



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:51 PM UTC

PDB ID : 1V0E / pdb_00001v0e
Title : Endosialidase of Bacteriophage K1F
Authors : Stummeyer, K.; Dickmanns, A.; Muehlenhoff, M.; Gerady-Schahn, R.; Ficner, R.
Deposited on : 2004-03-28
Resolution : 1.90 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

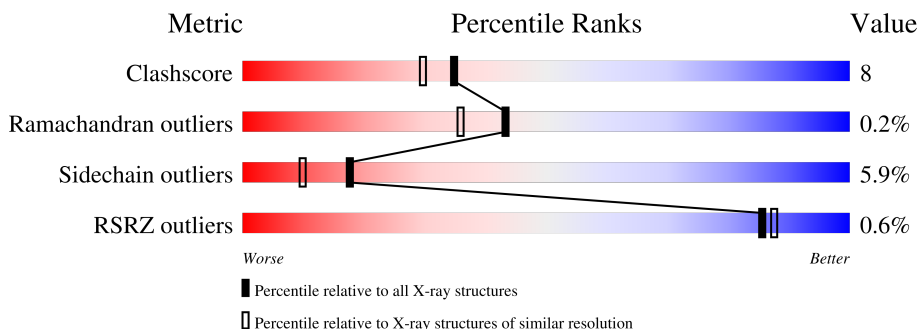
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	666	2% 84% 14% .
1	B	666	84% 13% ..
1	C	666	86% 12% .
1	D	666	82% 15% .
1	E	666	84% 13% .
1	F	666	83% 14% ..

2 Entry composition [i](#)

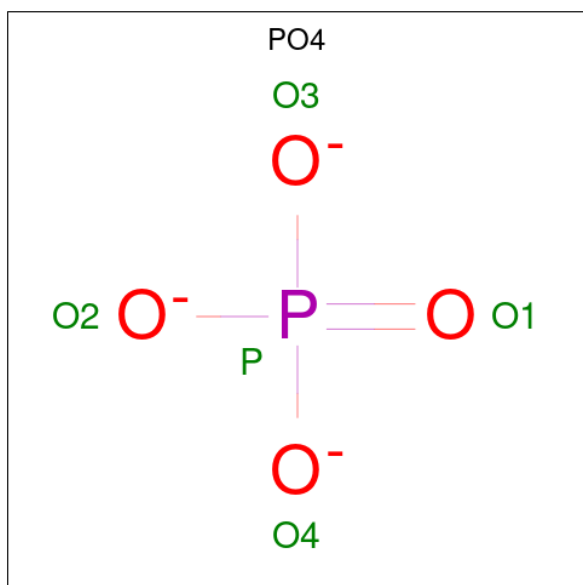
There are 3 unique types of molecules in this entry. The entry contains 34485 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENDO-ALPHA-SIALIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	B	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	C	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	D	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	E	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	F	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

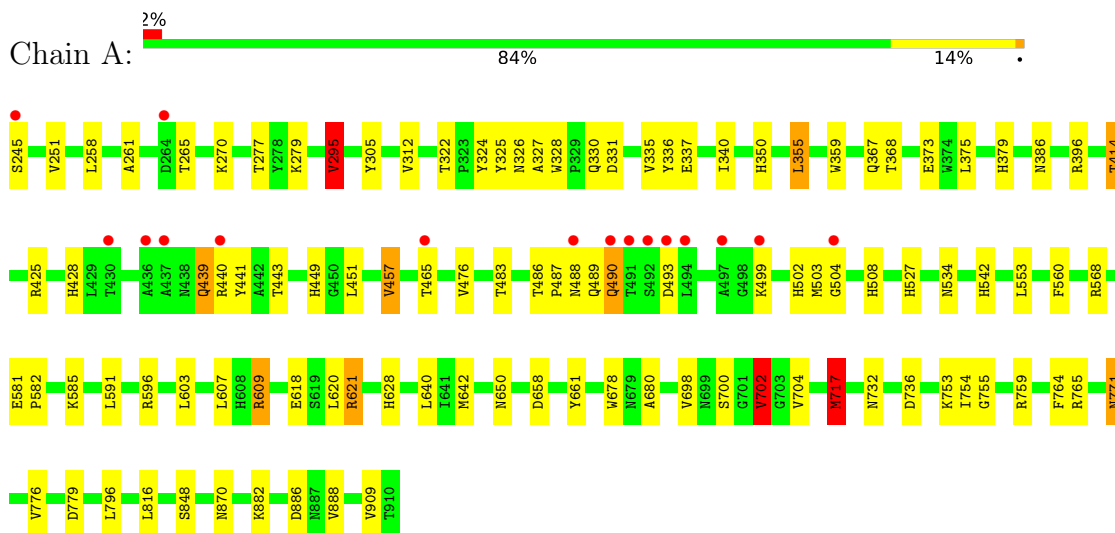
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	528	Total O 528 528	0	0
3	B	534	Total O 534 534	0	0
3	C	516	Total O 516 516	0	0
3	D	529	Total O 529 529	0	0
3	E	459	Total O 459 459	0	0
3	F	509	Total O 509 509	0	0

