Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:33 AM GMT

PDB ID	:	3F4N
Title	:	Crystal Structure of Pyridoxal Phosphate Biosynthetic Protein PdxJ from Yersinia pestis
Authors	:	Kim, Y.; Maltseva, N.; Stam, J.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2008-11-01
Resolution	:	2.40 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 (1)) were used in the production of this report:

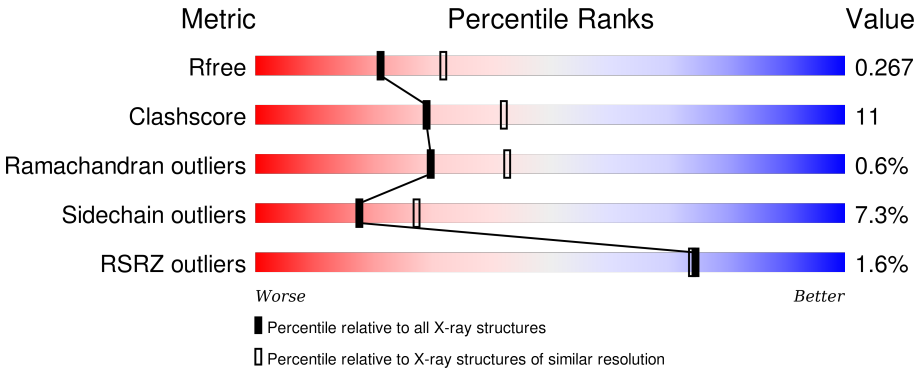
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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.



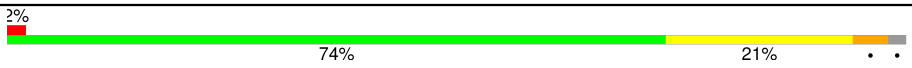
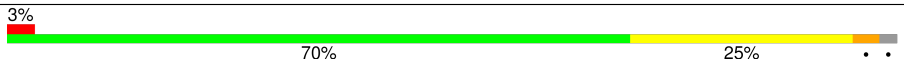
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	246	78% 17%
1	B	246	79% 15%
1	C	246	76% 19%
1	D	246	73% 23%
1	E	246	75% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	246	
1	G	246	
1	H	246	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15591 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 Pyridoxine 5'-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	3	0
			1863	1160	345	346	12			
1	B	238	Total	C	N	O	S	0	2	0
			1820	1134	335	339	12			
1	C	244	Total	C	N	O	S	0	1	0
			1855	1156	340	346	13			
1	D	242	Total	C	N	O	S	0	2	0
			1851	1153	340	346	12			
1	E	241	Total	C	N	O	S	0	3	0
			1858	1157	344	345	12			
1	F	242	Total	C	N	O	S	0	1	0
			1840	1147	335	346	12			
1	G	242	Total	C	N	O	S	0	1	0
			1841	1148	337	344	12			
1	H	241	Total	C	N	O	S	0	3	0
			1853	1154	338	349	12			

There are 24 discrepancies between the modelled and reference sequences:

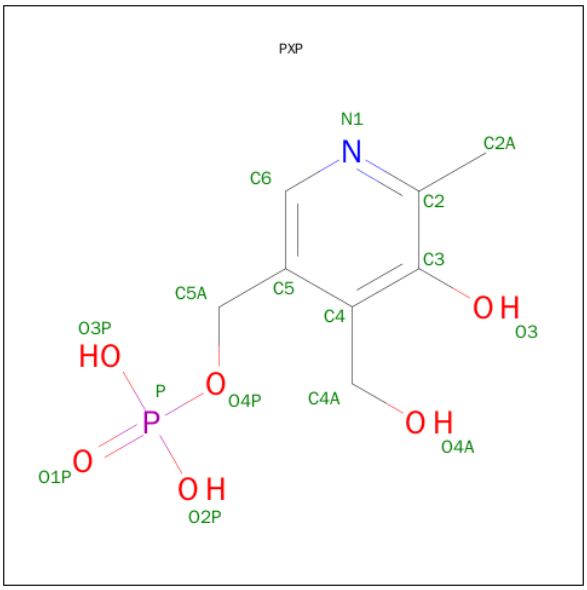
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q8ZCP4
A	-1	ASN	-	EXPRESSION TAG	UNP Q8ZCP4
A	0	ALA	-	EXPRESSION TAG	UNP Q8ZCP4
B	-2	SER	-	EXPRESSION TAG	UNP Q8ZCP4
B	-1	ASN	-	EXPRESSION TAG	UNP Q8ZCP4
B	0	ALA	-	EXPRESSION TAG	UNP Q8ZCP4
C	-2	SER	-	EXPRESSION TAG	UNP Q8ZCP4
C	-1	ASN	-	EXPRESSION TAG	UNP Q8ZCP4
C	0	ALA	-	EXPRESSION TAG	UNP Q8ZCP4
D	-2	SER	-	EXPRESSION TAG	UNP Q8ZCP4
D	-1	ASN	-	EXPRESSION TAG	UNP Q8ZCP4
D	0	ALA	-	EXPRESSION TAG	UNP Q8ZCP4
E	-2	SER	-	EXPRESSION TAG	UNP Q8ZCP4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	EXPRESSION TAG	UNP Q8ZCP4
E	0	ALA	-	EXPRESSION TAG	UNP Q8ZCP4
F	-2	SER	-	EXPRESSION TAG	UNP Q8ZCP4
F	-1	ASN	-	EXPRESSION TAG	UNP Q8ZCP4
F	0	ALA	-	EXPRESSION TAG	UNP Q8ZCP4
G	-2	SER	-	EXPRESSION TAG	UNP Q8ZCP4
G	-1	ASN	-	EXPRESSION TAG	UNP Q8ZCP4
G	0	ALA	-	EXPRESSION TAG	UNP Q8ZCP4
H	-2	SER	-	EXPRESSION TAG	UNP Q8ZCP4
H	-1	ASN	-	EXPRESSION TAG	UNP Q8ZCP4
H	0	ALA	-	EXPRESSION TAG	UNP Q8ZCP4

- Molecule 2 is PYRIDOXINE-5'-PHOSPHATE (three-letter code: PXP) (formula: $C_8H_{12}NO_6P$).



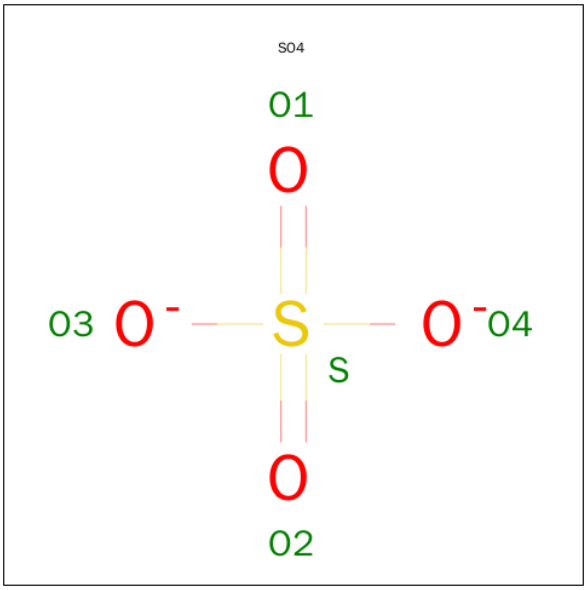
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	E	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	F	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C N O P 16 8 1 6 1	0	0
2	H	1	Total C N O P 16 8 1 6 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	104	Total O 104 104	0	0
4	B	79	Total O 79 79	0	0
4	C	99	Total O 99 99	0	0
4	D	74	Total O 74 74	0	0

Continued on next page...

Continued from previous page...

