN:HB3	1:E:147:VAL:HG22	1.79	0.64
1:A:276:TRP:HE1	1:A:278:ILE:HD12	1.62	0.63
1:B:247:THR:HB	1:B:276:TRP:HB2	1.78	0.63

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:TRP:O	1:A:47:TYR:HB2	1.99	0.63
1:B:64:GLY:O	1:B:68:GLN:HG2	1.98	0.62
1:H:331:GLU:HG3	1:H:332:ALA:N	2.13	0.62
1:A:233:MET:HB2	1:A:276:TRP:CH2	2.34	0.62
1:A:31:ALA:HB2	1:A:77:GLY:HA2	1.82	0.62
1:H:92:GLY:O	1:H:288:LYS:HB2	1.99	0.62
1:E:155:THR:HG21	1:G:196:ILE:CG2	2.30	0.62
1:E:32:GLY:O	1:E:60:ILE:HG13	2.00	0.62
1:E:244:SER:O	1:E:248:PHE:CD2	2.53	0.61
1:H:31:ALA:CB	1:H:77:GLY:HA2	2.29	0.61
1:B:28:VAL:HG11	1:B:298:ASN:CB	2.30	0.61
1:C:32:GLY:HA2	1:C:60:ILE:HG13	1.82	0.61
1:G:322:LEU:HB3	1:G:326:LEU:CD2	2.31	0.61
1:D:85:PRO:HG2	1:D:261:LYS:HG2	1.83	0.61
1:D:27:ASP:O	1:D:298:ASN:ND2	2.33	0.61
1:E:37:TYR:CD2	1:E:57:TYR:HE1	2.17	0.61
1:C:32:GLY:O	1:C:61:GLY:O	2.19	0.61
1:D:32:GLY:HA3	1:D:60:ILE:HG12	1.81	0.61
1:B:88:LEU:HD23	1:B:93:LEU:HB2	1.82	0.61
1:E:33:ALA:HB2	1:E:78:SER:O	2.01	0.61
1:G:48:ASN:O	1:G:51:THR:O	2.19	0.61
1:E:73:SER:OG	1:E:73:SER:O	2.14	0.61
1:B:52:LYS:H	1:B:53:LYS:CE	2.14	0.60
1:C:31:ALA:HB3	1:C:77:GLY:HA2	1.82	0.60
1:A:339:PRO:HB3	1:E:227:LYS:HD2	1.83	0.60
1:D:324:ASP:HA	1:D:327:VAL:HG22	1.83	0.60
1:G:63:GLY:O	1:G:65:GLY:HA2	2.01	0.60
1:H:31:ALA:HB1	1:H:77:GLY:HA2	1.82	0.60
1:B:33:ALA:HB2	1:B:78:SER:O	2.00	0.60
1:F:29:THR:OG1	1:F:75:ASP:N	2.33	0.60
1:B:165:THR:HG22	1:B:217:TYR:CE2	2.37	0.60
1:C:257:TRP:CH2	1:C:281:THR:HG21	2.36	0.60
1:D:234:LYS:HB2	1:D:240:PHE:CE1	2.36	0.60
1:E:35:PHE:HE2	1:E:219:GLU:CB	1.94	0.60
1:G:29:THR:CG2	1:G:75:ASP:OD1	2.49	0.60
1:E:32:GLY:HA2	1:E:58:GLN:O	2.02	0.60
1:B:61:GLY:O	1:B:63:GLY:HA2	2.02	0.60
1:B:61:GLY:C	1:B:63:GLY:HA2	2.23	0.59
1:C:184:VAL:HG12	1:C:190:VAL:HG11	1.83	0.59
1:C:32:GLY:HA2	1:C:60:ILE:CG1	2.32	0.59
1:E:114:ALA:O	1:E:230:TYR:O	2.20	0.59

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:ALA:HB1	1:H:36:ILE:CG1	2.32	0.59
1:B:248:PHE:CE1	1:B:276:TRP:CD1	2.90	0.59
1:B:109:VAL:CG1	1:B:135:TRP:CZ2	2.85	0.59
1:B:51:THR:CB	1:B:53:LYS:HE3	2.32	0.59
1:F:135:TRP:HZ3	1:F:154:ILE:HA	1.63	0.59
1:C:184:VAL:HG12	1:C:190:VAL:CG1	2.33	0.59
1:C:32:GLY:O	1:C:61:GLY:C	2.40	0.59
1:B:35:PHE:CZ	1:B:219:GLU:OE1	2.54	0.59
1:E:159:ARG:NH1	1:E:163:SER:CB	2.66	0.59
1:G:231:THR:HG22	1:G:232:ALA:O	2.03	0.59
1:E:31:ALA:HB3	1:E:76:PHE:O	1.99	0.59
1:F:132:VAL:O	1:F:132:VAL:HG23	2.01	0.59
1:A:172:TYR:HB2	1:A:278:ILE:CG2	2.33	0.58
1:A:172:TYR:O	1:A:176:VAL:HG23	2.03	0.58
1:C:36:ILE:HD11	1:C:99:VAL:CG1	2.33	0.58
1:C:63:GLY:HA3	2:E:402:PO4:O4	2.02	0.58
1:B:48:ASN:O	1:B:51:THR:O	2.22	0.58
1:H:114:ALA:O	1:H:230:TYR:O	2.20	0.58
1:H:34:SER:OG	1:H:201:ASN:HB2	2.04	0.58
1:E:35:PHE:CE2	1:E:219:GLU:CA	2.84	0.58
1:C:146:GLY:HA3	1:H:335:ALA:HB3	1.84	0.58
1:G:94:ALA:O	1:G:285:LEU:HA	2.02	0.58
1:G:29:THR:HG23	1:G:75:ASP:OD1	2.03	0.58
1:D:31:ALA:O	1:D:57:TYR:CZ	2.56	0.58
1:A:39:VAL:CG2	1:A:319:TYR:CE2	2.87	0.58
1:D:163:SER:OG	2:D:401:PO4:P	2.61	0.58
1:F:33:ALA:O	1:F:57:TYR:OH	2.12	0.58
1:G:333:TYR:O	1:G:337:ASN:CG	2.43	0.58
1:B:109:VAL:HG12	1:B:135:TRP:CE2	2.39	0.57
1:C:284:ILE:N	1:C:284:ILE:HD12	2.19	0.57
1:D:31:ALA:CB	1:D:77:GLY:HA2	2.34	0.57
1:E:28:VAL:HG22	1:E:298:ASN:HB3	1.85	0.57
1:F:170:THR:CG2	1:F:186:GLU:HA	2.34	0.57
1:A:103:VAL:HB	1:A:278:ILE:HD13	1.85	0.57
1:F:27:ASP:HB2	1:F:54:GLN:O	2.05	0.57
1:G:35:PHE:HD1	1:G:219:GLU:HB2	1.69	0.57
1:B:35:PHE:O	1:B:319:TYR:OH	2.10	0.57
2:C:402:PO4:O3	1:E:70:LYS:HD2	2.04	0.57
1:H:135:TRP:HE1	1:H:213:GLY:HA2	1.69	0.57
1:H:41:SER:HA	1:H:57:TYR:CE2	2.39	0.57
1:B:134:THR:O	1:B:154:ILE:HD11	2.04	0.57

