



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:09 PM UTC

PDB ID : 3F4N / pdb_00003f4n
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

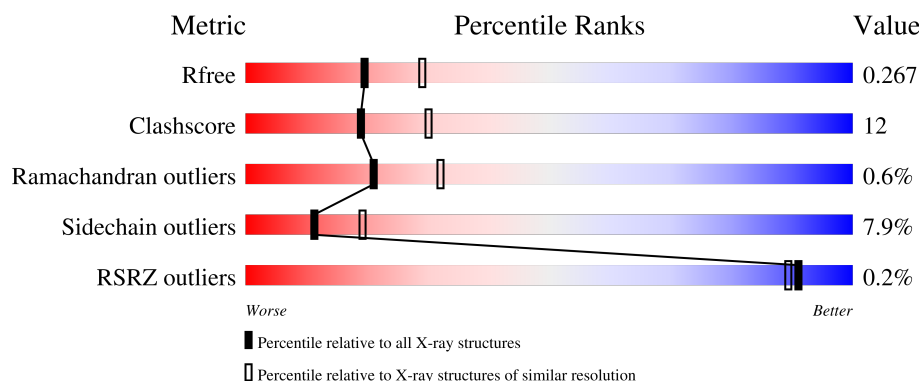
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	246	77% 18% ...
1	B	246	77% 17% ..
1	C	246	73% 23% ..
1	D	246	73% 22% ..
1	E	246	75% 19% ...

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

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	PXP	A	501	-	X	-	-

2 Entry composition

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:

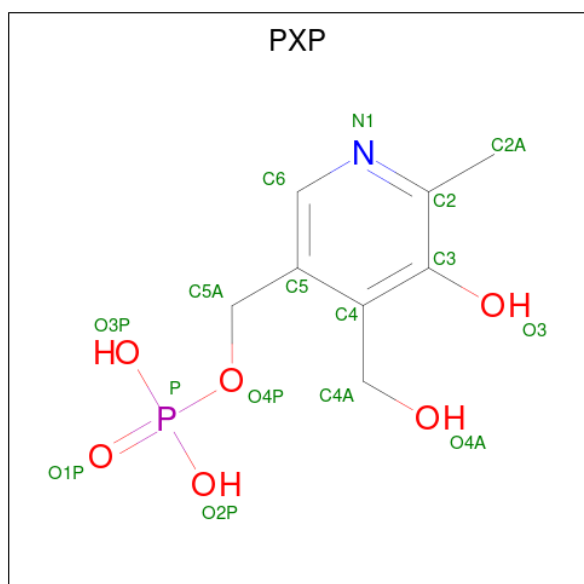
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8ZCP4
A	-1	ASN	-	expression tag	UNP Q8ZCP4
A	0	ALA	-	expression tag	UNP Q8ZCP4
B	-2	SER	-	expression tag	UNP Q8ZCP4
B	-1	ASN	-	expression tag	UNP Q8ZCP4
B	0	ALA	-	expression tag	UNP Q8ZCP4
C	-2	SER	-	expression tag	UNP Q8ZCP4
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

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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 (CCD ID: 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		

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is water.

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

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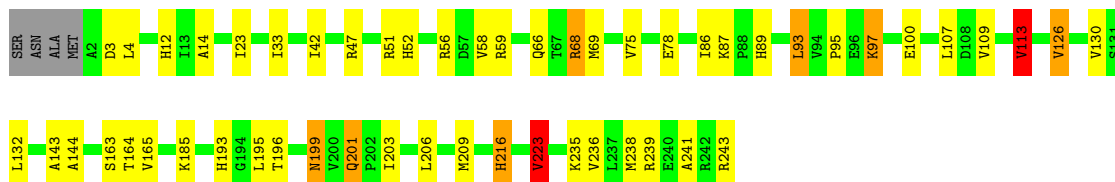
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	66	Total 66	O 66	0	0
4	F	78	Total 78	O 78	0	0
4	G	74	Total 74	O 74	0	0
4	H	93	Total 93	O 93	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

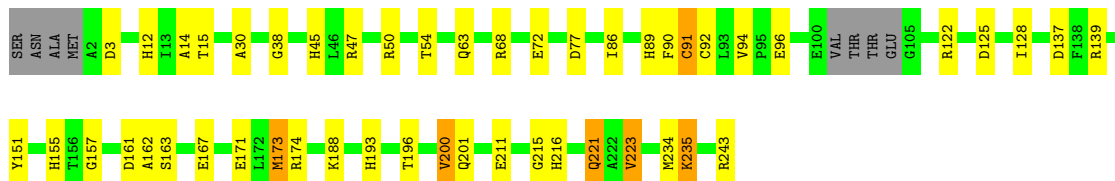
- Molecule 1: Pyridoxine 5'-phosphate synthase

Chain A: 



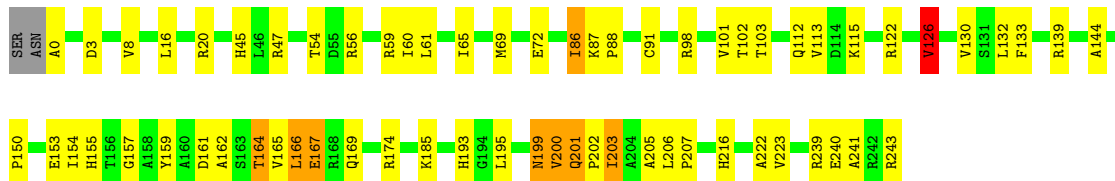
- Molecule 1: Pyridoxine 5'-phosphate synthase