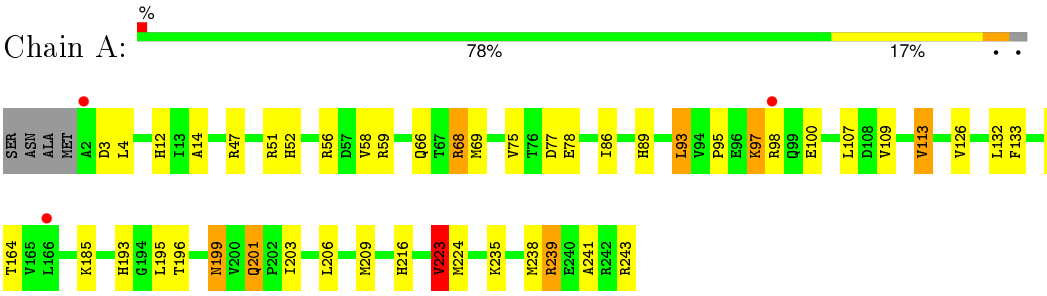
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	66	Total O 66 66	0	0
4	F	78	Total O 78 78	0	0
4	G	74	Total O 74 74	0	0
4	H	93	Total O 93 93	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

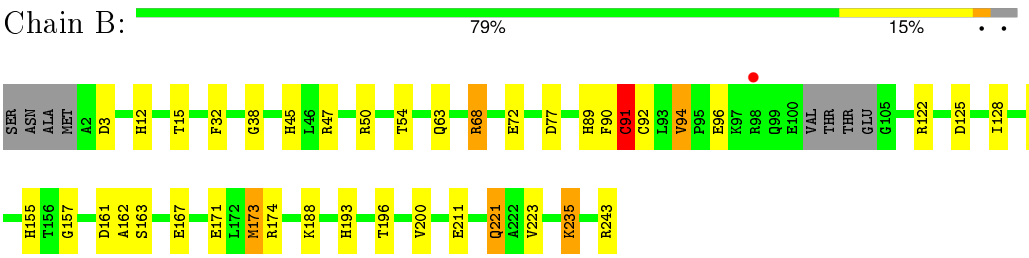
- Molecule 1: Pyridoxine 5'-phosphate synthase

Chain A:



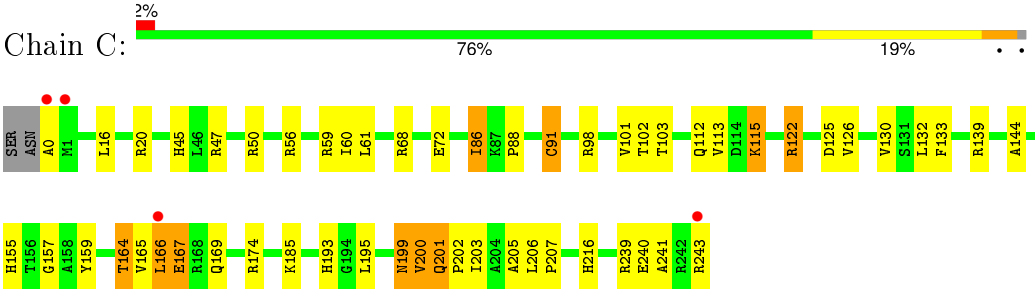
- Molecule 1: Pyridoxine 5'-phosphate synthase

Chain B:



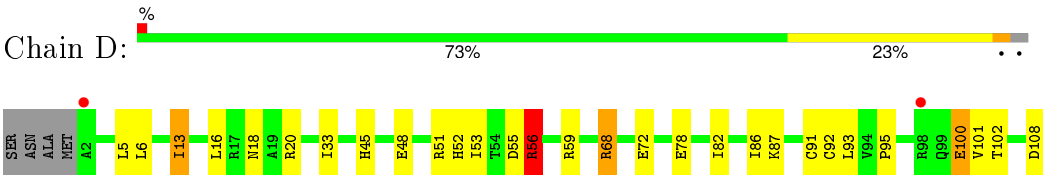
- Molecule 1: Pyridoxine 5'-phosphate synthase

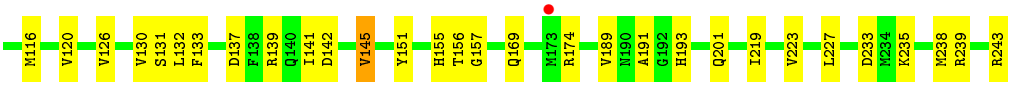
Chain C:



- Molecule 1: Pyridoxine 5'-phosphate synthase

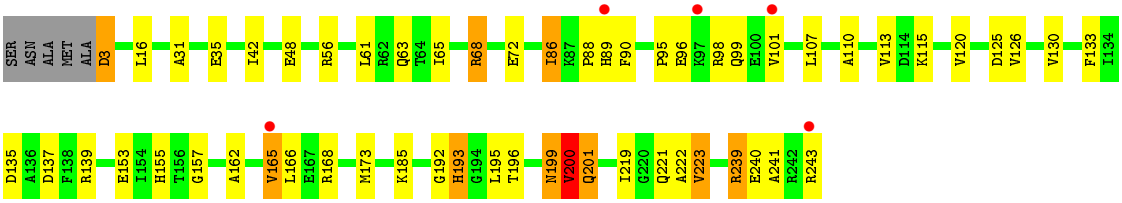
Chain D:





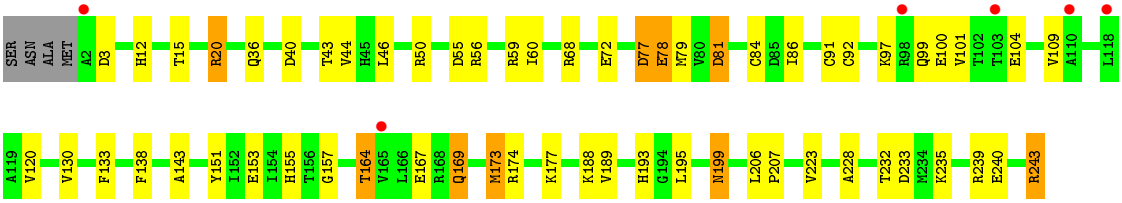
• Molecule 1: Pyridoxine 5'-phosphate synthase

Chain E:



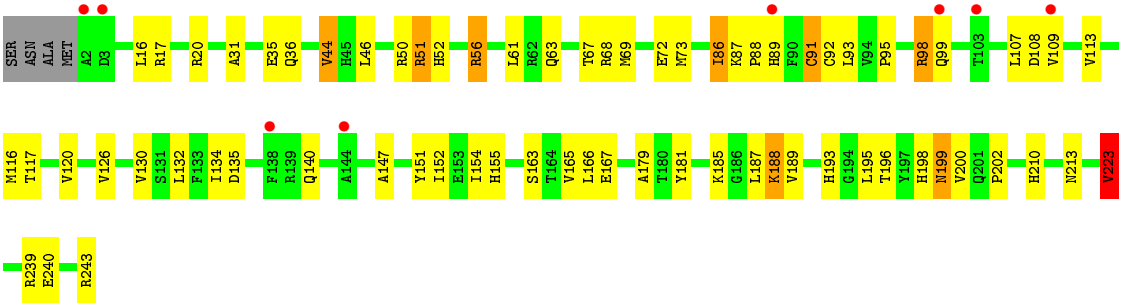
• Molecule 1: Pyridoxine 5'-phosphate synthase

Chain F:



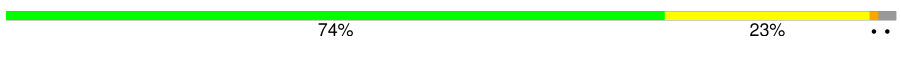
• Molecule 1: Pyridoxine 5'-phosphate synthase

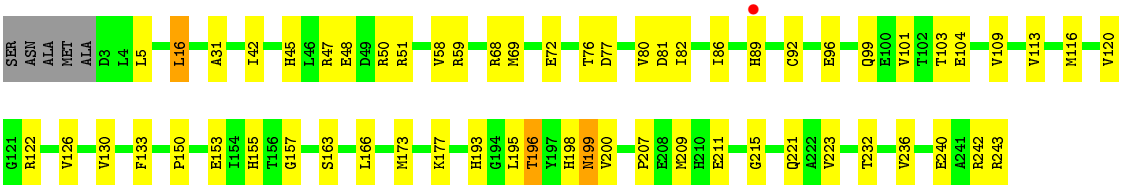
Chain G:



• Molecule 1: Pyridoxine 5'-phosphate synthase

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.63Å 114.82Å 154.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.81 – 2.40 34.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.6 (34.81-2.40) 94.6 (34.81-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.23 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.4	Depositor
R, R_{free}	0.191 , 0.266 0.193 , 0.267	Depositor DCC
R_{free} test set	3763 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.2	EDS
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 74940 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15591	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PXP, SO4