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:MET:HB2	1:D:276:TRP:CH2	2.39	0.57
1:B:62:SER:HG	1:B:79:SER:CA	2.16	0.57
1:B:134:THR:HG23	1:B:137:ASP:HB2	1.87	0.56
1:B:29:THR:HB	1:B:56:ASN:ND2	2.20	0.56
1:E:32:GLY:HA3	1:E:58:GLN:O	2.05	0.56
1:F:31:ALA:HB2	1:F:74:VAL:HG11	1.87	0.56
1:G:29:THR:HG21	1:G:75:ASP:N	2.19	0.56
1:A:241:VAL:O	1:A:276:TRP:HZ3	1.88	0.56
1:F:164:GLY:O	1:F:167:PHE:HB3	2.04	0.56
1:G:334:TRP:HA	1:G:337:ASN:HD21	1.70	0.56
1:E:212:LYS:O	1:E:212:LYS:HD3	2.05	0.56
1:F:66:ILE:HD13	1:F:83:LEU:HD21	1.88	0.56
1:D:163:SER:HG	2:D:401:PO4:P	2.28	0.56
1:G:80:ASP:HB3	1:G:164:GLY:HA3	1.87	0.56
1:H:44:SER:OG	1:H:57:TYR:HE2	1.88	0.56
1:A:276:TRP:NE1	1:A:278:ILE:HD12	2.21	0.56
1:F:96:PHE:CD2	1:F:334:TRP:CZ2	2.87	0.56
1:A:241:VAL:HG13	1:A:247:THR:HG21	1.87	0.56
1:C:122:LYS:HE3	1:D:259:THR:CG2	2.35	0.56
1:H:34:SER:O	1:H:222:TYR:OH	2.16	0.56
1:D:170:THR:HB	1:D:186:GLU:HA	1.87	0.56
1:F:96:PHE:CE2	1:F:334:TRP:CZ2	2.93	0.56
1:H:323:PRO:HG2	1:H:326:LEU:HD12	1.87	0.56
1:D:28:VAL:HG12	1:D:55:VAL:HG22	1.87	0.56
1:E:171:ASN:ND2	1:E:268:THR:OG1	2.39	0.56
1:A:172:TYR:CG	1:A:278:ILE:HG23	2.40	0.56
1:E:32:GLY:O	1:E:61:GLY:O	2.24	0.56
1:G:337:ASN:HD22	1:G:338:LEU:N	2.04	0.56
1:G:29:THR:HG21	1:G:75:ASP:H	1.71	0.56
1:A:31:ALA:O	1:A:58:GLN:O	2.23	0.55
1:D:208:VAL:CG1	1:D:228:MET:HE1	2.35	0.55
1:H:36:ILE:O	1:H:40:MET:N	2.39	0.55
1:G:98:SER:OG	1:G:284:ILE:HD11	2.06	0.55
1:A:170:THR:HG23	1:A:180:TRP:HE1	1.71	0.55
1:B:53:LYS:N	1:B:53:LYS:HE2	2.20	0.55
1:B:62:SER:O	1:B:163:SER:HA	2.07	0.55
1:F:137:ASP:OD1	1:F:138:PRO:HD2	2.07	0.55
1:G:29:THR:OG1	1:G:30:GLY:CA	2.54	0.55
1:A:42:LYS:HB2	1:A:313:GLN:HG2	1.88	0.55
1:C:36:ILE:HD11	1:C:99:VAL:HG12	1.87	0.55
1:G:65:GLY:C	1:G:67:ALA:N	2.56	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:TRP:CE3	1:B:265:LEU:HD13	2.42	0.55
1:B:33:ALA:HB3	1:B:57:TYR:OH	2.07	0.55
1:H:257:TRP:CE3	1:H:326:LEU:HB3	2.42	0.55
1:A:29:THR:OG1	1:A:75:ASP:N	2.34	0.55
1:H:174:SER:O	1:H:181:LYS:HG3	2.06	0.55
1:C:105:PRO:HG2	1:C:231:THR:OG1	2.07	0.54
1:H:61:GLY:O	1:H:62:SER:C	2.45	0.54
1:G:57:TYR:CD2	1:G:57:TYR:O	2.60	0.54
1:B:35:PHE:HZ	1:B:101:GLY:HA3	1.71	0.54
1:E:205:ALA:O	1:E:209:LYS:HG2	2.07	0.54
1:B:30:GLY:O	1:B:74:VAL:HB	2.08	0.54
1:F:96:PHE:CE2	1:F:334:TRP:HZ2	2.26	0.54
1:H:159:ARG:CD	1:H:200:GLY:O	2.56	0.54
1:C:257:TRP:HH2	1:C:281:THR:HG21	1.72	0.54
1:C:114:ALA:O	1:C:230:TYR:O	2.25	0.54
1:E:32:GLY:HA3	1:E:60:ILE:HG12	1.89	0.54
1:H:97:PRO:HB2	1:H:322:LEU:HD21	1.90	0.54
1:A:172:TYR:CB	1:A:278:ILE:CG2	2.86	0.53
1:G:28:VAL:HG12	1:G:29:THR:H	1.73	0.53
1:G:35:PHE:CE1	1:G:219:GLU:OE1	2.61	0.53
1:G:33:ALA:CB	1:G:57:TYR:HE2	2.18	0.53
1:B:35:PHE:CZ	1:B:101:GLY:HA3	2.44	0.53
1:B:127:ILE:HG23	1:B:154:ILE:HG21	1.91	0.53
1:G:29:THR:HG1	1:G:30:GLY:HA3	1.72	0.53
1:B:313:GLN:N	1:B:313:GLN:OE1	2.38	0.53
1:D:36:ILE:O	1:D:40:MET:HB2	2.09	0.53
1:D:147:VAL:O	1:D:147:VAL:HG13	2.09	0.53
1:E:159:ARG:NH1	1:E:163:SER:HB2	2.23	0.53
1:E:322:LEU:HD23	1:E:326:LEU:HD23	1.91	0.53
1:E:47:TYR:O	1:E:51:THR:HG23	2.09	0.52
1:G:28:VAL:HG21	1:G:55:VAL:HG23	1.83	0.52
1:C:47:TYR:HE1	1:C:305:TRP:HD1	1.57	0.52
1:F:241:VAL:HG12	1:F:242:GLN:N	2.24	0.52
1:G:235:ASN:HD22	1:G:237:ALA:HB3	1.73	0.52
1:G:322:LEU:HD13	1:G:326:LEU:HD21	1.92	0.52
1:H:100:ILE:CD1	1:H:281:THR:HG23	2.40	0.52
1:B:135:TRP:CH2	1:B:213:GLY:CA	2.88	0.52
1:D:29:THR:CG2	1:D:74:VAL:HG22	2.39	0.52
1:G:155:THR:O	1:G:214:GLY:HA2	2.09	0.52
1:E:135:TRP:HE1	1:E:213:GLY:CA	2.22	0.52
1:C:304:ARG:O	1:C:308:THR:OG1	2.27	0.52