Chain B: 



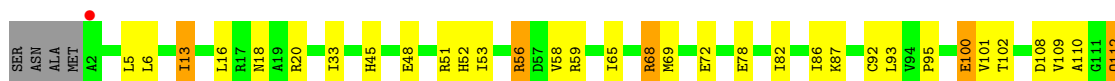
- Molecule 1: Pyridoxine 5'-phosphate synthase

Chain C: 



- Molecule 1: Pyridoxine 5'-phosphate synthase

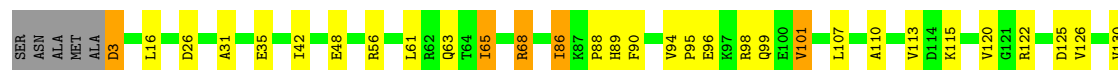
Chain D: 





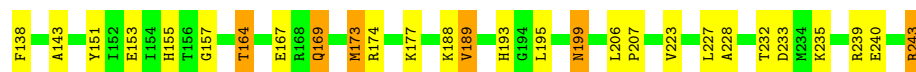
• Molecule 1: Pyridoxine 5'-phosphate synthase

Chain E: 75% 19% . . .



• Molecule 1: Pyridoxine 5'-phosphate synthase

Chain F: 74% 20% . .



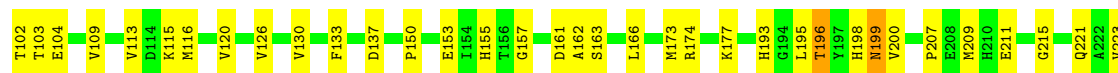
• Molecule 1: Pyridoxine 5'-phosphate synthase

Chain G: 66% 26% 6% .



• Molecule 1: Pyridoxine 5'-phosphate synthase

Chain H: 68% 28% . .



4 Data and refinement statistics

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) 94.5 (34.81-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.75%)	wwPDB-VP
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 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.16	3/1888 (0.2%)	1.24	10/2558 (0.4%)
1	B	1.12	1/1843 (0.1%)	1.17	5/2495 (0.2%)
1	C	1.16	3/1879 (0.2%)	1.23	8/2546 (0.3%)
1	D	1.11	0/1875	1.20	4/2541 (0.2%)
1	E	1.04	1/1883 (0.1%)	1.18	3/2551 (0.1%)
1	F	1.05	1/1864 (0.1%)	1.15	2/2527 (0.1%)
1	G	0.99	1/1866 (0.1%)	1.20	10/2530 (0.4%)
1	H	1.12	2/1878 (0.1%)	1.18	8/2546 (0.3%)
All	All	1.09	12/14976 (0.1%)	1.19	50/20294 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	8	VAL	CA-CB	6.88	1.62	1.54
1	A	23	ILE	CA-CB	6.53	1.62	1.54
1	F	189	VAL	CA-CB	5.87	1.61	1.54
1	C	154	ILE	CA-C	5.79	1.58	1.52
1	H	8	VAL	CA-CB	5.64	1.61	1.54
1	A	236	VAL	CA-CB	5.62	1.60	1.54
1	A	42	ILE	CA-CB	-5.62	1.47	1.54
1	G	141	ILE	CA-CB	5.58	1.60	1.54
1	E	94	VAL	CA-C	5.36	1.57	1.52
1	B	200	VAL	CA-CB	5.16	1.61	1.54
1	C	87	LYS	C-O	5.14	1.26	1.23
1	H	115	LYS	CA-C	5.09	1.59	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	VAL	CB-CA-C	-9.69	98.84	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	200	VAL	CB-CA-C	-9.28	99.81	112.24
1	G	75	VAL	N-CA-C	8.61	115.42	106.21
1	A	126	VAL	CB-CA-C	8.54	122.70	111.85
1	F	189	VAL	N-CA-C	8.51	120.18	107.75
1	A	223	VAL	CB-CA-C	-6.94	101.41	112.16
1	D	223	VAL	CB-CA-C	-6.73	102.23	112.05
1	G	149	ALA	CA-C-N	-6.72	112.78	120.04
1	G	149	ALA	C-N-CA	-6.72	112.78	120.04
1	G	37	ALA	N-CA-C	-6.67	104.28	112.88
1	G	223	VAL	CB-CA-C	-6.63	100.42	111.29
1	G	189	VAL	N-CA-C	6.56	117.57	108.12
1	E	223	VAL	CB-CA-C	-6.52	102.53	112.05
1	H	101	VAL	CB-CA-C	-6.42	102.39	111.38
1	A	33	ILE	N-CA-CB	6.38	117.59	110.51
1	H	7	GLY	N-CA-C	-6.25	101.15	110.71
1	A	33	ILE	CB-CA-C	-6.08	104.09	111.88
1	C	126	VAL	N-CA-C	-5.95	106.95	112.43
1	A	165	VAL	N-CA-C	5.89	116.63	110.62
1	F	227	LEU	N-CA-C	5.83	117.71	111.36
1	A	113	VAL	CB-CA-C	-5.79	104.47	111.88
1	A	68	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	C	222	ALA	N-CA-C	5.67	117.14	111.07
1	G	188	LYS	N-CA-C	-5.61	98.77	108.69
1	H	26	ASP	CA-C-N	5.55	125.22	119.05
1	H	26	ASP	C-N-CA	5.55	125.22	119.05
1	D	223	VAL	N-CA-CB	5.55	119.26	110.54
1	D	20	ARG	CA-C-N	-5.51	110.60	121.41
1	D	20	ARG	C-N-CA	-5.51	110.60	121.41
1	A	216	HIS	N-CA-C	5.47	117.94	111.33
1	A	130	VAL	N-CA-C	5.44	116.13	108.36
1	H	102	THR	CA-C-N	5.35	127.71	120.38
1	H	102	THR	C-N-CA	5.35	127.71	120.38
1	A	113	VAL	N-CA-C	5.33	115.95	110.36
1	E	122	ARG	N-CA-C	5.30	117.14	111.36
1	H	137	ASP	CB-CA-C	5.28	118.27	110.14
1	B	201	GLN	CA-C-N	-5.26	113.49	119.28
1	B	201	GLN	C-N-CA	-5.26	113.49	119.28
1	C	126	VAL	N-CA-CB	-5.17	105.44	112.16
1	G	223	VAL	N-CA-CB	5.13	119.70	111.23
1	B	223	VAL	CB-CA-C	-5.13	104.21	112.16
1	B	30	ALA	N-CA-C	-5.11	105.89	111.82
1	C	223	VAL	N-CA-CB	5.10	116.85	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	54	THR	CB-CA-C	-5.10	101.74	111.48
1	G	222	ALA	CA-C-O	-5.08	115.46	120.90
1	G	20	ARG	N-CA-C	-5.08	101.57	109.24
1	H	227	LEU	N-CA-C	5.05	117.52	111.71
1	B	234	MET	N-CA-C	-5.03	105.50	111.69
1	C	3	ASP	CA-C-N	-5.01	115.54	122.30
1	C	3	ASP	C-N-CA	-5.01	115.54	122.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1863	0	1888	42	0
1	B	1820	0	1843	35	0
1	C	1855	0	1887	46	0
1	D	1851	0	1877	35	0
1	E	1858	0	1883	54	0
1	F	1840	0	1863	45	0
1	G	1841	0	1864	66	0
1	H	1853	0	1867	52	0
2	A	16	0	8	0	0
2	B	16	0	8	0	0
2	C	16	0	8	2	0
2	D	16	0	9	1	0
2	E	16	0	8	1	0
2	F	16	0	8	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	353	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 12.