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	0.89	0/1888	0.95	6/2558 (0.2%)
1	B	0.88	2/1843 (0.1%)	0.89	0/2495
1	C	0.88	1/1879 (0.1%)	0.93	5/2546 (0.2%)
1	D	0.85	1/1875 (0.1%)	0.92	5/2541 (0.2%)
1	E	0.81	1/1883 (0.1%)	0.90	4/2551 (0.2%)
1	F	0.82	1/1864 (0.1%)	0.88	1/2527 (0.0%)
1	G	0.76	0/1866	0.85	2/2530 (0.1%)
1	H	0.86	0/1878	0.88	0/2546
All	All	0.85	6/14976 (0.0%)	0.90	23/20294 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	91	CYS	CB-SG	-7.29	1.69	1.82
1	B	91	CYS	CB-SG	-6.07	1.72	1.82
1	E	72	GLU	CB-CG	-5.33	1.42	1.52
1	F	84	CYS	CB-SG	-5.16	1.73	1.81
1	C	91	CYS	CB-SG	-5.14	1.73	1.81
1	B	32	PHE	CE1-CZ	5.03	1.47	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	68	ARG	NE-CZ-NH2	8.08	124.34	120.30
1	D	13	ILE	CG1-CB-CG2	-6.70	96.65	111.40
1	C	200	VAL	CB-CA-C	-6.61	98.84	111.40
1	A	68	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	E	68[A]	ARG	NE-CZ-NH1	-6.15	117.23	120.30
1	E	68[B]	ARG	NE-CZ-NH1	-6.15	117.23	120.30
1	E	200	VAL	CB-CA-C	-6.10	99.81	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	68	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	G	56	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	126	VAL	CB-CA-C	5.95	122.70	111.40
1	G	223	VAL	CB-CA-C	-5.78	100.42	111.40
1	D	233	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	55	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	77	ASP	CB-CG-OD1	5.58	123.32	118.30
1	D	20	ARG	C-N-CA	-5.57	110.60	122.30
1	F	173	MET	CG-SD-CE	5.53	109.05	100.20
1	C	125	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	223	VAL	CB-CA-C	-5.26	101.41	111.40
1	A	224	MET	CG-SD-CE	-5.21	91.86	100.20
1	C	50	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	C	122	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	E	195	LEU	CB-CG-CD1	-5.06	102.40	111.00
1	D	56	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1863	0	1888	42	0
1	B	1820	0	1843	34	0
1	C	1855	0	1887	45	0
1	D	1851	0	1877	35	0
1	E	1858	0	1883	54	0
1	F	1840	0	1863	44	0
1	G	1841	0	1864	65	0
1	H	1853	0	1867	46	0
2	A	16	0	8	1	0
2	B	16	0	8	1	0
2	C	16	0	8	3	0
2	D	16	0	9	2	0
2	E	16	0	8	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	16	0	8	2	0
2	G	16	0	8	0	0
2	H	16	0	8	2	0
3	C	5	0	0	0	0
3	E	10	0	0	0	0
4	A	104	0	0	8	0
4	B	79	0	0	7	0
4	C	99	0	0	5	0
4	D	74	0	0	1	0
4	E	66	0	0	0	0
4	F	78	0	0	8	0
4	G	74	0	0	7	0
4	H	93	0	0	4	0
All	All	15591	0	15037	343	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 11.