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:THR:HG22	1:F:259:THR:O	2.09	0.52
1:C:48:ASN:O	1:C:51:THR:O	2.28	0.52
1:D:43:TRP:CZ2	1:D:306:VAL:HG13	2.44	0.52
1:B:165:THR:HG22	1:B:217:TYR:CD2	2.45	0.52
1:A:60:ILE:HD11	1:A:65:GLY:N	2.25	0.52
1:B:127:ILE:CG2	1:B:154:ILE:HG21	2.39	0.52
1:B:43:TRP:CZ2	1:B:306:VAL:HG13	2.45	0.52
1:F:234:LYS:HB2	1:F:240:PHE:CE1	2.45	0.52
1:G:62:SER:O	1:G:66:ILE:HG13	2.09	0.52
1:D:29:THR:HG21	1:D:74:VAL:HG13	1.92	0.52
1:C:162:GLY:HA3	2:E:402:PO4:O4	2.10	0.51
1:F:184:VAL:CG1	1:F:190:VAL:HG13	2.39	0.51
1:G:256:ASP:OD2	1:G:259:THR:HG22	2.10	0.51
1:A:144:ASN:HB3	1:A:147:VAL:HG12	1.92	0.51
1:D:170:THR:HG21	1:D:190:VAL:HG21	1.92	0.51
1:E:155:THR:HG21	1:G:196:ILE:HG22	1.91	0.51
1:E:29:THR:HG21	1:E:74:VAL:HG12	1.92	0.51
1:B:165:THR:OG1	2:B:404:PO4:O3	2.26	0.51
1:G:196:ILE:HD11	1:G:211:ILE:HD11	1.92	0.51
1:C:223:ALA:HB1	1:C:228:MET:HB2	1.91	0.51
1:G:126:ASP:HA	1:G:129:LEU:HD12	1.92	0.51
1:F:77:GLY:O	1:F:285:LEU:N	2.41	0.51
1:G:284:ILE:HD12	1:G:284:ILE:N	2.26	0.51
1:A:65:GLY:HA2	1:A:68:GLN:OE1	2.11	0.51
1:B:28:VAL:HG11	1:B:298:ASN:HB2	1.91	0.51
1:C:31:ALA:CB	1:C:76:PHE:O	2.59	0.51
1:F:178:PRO:O	1:F:181:LYS:HB3	2.11	0.51
1:F:95:GLN:HA	1:F:284:ILE:O	2.11	0.51
1:E:233:MET:CE	1:E:278:ILE:HD11	2.40	0.50
1:C:66:ILE:CD1	1:C:83:LEU:HD21	2.41	0.50
1:E:135:TRP:HE1	1:E:213:GLY:HA3	1.76	0.50
1:E:118:LYS:HG2	1:E:232:ALA:HB3	1.92	0.50
1:A:35:PHE:CD1	1:A:219:GLU:HG3	2.47	0.50
1:A:83:LEU:O	1:A:95:GLN:NE2	2.44	0.50
1:C:106:VAL:HG21	1:C:228:MET:CE	2.41	0.50
1:E:103:VAL:HG22	1:E:165:THR:HG23	1.92	0.50
1:H:100:ILE:HD13	1:H:281:THR:HG23	1.93	0.50
1:C:245:ASP:OD1	1:C:320:VAL:HG22	2.12	0.50
1:D:28:VAL:CG1	1:D:55:VAL:HG22	2.41	0.50
1:E:69:ILE:HD13	1:E:285:LEU:HB2	1.91	0.50
1:B:165:THR:HG22	1:B:165:THR:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASN:HD22	1:B:48:ASN:C	2.15	0.50
1:D:29:THR:CG2	1:D:74:VAL:HG13	2.42	0.50
1:G:135:TRP:CD2	1:G:154:ILE:CD1	2.94	0.50
1:C:40:MET:HG2	1:C:57:TYR:CD2	2.47	0.50
1:D:322:LEU:HD12	1:D:326:LEU:HD23	1.94	0.50
1:D:32:GLY:HA3	1:D:60:ILE:CG1	2.41	0.50
1:E:244:SER:OG	1:E:245:ASP:N	2.43	0.50
1:G:28:VAL:CB	1:G:55:VAL:HG22	2.42	0.50
1:A:220:LEU:HD23	1:A:318:ASP:HB3	1.93	0.50
1:D:157:VAL:HG22	1:D:196:ILE:CG2	2.41	0.50
1:F:94:ALA:O	1:F:285:LEU:HA	2.12	0.49
1:H:95:GLN:CB	1:H:285:LEU:HD23	2.42	0.49
1:B:114:ALA:O	1:B:230:TYR:O	2.30	0.49
1:B:206:ALA:O	1:B:210:GLN:HG2	2.12	0.49
1:G:135:TRP:CE2	1:G:154:ILE:HD13	2.47	0.49
1:B:114:ALA:HA	1:B:229:ALA:HB1	1.93	0.49
1:B:31:ALA:CB	1:B:57:TYR:CE1	2.94	0.49
1:C:28:VAL:CG2	1:C:55:VAL:HG12	2.43	0.49
1:G:107:VAL:HG21	1:G:117:LEU:HD22	1.94	0.49
1:C:239:LYS:HG3	1:C:273:ASP:O	2.12	0.49
1:G:65:GLY:HA3	1:G:68:GLN:H	1.78	0.49
1:B:134:THR:O	1:B:154:ILE:CD1	2.61	0.49
1:G:135:TRP:CD1	1:G:154:ILE:HD13	2.48	0.49
1:A:140:ILE:O	1:A:144:ASN:N	2.41	0.49
1:C:37:TYR:O	1:C:38:PRO:C	2.48	0.49
1:E:136:ASN:OD1	1:E:150:PRO:C	2.51	0.49
1:D:108:ASN:ND2	1:D:211:ILE:O	2.45	0.49
1:F:261:LYS:O	1:F:262:ASP:C	2.51	0.49
1:A:244:SER:HB2	3:A:501:HOH:O	2.13	0.49
1:C:138:PRO:O	1:C:142:ALA:N	2.46	0.49
1:F:98:SER:OG	1:F:303:PHE:CE1	2.65	0.49
1:H:266:VAL:HG12	1:H:268:THR:OG1	2.13	0.49
1:H:101:GLY:O	1:H:279:THR:HG23	2.12	0.49
1:G:83:LEU:HB3	1:G:87:GLU:HB3	1.95	0.48
1:H:44:SER:HB3	1:H:55:VAL:HG13	1.94	0.48
1:A:255:ALA:HB1	1:A:265:LEU:HD21	1.95	0.48
1:B:233:MET:HB2	1:B:276:TRP:CZ3	2.48	0.48
1:B:62:SER:O	1:B:163:SER:C	2.52	0.48
1:C:159:ARG:HH12	1:C:200:GLY:HA2	1.78	0.48
1:E:108:ASN:O	1:E:212:LYS:C	2.49	0.48
1:F:126:ASP:HB3	1:F:132:VAL:HG13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:VAL:CG1	1:F:242:GLN:N	2.76	0.48
1:D:29:THR:HG23	1:D:74:VAL:HG22	1.96	0.48
1:F:132:VAL:O	1:F:154:ILE:HD12	2.12	0.48
1:G:106:VAL:HG12	1:G:230:TYR:HA	1.95	0.48
1:H:95:GLN:HB2	1:H:285:LEU:HD23	1.94	0.48
1:E:99:VAL:HG11	1:E:319:TYR:CD1	2.48	0.48
1:H:160:SER:O	1:H:199:LYS:HD3	2.11	0.48
1:B:52:LYS:H	1:B:53:LYS:HE2	1.69	0.48
1:C:71:ALA:O	1:C:72:ALA:HB3	2.14	0.48
1:D:127:ILE:HD11	1:D:140:ILE:HD11	1.95	0.48
1:D:61:GLY:O	1:D:62:SER:C	2.52	0.48
1:G:135:TRP:CE2	1:G:154:ILE:CD1	2.96	0.48
1:B:109:VAL:CG1	1:B:135:TRP:NE1	2.74	0.48
1:D:307:TYR:HB3	1:D:327:VAL:HG11	1.95	0.48
1:D:79:SER:OG	1:D:80:ASP:N	2.46	0.48
1:G:104:VAL:CG1	1:G:230:TYR:HB2	2.43	0.48
1:G:330:ILE:O	1:G:333:TYR:HB3	2.13	0.48
1:B:135:TRP:HZ3	1:B:153:LYS:O	1.96	0.48
1:C:106:VAL:HG21	1:C:228:MET:HE1	1.95	0.48
1:F:160:SER:OG	1:F:199:LYS:HD3	2.13	0.48
1:H:184:VAL:HG12	1:H:190:VAL:CG1	2.44	0.48
1:H:324:ASP:HA	1:H:327:VAL:HG12	1.95	0.48
1:C:112:ILE:HG21	1:C:117:LEU:HB2	1.96	0.48
1:D:28:VAL:HG13	1:D:55:VAL:HG13	1.93	0.48
1:B:109:VAL:HG11	1:B:135:TRP:CE2	2.46	0.48
1:D:83:LEU:O	1:D:95:GLN:NE2	2.47	0.48
1:F:121:GLY:HA3	1:F:176:VAL:HG21	1.96	0.48
1:F:262:ASP:OD1	1:F:333:TYR:OH	2.25	0.48
1:A:119:LEU:HD12	1:A:231:THR:HG21	1.94	0.47
1:A:136:ASN:ND2	1:A:150:PRO:O	2.47	0.47
1:D:313:GLN:N	1:D:313:GLN:OE1	2.44	0.47
1:H:28:VAL:HG12	1:H:29:THR:O	2.13	0.47
1:A:60:ILE:HG13	1:A:61:GLY:N	2.29	0.47
1:D:155:THR:O	1:D:214:GLY:HA2	2.14	0.47
1:G:40:MET:HG2	1:G:57:TYR:CD2	2.49	0.47
1:H:33:ALA:HB1	1:H:36:ILE:HG13	1.96	0.47
1:A:269:ASN:N	1:A:277:PRO:O	2.46	0.47
1:B:323:PRO:O	1:B:327:VAL:HG23	2.13	0.47
1:B:37:TYR:N	1:B:38:PRO:CD	2.78	0.47
1:D:221:SER:HG	1:D:221:SER:H	1.46	0.47