All (353) 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:D:174:ARG:HD3	4:D:1304:HOH:O	1.67	0.95
1:F:169:GLN:HG3	4:F:1257:HOH:O	1.65	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:G:73:MET:HE2	1:G:91:CYS:SG	2.16	0.86
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:E:199:ASN:C	1:E:199:ASN:HD22	1.87	0.83
1:F:243:ARG:NH2	1:H:240:GLU:OE2	2.12	0.82
1:F:199:ASN:C	1:F:199:ASN:HD22	1.86	0.81
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:C:199:ASN:C	1:C:199:ASN:HD22	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:173:MET:HE2	1:F:173:MET:HA	1.65	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: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:HG12	1:E:126:VAL:O	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:CG	1:E:68[B]:ARG:HH21	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:C:65:ILE:HD12	1:C:69:MET:HE3	1.74	0.69
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:H:199:ASN:C	1:H:199:ASN:HD22	2.02	0.68
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
1:G:199:ASN:C	1:G:199:ASN:HD22	2.03	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLN:HG3	1:A:241:ALA:HB2	1.78	0.66
1:B:68[B]:ARG:HD2	1:B:90:PHE:CE1	2.31	0.66
1:G:240:GLU:OE2	1:G:240:GLU:HA	1.94	0.66
1:A:199:ASN:C	1:A:199:ASN:HD22	2.04	0.65
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:CD2	1:E:89[B]:HIS:N	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:NH2	1:E:68[B]:ARG:HG3	2.11	0.64
1:H:58:VAL:HG11	1:H:86:ILE:HD13	1.78	0.64
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:CD2	1:A:89[B]:HIS:H	2.15	0.63
1:E:199:ASN:C	1:E:199:ASN:ND2	2.56	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:E:126:VAL:O	1:E:126:VAL:CG1	2.47	0.62
1:E:68[B]:ARG:HH21	1:E:68[B]:ARG:HG3	1.64	0.62
1:F:195:LEU:HA	1:F:199:ASN:HD21	1.65	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:F:228:ALA:O	1:F:232:THR:HG22	2.00	0.62
1:H:58:VAL:CG1	1:H:86:ILE:HD13	2.28	0.62
1:D:101:VAL:HG12	1:D:102:THR:O	2.00	0.61
1:E:89[A]:HIS:HD2	1:E:90:PHE:CE1	2.17	0.61
1:H:196:THR:CG2	1:H:198:HIS:H	2.13	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
1:F:77:ASP:O	1:F:81:ASP:OD2	2.20	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: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:59:ARG:NH2	4:A:1650:HOH:O	2.36	0.58
1:A:196:THR:H	1:A:199:ASN:ND2	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:VAL:HG13	1:D:69:MET:HE1	1.84	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:F:104[B]:GLU:CD	1:F:174:ARG:HH22	2.11	0.58
1:G:72:GLU:HG2	1:G:92:CYS:HB3	1.85	0.58
1:G:108:ASP:HA	1:G:140:GLN:HE22	1.67	0.58
1:G:126:VAL:HG12	1:G:126:VAL:O	2.03	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:F:55:ASP:O	1:F:59:ARG:HG3	2.04	0.57
1:H:196:THR:HG22	1:H:198:HIS:H	1.68	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:CD2	1:H:89[B]:HIS:N	2.68	0.56
1:A:195:LEU:HA	1:A:199:ASN:HD21	1.68	0.56
1:A:238:MET:HB2	1:A:239[B]:ARG:NH1	2.20	0.56
1:G:199:ASN:HD22	1:G:200:VAL:N	2.03	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: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:F:199:ASN:C	1:F:199:ASN:ND2	2.60	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
1:C:45:HIS:CE1	1:C:47[A]:ARG:HG2	2.42	0.55
1:H:82:ILE:CG2	1:H:86:ILE:HD12	2.37	0.55
1:C:126:VAL:O	1:C:126:VAL:CG1	2.55	0.54
1:A:66:GLN:NE2	4:A:1661:HOH:O	2.40	0.54
1:D:13:ILE:HD12	1:D:219:ILE:HD12	1.90	0.54
1:A:196:THR:H	1:A:199:ASN:HD21	1.54	0.54
1:F:173:MET:HE3	4:F:1327:HOH:O	2.06	0.54