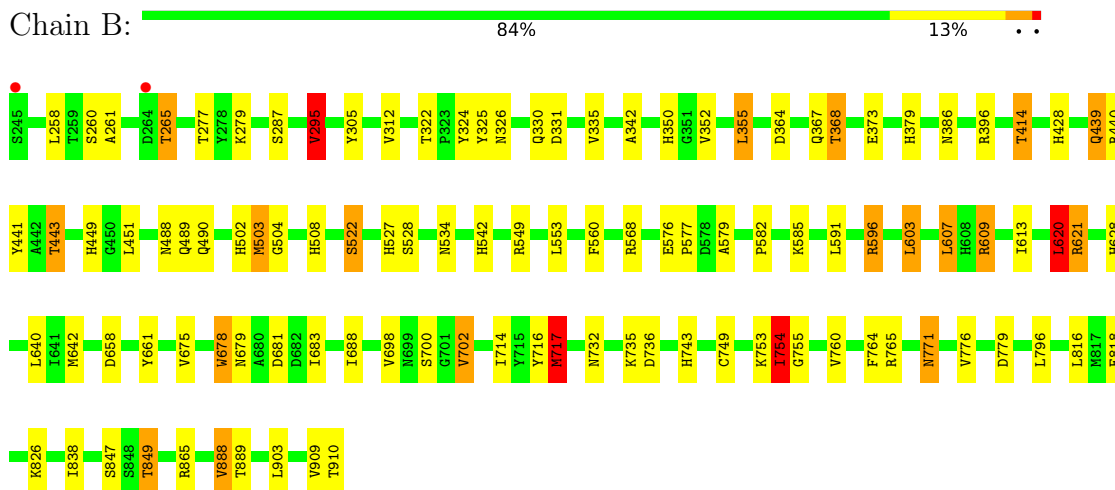
3 Residue-property plots [i](#)

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.

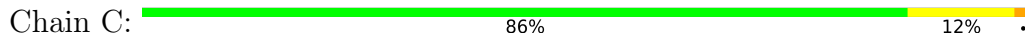
• Molecule 1: ENDO-ALPHA-SIALIDASE

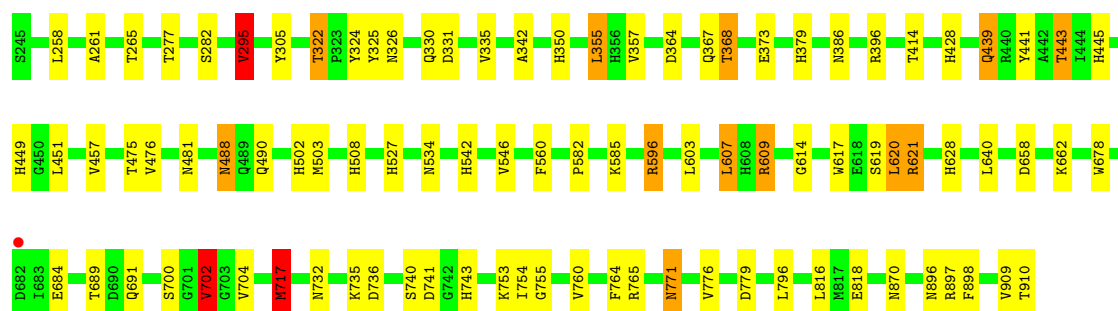


• Molecule 1: ENDO-ALPHA-SIALIDASE



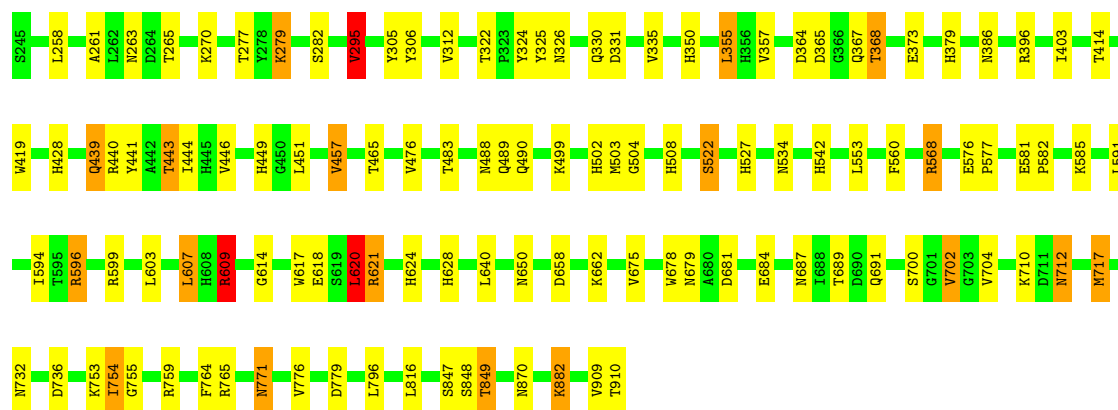
• Molecule 1: ENDO-ALPHA-SIALIDASE





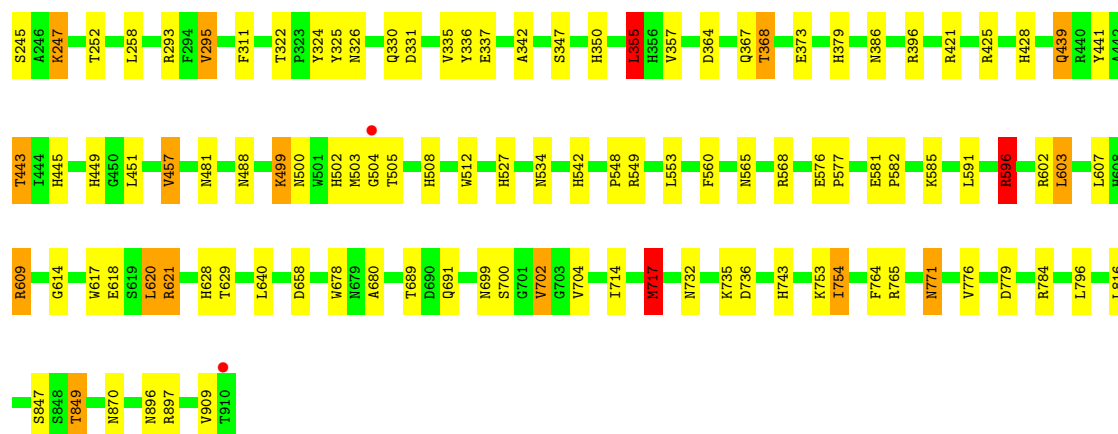
• Molecule 1: ENDO-ALPHA-SIALIDASE

Chain D: 82% 15% .