All (343) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:ARG:HD3	1:H:240:GLU:HG2	1.36	1.07
1:F:100:GLU:HG3	4:F:1292:HOH:O	1.60	1.02
1:A:58:VAL:HG12	1:A:86:ILE:HD13	1.44	0.98
1:B:155:HIS:HD2	1:B:157:GLY:H	1.12	0.96
1:F:169:GLN:HG3	4:F:1257:HOH:O	1.65	0.95
1:D:174:ARG:HD3	4:D:1304:HOH:O	1.67	0.95
1:F:155:HIS:HD2	1:F:157:GLY:H	1.06	0.95
1:E:196:THR:O	1:E:200:VAL:HG22	1.68	0.93
4:B:1481:HOH:O	1:G:198:HIS:HD2	1.51	0.92
1:B:243:ARG:HH11	1:G:243:ARG:NH1	1.67	0.91
1:E:201:GLN:HG3	1:E:241:ALA:HB2	1.53	0.91
1:E:223:VAL:HG13	1:F:223:VAL:HG12	1.52	0.91
1:F:155:HIS:CD2	1:F:157:GLY:H	1.88	0.90
1:D:52:HIS:HD2	1:D:53:ILE:H	1.21	0.88
1:C:59:ARG:HH12	1:E:63:GLN:HE22	1.20	0.87
1:D:52:HIS:CD2	1:D:53:ILE:H	1.95	0.84
1:G:117:THR:HG22	1:G:147:ALA:HA	1.56	0.84
1:B:155:HIS:CD2	1:B:157:GLY:H	1.95	0.84
1:C:205:ALA:HB3	4:C:1609:HOH:O	1.78	0.83
1:F:243:ARG:NH2	1:H:240:GLU:OE2	2.12	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89[B]:HIS:H	1:H:89[B]:HIS:CD2	1.95	0.81
1:C:165:VAL:HG12	1:C:169:GLN:OE1	1.81	0.80
1:G:196:THR:H	1:G:199:ASN:HD21	1.29	0.79
1:E:199:ASN:C	1:E:199:ASN:HD22	1.87	0.79
1:E:162:ALA:HB3	1:E:168:ARG:HG3	1.65	0.78
1:E:89[B]:HIS:CD2	1:E:89[B]:HIS:H	1.97	0.78
1:E:120:VAL:HG22	1:E:130:VAL:HG11	1.65	0.78
1:G:196:THR:H	1:G:199:ASN:ND2	1.82	0.78
1:E:196:THR:O	1:E:200:VAL:CG2	2.32	0.77
1:A:12:HIS:CD2	1:A:216:HIS:HD2	2.03	0.77
1:G:69:MET:H	1:G:89[B]:HIS:CD2	2.02	0.77
1:F:199:ASN:HD22	1:F:199:ASN:C	1.86	0.77
1:G:113:VAL:O	1:G:117:THR:HG23	1.86	0.76
1:A:58:VAL:CG1	1:A:86:ILE:HD13	2.14	0.76
1:C:199:ASN:HD22	1:C:199:ASN:C	1.90	0.74
1:C:98:ARG:HD3	4:C:1446:HOH:O	1.85	0.74
1:G:73:MET:CE	1:G:91:CYS:SG	2.76	0.73
1:B:137:ASP:OD1	1:B:139:ARG:HB3	1.88	0.73
1:G:210:HIS:HB2	4:G:1250:HOH:O	1.89	0.73
1:G:167:GLU:HB2	4:G:1641:HOH:O	1.88	0.72
1:C:155:HIS:CD2	1:C:157:GLY:H	2.08	0.72
1:B:243:ARG:HH11	1:G:243:ARG:HH12	1.35	0.72
1:G:16:LEU:HD13	1:H:16:LEU:HD22	1.70	0.72
1:B:63:GLN:HE22	1:H:59:ARG:HH12	1.37	0.72
1:E:126:VAL:O	1:E:126:VAL:HG12	1.89	0.72
1:G:95:PRO:HD3	1:G:107:LEU:HB2	1.72	0.71
1:B:38:GLY:O	1:B:235:LYS:HD3	1.90	0.71
1:A:69:MET:H	1:A:89[B]:HIS:CD2	2.09	0.70
1:A:58:VAL:HG12	1:A:86:ILE:CD1	2.20	0.70
1:E:68[B]:ARG:HH21	1:E:68[B]:ARG:CG	2.04	0.70
4:B:1481:HOH:O	1:G:198:HIS:CD2	2.33	0.70
1:D:13:ILE:CD1	1:D:219:ILE:HD12	2.21	0.70
1:F:3:ASP:HA	4:F:1277:HOH:O	1.91	0.69
1:G:120:VAL:HG22	1:G:130:VAL:HG11	1.73	0.69
1:A:223:VAL:HG13	1:B:223:VAL:HG12	1.73	0.69
1:A:238:MET:CB	1:A:239[B]:ARG:HH12	2.06	0.68
1:C:0:ALA:HB2	1:C:207:PRO:HA	1.75	0.68
1:E:31:ALA:O	1:E:35:GLU:HG3	1.93	0.68
1:D:137:ASP:O	1:D:141:ILE:HD12	1.94	0.68
1:C:159:TYR:CE1	1:C:203:ILE:CD1	2.77	0.68
1:G:98:ARG:H	1:G:98:ARG:HD2	1.59	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:LEU:HB2	1:H:211:GLU:HB2	1.75	0.67
1:A:238:MET:HB2	1:A:239[B]:ARG:HH12	1.58	0.67
1:E:155:HIS:CD2	1:E:157:GLY:H	2.13	0.67
1:C:130:VAL:O	1:C:150:PRO:HD2	1.94	0.67
1:A:201:GLN:HG3	1:A:241:ALA:HB2	1.78	0.66
1:G:240:GLU:HA	1:G:240:GLU:OE2	1.94	0.66
1:B:68[B]:ARG:HD2	1:B:90:PHE:CE1	2.31	0.66
1:A:97:LYS:O	1:A:100:GLU:HG2	1.97	0.65
1:H:153:GLU:OE1	2:H:508:PXP:N1	2.30	0.64
1:E:89[B]:HIS:N	1:E:89[B]:HIS:CD2	2.66	0.64
1:F:36:GLN:HG2	1:H:221:GLN:HE22	1.63	0.64
1:A:12:HIS:CD2	1:A:216:HIS:CD2	2.86	0.64
1:E:68[B]:ARG:HG3	1:E:68[B]:ARG:NH2	2.11	0.64
1:H:58:VAL:HG11	1:H:86:ILE:HD13	1.78	0.64
1:H:199:ASN:C	1:H:199:ASN:HD22	2.02	0.64
1:G:73:MET:HE1	1:G:91:CYS:SG	2.36	0.63
4:A:1456:HOH:O	1:D:56:ARG:HD2	1.98	0.63
1:A:109:VAL:HG12	1:A:143:ALA:HB1	1.81	0.63
1:C:201:GLN:HG3	1:C:241:ALA:HB2	1.79	0.63
1:E:243:ARG:HD3	1:G:243:ARG:NH1	2.13	0.63
1:A:89[B]:HIS:H	1:A:89[B]:HIS:CD2	2.15	0.63
1:E:221:GLN:HE22	1:G:36:GLN:HG2	1.63	0.63
1:E:201:GLN:HG3	1:E:241:ALA:CB	2.26	0.62
1:G:69:MET:H	1:G:89[B]:HIS:HD2	1.45	0.62
1:G:199:ASN:C	1:G:199:ASN:HD22	2.03	0.62
1:E:126:VAL:CG1	1:E:126:VAL:O	2.47	0.62
1:F:195:LEU:HA	1:F:199:ASN:HD21	1.65	0.62
1:E:68[B]:ARG:HH21	1:E:68[B]:ARG:HG3	1.64	0.62
1:A:75:VAL:HG22	1:A:93:LEU:HG	1.80	0.62
1:C:195:LEU:HA	1:C:199:ASN:HD21	1.65	0.62
1:H:58:VAL:CG1	1:H:86:ILE:HD13	2.28	0.62
1:F:228:ALA:O	1:F:232:THR:HG22	2.00	0.62
1:G:73:MET:HE2	1:G:91:CYS:SG	2.40	0.62
1:E:89[A]:HIS:HD2	1:E:90:PHE:CE1	2.17	0.61
1:D:101:VAL:HG12	1:D:102:THR:O	2.00	0.61
1:H:196:THR:CG2	1:H:198:HIS:H	2.13	0.61
1:A:199:ASN:C	1:A:199:ASN:HD22	2.04	0.61
1:A:239[A]:ARG:HD2	4:A:1004:HOH:O	2.00	0.61
1:H:242:ARG:NH2	4:H:1635:HOH:O	2.29	0.61
1:H:243:ARG:NH2	4:H:1364:HOH:O	2.33	0.60
1:D:239:ARG:HB3	1:D:243:ARG:HH21	1.67	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:ASP:O	1:F:81:ASP:OD2	2.20	0.59
1:E:133:PHE:CD2	2:E:505:PXP:H2A2	2.37	0.59
1:D:108:ASP:O	1:D:112:GLN:HG3	2.01	0.59
1:F:240:GLU:HA	1:F:243:ARG:HD2	1.84	0.59
1:H:133:PHE:CD2	2:H:508:PXP:H2A2	2.37	0.59
1:C:159:TYR:CE1	1:C:203:ILE:HD12	2.37	0.59
1:C:59:ARG:NH1	1:E:63:GLN:HE22	1.97	0.59
1:A:196:THR:H	1:A:199:ASN:ND2	2.01	0.58
1:A:59:ARG:NH2	4:A:1650:HOH:O	2.36	0.58
1:B:151:TYR:CZ	1:B:188:LYS:HD3	2.38	0.58
1:F:138:PHE:HB2	4:F:1662:HOH:O	2.02	0.58
1:D:131:SER:HA	1:D:151:TYR:O	2.03	0.58
1:G:126:VAL:HG12	1:G:126:VAL:O	2.03	0.58
1:G:108:ASP:HA	1:G:140:GLN:HE22	1.67	0.58
1:G:72:GLU:HG2	1:G:92:CYS:HB3	1.85	0.58
1:E:165:VAL:HG12	1:E:166:LEU:HD12	1.84	0.58
1:H:109:VAL:HG13	1:H:116:MET:HG3	1.84	0.58
1:E:196:THR:H	1:E:199:ASN:ND2	2.01	0.57
1:H:130:VAL:O	1:H:150:PRO:HD2	2.04	0.57
1:H:196:THR:HG22	1:H:198:HIS:H	1.68	0.57
1:F:55:ASP:O	1:F:59:ARG:HG3	2.04	0.57
1:F:133:PHE:CD2	2:F:506:PXP:H2A2	2.40	0.57
1:A:113:VAL:HG23	4:A:1468:HOH:O	2.03	0.57
1:B:77[B]:ASP:OD1	1:B:122:ARG:NH1	2.37	0.57
1:H:89[B]:HIS:N	1:H:89[B]:HIS:CD2	2.68	0.56
1:G:199:ASN:HD22	1:G:200:VAL:N	2.03	0.56
1:A:238:MET:HB2	1:A:239[B]:ARG:NH1	2.20	0.56
1:A:195:LEU:HA	1:A:199:ASN:HD21	1.68	0.56
1:H:155:HIS:CD2	1:H:157:GLY:H	2.24	0.56
1:H:207:PRO:O	4:H:1635:HOH:O	2.17	0.56
1:A:133:PHE:CD2	2:A:501:PXP:H2A2	2.40	0.56
1:C:47[A]:ARG:NH2	4:C:1206:HOH:O	2.37	0.56
1:E:48:GLU:HG2	1:E:96:GLU:OE1	2.06	0.56
1:D:87:LYS:HE3	1:D:126:VAL:CG1	2.37	0.55
1:D:109:VAL:HG13	1:D:116:MET:HG3	1.89	0.55
1:C:159:TYR:CD1	1:C:203:ILE:HD11	2.40	0.55
1:G:93:LEU:HD12	1:G:132:LEU:CD2	2.36	0.55
1:G:239:ARG:HG2	1:G:239:ARG:HH21	1.72	0.55
1:D:95:PRO:HB2	1:D:101:VAL:HG22	1.87	0.55
1:G:86:ILE:HG22	1:G:88:PRO:HD3	1.87	0.55
1:B:3:ASP:HB2	4:B:1372:HOH:O	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:HIS:CE1	1:C:47[A]:ARG:HG2	2.42	0.55
1:F:173:MET:HA	1:F:173:MET:CE	2.37	0.55
1:H:82:ILE:CG2	1:H:86:ILE:HD12	2.37	0.55
1:C:126:VAL:CG1	1:C:126:VAL:O	2.55	0.54
1:D:13:ILE:HD12	1:D:219:ILE:HD12	1.90	0.54
1:A:66:GLN:NE2	4:A:1661:HOH:O	2.40	0.54
1:A:196:THR:H	1:A:199:ASN:HD21	1.54	0.54
1:E:199:ASN:ND2	1:E:199:ASN:C	2.56	0.54
1:C:155:HIS:HD2	1:C:157:GLY:H	1.52	0.54
1:G:51:ARG:NH1	4:G:1276:HOH:O	2.41	0.54
1:C:239:ARG:HB3	1:C:243:ARG:NH2	2.22	0.54
1:D:93:LEU:HD12	1:D:132:LEU:CD2	2.38	0.53
1:C:133:PHE:CD2	2:C:503:PXP:H2A2	2.43	0.53
1:H:69:MET:H	1:H:89[B]:HIS:CD2	2.26	0.53
1:H:196:THR:H	1:H:199:ASN:ND2	2.07	0.53
1:G:31:ALA:O	1:G:35:GLU:HG3	2.07	0.53
1:F:138:PHE:N	1:F:138:PHE:CD1	2.76	0.53
1:F:104[B]:GLU:CD	1:F:174:ARG:HH22	2.11	0.53
1:F:138:PHE:N	1:F:138:PHE:HD1	2.06	0.53
1:C:86:ILE:HG22	1:C:88:PRO:HD3	1.90	0.53
1:D:100:GLU:HB3	1:D:112:GLN:HE22	1.73	0.53
1:G:17:ARG:O	1:G:20:ARG:O	2.26	0.53
1:C:159:TYR:CE1	1:C:203:ILE:HD11	2.44	0.53
1:D:133:PHE:CD2	2:D:504:PXP:H2A2	2.43	0.53
1:G:167:GLU:CB	4:G:1641:HOH:O	2.52	0.53
1:F:72:GLU:HG2	1:F:92:CYS:HB3	1.91	0.53
1:B:72:GLU:HG2	1:B:92:CYS:HB3	1.91	0.52
1:F:151:TYR:CZ	1:F:188:LYS:HD3	2.44	0.52
1:A:201:GLN:CG	1:A:241:ALA:HB2	2.39	0.52
1:F:199:ASN:C	1:F:199:ASN:ND2	2.60	0.52
1:D:5:LEU:HD13	1:D:68:ARG:HH12	1.75	0.52
1:G:213:ASN:HB3	4:G:1518:HOH:O	2.10	0.51
1:G:240:GLU:OE2	1:G:243:ARG:NE	2.43	0.51
1:C:126:VAL:HG13	1:C:126:VAL:O	2.10	0.51
1:B:91:CYS:HB2	1:B:128:ILE:HG21	1.93	0.51
1:C:0:ALA:HB2	1:C:207:PRO:CA	2.41	0.51
1:E:196:THR:H	1:E:199:ASN:HD21	1.59	0.51
1:F:153:GLU:OE1	2:F:506:PXP:N1	2.43	0.51
1:E:86:ILE:HG22	1:E:88:PRO:HD3	1.93	0.51
1:C:240:GLU:HA	1:C:243:ARG:HG3	1.92	0.50