1:C:155:HIS:HD2	1:C:157:GLY:H	1.52	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:31:ALA:O	1:G:35:GLU:HG3	2.07	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:C:199:ASN:C	1:C:199:ASN:ND2	2.63	0.53
1:F:138:PHE:N	1:F:138:PHE:CD1	2.76	0.53
1:C:86:ILE:HG22	1:C:88:PRO:HD3	1.90	0.53
1:F:138:PHE:N	1:F:138:PHE:HD1	2.06	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:F:72:GLU:HG2	1:F:92:CYS:HB3	1.91	0.53
1:G:167:GLU:CB	4:G:1641:HOH:O	2.52	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: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:B:91:CYS:HB2	1:B:128:ILE:HG21	1.93	0.51
1:C:126:VAL:O	1:C:126:VAL:HG13	2.10	0.51
1:G:240:GLU:OE2	1:G:243:ARG:NE	2.43	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:B:68[A]:ARG:HH21	1:B:89:HIS:CE1	2.29	0.50
1:E:89[A]:HIS:CD2	1:E:90:PHE:CE1	2.98	0.50
1:D:45:HIS:HA	1:D:72:GLU:HB2	1.94	0.50
1:F:59:ARG:HG2	1:F:86:ILE:HD11	1.93	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:A:235:LYS:HD2	1:A:239[B]:ARG:NH1	2.28	0.49
1:B:161:ASP:O	1:B:162:ALA:C	2.55	0.49
1:E:243:ARG:HH12	1:G:239:ARG:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:201:GLN:HE22	1:E:239[A]:ARG:HH12	1.60	0.49
1:H:209:MET:O	4:H:1635:HOH:O	2.20	0.49
1:E:153:GLU:OE1	1:E:192:GLY:HA3	2.12	0.49
1:F:173:MET:HA	1:F:173:MET:CE	2.37	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:C:59:ARG:HG2	1:C:59:ARG:HH11	1.78	0.49
1:C:164:THR:OG1	1:C:167:GLU:HB2	2.13	0.49
1:G:89[B]:HIS:CD2	1:G:89[B]:HIS:H	2.30	0.49
1:C:239:ARG:HB3	1:C:243:ARG:HH22	1.78	0.48
1:G:109:VAL:HG13	1:G:116:MET:HG3	1.95	0.48
1:G:135:ASP:OD2	4:G:1127:HOH:O	2.19	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:A:69:MET:H	1:A:89[B]:HIS:HD2	1.60	0.47
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:E:199:ASN:HD22	1:E:200:VAL:N	2.10	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
1:D:239:ARG:HB3	1:D:243:ARG:NH2	2.29	0.47
1:E:223:VAL:HG13	1:F:223:VAL:CG1	2.33	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:C:60:ILE:O	1:C:61:LEU:C	2.57	0.47
1:G:199:ASN:ND2	1:G:199:ASN:C	2.72	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:D:33:ILE:HG21	1:D:227:LEU:HB3	1.97	0.47
1:F:43:THR:HG22	1:F:44:VAL:N	2.30	0.47
1:E:31:ALA:HA	1:E:42:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:197:TYR:CE2	1:G:234:MET:HE2	2.50	0.47
1:A:4:LEU:HB3	1:A:239[B]:ARG:HH22	1.80	0.46
1:H:89[B]:HIS:H	1:H:89[B]:HIS:HD2	1.57	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:101:VAL:HG22	1:C:102:THR:O	2.15	0.46
1:C:153:GLU:OE1	2:C:503:PXP:N1	2.48	0.46
1:E:95:PRO:HG3	1:E:107:LEU:HA	1.98	0.46
1:H:133:PHE:CD2	2:H:508:PXP:H2A1	2.51	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:221:GLN:CD	4:B:1615:HOH:O	2.58	0.45
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:E:56:ARG:HD3	1:E:56:ARG:C	2.41	0.45
1:C:216:HIS:HE1	1:D:16:LEU:O	2.00	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:G:87:LYS:HG2	1:G:126:VAL:CG1	2.47	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:A:78:GLU:HG3	4:A:1459:HOH:O	2.16	0.45
1:A:59:ARG:HG2	4:A:1454:HOH:O	2.17	0.45
1:D:141:ILE:O	1:D:145:VAL:HG22	2.16	0.45
1:B:14:ALA:O	1:B:15:THR:C	2.60	0.44
1:G:239:ARG:HH21	1:G:239:ARG:CG	2.30	0.44
1:A:56:ARG:HD3	1:A:56:ARG:C	2.43	0.44
1:B:167:GLU:O	1:B:171:GLU:HG2	2.17	0.44
1:C:0:ALA:HB2	1:C:207:PRO:HB3	1.99	0.44
1:F:164:THR:HB	1:F:167:GLU:H	1.82	0.44
1:G:134:ILE:HD12	1:G:135:ASP:O	2.17	0.44
1:H:48[A]:GLU:HG2	1:H:96:GLU:OE1	2.17	0.44