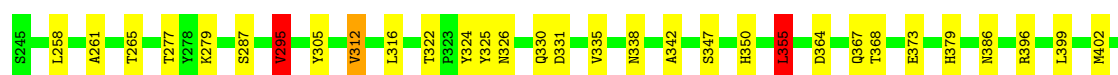
• Molecule 1: ENDO-ALPHA-SIALIDASE

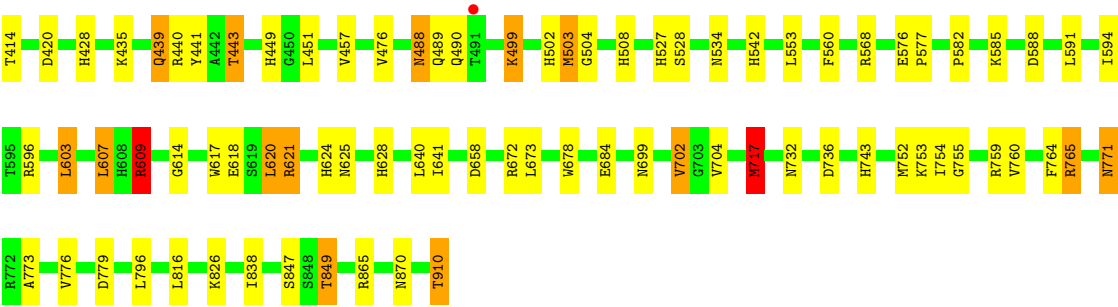
Chain E: 84% 13% .



• Molecule 1: ENDO-ALPHA-SIALIDASE

Chain F: 83% 14% ..





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.65Å 131.25Å 346.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.7 (30.00-1.90) 93.9 (30.00-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.166 , 0.202 0.187 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34485	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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 [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	0.69	3/5376 (0.1%)	0.93	5/7325 (0.1%)
1	B	0.68	2/5376 (0.0%)	0.94	4/7325 (0.1%)
1	C	0.63	2/5376 (0.0%)	0.91	5/7325 (0.1%)
1	D	0.66	1/5376 (0.0%)	0.92	7/7325 (0.1%)
1	E	0.65	1/5376 (0.0%)	0.89	5/7325 (0.1%)
1	F	0.65	3/5376 (0.1%)	0.90	5/7325 (0.1%)
All	All	0.66	12/32256 (0.0%)	0.91	31/43950 (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	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	717	MET	SD-CE	-8.95	1.57	1.79
1	B	717	MET	SD-CE	-8.47	1.58	1.79
1	A	702	VAL	CA-CB	7.65	1.62	1.54
1	C	717	MET	SD-CE	-7.44	1.60	1.79
1	E	717	MET	SD-CE	-7.00	1.62	1.79
1	D	717	MET	SD-CE	-6.28	1.63	1.79
1	B	642	MET	SD-CE	-5.88	1.64	1.79
1	C	702	VAL	CA-CB	5.37	1.60	1.54
1	F	717	MET	SD-CE	-5.29	1.66	1.79
1	F	402	MET	SD-CE	5.28	1.92	1.79
1	A	642	MET	SD-CE	-5.23	1.66	1.79
1	F	702	VAL	CA-CB	5.11	1.60	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	VAL	CB-CA-C	-8.41	98.30	110.83
1	A	596	ARG	NE-CZ-NH2	7.83	126.25	119.20
1	B	295	VAL	CB-CA-C	-6.72	100.60	110.81
1	F	295	VAL	CB-CA-C	-6.65	100.93	110.83
1	C	295	VAL	CB-CA-C	-6.52	101.11	110.83
1	D	295	VAL	CB-CA-C	-6.43	101.25	110.83
1	B	596	ARG	NE-CZ-NH2	6.35	124.92	119.20
1	E	295	VAL	CB-CA-C	-6.28	101.27	110.81
1	D	609	ARG	NE-CZ-NH2	5.89	124.50	119.20
1	C	503	MET	O-C-N	-5.86	116.08	123.17
1	F	609	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	A	596	ARG	NE-CZ-NH1	-5.74	115.76	121.50
1	D	357	VAL	N-CA-C	-5.61	102.28	109.30
1	E	505	THR	N-CA-C	5.57	118.77	110.14
1	F	624	HIS	N-CA-C	5.56	119.37	111.92
1	A	503	MET	O-C-N	-5.51	116.88	123.27
1	D	355	LEU	CA-CB-CG	5.42	135.26	116.30
1	D	596	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	F	503	MET	O-C-N	-5.40	117.01	123.27
1	C	357	VAL	N-CA-C	-5.40	102.56	109.30
1	A	355	LEU	CA-CB-CG	5.35	135.02	116.30
1	C	355	LEU	CA-CB-CG	5.32	134.93	116.30
1	E	355	LEU	CA-CB-CG	5.25	134.67	116.30
1	B	620	LEU	CA-CB-CG	5.21	134.52	116.30
1	B	754	ILE	N-CA-CB	-5.20	106.14	112.33
1	D	624	HIS	N-CA-C	5.20	118.76	111.74
1	D	620	LEU	CA-CB-CG	5.20	134.49	116.30
1	F	355	LEU	CA-CB-CG	5.13	134.25	116.30
1	C	596	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	E	596	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	E	357	VAL	N-CA-C	-5.06	102.98	109.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	503	MET	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5230	0	4942	74	0
1	B	5230	0	4942	79	0
1	C	5230	0	4942	72	0
1	D	5230	0	4942	86	0
1	E	5230	0	4942	92	0
1	F	5230	0	4942	85	0
2	B	5	0	0	1	0
2	C	10	0	0	1	0
2	D	5	0	0	0	0
2	F	10	0	0	0	0
3	A	528	0	0	13	0
3	B	534	0	0	14	0
3	C	516	0	0	11	0
3	D	529	0	0	12	0
3	E	459	0	0	18	0
3	F	509	0	0	19	0
All	All	34485	0	29652	460	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 8.