1:F:109:VAL:HG21	1:F:135:TRP:NE1	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:GLY:O	1:F:66:ILE:C	2.50	0.47
1:F:135:TRP:C	1:F:137:ASP:H	2.18	0.47
1:G:93:LEU:C	1:G:288:LYS:NZ	2.68	0.47
1:G:28:VAL:CG2	1:G:55:VAL:HG23	2.42	0.47
1:A:72:ALA:CB	1:A:291:LYS:HE2	2.44	0.47
1:F:36:ILE:O	1:F:40:MET:HB2	2.15	0.47
1:H:208:VAL:HG11	1:H:228:MET:HE1	1.97	0.47
1:A:172:TYR:HB2	1:A:278:ILE:HG22	1.97	0.47
1:H:160:SER:OG	1:H:199:LYS:HB3	2.14	0.47
1:H:28:VAL:HB	1:H:55:VAL:HG23	1.97	0.47
1:D:136:ASN:ND2	1:D:151:GLU:HA	2.30	0.47
1:D:332:ALA:O	1:D:335:ALA:HB3	2.15	0.47
1:F:157:VAL:HG22	1:F:196:ILE:CD1	2.37	0.47
1:G:95:GLN:HA	1:G:284:ILE:O	2.14	0.47
1:A:129:LEU:HD11	1:A:180:TRP:HB2	1.97	0.47
1:A:284:ILE:HG13	1:A:303:PHE:CZ	2.49	0.47
1:D:278:ILE:O	1:D:278:ILE:HG12	2.14	0.47
1:F:80:ASP:O	1:F:81:ALA:C	2.53	0.47
1:C:80:ASP:HB2	1:C:164:GLY:HA3	1.97	0.47
1:G:108:ASN:ND2	1:G:211:ILE:O	2.48	0.47
1:G:303:PHE:O	1:G:307:TYR:CD2	2.68	0.47
1:E:135:TRP:HZ2	1:E:213:GLY:O	1.98	0.47
1:E:159:ARG:NH1	1:E:163:SER:OG	2.48	0.47
1:A:96:PHE:O	1:A:284:ILE:N	2.49	0.46
1:C:55:VAL:HG23	1:C:55:VAL:O	2.13	0.46
1:E:33:ALA:HA	1:E:60:ILE:O	2.15	0.46
1:F:81:ALA:HB2	1:F:167:PHE:CG	2.50	0.46
1:A:106:VAL:O	1:A:215:ILE:HA	2.15	0.46
1:E:163:SER:O	1:E:188:THR:HA	2.16	0.46
1:F:276:TRP:CE3	1:F:277:PRO:HD2	2.50	0.46
1:G:29:THR:CB	1:G:30:GLY:CA	2.93	0.46
1:F:207:TYR:O	1:F:211:ILE:HD12	2.14	0.46
1:F:33:ALA:N	1:F:57:TYR:OH	2.48	0.46
1:H:135:TRP:O	1:H:149:LEU:HD21	2.15	0.46
1:H:300:LEU:HG	1:H:334:TRP:CD2	2.49	0.46
1:E:166:SER:OG	1:E:192:TRP:CZ2	2.68	0.46
1:E:60:ILE:HD12	1:E:64:GLY:HA3	1.97	0.46
1:A:218:VAL:CG2	1:A:222:TYR:HB2	2.46	0.46
1:A:31:ALA:CB	1:A:77:GLY:HA2	2.46	0.46
1:B:47:TYR:CE2	1:B:53:LYS:CG	2.98	0.46
1:F:234:LYS:HD3	1:F:240:PHE:CZ	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LYS:HE3	1:A:298:ASN:HD22	1.80	0.46
1:C:159:ARG:NH1	1:C:161:ASP:OD1	2.48	0.46
1:E:166:SER:OG	1:E:192:TRP:CH2	2.68	0.46
1:G:159:ARG:HH21	1:G:200:GLY:HA2	1.80	0.46
1:C:174:SER:HB3	1:C:181:LYS:HB2	1.98	0.46
1:C:67:ALA:HA	2:C:402:PO4:O2	2.16	0.46
1:E:210:GLN:NE2	1:G:160:SER:OG	2.49	0.46
1:G:98:SER:HB3	1:G:284:ILE:HD11	1.97	0.46
1:G:65:GLY:CA	1:G:67:ALA:H	2.29	0.46
1:A:172:TYR:CG	1:A:278:ILE:CG2	2.99	0.46
1:B:135:TRP:CZ3	1:B:153:LYS:O	2.69	0.46
1:D:208:VAL:CG1	1:D:228:MET:CE	2.93	0.45
1:D:257:TRP:CZ3	1:D:265:LEU:HB3	2.50	0.45
1:E:137:ASP:OD1	1:E:138:PRO:HD2	2.16	0.45
1:F:312:ALA:HA	1:F:315:LYS:HD2	1.98	0.45
1:C:97:PRO:HA	1:C:282:ASN:O	2.15	0.45
1:C:284:ILE:HG12	1:C:303:PHE:CZ	2.51	0.45
1:F:233:MET:HB3	1:F:277:PRO:HG2	1.98	0.45
1:B:315:LYS:NZ	1:B:316:GLN:OE1	2.49	0.45
1:B:56:ASN:C	1:B:56:ASN:ND2	2.69	0.45
1:C:326:LEU:HD22	1:C:330:ILE:HD11	1.97	0.45
1:B:257:TRP:CH2	1:B:281:THR:HG21	2.51	0.45
1:D:72:ALA:HB1	1:D:291:LYS:HD3	1.99	0.45
1:E:120:ASP:OD1	1:E:123:THR:HB	2.16	0.45
1:E:144:ASN:HB3	1:E:147:VAL:CG2	2.45	0.45
1:A:124:LEU:HD22	1:A:233:MET:HE1	1.97	0.45
1:B:159:ARG:HB3	1:B:217:TYR:OH	2.17	0.45
1:B:28:VAL:HG11	1:B:298:ASN:HB3	1.99	0.45
1:E:210:GLN:HG3	1:G:199:LYS:CA	2.46	0.45
1:E:252:ALA:O	1:E:253:ASN:C	2.54	0.45
1:F:34:SER:OG	2:F:402:PO4:O2	2.25	0.45
1:F:79:SER:O	1:F:283:PHE:N	2.44	0.45
1:F:39:VAL:HB	1:F:319:TYR:CE2	2.52	0.45
1:F:32:GLY:O	1:F:60:ILE:O	2.35	0.45
1:F:81:ALA:O	1:F:82:PRO:C	2.52	0.45
1:H:31:ALA:O	1:H:58:GLN:O	2.35	0.45
1:D:60:ILE:CD1	1:D:64:GLY:HA3	2.44	0.45
1:E:37:TYR:CD2	1:E:57:TYR:CE1	3.03	0.45
1:G:80:ASP:CB	1:G:164:GLY:HA3	2.46	0.45
1:H:32:GLY:HA2	1:H:60:ILE:HG13	1.98	0.45
1:E:196:ILE:HG22	1:G:211:ILE:HG13	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:233:MET:HB2	1:G:276:TRP:CH2	2.52	0.45
1:G:118:LYS:HD2	1:G:240:PHE:CD1	2.52	0.45
1:B:104:VAL:HG12	1:B:276:TRP:CZ2	2.53	0.44
1:B:128:PHE:HA	1:B:156:VAL:HG21	1.99	0.44
1:C:102:GLY:HA3	1:C:248:PHE:CZ	2.52	0.44
1:F:103:VAL:HB	1:F:278:ILE:CG2	2.47	0.44
1:H:159:ARG:HD2	1:H:163:SER:CB	2.46	0.44
1:B:34:SER:HB2	1:B:59:SER:HB2	1.99	0.44
1:D:157:VAL:HG22	1:D:196:ILE:HG23	1.99	0.44
1:F:30:GLY:CA	1:F:56:ASN:O	2.66	0.44
1:G:209:LYS:HE3	1:G:226:ASN:O	2.17	0.44
1:G:233:MET:HB2	1:G:276:TRP:CZ3	2.52	0.44
1:B:159:ARG:HD3	1:B:163:SER:OG	2.17	0.44
1:B:172:TYR:CD2	1:B:278:ILE:HG12	2.52	0.44
1:E:106:VAL:O	1:E:215:ILE:HA	2.18	0.44
1:E:244:SER:O	1:E:248:PHE:CG	2.71	0.44
1:E:307:TYR:O	1:E:311:ASP:OD1	2.35	0.44
1:F:134:THR:O	1:F:137:ASP:HB2	2.17	0.44
1:G:57:TYR:CG	1:G:57:TYR:O	2.69	0.44
1:G:93:LEU:O	1:G:288:LYS:NZ	2.46	0.44
1:D:44:SER:O	1:D:48:ASN:HB2	2.18	0.44
1:F:257:TRP:O	1:F:258:GLY:C	2.55	0.44
1:H:144:ASN:ND2	1:H:144:ASN:O	2.46	0.44
1:B:35:PHE:CD2	1:B:219:GLU:CB	2.95	0.44
1:B:61:GLY:C	1:B:63:GLY:CA	2.85	0.44
1:D:211:ILE:HG22	1:D:212:LYS:O	2.18	0.44
1:E:28:VAL:HG13	1:E:299:THR:OG1	2.18	0.44
1:H:129:LEU:HD11	1:H:183:LYS:HD2	1.98	0.44
1:H:199:LYS:HA	1:H:200:GLY:HA2	1.78	0.44
1:A:32:GLY:O	1:A:78:SER:O	2.36	0.44
1:B:108:ASN:ND2	1:B:211:ILE:O	2.50	0.44
1:B:55:VAL:HG12	1:B:55:VAL:O	2.18	0.44
1:C:126:ASP:HA	1:C:129:LEU:HB2	1.99	0.44
1:H:159:ARG:HD3	1:H:200:GLY:O	2.17	0.44
1:B:118:LYS:NZ	1:B:143:LEU:O	2.45	0.44
1:H:158:HIS:HA	1:H:217:TYR:CE2	2.53	0.44
1:A:284:ILE:HG13	1:A:303:PHE:CE1	2.52	0.44
1:A:75:ASP:O	1:A:286:VAL:HG12	2.17	0.44
1:F:109:VAL:HG21	1:F:135:TRP:CE2	2.53	0.44
1:G:135:TRP:CD2	1:G:154:ILE:HD13	2.53	0.44
1:G:235:ASN:ND2	1:G:237:ALA:HB3	2.33	0.44