1:H:104:GLU:CD	1:H:174:ARG:HH22	2.26	0.44
1:A:4:LEU:HB3	1:A:239[B]:ARG:NH2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89[B]:HIS:CD2	1:A:89[B]:HIS:N	2.85	0.44
1:A:206:LEU:HB2	1:A:209:MET:HG2	1.98	0.44
1:B:196:THR:O	1:B:200:VAL:HB	2.18	0.44
1:C:240:GLU:HA	1:C:243:ARG:CG	2.48	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:G:154:ILE:HD11	1:G:179:ALA:HB2	1.98	0.43
1:H:196:THR:O	1:H:200:VAL:HB	2.18	0.43
1:E:89[B]:HIS:H	1:E:89[B]:HIS:HD2	1.55	0.43
1:F:20:ARG:HA	1:F:20:ARG:HD3	1.76	0.43
1:F:99:GLN:HB2	4:F:1292:HOH:O	2.18	0.43
1:C:133:PHE:CD2	2:C:503:PXP:H2A1	2.53	0.43
1:E:16:LEU:CD2	1:F:223:VAL:HG11	2.49	0.43
1:E:240:GLU:HG2	1:E:243:ARG:HH11	1.82	0.43
1:B:125:ASP:HA	4:B:1398:HOH:O	2.18	0.43
1:C:166:LEU:HD12	4:C:1217:HOH:O	2.18	0.43
1:G:223:VAL:HG13	1:H:223:VAL:HG12	2.00	0.43
1:H:31:ALA:HB1	1:H:42:ILE:HG13	2.01	0.43
1:E:110:ALA:O	1:E:113:VAL:HG23	2.19	0.42
1:D:6:LEU:HD13	1:D:238:MET:SD	2.59	0.42
1:E:110:ALA:HB1	1:E:139:ARG:NH2	2.34	0.42
1:H:15:THR:O	1:H:16:LEU:C	2.62	0.42
1:F:155:HIS:CD2	1:F:157:GLY:N	2.71	0.42
1:H:126:VAL:HG12	1:H:126:VAL:O	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:H:56:ARG:HD3	1:H:56:ARG:C	2.45	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:H:161:ASP:O	1:H:162:ALA:C	2.63	0.42
1:D:52:HIS:CD2	1:D:53:ILE:N	2.77	0.42
1:G:152:ILE:CG2	1:G:187:LEU:HD13	2.50	0.42
1:G:152:ILE:HG23	1:G:187:LEU:HD13	2.01	0.42
1:H:61:LEU:HB3	1:H:69:MET:HE3	2.01	0.42
1:C:112:GLN:OE1	1:C:115:LYS:NZ	2.46	0.42
1:C:206:LEU:HA	1:C:207:PRO:HD3	1.76	0.42
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:H:199:ASN:HD22	1:H:200:VAL:N	2.17	0.42
1:B:215:GLY:O	1:B:216:HIS:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ARG:HH22	2:D:504:PXP:P	2.43	0.41
1:F:155:HIS:CD2	1:F:155:HIS:C	2.98	0.41
1:G:164:THR:O	1:G:165:VAL:C	2.63	0.41
1:A:95:PRO:HD3	1:A:107:LEU:HB2	2.01	0.41
1:D:110:ALA:HB1	1:D:139[A]:ARG:HH21	1.86	0.41
1:F:46:LEU:HD11	1:F:50:ARG:HD2	2.01	0.41
1:G:46:LEU:HD11	1:G:50:ARG:CD	2.50	0.41
1:F:60:ILE:HD11	1:G:63:GLN:NE2	2.34	0.41
1:G:169:GLN:HE21	1:G:173:MET:HE1	1.85	0.41
1:E:61:LEU:HB3	1:E:65:ILE:HD12	2.02	0.41
1:E:86:ILE:HD13	1:E:86:ILE:N	2.36	0.41
1:B:47:ARG:O	1:B:50:ARG:HD3	2.21	0.41
1:C:202:PRO:HA	4:C:1609:HOH:O	2.18	0.41
1:E:26:ASP:OD1	1:E:26:ASP:C	2.64	0.41
1:E:153:GLU:OE1	2:E:505:PXP:N1	2.54	0.41
1:H:196:THR:HG22	1:H:198:HIS:N	2.34	0.41
1:G:87:LYS:HG2	1:G:126:VAL:HG12	2.03	0.41
1:B:91:CYS:HB2	1:B:128:ILE:CG2	2.51	0.41
1:C:161:ASP:O	1:C:162:ALA:C	2.63	0.41
1:D:156:THR:CG2	1:D:191:ALA:HB1	2.51	0.41
1:F:120:VAL:HG22	1:F:130:VAL:HG11	2.02	0.41
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:E:16:LEU:HD12	1:E:16:LEU:HA	1.89	0.40
1:D:120:VAL:HG22	1:D:130:VAL:HG11	2.04	0.40
1:D:156:THR:HG23	1:D:191:ALA:HB1	2.03	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:C:164:THR:HG23	1:C:167:GLU:HG3	2.04	0.40
1:D:18:ASN:ND2	1:D:52:HIS:HA	2.36	0.40
1:F:40:ASP:OD2	1:F:235:LYS:NZ	2.54	0.40
1:H:9:ASN:OD1	1:H:9:ASN:C	2.64	0.40
1:H:103:THR:HG23	1:H:104:GLU:N	2.36	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%)	30	43
1	B	236/246 (96%)	223 (94%)	12 (5%)	1 (0%)	30	43
1	C	243/246 (99%)	232 (96%)	9 (4%)	2 (1%)	16	25
1	D	242/246 (98%)	230 (95%)	11 (4%)	1 (0%)	30	43
1	E	242/246 (98%)	234 (97%)	7 (3%)	1 (0%)	30	43
1	F	241/246 (98%)	226 (94%)	14 (6%)	1 (0%)	30	43
1	G	241/246 (98%)	226 (94%)	13 (5%)	2 (1%)	16	25
1	H	242/246 (98%)	230 (95%)	10 (4%)	2 (1%)	16	25
All	All	1930/1968 (98%)	1832 (95%)	87 (4%)	11 (1%)	21	32