All (460) 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:D:263:ASN:HB3	3:D:2012:HOH:O	1.36	1.19
1:A:449:HIS:HD2	1:A:451:LEU:H	1.03	1.00
1:B:490:GLN:HG3	3:B:2170:HOH:O	1.61	0.99
1:E:499:LYS:HE3	1:E:500:ASN:H	1.27	0.98
3:A:2050:HOH:O	1:B:368:THR:HG21	1.65	0.96
1:B:261:ALA:O	1:B:265:THR:HG23	1.71	0.91
1:C:475:THR:HB	3:C:2195:HOH:O	1.69	0.90
1:F:449:HIS:HD2	1:F:451:LEU:H	1.14	0.90
1:E:565:ASN:HB3	3:E:2222:HOH:O	1.73	0.89
1:C:449:HIS:HD2	1:C:451:LEU:H	1.20	0.89
1:B:449:HIS:HD2	1:B:451:LEU:H	1.18	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:ARG:HH12	1:C:367:GLN:HE21	1.24	0.86
1:D:765:ARG:HH12	1:E:367:GLN:HE21	1.21	0.85
1:D:449:HIS:HD2	1:D:451:LEU:H	1.22	0.85
1:D:367:GLN:HE22	1:D:764:PHE:H	1.25	0.84
1:F:609:ARG:HG2	1:F:678:TRP:CH2	2.12	0.84
1:A:449:HIS:CD2	1:A:451:LEU:H	1.93	0.83
1:A:368:THR:HG21	3:C:2043:HOH:O	1.78	0.83
1:C:295:VAL:HG13	1:C:305:TYR:CE2	2.15	0.82
1:B:367:GLN:HE21	1:C:765:ARG:HH12	1.28	0.82
1:E:449:HIS:HD2	1:E:451:LEU:H	1.24	0.81
1:E:367:GLN:HE22	1:E:764:PHE:H	1.27	0.81
1:B:295:VAL:HG13	1:B:305:TYR:CE2	2.16	0.80
1:D:295:VAL:HG13	1:D:305:TYR:CE2	2.16	0.80
1:F:621:ARG:HD2	3:F:2297:HOH:O	1.81	0.80
1:A:620:LEU:HD21	1:A:680:ALA:HB2	1.63	0.79
1:A:367:GLN:HE21	1:B:765:ARG:HH12	1.27	0.79
1:A:295:VAL:HG13	1:A:305:TYR:CE2	2.18	0.78
1:B:440:ARG:HE	1:B:489:GLN:HE21	1.29	0.78
1:E:765:ARG:HH12	1:F:367:GLN:HE21	1.29	0.78
1:D:553:LEU:HD22	1:D:591:LEU:HD21	1.66	0.78
1:B:322:THR:HG21	3:B:2054:HOH:O	1.83	0.78
1:A:261:ALA:O	1:A:265:THR:HG23	1.83	0.77
1:C:342:ALA:HB2	1:C:717:MET:HE2	1.65	0.77
1:C:367:GLN:HE22	1:C:764:PHE:H	1.31	0.77
1:A:367:GLN:HE22	1:A:764:PHE:H	1.32	0.77
1:C:609:ARG:HG2	1:C:678:TRP:CH2	2.19	0.76
1:F:367:GLN:HE22	1:F:764:PHE:H	1.33	0.76
1:F:443:THR:HG21	3:F:2118:HOH:O	1.86	0.75
1:E:503:MET:HG2	1:E:504:GLY:HA3	1.69	0.75
1:B:367:GLN:HE22	1:B:764:PHE:H	1.35	0.74
1:E:609:ARG:HG2	1:E:678:TRP:CH2	2.21	0.74
1:C:443:THR:HG22	3:C:2161:HOH:O	1.87	0.74
1:B:847:SER:OG	1:B:849:THR:HB	1.88	0.73
1:B:449:HIS:CD2	1:B:451:LEU:H	2.04	0.73
1:E:245:SER:HB3	3:E:2001:HOH:O	1.88	0.73
1:E:322:THR:HG22	1:E:324:TYR:H	1.52	0.72
1:F:449:HIS:CD2	1:F:451:LEU:H	2.03	0.72
1:F:364:ASP:OD1	1:F:368:THR:HG22	1.90	0.71
1:B:443:THR:HG21	3:B:2183:HOH:O	1.91	0.71
1:E:499:LYS:CE	1:E:500:ASN:H	2.02	0.71
1:D:449:HIS:CD2	1:D:451:LEU:H	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2047:HOH:O	1:C:368:THR:HG21	1.92	0.70
1:F:322:THR:HG22	1:F:324:TYR:H	1.56	0.70
1:D:609:ARG:HG2	1:D:678:TRP:CZ2	2.25	0.70
1:B:364:ASP:OD1	1:B:368:THR:HB	1.92	0.70
1:C:322:THR:HG22	1:C:324:TYR:H	1.56	0.70
1:C:373:GLU:OE2	1:C:508:HIS:HE1	1.75	0.70
1:D:440:ARG:HE	1:D:489:GLN:HE21	1.37	0.70
1:F:295:VAL:HG13	1:F:305:TYR:CE2	2.26	0.69
1:F:322:THR:HG21	3:F:2048:HOH:O	1.90	0.69
1:C:277:THR:HG22	1:C:295:VAL:HG22	1.75	0.69
1:A:322:THR:HG21	3:A:2056:HOH:O	1.91	0.69
1:A:771:ASN:HD21	1:A:776:VAL:H	1.40	0.69
1:F:588:ASP:HB3	3:F:2278:HOH:O	1.92	0.69
3:D:2051:HOH:O	1:F:368:THR:HG21	1.91	0.69
1:D:553:LEU:CD2	1:D:591:LEU:HD21	2.23	0.68
1:A:553:LEU:HD22	1:A:591:LEU:HD21	1.74	0.68