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:VAL:HG13	1:B:247:THR:CG2	2.46	0.43
1:H:135:TRP:CZ2	1:H:154:ILE:HG22	2.52	0.43
1:B:132:VAL:HG12	1:B:137:ASP:OD2	2.17	0.43
1:C:28:VAL:HG12	1:C:29:THR:N	2.33	0.43
1:C:64:GLY:O	1:C:68:GLN:HB2	2.17	0.43
1:E:28:VAL:CG1	1:E:299:THR:OG1	2.66	0.43
1:E:69:ILE:CD1	1:E:285:LEU:CB	2.93	0.43
1:G:311:ASP:O	1:G:315:LYS:HG3	2.18	0.43
1:H:196:ILE:HG22	1:H:197:GLY:H	1.83	0.43
1:D:29:THR:HG21	1:D:74:VAL:CA	2.49	0.43
1:E:163:SER:OG	1:E:166:SER:HB2	2.18	0.43
1:F:32:GLY:C	1:F:57:TYR:OH	2.56	0.43
1:G:313:GLN:OE1	1:G:313:GLN:N	2.51	0.43
1:G:33:ALA:N	1:G:57:TYR:OH	2.51	0.43
1:H:135:TRP:HE1	1:H:213:GLY:CA	2.31	0.43
1:D:33:ALA:HB2	1:D:78:SER:O	2.17	0.43
1:E:160:SER:OG	1:E:198:GLY:C	2.56	0.43
1:G:135:TRP:O	1:G:149:LEU:HD13	2.18	0.43
1:B:166:SER:O	1:B:170:THR:HG23	2.19	0.43
1:F:196:ILE:HD12	1:F:196:ILE:O	2.18	0.43
1:A:97:PRO:HG2	1:A:330:ILE:HD11	2.00	0.43
1:C:122:LYS:HE3	1:D:259:THR:HG23	2.01	0.43
1:D:144:ASN:HB3	1:D:147:VAL:CG1	2.43	0.43
1:G:82:PRO:HB3	1:G:283:PHE:CE2	2.52	0.43
1:H:140:ILE:HG22	1:H:144:ASN:OD1	2.18	0.43
1:H:208:VAL:CG1	1:H:228:MET:HE1	2.49	0.43
1:A:234:LYS:HE2	1:A:238:GLY:O	2.19	0.43
1:B:62:SER:O	1:B:163:SER:CA	2.67	0.43
1:E:271:ALA:HA	1:F:271:ALA:HB1	2.00	0.43
1:H:124:LEU:HD22	1:H:233:MET:CE	2.48	0.43
1:A:136:ASN:N	1:A:136:ASN:ND2	2.67	0.43
1:D:133:SER:HB3	1:G:151:GLU:HG2	2.01	0.43
1:D:34:SER:HB2	2:D:401:PO4:P	2.58	0.43
1:H:99:VAL:HA	1:H:322:LEU:HD13	2.00	0.43
1:A:120:ASP:O	1:A:121:GLY:C	2.56	0.43
1:A:43:TRP:O	1:A:47:TYR:CB	2.66	0.43
1:D:184:VAL:HG12	1:D:190:VAL:HG11	2.01	0.43
1:D:276:TRP:HA	1:D:277:PRO:HD3	1.92	0.43
1:E:35:PHE:CD2	1:E:219:GLU:CB	2.80	0.43
1:F:296:LEU:HD11	1:F:338:LEU:HD22	2.00	0.43
1:G:151:GLU:OE1	1:G:151:GLU:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:GLY:HA2	1:G:65:GLY:HA2	1.69	0.43
1:H:106:VAL:HA	1:H:229:ALA:O	2.18	0.43
1:H:210:GLN:HE21	1:H:210:GLN:N	2.16	0.43
1:B:184:VAL:HG21	1:B:193:PRO:CG	2.48	0.42
1:D:61:GLY:O	1:D:64:GLY:N	2.50	0.42
1:E:121:GLY:HA3	1:E:176:VAL:HG21	2.00	0.42
1:F:196:ILE:HD13	1:F:207:TYR:HD2	1.84	0.42
1:H:133:SER:HA	1:H:154:ILE:HD11	2.01	0.42
1:H:325:THR:C	1:H:328:THR:CG2	2.87	0.42
1:G:334:TRP:HA	1:G:337:ASN:ND2	2.32	0.42
1:H:138:PRO:HA	1:H:141:ALA:HB3	2.00	0.42
1:H:91:ALA:HB1	1:H:93:LEU:HG	2.01	0.42
1:A:109:VAL:HB	1:A:112:ILE:HG13	2.01	0.42
1:B:28:VAL:O	1:B:28:VAL:HG23	2.19	0.42
1:C:107:VAL:O	1:C:229:ALA:HB3	2.20	0.42
1:F:265:LEU:C	1:F:265:LEU:HD23	2.40	0.42
1:B:159:ARG:HH22	1:B:201:ASN:N	2.17	0.42
1:E:212:LYS:O	1:E:212:LYS:CD	2.67	0.42
1:A:330:ILE:O	1:A:333:TYR:HB3	2.19	0.42
1:D:104:VAL:HG11	1:D:243:PRO:HG3	2.02	0.42
1:E:323:PRO:HB2	1:E:325:THR:HG22	2.02	0.42
1:G:256:ASP:CG	1:G:256:ASP:O	2.58	0.42
1:H:135:TRP:CE2	1:H:154:ILE:HG23	2.55	0.42
1:A:34:SER:O	1:A:222:TYR:OH	2.35	0.42
1:B:165:THR:HG22	1:B:217:TYR:HE2	1.81	0.42
1:B:163:SER:HG	1:B:166:SER:H	1.66	0.42
1:B:43:TRP:CH2	1:B:306:VAL:HG13	2.54	0.42
1:B:99:VAL:HA	1:B:322:LEU:CD1	2.50	0.42
1:D:82:PRO:HG2	1:D:264:TYR:CE1	2.55	0.42
1:E:83:LEU:HD11	1:E:285:LEU:HD21	2.01	0.42
1:G:234:LYS:HD3	1:G:240:PHE:CE1	2.53	0.42
1:H:155:THR:HG21	1:H:211:ILE:CG2	2.49	0.42
1:B:33:ALA:HB3	1:B:57:TYR:HH	1.85	0.42
1:B:52:LYS:H	1:B:53:LYS:NZ	2.17	0.42
1:B:62:SER:OG	1:B:79:SER:C	2.57	0.42
1:D:158:HIS:CE1	1:D:192:TRP:CD1	3.08	0.42
1:D:332:ALA:O	1:D:335:ALA:N	2.53	0.42
1:D:43:TRP:HH2	1:D:99:VAL:HG13	1.85	0.42
1:E:79:SER:O	1:E:283:PHE:HB2	2.19	0.42
1:H:135:TRP:CZ2	1:H:154:ILE:CG2	3.03	0.42
1:H:44:SER:OG	1:H:57:TYR:CE2	2.70	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:TRP:CZ2	1:C:306:VAL:HG13	2.55	0.42
1:D:37:TYR:O	1:D:41:SER:OG	2.33	0.42
1:E:110:PRO:HD3	1:E:212:LYS:HE3	2.01	0.42
1:A:336:LYS:HB3	1:E:111:GLY:HA2	2.01	0.42
1:D:169:PHE:HA	1:D:278:ILE:CD1	2.49	0.42
1:D:232:ALA:HB2	1:D:242:GLN:OE1	2.19	0.42
1:F:177:ASN:O	1:F:180:TRP:HB3	2.20	0.42
1:B:257:TRP:HH2	1:B:281:THR:HG21	1.83	0.42
1:E:243:PRO:N	1:E:276:TRP:CZ3	2.88	0.42
1:G:184:VAL:HG12	1:G:190:VAL:CG1	2.50	0.42
1:G:288:LYS:HE2	1:G:288:LYS:HB2	1.86	0.42
1:H:31:ALA:HB2	1:H:77:GLY:HA2	2.02	0.42
1:G:235:ASN:HB2	1:G:239:LYS:O	2.19	0.41
1:G:63:GLY:O	1:G:66:ILE:N	2.53	0.41
1:H:243:PRO:HB3	1:H:276:TRP:CZ2	2.55	0.41
1:C:118:LYS:HA	1:C:232:ALA:HB3	2.02	0.41
1:A:268:THR:HG22	1:A:278:ILE:HG22	2.03	0.41
1:F:119:LEU:HB2	1:F:233:MET:HE1	2.02	0.41
1:H:244:SER:O	1:H:245:ASP:C	2.59	0.41
1:A:167:PHE:O	1:A:171:ASN:HB2	2.19	0.41
1:B:52:LYS:H	1:B:53:LYS:HZ1	1.69	0.41
1:C:233:MET:HB3	1:C:276:TRP:CZ3	2.55	0.41
1:C:122:LYS:CE	1:D:259:THR:CG2	2.98	0.41
1:F:109:VAL:CG2	1:F:135:TRP:CE2	3.03	0.41
1:H:135:TRP:CE2	1:H:154:ILE:CG2	3.03	0.41
1:B:172:TYR:CD2	1:B:278:ILE:HD11	2.55	0.41
1:B:159:ARG:CB	1:B:217:TYR:OH	2.69	0.41
1:B:36:ILE:HD11	1:B:78:SER:HG	1.85	0.41
1:C:119:LEU:HD13	1:C:124:LEU:HD12	2.03	0.41
1:C:83:LEU:N	1:C:83:LEU:HD23	2.36	0.41
1:D:122:LYS:HD3	1:D:122:LYS:O	2.20	0.41
1:D:29:THR:HG21	1:D:74:VAL:CB	2.51	0.41
1:H:325:THR:C	1:H:328:THR:HG22	2.41	0.41
1:A:170:THR:CG2	1:A:186:GLU:HA	2.46	0.41
1:B:35:PHE:HZ	1:B:102:GLY:N	2.19	0.41
1:E:166:SER:O	1:E:170:THR:HG23	2.21	0.41
1:E:257:TRP:HH2	1:E:281:THR:HG21	1.85	0.41
1:G:82:PRO:HB3	1:G:283:PHE:CD2	2.55	0.41
1:A:135:TRP:CD2	1:A:154:ILE:HG12	2.56	0.41
1:A:331:GLU:HG2	1:A:334:TRP:CE3	2.56	0.41
1:C:84:LYS:O	1:C:85:PRO:C	2.57	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:ILE:HG23	1:E:154:ILE:HG21	2.02	0.41
1:F:184:VAL:CG1	1:F:190:VAL:CG1	2.99	0.41
1:A:139:ALA:O	1:A:143:LEU:HD12	2.20	0.41
1:A:66:ILE:HG22	1:A:70:LYS:HE3	2.03	0.41
1:B:27:ASP:HB3	1:B:54:GLN:HB3	2.02	0.41
1:C:28:VAL:HB	1:C:55:VAL:HG12	2.02	0.41
1:G:105:PRO:HG2	1:G:233:MET:CE	2.51	0.41
1:G:338:LEU:HB3	1:G:339:PRO:HD2	2.02	0.41
1:H:226:ASN:HB2	1:H:228:MET:HG3	2.03	0.41
1:E:159:ARG:HE	1:E:200:GLY:CA	2.34	0.41
1:D:133:SER:HB3	1:G:151:GLU:OE2	2.21	0.41
1:G:98:SER:N	1:G:284:ILE:CD1	2.84	0.41
1:A:241:VAL:CG1	1:A:247:THR:CG2	2.96	0.41
1:B:117:LEU:HD23	1:B:118:LYS:N	2.36	0.41
1:C:98:SER:HB3	1:C:284:ILE:HD11	2.02	0.41
1:D:31:ALA:HB2	1:D:77:GLY:HA2	2.01	0.41
1:G:65:GLY:HA3	1:G:68:GLN:N	2.36	0.41
1:A:102:GLY:O	1:A:219:GLU:HA	2.20	0.40
1:A:68:GLN:O	1:A:73:SER:HB3	2.21	0.40
1:C:201:ASN:OD1	1:C:218:VAL:HG12	2.21	0.40
1:E:255:ALA:HB1	1:E:265:LEU:HD21	2.03	0.40
1:G:33:ALA:HB1	1:G:36:ILE:HG12	2.04	0.40
1:G:80:ASP:HB3	1:G:164:GLY:CA	2.52	0.40
1:C:86:GLU:HB3	1:E:191:GLN:HG2	2.02	0.40
1:D:335:ALA:HA	1:D:340:HIS:NE2	2.37	0.40
1:G:171:ASN:OD1	1:G:171:ASN:C	2.60	0.40
1:B:172:TYR:HD2	1:B:278:ILE:HD11	1.86	0.40
1:D:115:GLY:HA3	1:D:242:GLN:HE22	1.87	0.40
1:B:61:GLY:O	1:B:64:GLY:N	2.53	0.40
1:F:82:PRO:HG2	1:F:264:TYR:CD1	2.57	0.40
1:E:210:GLN:HG3	1:G:199:LYS:HA	2.04	0.40
1:E:179:ASP:HB3	1:E:183:LYS:HD2	2.04	0.40
1:E:242:GLN:C	1:E:276:TRP:CZ3	2.95	0.40
1:E:336:LYS:HG3	1:E:337:ASN:ND2	2.37	0.40
1:F:320:VAL:HG12	1:F:321:PRO:O	2.21	0.40
1:G:135:TRP:CG	1:G:154:ILE:HD13	2.57	0.40
1:G:33:ALA:HB1	1:G:36:ILE:CG1	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LYS:NZ	2:H:403:PO4:O2[1_554]	1.71	0.49