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%)	176 (93%)	14 (7%)	13	22
1	B	185/190 (97%)	178 (96%)	7 (4%)	29	49
1	C	189/190 (100%)	172 (91%)	17 (9%)	9	15
1	D	189/190 (100%)	171 (90%)	18 (10%)	8	13
1	E	190/190 (100%)	172 (90%)	18 (10%)	8	13
1	F	188/190 (99%)	172 (92%)	16 (8%)	10	16
1	G	188/190 (99%)	169 (90%)	19 (10%)	7	11
1	H	190/190 (100%)	177 (93%)	13 (7%)	14	25
All	All	1509/1520 (99%)	1387 (92%)	122 (8%)	11	18

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	68	ARG
1	A	87	LYS
1	A	93	LEU
1	A	97	LYS
1	A	113	VAL
1	A	126	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	243	ARG
1	B	86	ILE
1	B	91	CYS
1	B	94	VAL
1	B	163	SER
1	B	173	MET
1	B	221	GLN
1	B	235	LYS
1	C	16	LEU
1	C	56	ARG
1	C	86	ILE

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Mol	Chain	Res	Type
1	C	91	CYS
1	C	113	VAL
1	C	122	ARG
1	C	126	VAL
1	C	139	ARG
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	C	203	ILE
1	D	13	ILE
1	D	48	GLU
1	D	51	ARG
1	D	56	ARG
1	D	59	ARG
1	D	65	ILE
1	D	68	ARG
1	D	86	ILE
1	D	100	GLU
1	D	112	GLN
1	D	141	ILE
1	D	145	VAL
1	D	165	VAL
1	D	169[A]	GLN
1	D	169[B]	GLN
1	D	180	THR
1	D	189	VAL
1	D	223	VAL
1	E	3	ASP
1	E	65	ILE
1	E	68[A]	ARG
1	E	68[B]	ARG
1	E	86	ILE
1	E	99	GLN
1	E	101	VAL
1	E	115	LYS
1	E	125	ASP
1	E	165	VAL

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Mol	Chain	Res	Type
1	E	173	MET
1	E	185	LYS
1	E	199	ASN
1	E	200	VAL
1	E	201	GLN
1	E	223	VAL
1	E	239[A]	ARG
1	E	239[B]	ARG
1	F	20	ARG
1	F	68	ARG
1	F	78	GLU
1	F	91	CYS
1	F	97	LYS
1	F	101	VAL
1	F	104[A]	GLU
1	F	104[B]	GLU
1	F	126	VAL
1	F	164	THR
1	F	169	GLN
1	F	173	MET
1	F	177	LYS
1	F	189	VAL
1	F	199	ASN
1	F	243	ARG
1	G	16	LEU
1	G	44	VAL
1	G	51	ARG
1	G	56	ARG
1	G	65	ILE
1	G	86	ILE
1	G	91	CYS
1	G	98	ARG
1	G	99	GLN
1	G	113	VAL
1	G	117	THR
1	G	141	ILE
1	G	163	SER
1	G	166	LEU
1	G	167	GLU
1	G	168	ARG
1	G	189	VAL
1	G	199	ASN

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	66	GLN
1	A	70	ASN
1	A	199	ASN
1	A	210	HIS
1	A	216	HIS
1	B	12	HIS
1	B	63	GLN
1	B	70	ASN
1	B	89	HIS
1	B	155	HIS
1	B	210	HIS
1	B	221	GLN
1	C	63	GLN
1	C	70	ASN
1	C	155	HIS
1	C	199	ASN
1	C	201	GLN
1	D	12	HIS
1	D	52	HIS
1	D	70	ASN
1	D	89	HIS
1	D	112	GLN
1	D	201	GLN