1:F:732:ASN:HD21	1:F:736:ASP:H	1.41	0.68
1:D:322:THR:HG21	3:D:2056:HOH:O	1.93	0.68
1:F:553:LEU:CD2	1:F:591:LEU:HD21	2.24	0.68
1:A:621:ARG:HD3	3:A:2307:HOH:O	1.93	0.67
1:A:620:LEU:HD21	1:A:680:ALA:CB	2.24	0.67
1:A:621:ARG:CD	3:A:2307:HOH:O	2.41	0.67
1:B:443:THR:HG22	3:B:2182:HOH:O	1.93	0.67
1:F:396:ARG:HD3	1:F:534:ASN:O	1.93	0.67
1:E:771:ASN:HD21	1:E:776:VAL:H	1.42	0.67
1:E:449:HIS:CD2	1:E:451:LEU:H	2.10	0.66
1:A:414:THR:HG21	3:A:2141:HOH:O	1.96	0.66
1:F:847:SER:OG	1:F:849:THR:HB	1.95	0.66
1:E:499:LYS:HG3	3:E:2149:HOH:O	1.96	0.66
1:E:603:LEU:HG	1:E:621:ARG:HD3	1.77	0.66
1:D:771:ASN:HD21	1:D:776:VAL:H	1.43	0.66
1:D:732:ASN:HD21	1:D:736:ASP:H	1.43	0.65
1:B:771:ASN:HD21	1:B:776:VAL:H	1.45	0.65
1:E:342:ALA:HB2	1:E:717:MET:HE2	1.79	0.65
1:E:439:GLN:HE22	1:E:441:TYR:HB2	1.62	0.65
1:F:542:HIS:HD2	3:F:2235:HOH:O	1.81	0.64
1:E:897:ARG:CZ	3:E:2451:HOH:O	2.46	0.64
1:D:609:ARG:HG2	1:D:678:TRP:CH2	2.32	0.64
1:D:882:LYS:HD2	1:E:896:ASN:HB2	1.80	0.64
1:A:325:TYR:OH	1:A:350:HIS:HE1	1.80	0.63
1:F:439:GLN:HE22	1:F:441:TYR:HB2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:GLN:HB2	1:C:527:HIS:HE1	1.63	0.63
1:D:367:GLN:HE21	1:F:765:ARG:HH12	1.46	0.63
1:D:396:ARG:HD3	1:D:534:ASN:O	1.99	0.63
1:A:367:GLN:HE21	1:B:765:ARG:NH1	1.96	0.63
1:D:628:HIS:HE1	1:D:658:ASP:OD1	1.82	0.63
1:A:553:LEU:CD2	1:A:591:LEU:HD21	2.29	0.63
1:A:765:ARG:NH1	1:C:367:GLN:HE21	1.95	0.63
1:E:620:LEU:HD21	1:E:680:ALA:HB2	1.80	0.63
1:E:549:ARG:HG3	3:E:2207:HOH:O	1.99	0.62
1:A:443:THR:HG22	1:A:483:THR:HG22	1.81	0.62
1:B:428:HIS:ND1	1:B:502:HIS:HD2	1.96	0.62
1:E:330:GLN:HB2	1:E:527:HIS:HE1	1.64	0.62
1:A:396:ARG:HD3	1:A:534:ASN:O	1.99	0.62
1:D:364:ASP:OD1	1:D:368:THR:HG22	2.00	0.62
1:C:428:HIS:ND1	1:C:502:HIS:HD2	1.97	0.62
1:F:771:ASN:HD21	1:F:776:VAL:H	1.48	0.62
1:B:396:ARG:HD3	1:B:534:ASN:O	2.00	0.61
1:A:367:GLN:NE2	1:B:765:ARG:HH12	1.97	0.61
1:B:342:ALA:HB2	1:B:717:MET:HE2	1.82	0.61
1:F:347:SER:HB3	1:F:355:LEU:HB2	1.82	0.61
1:F:428:HIS:ND1	1:F:502:HIS:HD2	1.98	0.61
1:B:373:GLU:OE2	1:B:508:HIS:HE1	1.82	0.61
1:C:439:GLN:NE2	1:C:441:TYR:H	1.98	0.61
1:C:449:HIS:CD2	1:C:451:LEU:H	2.09	0.61
1:C:277:THR:CG2	1:C:295:VAL:HG22	2.31	0.60
1:D:712:ASN:HD22	1:D:712:ASN:H	1.49	0.60
1:C:322:THR:HG21	3:C:2049:HOH:O	2.00	0.60
1:C:325:TYR:OH	1:C:350:HIS:HE1	1.84	0.60
1:D:443:THR:HG22	3:D:2158:HOH:O	2.01	0.60
1:D:765:ARG:NH1	1:E:367:GLN:HE21	1.95	0.59
1:B:527:HIS:HD2	1:B:582:PRO:O	1.84	0.59
1:A:732:ASN:HD21	1:A:736:ASP:H	1.49	0.59
1:D:350:HIS:HD2	3:D:2192:HOH:O	1.85	0.59
1:A:527:HIS:HD2	1:A:582:PRO:O	1.84	0.59
1:C:771:ASN:HD21	1:C:776:VAL:H	1.50	0.59
1:F:553:LEU:HD22	1:F:591:LEU:HD21	1.83	0.59
1:B:396:ARG:HB3	1:B:560:PHE:CZ	2.37	0.59
1:C:527:HIS:HD2	1:C:582:PRO:O	1.85	0.59
1:C:609:ARG:HG2	1:C:678:TRP:CZ2	2.38	0.59
1:B:771:ASN:ND2	1:B:776:VAL:H	2.00	0.59
1:D:847:SER:OG	1:D:849:THR:HB	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:439:GLN:NE2	1:E:441:TYR:H	2.00	0.59
1:D:527:HIS:HD2	1:D:582:PRO:O	1.84	0.59
1:F:261:ALA:O	1:F:265:THR:HG23	2.03	0.58
1:A:771:ASN:ND2	1:A:776:VAL:H	2.00	0.58
1:F:373:GLU:OE2	1:F:508:HIS:HE1	1.86	0.58