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	312/335 (93%)	286 (92%)	25 (8%)	1 (0%)	44	80
1	B	312/335 (93%)	277 (89%)	33 (11%)	2 (1%)	28	68
1	C	308/335 (92%)	279 (91%)	27 (9%)	2 (1%)	28	68
1	D	312/335 (93%)	287 (92%)	23 (7%)	2 (1%)	28	68
1	E	312/335 (93%)	285 (91%)	27 (9%)	0	100	100
1	F	312/335 (93%)	284 (91%)	27 (9%)	1 (0%)	44	80
1	G	312/335 (93%)	275 (88%)	36 (12%)	1 (0%)	44	80
1	H	308/335 (92%)	284 (92%)	21 (7%)	3 (1%)	18	57
All	All	2488/2680 (93%)	2257 (91%)	219 (9%)	12 (0%)	32	72

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	150	PRO
1	C	193	PRO
1	H	60	ILE
1	D	237	ALA
1	F	136	ASN
1	H	52	LYS
1	B	138	PRO
1	D	151	GLU
1	A	145	PRO
1	H	323	PRO
1	G	66	ILE
1	B	38	PRO

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	238/255 (93%)	218 (92%)	20 (8%)	13	41
1	B	238/255 (93%)	220 (92%)	18 (8%)	15	47
1	C	236/255 (92%)	207 (88%)	29 (12%)	5	22
1	D	238/255 (93%)	216 (91%)	22 (9%)	11	37
1	E	238/255 (93%)	207 (87%)	31 (13%)	5	20
1	F	238/255 (93%)	202 (85%)	36 (15%)	3	14
1	G	238/255 (93%)	200 (84%)	38 (16%)	3	13
1	H	234/255 (92%)	196 (84%)	38 (16%)	3	12
All	All	1898/2040 (93%)	1666 (88%)	232 (12%)	6	23

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LYS
1	A	46	ASP
1	A	60	ILE
1	A	99	VAL
1	A	116	THR
1	A	123	THR
1	A	126	ASP
1	A	129	LEU
1	A	136	ASN
1	A	143	LEU
1	A	174	SER
1	A	201	ASN
1	A	210	GLN
1	A	215	ILE
1	A	225	GLN
1	A	227	LYS
1	A	259	THR
1	A	266	VAL
1	A	309	LYS

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type
1	A	316	GLN
1	B	48	ASN
1	B	53	LYS
1	B	56	ASN
1	B	60	ILE
1	B	62	SER
1	B	96	PHE
1	B	118	LYS
1	B	135	TRP
1	B	137	ASP
1	B	153	LYS
1	B	176	VAL
1	B	226	ASN
1	B	247	THR
1	B	281	THR
1	B	297	LYS
1	B	309	LYS
1	B	315	LYS
1	B	328	THR
1	C	42	LYS
1	C	98	SER
1	C	118	LYS
1	C	122	LYS
1	C	123	THR
1	C	124	LEU
1	C	133	SER
1	C	137	ASP
1	C	150	PRO
1	C	151	GLU
1	C	153	LYS
1	C	183	LYS
1	C	191	GLN
1	C	194	THR
1	C	211	ILE
1	C	227	LYS
1	C	261	LYS
1	C	273	ASP
1	C	279	THR
1	C	287	GLN
1	C	289	LYS
1	C	297	LYS
1	C	308	THR

Continued from previous page...