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Mol	Chain	Res	Type
1	E	63	GLN
1	E	66	GLN
1	E	155	HIS
1	E	198	HIS
1	E	199	ASN
1	E	216	HIS
1	E	221	GLN
1	F	12	HIS
1	F	89	HIS
1	F	155	HIS
1	F	199	ASN
1	F	213	ASN
1	G	63	GLN
1	G	70	ASN
1	G	99	GLN
1	G	112	GLN
1	G	169	GLN
1	G	198	HIS
1	G	199	ASN
1	H	70	ASN
1	H	155	HIS
1	H	198	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 oligosaccharides 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
3	SO4	E	603	-	4,4,4	0.25	0	6,6,6	0.49	0
2	PXP	B	502	-	16,16,16	2.85	5 (31%)	22,23,23	1.69	6 (27%)
2	PXP	H	508	-	16,16,16	2.91	4 (25%)	22,23,23	1.77	4 (18%)
2	PXP	G	507	-	16,16,16	3.75	4 (25%)	22,23,23	2.02	4 (18%)
2	PXP	D	504	-	16,16,16	3.35	5 (31%)	22,23,23	1.26	3 (13%)
2	PXP	E	505	-	16,16,16	3.54	5 (31%)	22,23,23	2.02	7 (31%)
3	SO4	E	602	-	4,4,4	0.20	0	6,6,6	0.19	0
2	PXP	A	501	-	16,16,16	2.73	5 (31%)	22,23,23	1.95	11 (50%)
2	PXP	F	506	-	16,16,16	2.88	5 (31%)	22,23,23	2.04	5 (22%)
2	PXP	C	503	-	16,16,16	2.86	5 (31%)	22,23,23	2.06	6 (27%)
3	SO4	C	601	-	4,4,4	0.36	0	6,6,6	0.42	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	PXP	B	502	-	-	0/8/8/8	0/1/1/1
2	PXP	H	508	-	-	1/8/8/8	0/1/1/1
2	PXP	G	507	-	-	0/8/8/8	0/1/1/1
2	PXP	D	504	-	-	6/8/8/8	0/1/1/1
2	PXP	E	505	-	-	0/8/8/8	0/1/1/1
2	PXP	A	501	-	-	4/8/8/8	0/1/1/1
2	PXP	F	506	-	-	0/8/8/8	0/1/1/1
2	PXP	C	503	-	-	2/8/8/8	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	507	PXP	C3-C2	10.38	1.51	1.41
2	E	505	PXP	C3-C2	9.47	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	504	PXP	C3-C2	7.72	1.49	1.41
2	G	507	PXP	C5-C4	7.04	1.50	1.40
2	B	502	PXP	C5-C4	6.88	1.50	1.40
2	D	504	PXP	C3-C4	6.76	1.50	1.40
2	C	503	PXP	C3-C2	6.64	1.47	1.41
2	H	508	PXP	C5-C4	6.60	1.49	1.40
2	F	506	PXP	C5-C4	6.49	1.49	1.40
2	D	504	PXP	C5-C4	6.22	1.49	1.40
2	H	508	PXP	C3-C2	6.17	1.47	1.41
2	E	505	PXP	C5-C4	6.15	1.49	1.40
2	G	507	PXP	C3-C4	6.13	1.49	1.40
2	A	501	PXP	C5-C4	5.80	1.48	1.40
2	C	503	PXP	C5-C4	5.66	1.48	1.40
2	E	505	PXP	C3-C4	5.43	1.48	1.40
2	F	506	PXP	C3-C4	5.39	1.47	1.40
2	A	501	PXP	C3-C2	5.07	1.46	1.41
2	F	506	PXP	C3-C2	5.06	1.46	1.41
2	H	508	PXP	C3-C4	4.91	1.47	1.40
2	B	502	PXP	C4A-C4	-4.77	1.46	1.51
2	E	505	PXP	O4A-C4A	-4.75	1.21	1.41
2	B	502	PXP	O4A-C4A	-4.68	1.21	1.41
2	C	503	PXP	O4A-C4A	-4.64	1.21	1.41
2	G	507	PXP	O4A-C4A	-4.53	1.22	1.41
2	H	508	PXP	O4A-C4A	-4.53	1.22	1.41
2	D	504	PXP	O4A-C4A	-4.50	1.22	1.41
2	B	502	PXP	C3-C2	4.40	1.45	1.41
2	A	501	PXP	C4A-C4	-4.38	1.46	1.51
2	A	501	PXP	O4A-C4A	-4.34	1.23	1.41
2	A	501	PXP	C3-C4	4.30	1.46	1.40
2	F	506	PXP	O4A-C4A	-4.17	1.23	1.41
2	C	503	PXP	C4A-C4	-3.72	1.47	1.51
2	E	505	PXP	C4A-C4	-3.63	1.47	1.51
2	C	503	PXP	C3-C4	3.49	1.45	1.40
2	F	506	PXP	C4A-C4	-3.27	1.48	1.51
2	D	504	PXP	C4A-C4	-3.13	1.48	1.51
2	B	502	PXP	C3-C4	2.92	1.44	1.40