1:A:609:ARG:HG2	1:A:678:TRP:CH2	2.38	0.58
1:F:443:THR:HG22	3:F:2156:HOH:O	2.03	0.58
1:B:330:GLN:HB2	1:B:527:HIS:HE1	1.69	0.58
1:E:445:HIS:HD2	1:E:481:ASN:HD21	1.51	0.58
1:E:847:SER:OG	1:E:849:THR:HB	2.04	0.58
1:D:295:VAL:HG13	1:D:305:TYR:CD2	2.39	0.58
1:E:527:HIS:HD2	1:E:582:PRO:O	1.87	0.58
1:F:457:VAL:HA	1:F:504:GLY:O	2.04	0.58
1:E:379:HIS:H	1:E:386:ASN:ND2	2.00	0.58
1:A:428:HIS:ND1	1:A:502:HIS:HD2	2.01	0.58
1:D:322:THR:HG22	1:D:324:TYR:H	1.69	0.58
1:E:771:ASN:ND2	1:E:776:VAL:H	2.02	0.57
1:F:277:THR:HG22	1:F:295:VAL:HG22	1.84	0.57
1:E:322:THR:HB	1:E:326:ASN:OD1	2.03	0.57
1:F:490:GLN:HG2	3:F:2196:HOH:O	2.04	0.57
1:A:449:HIS:HD2	1:A:451:LEU:N	1.87	0.57
1:E:396:ARG:HD3	1:E:534:ASN:O	2.04	0.57
1:E:368:THR:HG21	3:F:2041:HOH:O	2.04	0.57
1:C:628:HIS:HE1	1:C:658:ASP:OD1	1.88	0.57
1:F:779:ASP:HB2	3:F:2423:HOH:O	2.04	0.57
1:C:330:GLN:HE21	1:C:527:HIS:CE1	2.23	0.56
1:F:330:GLN:HE21	1:F:527:HIS:CE1	2.23	0.56
1:B:322:THR:HG22	1:B:324:TYR:H	1.70	0.56
1:F:527:HIS:HD2	1:F:582:PRO:O	1.88	0.56
1:B:609:ARG:HG2	1:B:678:TRP:CZ2	2.41	0.56
1:C:364:ASP:OD1	1:C:368:THR:HB	2.05	0.56
1:D:771:ASN:ND2	1:D:776:VAL:H	2.03	0.56
1:F:779:ASP:HB2	3:F:2426:HOH:O	2.05	0.56
1:C:621:ARG:HD2	3:C:2307:HOH:O	2.04	0.56
1:E:553:LEU:CD2	1:E:591:LEU:HD21	2.36	0.56
1:D:279:LYS:HA	1:D:295:VAL:HG23	1.87	0.56
1:A:279:LYS:HA	1:A:295:VAL:HG23	1.88	0.56
1:E:373:GLU:OE2	1:E:508:HIS:HE1	1.89	0.55
1:E:621:ARG:HD2	3:E:2254:HOH:O	2.07	0.55
1:F:338:ASN:ND2	3:F:2059:HOH:O	2.40	0.55
1:A:609:ARG:HG2	1:A:678:TRP:CZ2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2103:HOH:O	1:C:779:ASP:HB2	2.05	0.55
1:B:277:THR:HG22	1:B:295:VAL:HG22	1.88	0.55
1:B:542:HIS:HD2	3:B:2263:HOH:O	1.89	0.55
1:E:364:ASP:OD1	1:E:368:THR:HB	2.06	0.55
1:A:322:THR:HG22	1:A:324:TYR:H	1.71	0.55
1:A:765:ARG:HH12	1:C:367:GLN:NE2	2.00	0.55
1:B:621:ARG:CD	3:B:2325:HOH:O	2.54	0.55
1:B:732:ASN:HD21	1:B:736:ASP:H	1.54	0.55
1:B:826:LYS:HB2	1:B:838:ILE:HG13	1.89	0.55
1:E:457:VAL:HA	1:E:504:GLY:O	2.07	0.55
1:C:261:ALA:O	1:C:265:THR:HG23	2.07	0.55
1:F:594:ILE:HG12	1:F:607:LEU:HD23	1.88	0.55
1:C:700:SER:OG	1:C:702:VAL:HG13	2.07	0.55
1:B:753:LYS:HE2	1:B:755:GLY:O	2.07	0.55
1:D:368:THR:HG21	3:E:2041:HOH:O	2.07	0.55
1:C:330:GLN:HE21	1:C:527:HIS:HE1	1.54	0.54
1:B:628:HIS:HE1	1:B:658:ASP:OD1	1.90	0.54
1:F:534:ASN:HB2	3:F:2242:HOH:O	2.07	0.54
1:C:396:ARG:HD3	1:C:534:ASN:O	2.07	0.54
1:D:373:GLU:OE2	1:D:508:HIS:HE1	1.89	0.54
3:D:2359:HOH:O	1:F:759:ARG:HD3	2.06	0.54
1:E:439:GLN:NE2	3:E:2131:HOH:O	2.40	0.54
1:F:603:LEU:HG	1:F:621:ARG:HD3	1.90	0.54
1:B:609:ARG:NH1	1:B:675:VAL:O	2.40	0.54
1:B:621:ARG:HD2	3:B:2325:HOH:O	2.07	0.54
1:B:679:ASN:HD21	1:B:681:ASP:CG	2.17	0.54
1:B:503:MET:HG2	1:B:504:GLY:HA2	1.90	0.53
1:C:439:GLN:HE22	1:C:441:TYR:H	1.56	0.53
1:F:322:THR:HB	1:F:326:ASN:OD1	2.08	0.53
1:E:396:ARG:HB3	1:E:560:PHE:CZ	2.44	0.53
1:F:379:HIS:H	1:F:386:ASN:ND2	2.06	0.53
1:A:396:ARG:HB3	1:A:560:PHE:CZ	2.44	0.53
1:D:305:TYR:CZ	1:D:684:GLU:HG2	2.43	0.53
1:E:765:ARG:HH12	1:F:367:GLN:NE2	2.04	0.53
1:B:503:MET:HG2	1:B:504:GLY:CA	2.38	0.53