Mol	Chain	Res	Type
1	C	309	LYS
1	C	311	ASP
1	C	316	GLN
1	C	318	ASP
1	C	325	THR
1	C	326	LEU
1	D	29	THR
1	D	34	SER
1	D	58	GLN
1	D	99	VAL
1	D	116	THR
1	D	122	LYS
1	D	123	THR
1	D	136	ASN
1	D	137	ASP
1	D	159	ARG
1	D	160	SER
1	D	170	THR
1	D	199	LYS
1	D	221	SER
1	D	224	LEU
1	D	241	VAL
1	D	261	LYS
1	D	315	LYS
1	D	318	ASP
1	D	322	LEU
1	D	324	ASP
1	D	325	THR
1	E	29	THR
1	E	34	SER
1	E	48	ASN
1	E	51	THR
1	E	53	LYS
1	E	54	GLN
1	E	59	SER
1	E	62	SER
1	E	68	GLN
1	E	69	ILE
1	E	119	LEU
1	E	122	LYS
1	E	131	LYS
1	E	133	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	136	ASN
1	E	166	SER
1	E	174	SER
1	E	212	LYS
1	E	227	LYS
1	E	245	ASP
1	E	259	THR
1	E	278	ILE
1	E	279	THR
1	E	281	THR
1	E	287	GLN
1	E	291	LYS
1	E	296	LEU
1	E	297	LYS
1	E	300	LEU
1	E	301	GLU
1	E	317	LEU
1	F	52	LYS
1	F	54	GLN
1	F	58	GLN
1	F	70	LYS
1	F	73	SER
1	F	84	LYS
1	F	97	PRO
1	F	98	SER
1	F	116	THR
1	F	122	LYS
1	F	123	THR
1	F	124	LEU
1	F	135	TRP
1	F	137	ASP
1	F	148	LYS
1	F	153	LYS
1	F	159	ARG
1	F	163	SER
1	F	183	LYS
1	F	188	THR
1	F	194	THR
1	F	233	MET
1	F	242	GLN
1	F	245	ASP
1	F	254	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	261	LYS
1	F	262	ASP
1	F	277	PRO
1	F	287	GLN
1	F	289	LYS
1	F	292	ASN
1	F	311	ASP
1	F	324	ASP
1	F	328	THR
1	F	338	LEU
1	F	340	HIS
1	G	27	ASP
1	G	34	SER
1	G	41	SER
1	G	55	VAL
1	G	58	GLN
1	G	60	ILE
1	G	70	LYS
1	G	73	SER
1	G	78	SER
1	G	80	ASP
1	G	87	GLU
1	G	106	VAL
1	G	116	THR
1	G	138	PRO
1	G	153	LYS
1	G	161	ASP
1	G	163	SER
1	G	166	SER
1	G	188	THR
1	G	194	THR
1	G	199	LYS
1	G	227	LYS
1	G	233	MET
1	G	247	THR
1	G	254	SER
1	G	256	ASP
1	G	259	THR
1	G	273	ASP
1	G	278	ILE
1	G	281	THR
1	G	288	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	291	LYS
1	G	292	ASN
1	G	300	LEU
1	G	325	THR
1	G	326	LEU
1	G	336	LYS
1	G	337	ASN
1	H	27	ASP
1	H	44	SER
1	H	52	LYS
1	H	57	TYR
1	H	59	SER
1	H	80	ASP
1	H	99	VAL
1	H	118	LYS
1	H	119	LEU
1	H	122	LYS
1	H	126	ASP
1	H	133	SER
1	H	144	ASN
1	H	148	LYS
1	H	149	LEU
1	H	151	GLU
1	H	155	THR
1	H	163	SER
1	H	199	LYS
1	H	210	GLN
1	H	224	LEU
1	H	227	LYS
1	H	231	THR
1	H	233	MET
1	H	242	GLN
1	H	245	ASP
1	H	261	LYS
1	H	265	LEU
1	H	268	THR
1	H	289	LYS
1	H	309	LYS
1	H	315	LYS
1	H	316	GLN
1	H	318	ASP
1	H	324	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	328	THR
1	H	331	GLU
1	H	336	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	298	ASN
1	A	313	GLN
1	B	48	ASN
1	B	56	ASN
1	B	58	GLN
1	B	136	ASN
1	B	158	HIS
1	C	144	ASN
1	C	242	GLN
1	C	282	ASN
1	C	329	GLN
1	D	95	GLN
1	D	136	ASN
1	E	48	ASN
1	E	171	ASN
1	E	210	GLN
1	E	337	ASN
1	F	242	GLN
1	F	337	ASN
1	G	316	GLN
1	G	337	ASN
1	H	210	GLN
1	H	253	ASN
1	H	287	GLN

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)

34 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	PO4	A	401	-	4,4,4	0.84	0	6,6,6	0.70	0
2	PO4	A	402	-	4,4,4	0.85	0	6,6,6	0.84	0
2	PO4	A	403	-	4,4,4	0.62	0	6,6,6	1.53	2 (33%)
2	PO4	A	404	-	4,4,4	1.12	0	6,6,6	0.67	0
2	PO4	B	401	-	4,4,4	0.77	0	6,6,6	0.93	0
2	PO4	B	402	-	4,4,4	0.75	0	6,6,6	1.42	1 (16%)
2	PO4	B	403	-	4,4,4	0.62	0	6,6,6	0.64	0
2	PO4	B	404	-	4,4,4	0.78	0	6,6,6	0.96	0
2	PO4	B	405	-	4,4,4	0.78	0	6,6,6	1.11	1 (16%)
2	PO4	C	401	-	4,4,4	0.93	0	6,6,6	2.16	3 (50%)
2	PO4	C	402	-	4,4,4	1.74	1 (25%)	6,6,6	1.30	2 (33%)
2	PO4	C	403	-	4,4,4	1.00	0	6,6,6	1.66	2 (33%)
2	PO4	C	404	-	4,4,4	0.94	0	6,6,6	0.78	0
2	PO4	D	401	-	4,4,4	0.76	0	6,6,6	1.19	0
2	PO4	D	402	-	4,4,4	0.96	0	6,6,6	3.10	3 (50%)
2	PO4	D	403	-	4,4,4	0.36	0	6,6,6	2.59	2 (33%)
2	PO4	D	404	-	4,4,4	0.99	0	6,6,6	0.72	0
2	PO4	D	405	-	4,4,4	1.09	0	6,6,6	0.84	0
2	PO4	E	401	-	4,4,4	0.80	0	6,6,6	0.85	0
2	PO4	E	402	-	4,4,4	0.69	0	6,6,6	1.50	0
2	PO4	E	403	-	4,4,4	0.71	0	6,6,6	1.01	0
2	PO4	E	404	-	4,4,4	1.09	0	6,6,6	2.34	3 (50%)
2	PO4	E	405	-	4,4,4	0.84	0	6,6,6	0.96	0
2	PO4	F	401	-	4,4,4	0.88	0	6,6,6	1.47	1 (16%)
2	PO4	F	402	-	4,4,4	0.89	0	6,6,6	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	PO4	F	403	-	4,4,4	0.97	0	6,6,6	1.22	0
2	PO4	F	404	-	4,4,4	1.00	0	6,6,6	1.09	0
2	PO4	F	405	-	4,4,4	1.15	0	6,6,6	0.60	0
2	PO4	F	406	-	4,4,4	0.93	0	6,6,6	1.27	1 (16%)
2	PO4	G	401	-	4,4,4	0.92	0	6,6,6	1.08	0
2	PO4	G	402	-	4,4,4	0.77	0	6,6,6	1.50	1 (16%)
2	PO4	H	401	-	4,4,4	0.96	0	6,6,6	0.41	0
2	PO4	H	402	-	4,4,4	1.21	0	6,6,6	1.53	1 (16%)
2	PO4	H	403	-	4,4,4	0.70	0	6,6,6	1.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	401	-	-	0/0/0/0	0/0/0/0
2	PO4	A	402	-	-	0/0/0/0	0/0/0/0
2	PO4	A	403	-	-	0/0/0/0	0/0/0/0
2	PO4	A	404	-	-	0/0/0/0	0/0/0/0
2	PO4	B	401	-	-	0/0/0/0	0/0/0/0
2	PO4	B	402	-	-	0/0/0/0	0/0/0/0
2	PO4	B	403	-	-	0/0/0/0	0/0/0/0
2	PO4	B	404	-	-	0/0/0/0	0/0/0/0
2	PO4	B	405	-	-	0/0/0/0	0/0/0/0
2	PO4	C	401	-	-	0/0/0/0	0/0/0/0
2	PO4	C	402	-	-	0/0/0/0	0/0/0/0
2	PO4	C	403	-	-	0/0/0/0	0/0/0/0
2	PO4	C	404	-	-	0/0/0/0	0/0/0/0
2	PO4	D	401	-	-	0/0/0/0	0/0/0/0
2	PO4	D	402	-	-	0/0/0/0	0/0/0/0
2	PO4	D	403	-	-	0/0/0/0	0/0/0/0
2	PO4	D	404	-	-	0/0/0/0	0/0/0/0
2	PO4	D	405	-	-	0/0/0/0	0/0/0/0
2	PO4	E	401	-	-	0/0/0/0	0/0/0/0
2	PO4	E	402	-	-	0/0/0/0	0/0/0/0
2	PO4	E	403	-	-	0/0/0/0	0/0/0/0
2	PO4	E	404	-	-	0/0/0/0	0/0/0/0
2	PO4	E	405	-	-	0/0/0/0	0/0/0/0
2	PO4	F	401	-	-	0/0/0/0	0/0/0/0
2	PO4	F	402	-	-	0/0/0/0	0/0/0/0
2	PO4	F	403	-	-	0/0/0/0	0/0/0/0