1:E:89[A]:HIS:CD2	1:E:90:PHE:CE1	2.98	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ASN:ND2	1:C:199:ASN:C	2.63	0.50
1:B:68[A]:ARG:HH21	1:B:89:HIS:CE1	2.29	0.50
1:F:59:ARG:HG2	1:F:86:ILE:HD11	1.93	0.50
1:D:45:HIS:HA	1:D:72:GLU:HB2	1.94	0.50
1:G:196:THR:O	1:G:200:VAL:HB	2.10	0.50
1:H:82:ILE:HG23	1:H:86:ILE:HD12	1.93	0.50
1:H:155:HIS:HD2	1:H:157:GLY:H	1.59	0.50
1:A:47[A]:ARG:NH2	4:A:1619:HOH:O	2.41	0.50
1:B:12:HIS:HA	1:B:15:THR:OG1	2.12	0.50
1:G:117:THR:HG21	4:G:1642:HOH:O	2.12	0.49
1:E:243:ARG:HH12	1:G:239:ARG:HB3	1.77	0.49
1:A:235:LYS:HD2	1:A:239[B]:ARG:NH1	2.28	0.49
1:G:44:VAL:HG21	1:G:61:LEU:HD13	1.93	0.49
1:B:68[B]:ARG:HD2	1:B:90:PHE:HE1	1.76	0.49
1:H:209:MET:O	4:H:1635:HOH:O	2.20	0.49
1:D:201:GLN:HE22	1:E:239[A]:ARG:HH12	1.60	0.49
1:E:153:GLU:OE1	1:E:192:GLY:HA3	2.12	0.49
1:G:195:LEU:HA	1:G:199:ASN:HD21	1.78	0.49
1:A:14:ALA:HB3	1:A:52:HIS:HB2	1.95	0.49
1:G:196:THR:N	1:G:199:ASN:HD21	2.04	0.49
1:G:35:GLU:OE2	1:G:67:THR:OG1	2.21	0.49
1:C:59:ARG:HH11	1:C:59:ARG:HG2	1.78	0.49
1:G:89[B]:HIS:CD2	1:G:89[B]:HIS:H	2.30	0.49
1:C:164:THR:OG1	1:C:167:GLU:HB2	2.13	0.49
1:E:199:ASN:HD22	1:E:200:VAL:N	2.10	0.48
1:C:239:ARG:HB3	1:C:243:ARG:HH22	1.78	0.48
1:G:135:ASP:OD2	4:G:1127:HOH:O	2.19	0.48
1:G:109:VAL:HG13	1:G:116:MET:HG3	1.95	0.48
1:B:94:VAL:HG21	2:B:502:PXP:H2A1	1.95	0.48
1:H:196:THR:H	1:H:199:ASN:HD21	1.61	0.48
1:A:132:LEU:HD12	1:A:144:ALA:CB	2.44	0.48
1:H:76:THR:O	1:H:80:VAL:HG23	2.14	0.48
1:E:3:ASP:OD1	1:E:239[A]:ARG:NH1	2.42	0.48
1:G:134:ILE:HD11	1:G:152:ILE:HD12	1.96	0.48
1:G:151:TYR:CZ	1:G:188:LYS:HG2	2.48	0.48
1:E:135:ASP:O	1:E:137:ASP:N	2.46	0.48
1:B:243:ARG:NH1	1:G:243:ARG:NH1	2.50	0.47
1:G:199:ASN:O	1:G:202:PRO:HD2	2.14	0.47
1:A:69:MET:H	1:A:89[B]:HIS:HD2	1.60	0.47
1:G:46:LEU:HD11	1:G:50:ARG:HD2	1.95	0.47
1:B:45:HIS:NE2	1:B:96:GLU:OE2	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:VAL:HG13	1:F:223:VAL:CG1	2.33	0.47
1:D:239:ARG:HB3	1:D:243:ARG:NH2	2.29	0.47
1:F:12:HIS:HD2	1:F:15:THR:OG1	1.97	0.47
1:A:238:MET:HB3	1:A:239[B]:ARG:HH12	1.78	0.47
1:B:68[B]:ARG:HG3	1:B:68[B]:ARG:HH11	1.79	0.47
1:E:68[A]:ARG:HE	1:E:68[A]:ARG:HB2	1.21	0.47
1:E:98:ARG:HA	1:E:101:VAL:HG12	1.97	0.47
1:A:58:VAL:CG1	1:A:86:ILE:CD1	2.87	0.47
1:F:43:THR:HG22	1:F:44:VAL:N	2.30	0.47
1:D:33:ILE:HG21	1:D:227:LEU:HB3	1.97	0.47
1:E:31:ALA:HA	1:E:42:ILE:HD12	1.97	0.47
1:G:68:ARG:HE	1:G:68:ARG:HB2	1.21	0.47
1:D:142:ASP:O	1:D:145:VAL:HG23	2.15	0.47
1:H:89[B]:HIS:H	1:H:89[B]:HIS:HD2	1.57	0.46
1:A:4:LEU:HB3	1:A:239[B]:ARG:HH22	1.80	0.46
1:F:233:ASP:HB3	4:F:1433:HOH:O	2.14	0.46
1:A:238:MET:CB	1:A:239[B]:ARG:NH1	2.74	0.46
1:C:153:GLU:OE1	2:C:503:PXP:N1	2.48	0.46
1:C:101:VAL:HG22	1:C:102:THR:O	2.15	0.46
1:E:95:PRO:HG3	1:E:107:LEU:HA	1.98	0.46
1:A:47[B]:ARG:HD3	1:A:51:ARG:HG2	1.98	0.46
1:E:137:ASP:OD1	1:E:139:ARG:HB2	2.15	0.46
1:H:232:THR:O	1:H:236:VAL:HG23	2.16	0.46
1:B:221:GLN:HB2	4:B:1615:HOH:O	2.16	0.46
1:B:173:MET:HG3	1:B:174:ARG:N	2.31	0.45
1:B:68[B]:ARG:NH2	1:B:211:GLU:OE1	2.49	0.45
1:G:87:LYS:HG2	1:G:126:VAL:CG1	2.47	0.45
1:D:155:HIS:CE1	1:D:157:GLY:HA3	2.50	0.45
1:F:78:GLU:HG3	1:F:79:MET:N	2.32	0.45
1:C:216:HIS:HE1	1:D:16:LEU:O	2.00	0.45
1:F:109:VAL:HG12	1:F:143:ALA:HB1	1.97	0.45
1:G:181:TYR:O	1:G:185:LYS:HG2	2.17	0.45
1:B:54:THR:HB	4:B:1022:HOH:O	2.17	0.45
1:H:177:LYS:HB3	1:H:177:LYS:HE3	1.64	0.45
1:H:195:LEU:HA	1:H:199:ASN:HD21	1.81	0.45
1:B:161:ASP:O	1:B:162:ALA:C	2.55	0.45
1:A:78:GLU:HG3	4:A:1459:HOH:O	2.16	0.45
1:D:141:ILE:O	1:D:145:VAL:HG22	2.16	0.45
1:A:59:ARG:HG2	4:A:1454:HOH:O	2.17	0.45
1:G:239:ARG:HH21	1:G:239:ARG:CG	2.30	0.44
1:C:0:ALA:HB2	1:C:207:PRO:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:ILE:HD12	1:G:135:ASP:O	2.17	0.44
1:B:167:GLU:O	1:B:171:GLU:HG2	2.17	0.44
1:F:164:THR:HB	1:F:167:GLU:H	1.82	0.44
1:C:133:PHE:CE2	2:C:503:PXP:H2A2	2.53	0.44
1:H:48[A]:GLU:HG2	1:H:96:GLU:OE1	2.17	0.44
1:A:89[B]:HIS:N	1:A:89[B]:HIS:CD2	2.85	0.44
1:A:4:LEU:HB3	1:A:239[B]:ARG:NH2	2.33	0.44
1:F:173:MET:HE3	4:F:1327:HOH:O	2.18	0.44
1:C:240:GLU:HA	1:C:243:ARG:CG	2.48	0.44
1:B:196:THR:O	1:B:200:VAL:HB	2.18	0.44
1:A:206:LEU:HB2	1:A:209:MET:HG2	1.98	0.44
1:B:63:GLN:NE2	1:H:59:ARG:HH12	2.11	0.44
1:H:120:VAL:HG22	1:H:130:VAL:HG11	2.00	0.44
1:C:132:LEU:HD12	1:C:144:ALA:HA	1.99	0.43
1:H:196:THR:O	1:H:200:VAL:HB	2.18	0.43
1:G:154:ILE:HD11	1:G:179:ALA:HB2	1.98	0.43
1:E:89[B]:HIS:HD2	1:E:89[B]:HIS:H	1.55	0.43
1:F:99:GLN:HB2	4:F:1292:HOH:O	2.18	0.43
1:F:20:ARG:HA	1:F:20:ARG:HD3	1.76	0.43
1:E:240:GLU:HG2	1:E:243:ARG:HH11	1.82	0.43
1:E:16:LEU:CD2	1:F:223:VAL:HG11	2.49	0.43
1:C:166:LEU:HD12	4:C:1217:HOH:O	2.18	0.43
1:B:125:ASP:HA	4:B:1398:HOH:O	2.18	0.43
1:H:31:ALA:HB1	1:H:42:ILE:HG13	2.01	0.43
1:G:223:VAL:HG13	1:H:223:VAL:HG12	2.00	0.43
1:E:110:ALA:O	1:E:113:VAL:HG23	2.19	0.42
1:C:60:ILE:O	1:C:61:LEU:C	2.57	0.42
1:E:110:ALA:HB1	1:E:139:ARG:NH2	2.34	0.42
1:D:6:LEU:HD13	1:D:238:MET:SD	2.59	0.42
1:F:155:HIS:CD2	1:F:157:GLY:N	2.71	0.42
1:H:126:VAL:O	1:H:126:VAL:HG12	2.19	0.42
1:D:72:GLU:HG2	1:D:92:CYS:HB3	2.01	0.42
1:H:45:HIS:HA	1:H:72:GLU:HB2	2.02	0.42
1:G:98:ARG:H	1:G:98:ARG:CD	2.30	0.42
1:H:72:GLU:HG2	1:H:92:CYS:HB3	2.01	0.42
1:D:52:HIS:CD2	1:D:53:ILE:N	2.77	0.42
1:G:152:ILE:HG23	1:G:187:LEU:HD13	2.01	0.42
1:G:152:ILE:CG2	1:G:187:LEU:HD13	2.50	0.42
1:C:206:LEU:HA	1:C:207:PRO:HD3	1.76	0.42
1:C:112:GLN:OE1	1:C:115:LYS:NZ	2.46	0.42
1:H:199:ASN:HD22	1:H:200:VAL:N	2.17	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:HIS:HA	1:C:72:GLU:O	2.20	0.42
1:E:219:ILE:O	1:E:222:ALA:HB3	2.19	0.42
1:C:20:ARG:HH22	2:D:504:PXP:P	2.43	0.41
1:G:199:ASN:ND2	1:G:199:ASN:C	2.72	0.41
1:G:46:LEU:HD11	1:G:50:ARG:CD	2.50	0.41
1:F:46:LEU:HD11	1:F:50:ARG:HD2	2.01	0.41
1:D:110:ALA:HB1	1:D:139[A]:ARG:HH21	1.86	0.41
1:A:95:PRO:HD3	1:A:107:LEU:HB2	2.01	0.41
1:F:60:ILE:HD11	1:G:63:GLN:NE2	2.34	0.41
1:E:86:ILE:HD13	1:E:86:ILE:N	2.36	0.41
1:E:61:LEU:HB3	1:E:65:ILE:HD12	2.02	0.41
1:C:202:PRO:HA	4:C:1609:HOH:O	2.18	0.41
1:H:196:THR:HG22	1:H:198:HIS:N	2.34	0.41
1:E:153:GLU:OE1	2:E:505:PXP:N1	2.54	0.41
1:B:47:ARG:O	1:B:50:ARG:HD3	2.21	0.41
1:G:87:LYS:HG2	1:G:126:VAL:HG12	2.03	0.41
1:B:221:GLN:CD	4:B:1615:HOH:O	2.58	0.41
1:B:91:CYS:HB2	1:B:128:ILE:CG2	2.51	0.41
1:E:56:ARG:C	1:E:56:ARG:HD3	2.41	0.41
1:F:120:VAL:HG22	1:F:130:VAL:HG11	2.02	0.41
1:D:156:THR:CG2	1:D:191:ALA:HB1	2.51	0.41
1:E:16:LEU:HD12	1:E:16:LEU:HA	1.89	0.40
1:C:59:ARG:NH1	1:C:59:ARG:HG2	2.36	0.40
1:D:78:GLU:O	1:D:82:ILE:HG12	2.21	0.40
1:D:156:THR:HG23	1:D:191:ALA:HB1	2.03	0.40
1:D:120:VAL:HG22	1:D:130:VAL:HG11	2.04	0.40
1:H:47:ARG:NH1	1:H:51:ARG:HH21	2.19	0.40
1:F:232:THR:HB	4:F:1666:HOH:O	2.21	0.40
1:A:195:LEU:HD21	1:A:203:ILE:HG13	2.03	0.40
1:B:12:HIS:HD2	1:B:15:THR:OG1	2.04	0.40
1:F:206:LEU:HA	1:F:207:PRO:HD3	1.88	0.40
1:D:18:ASN:ND2	1:D:52:HIS:HA	2.36	0.40
1:C:164:THR:HG23	1:C:167:GLU:HG3	2.04	0.40
1:H:103:THR:HG23	1:H:104:GLU:N	2.36	0.40
1:F:40:ASP:OD2	1:F:235:LYS:NZ	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	243/246 (99%)	231 (95%)	11 (4%)	1 (0%)	39	56
1	B	236/246 (96%)	223 (94%)	12 (5%)	1 (0%)	39	56
1	C	243/246 (99%)	232 (96%)	9 (4%)	2 (1%)	24	35
1	D	242/246 (98%)	230 (95%)	11 (4%)	1 (0%)	39	56
1	E	242/246 (98%)	234 (97%)	7 (3%)	1 (0%)	39	56
1	F	241/246 (98%)	226 (94%)	14 (6%)	1 (0%)	39	56
1	G	241/246 (98%)	226 (94%)	13 (5%)	2 (1%)	24	35
1	H	242/246 (98%)	230 (95%)	10 (4%)	2 (1%)	24	35
All	All	1930/1968 (98%)	1832 (95%)	87 (4%)	11 (1%)	30	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	193	HIS
1	G	165	VAL
1	A	193	HIS
1	C	193	HIS
1	D	193	HIS
1	E	193	HIS
1	F	193	HIS
1	G	193	HIS
1	H	193	HIS
1	C	103	THR
1	H	215	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/190 (100%)	174 (92%)	16 (8%)	14	20
1	B	185/190 (97%)	177 (96%)	8 (4%)	35	55
1	C	189/190 (100%)	172 (91%)	17 (9%)	12	17
1	D	189/190 (100%)	176 (93%)	13 (7%)	19	30
1	E	190/190 (100%)	175 (92%)	15 (8%)	15	23
1	F	188/190 (99%)	173 (92%)	15 (8%)	15	23
1	G	188/190 (99%)	173 (92%)	15 (8%)	15	23
1	H	190/190 (100%)	176 (93%)	14 (7%)	17	26
All	All	1509/1520 (99%)	1396 (92%)	113 (8%)	17	26