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	506	PXP	O2P-P-O4P	-5.79	91.56	106.67
2	G	507	PXP	C6-C5-C4	4.62	121.56	118.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	PXP	C4A-C4-C5	4.40	126.62	119.91
2	E	505	PXP	O3-C3-C2	4.29	126.47	117.58
2	G	507	PXP	O4A-C4A-C4	4.26	122.54	111.60
2	H	508	PXP	O4A-C4A-C4	4.15	122.26	111.60
2	G	507	PXP	C3-C4-C5	-4.02	115.09	118.73
2	C	503	PXP	O2P-P-O4P	-4.00	96.24	106.67
2	C	503	PXP	O4A-C4A-C4	3.90	121.63	111.60
2	E	505	PXP	C3-C4-C5	-3.79	115.29	118.73
2	C	503	PXP	C3-C4-C5	-3.67	115.40	118.73
2	E	505	PXP	C4A-C4-C5	3.66	125.50	119.91
2	C	503	PXP	C4A-C4-C5	3.42	125.13	119.91
2	F	506	PXP	C6-N1-C2	3.22	125.04	119.20
2	A	501	PXP	C6-N1-C2	3.22	125.03	119.20
2	A	501	PXP	C2A-C2-C3	-3.22	117.03	120.80
2	C	503	PXP	C6-C5-C4	3.21	120.49	118.06
2	H	508	PXP	C4A-C4-C5	3.15	124.72	119.91
2	H	508	PXP	O3-C3-C2	3.08	123.95	117.58
2	B	502	PXP	C3-C4-C5	-3.04	115.98	118.73
2	E	505	PXP	O3P-P-O2P	2.94	118.83	107.80
2	F	506	PXP	C4A-C4-C5	2.92	124.36	119.91
2	A	501	PXP	O2P-P-O4P	-2.77	99.44	106.67
2	E	505	PXP	O3P-P-O4P	-2.76	99.48	106.67
2	A	501	PXP	O3-C3-C2	2.74	123.27	117.58
2	E	505	PXP	C2A-C2-C3	2.72	123.97	120.80
2	A	501	PXP	C4A-C4-C5	2.63	123.93	119.91
2	H	508	PXP	C3-C4-C5	-2.63	116.35	118.73
2	G	507	PXP	O3-C3-C2	2.60	122.97	117.58
2	D	504	PXP	O4P-P-O1P	-2.54	99.58	106.44
2	A	501	PXP	C2A-C2-N1	2.41	122.18	117.64
2	A	501	PXP	C4-C3-C2	-2.35	116.36	119.91
2	B	502	PXP	O3-C3-C2	2.34	122.44	117.58
2	D	504	PXP	C6-N1-C2	2.31	123.39	119.20
2	B	502	PXP	C4A-C4-C3	-2.31	117.38	121.54
2	B	502	PXP	O2P-P-O1P	2.29	119.77	110.83
2	A	501	PXP	C5-C6-N1	-2.28	120.13	123.83
2	A	501	PXP	C4A-C4-C3	-2.25	117.47	121.54
2	B	502	PXP	O4P-P-O1P	-2.25	100.37	106.44
2	C	503	PXP	O3-C3-C2	2.21	122.17	117.58
2	E	505	PXP	C6-N1-C2	2.20	123.19	119.20
2	D	504	PXP	C3-C4-C5	-2.19	116.74	118.73
2	A	501	PXP	C5A-C5-C4	-2.16	118.12	122.67
2	F	506	PXP	C2A-C2-N1	2.13	121.65	117.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PXP	C5A-C5-C6	2.06	122.71	119.36
2	F	506	PXP	C4A-C4-C3	-2.05	117.84	121.54

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PXP	C5A-O4P-P-O1P
2	D	504	PXP	C4-C5-C5A-O4P
2	D	504	PXP	C5A-O4P-P-O2P
2	D	504	PXP	C5A-O4P-P-O3P
2	C	503	PXP	C3-C4-C4A-O4A
2	D	504	PXP	C5A-O4P-P-O1P
2	A	501	PXP	C6-C5-C5A-O4P
2	D	504	PXP	C6-C5-C5A-O4P
2	A	501	PXP	C5A-O4P-P-O2P
2	A	501	PXP	C4-C5-C5A-O4P
2	C	503	PXP	C5-C4-C4A-O4A
2	H	508	PXP	C5A-O4P-P-O2P
2	D	504	PXP	C5-C4-C4A-O4A

There are no ring outliers.

5 monomers are involved in 7 short contacts:

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

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	242/246 (98%)	-0.55	0	100 100	8, 20, 40, 49	3 (1%)
1	B	238/246 (96%)	-0.46	0	100 100	8, 19, 32, 55	2 (0%)
1	C	244/246 (99%)	-0.44	0	100 100	8, 18, 35, 51	1 (0%)
1	D	242/246 (98%)	-0.43	1 (0%)	88 86	9, 22, 39, 48	2 (0%)
1	E	241/246 (97%)	-0.38	0	100 100	10, 24, 39, 50	3 (1%)
1	F	242/246 (98%)	-0.37	1 (0%)	88 86	12, 23, 36, 46	1 (0%)
1	G	242/246 (98%)	-0.04	1 (0%)	88 86	15, 30, 47, 51	1 (0%)
1	H	241/246 (97%)	-0.57	0	100 100	9, 18, 32, 42	3 (1%)
All	All	1932/1968 (98%)	-0.40	3 (0%)	91 89	8, 21, 40, 55	16 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	89[A]	HIS	2.9
1	F	2	ALA	2.6
1	D	2	ALA	2.3

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å ²)	Q<0.9
3	SO4	E	603	5/5	0.73	0.15	73,73,75,76	0
3	SO4	E	602	5/5	0.75	0.15	83,83,83,84	0
3	SO4	C	601	5/5	0.75	0.14	73,74,75,75	0
2	PXP	H	508	16/16	0.96	0.08	14,19,28,28	0
2	PXP	B	502	16/16	0.96	0.07	9,21,28,29	0
2	PXP	C	503	16/16	0.96	0.07	19,23,30,32	0
2	PXP	E	505	16/16	0.96	0.07	21,29,33,35	0
2	PXP	F	506	16/16	0.97	0.07	13,23,32,36	0
2	PXP	G	507	16/16	0.97	0.06	27,35,37,38	0
2	PXP	D	504	16/16	0.97	0.08	19,39,44,47	0
2	PXP	A	501	16/16	0.98	0.06	11,23,27,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.