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	F	404	-	-	0/0/0/0	0/0/0/0
2	PO4	F	405	-	-	0/0/0/0	0/0/0/0
2	PO4	F	406	-	-	0/0/0/0	0/0/0/0
2	PO4	G	401	-	-	0/0/0/0	0/0/0/0
2	PO4	G	402	-	-	0/0/0/0	0/0/0/0
2	PO4	H	401	-	-	0/0/0/0	0/0/0/0
2	PO4	H	402	-	-	0/0/0/0	0/0/0/0
2	PO4	H	403	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	402	PO4	P-O4	-2.11	1.46	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	402	PO4	O4-P-O1	-4.70	90.96	110.97
2	D	403	PO4	O2-P-O1	-3.26	97.09	110.97
2	E	404	PO4	O4-P-O2	-3.01	96.83	107.90
2	C	401	PO4	O4-P-O2	-2.99	96.93	107.90
2	E	404	PO4	O3-P-O1	-2.83	98.94	110.97
2	D	402	PO4	O3-P-O1	-2.72	99.38	110.97
2	F	401	PO4	O4-P-O1	-2.33	101.06	110.97
2	C	402	PO4	O2-P-O1	-2.05	102.26	110.97
2	G	402	PO4	O4-P-O2	-2.04	100.42	107.90
2	A	403	PO4	O4-P-O2	-2.03	100.44	107.90
2	C	403	PO4	O4-P-O1	-2.00	102.44	110.97
2	F	406	PO4	O4-P-O3	2.00	115.25	107.90
2	A	403	PO4	O4-P-O3	2.07	115.49	107.90
2	C	402	PO4	O4-P-O2	2.20	115.99	107.90
2	H	402	PO4	O4-P-O2	2.27	116.23	107.90
2	B	405	PO4	O4-P-O2	2.44	116.87	107.90
2	B	402	PO4	O4-P-O2	2.49	117.04	107.90
2	C	401	PO4	O4-P-O1	2.72	122.55	110.97
2	C	403	PO4	O4-P-O2	3.01	118.96	107.90
2	C	401	PO4	O3-P-O2	3.03	119.03	107.90
2	E	404	PO4	O4-P-O3	3.10	119.30	107.90
2	D	403	PO4	O3-P-O2	4.95	126.08	107.90
2	D	402	PO4	O3-P-O2	5.11	126.66	107.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	404	PO4	1	0
2	C	402	PO4	2	0
2	D	401	PO4	3	0
2	D	402	PO4	1	0
2	E	402	PO4	2	0
2	F	402	PO4	1	0
2	H	403	PO4	0	1

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	314/335 (93%)	0.12	11 (3%)	44	26	35, 53, 72, 97	0
1	B	314/335 (93%)	0.09	9 (2%)	52	32	30, 49, 75, 91	0
1	C	312/335 (93%)	-0.20	5 (1%)	72	51	23, 35, 55, 65	0
1	D	314/335 (93%)	-0.17	5 (1%)	72	51	24, 35, 60, 74	0
1	E	314/335 (93%)	-0.15	7 (2%)	62	41	28, 38, 61, 73	0
1	F	314/335 (93%)	-0.29	8 (2%)	58	37	20, 32, 55, 85	0
1	G	314/335 (93%)	0.05	14 (4%)	34	19	29, 47, 72, 91	0
1	H	310/335 (92%)	0.05	9 (2%)	52	32	31, 49, 83, 101	0
All	All	2506/2680 (93%)	-0.06	68 (2%)	55	34	20, 43, 69, 101	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	ASN	4.4
1	H	151	GLU	4.4
1	B	29	THR	4.1
1	G	324	ASP	4.0
1	F	340	HIS	3.9
1	G	59	SER	3.9
1	A	211	ILE	3.8
1	G	54	GLN	3.8
1	B	207	TYR	3.8
1	A	50	ALA	3.7
1	G	111	GLY	3.6
1	F	324	ASP	3.4
1	B	153	LYS	3.3
1	G	258	GLY	3.2
1	H	152	GLY	3.2
1	D	340	HIS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	152	GLY	3.1
1	G	58	GLN	3.0
1	B	145	PRO	2.9
1	G	73	SER	2.9
1	B	30	GLY	2.8
1	B	27	ASP	2.8
1	D	50	ALA	2.8
1	A	27	ASP	2.8
1	E	35	PHE	2.8
1	G	339	PRO	2.7
1	E	258	GLY	2.7
1	G	337	ASN	2.7
1	B	50	ALA	2.6
1	E	34	SER	2.6
1	A	246	GLU	2.6
1	C	292	ASN	2.5
1	E	29	THR	2.5
1	H	136	ASN	2.5
1	E	259	THR	2.5
1	H	144	ASN	2.5
1	C	316	GLN	2.4
1	A	308	THR	2.4
1	G	64	GLY	2.4
1	H	176	VAL	2.4
1	D	48	ASN	2.4
1	A	33	ALA	2.3
1	B	166	SER	2.3
1	C	291	LYS	2.3
1	A	212	LYS	2.3
1	H	325	THR	2.3
1	G	340	HIS	2.3
1	G	290	PRO	2.3
1	C	73	SER	2.3
1	A	49	ALA	2.2
1	A	340	HIS	2.2
1	H	54	GLN	2.2
1	A	160	SER	2.2
1	D	37	TYR	2.2
1	B	60	ILE	2.2
1	F	151	GLU	2.1
1	F	148	LYS	2.1
1	C	27	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	315	LYS	2.1
1	H	200	GLY	2.1
1	E	308	THR	2.1
1	F	145	PRO	2.1
1	H	150	PRO	2.1
1	E	328	THR	2.1
1	G	139	ALA	2.1
1	F	50	ALA	2.0
1	F	292	ASN	2.0
1	F	46	ASP	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. 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
2	PO4	A	403	5/5	0.91	0.22	1.70	41,51,51,55	0
2	PO4	D	403	5/5	0.94	0.20	1.16	24,32,33,35	0
2	PO4	C	403	5/5	0.95	0.19	0.52	33,37,39,39	0
2	PO4	B	402	5/5	0.97	0.17	0.02	26,26,30,30	0
2	PO4	F	401	5/5	0.94	0.16	-0.06	30,30,36,36	0
2	PO4	F	402	5/5	0.98	0.15	-0.10	35,38,40,41	0
2	PO4	B	405	5/5	0.97	0.18	-0.15	32,32,34,36	0
2	PO4	E	405	5/5	0.96	0.17	-0.28	33,34,37,40	0
2	PO4	E	401	5/5	0.97	0.20	-0.31	29,29,30,31	0
2	PO4	H	403	5/5	0.95	0.17	-0.34	35,47,47,52	0
2	PO4	E	403	5/5	0.97	0.13	-0.78	34,38,40,40	0

Full wwPDB X-ray Structure Validation Report 5I84

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
2	PO4	D	401	5/5	0.97	0.14	-0.79	30,32,34,39	0
2	PO4	F	404	5/5	0.98	0.13	-0.87	23,24,25,26	0
2	PO4	C	401	5/5	0.98	0.14	-0.91	19,21,21,22	0
2	PO4	F	405	5/5	0.99	0.10	-0.92	21,22,24,25	0
2	PO4	A	402	5/5	0.97	0.15	-0.97	35,35,37,44	0
2	PO4	E	402	5/5	0.98	0.09	-1.09	17,18,19,19	0
2	PO4	A	401	5/5	0.98	0.12	-1.34	36,38,39,41	0
2	PO4	D	402	5/5	0.99	0.11	-1.41	2,2,2,2	0
2	PO4	B	403	5/5	0.97	0.17	-1.45	50,50,53,54	0
2	PO4	H	402	5/5	0.99	0.11	-1.49	19,21,22,24	0
2	PO4	F	403	5/5	0.99	0.10	-1.54	21,23,25,25	0
2	PO4	C	402	5/5	0.99	0.10	-1.60	7,7,8,8	0
2	PO4	H	401	5/5	0.97	0.13	-1.75	39,41,42,43	0
2	PO4	G	402	5/5	0.99	0.09	-1.76	19,20,21,21	0
2	PO4	D	405	5/5	0.97	0.12	-1.78	32,33,38,42	0
2	PO4	G	401	5/5	0.97	0.12	-1.81	50,50,54,57	0
2	PO4	E	404	5/5	0.98	0.12	-1.90	19,20,22,23	0
2	PO4	A	404	5/5	0.98	0.10	-2.20	26,26,29,30	0
2	PO4	B	404	5/5	0.99	0.08	-2.35	32,32,34,34	0
2	PO4	C	404	5/5	0.98	0.10	-	33,33,35,37	0
2	PO4	B	401	5/5	0.96	0.25	-	45,54,56,59	0
2	PO4	F	406	5/5	0.98	0.15	-	23,23,24,24	0
2	PO4	D	404	5/5	0.97	0.14	-	31,35,37,41	0

6.5 Other polymers (i)

There are no such residues in this entry.