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	56	ARG
1	A	68	ARG
1	A	93	LEU
1	A	97	LYS
1	A	98	ARG
1	A	113	VAL
1	A	163	SER
1	A	164	THR
1	A	185	LYS
1	A	199	ASN
1	A	201	GLN
1	A	223	VAL
1	A	239[A]	ARG
1	A	239[B]	ARG
1	A	243	ARG
1	B	68[A]	ARG
1	B	68[B]	ARG
1	B	91	CYS
1	B	94	VAL
1	B	163	SER
1	B	173	MET
1	B	221	GLN
1	B	235	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	16	LEU
1	C	56	ARG
1	C	86	ILE
1	C	91	CYS
1	C	113	VAL
1	C	115	LYS
1	C	122	ARG
1	C	139	ARG
1	C	150	PRO
1	C	164	THR
1	C	166	LEU
1	C	167	GLU
1	C	174	ARG
1	C	185	LYS
1	C	199	ASN
1	C	200	VAL
1	C	201	GLN
1	D	48	GLU
1	D	51	ARG
1	D	56	ARG
1	D	59	ARG
1	D	68	ARG
1	D	86	ILE
1	D	100	GLU
1	D	145	VAL
1	D	169[A]	GLN
1	D	169[B]	GLN
1	D	189	VAL
1	D	223	VAL
1	D	235	LYS
1	E	3	ASP
1	E	86	ILE
1	E	99	GLN
1	E	115	LYS
1	E	125	ASP
1	E	165	VAL
1	E	173	MET
1	E	185	LYS
1	E	193	HIS
1	E	199	ASN
1	E	200	VAL
1	E	201	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	223	VAL
1	E	239[A]	ARG
1	E	239[B]	ARG
1	F	20	ARG
1	F	56	ARG
1	F	68	ARG
1	F	77	ASP
1	F	78	GLU
1	F	81	ASP
1	F	91	CYS
1	F	97	LYS
1	F	101	VAL
1	F	164	THR
1	F	169	GLN
1	F	177	LYS
1	F	189	VAL
1	F	199	ASN
1	F	243	ARG
1	G	44	VAL
1	G	51	ARG
1	G	52	HIS
1	G	56	ARG
1	G	86	ILE
1	G	91	CYS
1	G	98	ARG
1	G	99	GLN
1	G	155	HIS
1	G	163	SER
1	G	166	LEU
1	G	188	LYS
1	G	189	VAL
1	G	199	ASN
1	G	223	VAL
1	H	16	LEU
1	H	50	ARG
1	H	68	ARG
1	H	77	ASP
1	H	81	ASP
1	H	99	GLN
1	H	101	VAL
1	H	113	VAL
1	H	122	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	163	SER
1	H	166	LEU
1	H	173	MET
1	H	196	THR
1	H	199	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	66	GLN
1	A	199	ASN
1	A	201	GLN
1	A	210	HIS
1	A	216	HIS
1	B	12	HIS
1	B	63	GLN
1	B	89	HIS
1	B	155	HIS
1	B	210	HIS
1	C	63	GLN
1	C	155	HIS
1	C	199	ASN
1	C	201	GLN
1	D	12	HIS
1	D	52	HIS
1	D	89	HIS
1	D	112	GLN
1	D	201	GLN
1	E	45	HIS
1	E	63	GLN
1	E	66	GLN
1	E	155	HIS
1	E	198	HIS
1	E	199	ASN
1	E	221	GLN
1	F	12	HIS
1	F	89	HIS
1	F	155	HIS
1	F	199	ASN
1	G	63	GLN
1	G	66	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	99	GLN
1	G	169	GLN
1	G	198	HIS
1	G	199	ASN
1	G	201	GLN
1	H	155	HIS
1	H	199	ASN
1	H	221	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