1:E:342:ALA:HB2	1:E:717:MET:CE	2.39	0.53
1:F:342:ALA:HB2	1:F:717:MET:HE2	1.90	0.53
1:F:440:ARG:HE	1:F:489:GLN:HE21	1.55	0.53
1:A:336:TYR:CE2	1:A:337:GLU:HG3	2.43	0.53
1:E:439:GLN:HE22	1:E:441:TYR:H	1.56	0.53
1:A:368:THR:HG23	3:A:2099:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:VAL:HA	1:A:504:GLY:O	2.09	0.52
1:E:620:LEU:HD21	1:E:680:ALA:CB	2.39	0.52
1:A:628:HIS:HE1	1:A:658:ASP:OD1	1.92	0.52
1:F:325:TYR:OH	1:F:350:HIS:HE1	1.93	0.52
1:F:628:HIS:HE1	1:F:658:ASP:OD1	1.93	0.52
1:B:325:TYR:OH	1:B:350:HIS:HE1	1.92	0.52
1:F:771:ASN:ND2	1:F:776:VAL:H	2.08	0.52
1:C:368:THR:HG22	3:C:2081:HOH:O	2.09	0.52
1:E:870:ASN:C	1:E:870:ASN:HD22	2.18	0.52
1:C:396:ARG:HB3	1:C:560:PHE:CZ	2.45	0.52
1:A:277:THR:HG22	1:A:295:VAL:HG22	1.92	0.52
1:C:325:TYR:OH	1:C:350:HIS:CE1	2.62	0.52
1:D:396:ARG:HB3	1:D:560:PHE:CZ	2.44	0.52
1:E:428:HIS:ND1	1:E:502:HIS:HD2	2.07	0.52
1:B:367:GLN:HE21	1:C:765:ARG:NH1	2.03	0.51
1:A:542:HIS:HE1	3:A:2159:HOH:O	1.92	0.51
1:D:261:ALA:O	1:D:265:THR:HG23	2.10	0.51
1:A:325:TYR:OH	1:A:350:HIS:CE1	2.61	0.51
1:A:886:ASP:OD2	1:C:897:ARG:NH1	2.43	0.51
1:D:457:VAL:HA	1:D:504:GLY:O	2.11	0.51
1:D:765:ARG:HH12	1:E:367:GLN:NE2	1.99	0.51
1:D:542:HIS:HD2	3:D:2237:HOH:O	1.94	0.51
1:E:732:ASN:HD21	1:E:736:ASP:H	1.59	0.51
1:B:279:LYS:HA	1:B:295:VAL:HG23	1.93	0.51
1:B:818:GLU:HB3	2:B:1685:PO4:O2	2.11	0.51
1:A:779:ASP:HB2	3:C:2102:HOH:O	2.10	0.50
1:B:607:LEU:HB3	1:B:620:LEU:HD22	1.92	0.50
1:F:628:HIS:HD2	3:F:2283:HOH:O	1.93	0.50
1:A:330:GLN:HB2	1:A:527:HIS:HE1	1.76	0.50
1:C:771:ASN:ND2	1:C:776:VAL:H	2.09	0.50
1:E:325:TYR:OH	1:E:350:HIS:HE1	1.95	0.50
1:E:714:ILE:HG22	1:E:754:ILE:HD13	1.92	0.50
1:E:628:HIS:HE1	1:E:658:ASP:OD1	1.94	0.50
1:A:650:ASN:ND2	3:A:2325:HOH:O	2.44	0.50
1:C:445:HIS:HD2	1:C:481:ASN:HD21	1.60	0.50
1:C:818:GLU:HB3	2:C:1685:PO4:O4	2.11	0.50
1:E:396:ARG:HD2	1:E:534:ASN:ND2	2.26	0.50
1:E:553:LEU:HD22	1:E:591:LEU:HD21	1.93	0.50
1:A:661:TYR:CZ	1:A:698:VAL:HB	2.47	0.50
1:D:330:GLN:HE21	1:D:527:HIS:CE1	2.30	0.50
1:D:325:TYR:OH	1:D:350:HIS:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2109:HOH:O	1:B:779:ASP:HB2	2.11	0.49
1:F:350:HIS:CE1	1:F:699:ASN:HB3	2.46	0.49
1:F:743:HIS:HD2	3:F:2391:HOH:O	1.94	0.49
1:D:379:HIS:H	1:D:386:ASN:ND2	2.11	0.49
1:B:330:GLN:HE21	1:B:527:HIS:CE1	2.30	0.49
1:B:379:HIS:H	1:B:386:ASN:ND2	2.10	0.49
1:F:621:ARG:CD	3:F:2297:HOH:O	2.49	0.49
1:D:428:HIS:ND1	1:D:502:HIS:HD2	2.10	0.49
1:E:897:ARG:NE	3:E:2451:HOH:O	2.45	0.49
1:B:295:VAL:HG13	1:B:305:TYR:CD2	2.47	0.49
1:D:295:VAL:CG1	1:D:305:TYR:CE2	2.94	0.49
1:E:445:HIS:CD2	1:E:481:ASN:HD21	2.30	0.49
1:B:700:SER:OG	1:B:702:VAL:HG13	2.13	0.49
1:C:488:ASN:ND2	1:C:490:GLN:HE22	2.11	0.49
1:E:499:LYS:HE3	1:E:500:ASN:N	2.11	0.49
1:C:295:VAL:HG13	1:C:305:TYR:CD2	2.48	0.49
1:E:330:GLN:HB2	1:E:527:HIS:CE1	2.45	0.49
1:F:826:LYS:HB2	1:F:838:ILE:HG13	1.95	0.49
1:E:765:ARG:NH1	1:F:367:GLN:HE21	2.05	0.48
1:C:330:GLN:HB2	1:C:527:HIS:CE1	2.44	0.48
1:B:522:SER:O	1:B:522:SER:OG	2.32	0.48
1:C:542:HIS:HD2	3:C:2248:HOH:O	1.95	0.48
1:B:576:GLU:N	1:B:577:PRO:CD	2.77	0.48