11 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	PXP	A	501	-	16,16,16	3.00	5 (31%)	20,23,23	1.84	7 (35%)
2	PXP	B	502	-	16,16,16	3.00	5 (31%)	20,23,23	1.43	4 (20%)
2	PXP	C	503	-	16,16,16	3.37	5 (31%)	20,23,23	1.88	5 (25%)
3	SO4	C	601	-	4,4,4	0.20	0	6,6,6	0.33	0
2	PXP	D	504	-	16,16,16	3.95	5 (31%)	20,23,23	1.28	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PXP	E	505	-	16,16,16	4.40	5 (31%)	20,23,23	1.93	5 (25%)
3	SO4	E	602	-	4,4,4	0.19	0	6,6,6	0.23	0
3	SO4	E	603	-	4,4,4	0.24	0	6,6,6	0.41	0
2	PXP	F	506	-	16,16,16	3.15	5 (31%)	20,23,23	1.89	4 (20%)
2	PXP	G	507	-	16,16,16	4.75	4 (25%)	20,23,23	1.99	4 (20%)
2	PXP	H	508	-	16,16,16	3.38	4 (25%)	20,23,23	1.62	3 (15%)

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	PXP	A	501	-	-	0/8/8/8	0/1/1/1
2	PXP	B	502	-	-	0/8/8/8	0/1/1/1
2	PXP	C	503	-	-	0/8/8/8	0/1/1/1
3	SO4	C	601	-	-	0/0/0/0	0/0/0/0
2	PXP	D	504	-	-	0/8/8/8	0/1/1/1
2	PXP	E	505	-	-	0/8/8/8	0/1/1/1
3	SO4	E	602	-	-	0/0/0/0	0/0/0/0
3	SO4	E	603	-	-	0/0/0/0	0/0/0/0
2	PXP	F	506	-	-	0/8/8/8	0/1/1/1
2	PXP	G	507	-	-	0/8/8/8	0/1/1/1
2	PXP	H	508	-	-	0/8/8/8	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	505	PXP	O4A-C4A	-4.72	1.21	1.41
2	B	502	PXP	O4A-C4A	-4.65	1.21	1.41
2	C	503	PXP	O4A-C4A	-4.61	1.21	1.41
2	G	507	PXP	O4A-C4A	-4.50	1.22	1.41
2	H	508	PXP	O4A-C4A	-4.50	1.22	1.41
2	D	504	PXP	O4A-C4A	-4.47	1.22	1.41
2	A	501	PXP	O4A-C4A	-4.31	1.23	1.41
2	F	506	PXP	O4A-C4A	-4.15	1.23	1.41
2	B	502	PXP	C4A-C4	-3.47	1.46	1.51
2	A	501	PXP	C4A-C4	-3.19	1.46	1.51
2	C	503	PXP	C4A-C4	-2.71	1.47	1.51
2	E	505	PXP	C4A-C4	-2.65	1.47	1.51
2	F	506	PXP	C4A-C4	-2.38	1.48	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	504	PXP	C4A-C4	-2.28	1.48	1.51
2	B	502	PXP	C3-C4	2.75	1.44	1.40
2	C	503	PXP	C3-C4	3.29	1.45	1.40
2	A	501	PXP	C3-C4	4.06	1.46	1.40
2	H	508	PXP	C3-C4	4.64	1.47	1.40
2	F	506	PXP	C3-C4	5.09	1.47	1.40
2	E	505	PXP	C3-C4	5.13	1.48	1.40
2	C	503	PXP	C5-C4	5.59	1.48	1.40
2	A	501	PXP	C5-C4	5.73	1.48	1.40
2	G	507	PXP	C3-C4	5.80	1.49	1.40
2	E	505	PXP	C5-C4	6.08	1.49	1.40
2	D	504	PXP	C5-C4	6.14	1.49	1.40
2	D	504	PXP	C3-C4	6.39	1.50	1.40
2	F	506	PXP	C5-C4	6.41	1.49	1.40
2	H	508	PXP	C5-C4	6.52	1.49	1.40
2	B	502	PXP	C5-C4	6.79	1.50	1.40
2	B	502	PXP	C3-C2	6.89	1.45	1.40
2	G	507	PXP	C5-C4	6.95	1.50	1.40
2	F	506	PXP	C3-C2	7.87	1.46	1.40
2	A	501	PXP	C3-C2	7.89	1.46	1.40
2	H	508	PXP	C3-C2	9.54	1.47	1.40
2	C	503	PXP	C3-C2	10.26	1.47	1.40
2	D	504	PXP	C3-C2	11.87	1.49	1.40
2	E	505	PXP	C3-C2	14.50	1.50	1.40
2	G	507	PXP	C3-C2	15.87	1.51	1.40

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	506	PXP	O2P-P-O4P	-5.21	91.56	106.56
2	C	503	PXP	O2P-P-O4P	-3.59	96.24	106.56
2	G	507	PXP	C3-C4-C5	-3.54	115.09	118.82
2	E	505	PXP	C3-C4-C5	-3.35	115.29	118.82
2	A	501	PXP	C2A-C2-C3	-3.32	117.03	121.04
2	C	503	PXP	C3-C4-C5	-3.24	115.40	118.82
2	D	504	PXP	O4P-P-O1P	-2.97	99.58	107.14
2	B	502	PXP	C3-C4-C5	-2.70	115.98	118.82
2	B	502	PXP	O4P-P-O1P	-2.66	100.37	107.14
2	A	501	PXP	O2P-P-O4P	-2.47	99.44	106.56
2	E	505	PXP	O3P-P-O4P	-2.46	99.48	106.56
2	H	508	PXP	C3-C4-C5	-2.34	116.35	118.82
2	A	501	PXP	C5-C6-N1	-2.15	120.13	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	PXP	C4-C3-C2	-2.03	116.36	120.03
2	D	504	PXP	C6-N1-C2	2.01	123.39	119.28
2	F	506	PXP	O3-C3-C2	2.03	121.18	117.66
2	A	501	PXP	O3P-P-O2P	2.05	115.18	107.38
2	F	506	PXP	O2P-P-O1P	2.24	117.78	110.58
2	E	505	PXP	C2A-C2-C3	2.44	123.97	121.04
2	C	503	PXP	O3-C3-C2	2.59	122.17	117.66
2	B	502	PXP	O3-C3-C2	2.75	122.44	117.66
2	A	501	PXP	C6-N1-C2	2.82	125.03	119.28
2	F	506	PXP	C6-N1-C2	2.83	125.04	119.28
2	B	502	PXP	O2P-P-O1P	2.85	119.77	110.58
2	E	505	PXP	O3P-P-O2P	3.01	118.83	107.38
2	G	507	PXP	O3-C3-C2	3.05	122.97	117.66
2	C	503	PXP	O4A-C4A-C4	3.17	121.63	111.64
2	C	503	PXP	C6-C5-C4	3.21	120.49	118.09
2	A	501	PXP	O3-C3-C2	3.23	123.27	117.66
2	H	508	PXP	O4A-C4A-C4	3.37	122.26	111.64
2	G	507	PXP	O4A-C4A-C4	3.46	122.54	111.64
2	H	508	PXP	O3-C3-C2	3.62	123.95	117.66
2	G	507	PXP	C6-C5-C4	4.64	121.56	118.09
2	E	505	PXP	O3-C3-C2	5.07	126.47	117.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PXP	1	0
2	B	502	PXP	1	0
2	C	503	PXP	3	0
2	D	504	PXP	2	0
2	E	505	PXP	2	0
2	F	506	PXP	2	0
2	H	508	PXP	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	242/246 (98%)	-0.33	3 (1%)	81	81	8, 20, 40, 49	0
1	B	238/246 (96%)	-0.49	1 (0%)	93	93	9, 19, 32, 55	0
1	C	244/246 (99%)	-0.25	4 (1%)	74	74	8, 18, 35, 51	0
1	D	242/246 (98%)	-0.35	3 (1%)	81	81	9, 22, 39, 48	0
1	E	241/246 (97%)	-0.31	5 (2%)	67	66	11, 24, 39, 50	0
1	F	242/246 (98%)	-0.33	6 (2%)	61	60	12, 23, 36, 46	0
1	G	242/246 (98%)	-0.02	8 (3%)	50	50	17, 30, 47, 51	0
1	H	241/246 (97%)	-0.35	1 (0%)	93	93	10, 18, 32, 42	0
All	All	1932/1968 (98%)	-0.30	31 (1%)	74	74	8, 21, 40, 55	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2	ALA	4.9
1	C	1	MET	4.2
1	D	2	ALA	4.0
1	G	103	THR	3.8
1	A	166	LEU	3.8
1	F	98	ARG	3.6
1	C	0	ALA	3.3
1	C	243	ARG	3.0
1	E	243	ARG	3.0
1	G	2	ALA	3.0
1	G	144	ALA	3.0
1	G	99	GLN	2.9
1	B	98	ARG	2.9
1	F	110	ALA	2.6
1	G	109	VAL	2.6
1	D	98	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	165	VAL	2.6
1	E	101	VAL	2.4
1	F	165	VAL	2.4
1	D	173	MET	2.4
1	C	166	LEU	2.4
1	A	2	ALA	2.3
1	E	97	LYS	2.3
1	G	3	ASP	2.3
1	E	89[A]	HIS	2.3
1	G	89[A]	HIS	2.3
1	A	98	ARG	2.3
1	G	138	PHE	2.2
1	F	118	LEU	2.2
1	F	103	THR	2.2
1	H	89[A]	HIS	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, 95^{th} 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
3	SO4	E	603	5/5	0.84	0.17	1.01	73,73,75,76	0
3	SO4	E	602	5/5	0.88	0.17	0.57	83,83,83,84	0
3	SO4	C	601	5/5	0.89	0.16	-0.04	73,74,75,75	0
2	PXP	H	508	16/16	0.96	0.14	-0.53	14,19,28,28	0
2	PXP	A	501	16/16	0.98	0.11	-0.88	11,23,27,31	0
2	PXP	C	503	16/16	0.96	0.12	-0.93	19,23,30,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	PXP	B	502	16/16	0.97	0.09	-0.97	9,21,28,29	0
2	PXP	D	504	16/16	0.97	0.09	-1.00	19,39,44,47	0
2	PXP	E	505	16/16	0.97	0.10	-1.73	21,29,33,35	0
2	PXP	F	506	16/16	0.98	0.09	-1.85	13,23,32,36	0
2	PXP	G	507	16/16	0.97	0.10	-1.87	27,35,37,38	0

6.5 Other polymers

There are no such residues in this entry.