1:E:336:TYR:CE2	1:E:337:GLU:HG3	2.49	0.48
1:A:359:TRP:CE3	1:A:375:LEU:HD11	2.49	0.48
1:F:330:GLN:HB2	1:F:527:HIS:HE1	1.79	0.48
1:D:440:ARG:HE	1:D:489:GLN:NE2	2.09	0.48
1:A:330:GLN:HE21	1:A:527:HIS:CE1	2.32	0.48
1:A:340:ILE:CG2	1:A:717:MET:HE1	2.44	0.47
1:B:743:HIS:HD2	3:B:2423:HOH:O	1.97	0.47
1:E:714:ILE:CG2	1:E:754:ILE:HD13	2.44	0.47
1:A:489:GLN:O	1:E:548:PRO:HG3	2.14	0.47
1:A:618:GLU:HG2	1:A:678:TRP:NE1	2.30	0.47
1:B:628:HIS:HD2	3:B:2311:HOH:O	1.98	0.47
1:E:368:THR:HG22	3:E:2072:HOH:O	2.13	0.47
1:F:312:VAL:HG21	1:F:752:MET:HE2	1.97	0.47
1:A:621:ARG:HD2	3:A:2307:HOH:O	2.10	0.47
1:D:350:HIS:CD2	3:D:2192:HOH:O	2.65	0.47
1:A:465:THR:HB	1:A:490:GLN:HE22	1.80	0.47
1:E:735:LYS:O	1:E:743:HIS:HE1	1.98	0.47
1:E:443:THR:HG22	3:E:2135:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:689:THR:HG23	1:E:691:GLN:HE22	1.80	0.47
1:D:753:LYS:HE2	1:D:755:GLY:O	2.15	0.47
1:E:247:LYS:HG3	1:E:252:THR:HG21	1.96	0.47
1:A:396:ARG:HD2	1:A:534:ASN:ND2	2.30	0.47
1:B:439:GLN:HE22	1:B:441:TYR:HB2	1.80	0.47
1:D:335:VAL:HG11	3:D:2373:HOH:O	2.16	0.47
1:D:576:GLU:N	1:D:577:PRO:CD	2.78	0.47
1:D:607:LEU:HB3	1:D:620:LEU:HD22	1.96	0.47
1:E:379:HIS:H	1:E:386:ASN:HD22	1.62	0.47
1:E:576:GLU:N	1:E:577:PRO:CD	2.78	0.47
1:A:322:THR:HB	1:A:326:ASN:OD1	2.15	0.46
1:F:305:TYR:CZ	1:F:684:GLU:HG2	2.50	0.46
1:F:364:ASP:OD1	1:F:368:THR:CG2	2.63	0.46
1:A:628:HIS:HD2	3:A:2288:HOH:O	1.98	0.46
1:B:735:LYS:O	1:B:743:HIS:HE1	1.98	0.46
1:F:279:LYS:HE2	3:F:2002:HOH:O	2.13	0.46
1:B:888:VAL:HG12	1:B:889:THR:HG23	1.96	0.46
1:E:609:ARG:HG2	1:E:678:TRP:CZ2	2.50	0.46
1:B:330:GLN:HB2	1:B:527:HIS:CE1	2.50	0.46
1:D:542:HIS:HE1	3:D:2153:HOH:O	1.97	0.46
1:A:330:GLN:HE21	1:A:527:HIS:HE1	1.62	0.46
1:B:325:TYR:OH	1:B:350:HIS:CE1	2.68	0.46
1:A:542:HIS:HD2	3:A:2233:HOH:O	1.98	0.46
1:D:367:GLN:HE21	1:F:765:ARG:NH1	2.11	0.46
1:B:367:GLN:NE2	1:C:765:ARG:HH12	2.04	0.46
1:D:759:ARG:HD3	3:E:2293:HOH:O	2.15	0.46
1:B:330:GLN:HE21	1:B:527:HIS:HE1	1.62	0.45
1:D:689:THR:HG23	1:D:691:GLN:HE22	1.81	0.45
1:E:779:ASP:HB2	3:F:2099:HOH:O	2.15	0.45
1:D:439:GLN:HE22	1:D:441:TYR:HB2	1.81	0.45
1:F:396:ARG:HB3	1:F:560:PHE:CZ	2.52	0.45
1:A:848:SER:O	1:B:865:ARG:NE	2.50	0.45
1:D:330:GLN:HB2	1:D:527:HIS:HE1	1.82	0.45
1:D:503:MET:HG2	1:D:504:GLY:HA3	1.98	0.45
1:E:542:HIS:CD2	1:E:581:GLU:H	2.35	0.45
1:D:870:ASN:C	1:D:870:ASN:HD22	2.25	0.45
1:F:576:GLU:N	1:F:577:PRO:CD	2.80	0.45
1:A:373:GLU:OE2	1:A:508:HIS:HE1	1.98	0.45
1:D:679:ASN:ND2	1:D:681:ASP:H	2.15	0.45
1:B:568:ARG:HD2	3:B:2288:HOH:O	2.16	0.45
1:C:322:THR:HG22	1:C:324:TYR:N	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:700:SER:HG	1:C:702:VAL:HG13	1.82	0.45
1:D:403:ILE:HG13	1:D:419:TRP:CD2	2.52	0.45
1:F:330:GLN:HA	1:F:331:ASP:HA	1.83	0.45
1:F:331:ASP:HB3	1:F:528:SER:HA	1.99	0.45
1:F:553:LEU:HD21	1:F:591:LEU:HD21	1.96	0.45
1:A:379:HIS:H	1:A:386:ASN:ND2	2.16	0.44
1:B:322:THR:HB	1:B:326:ASN:OD1	2.17	0.44
1:C:740:SER:OG	1:C:741:ASP:N	2.47	0.44
1:D:700:SER:OG	1:D:702:VAL:HG13	2.17	0.44
1:C:330:GLN:HA	1:C:331:ASP:HA	1.75	0.44
1:A:870:ASN:C	1:A:870:ASN:HD22	2.25	0.44
3:B:2047:HOH:O	1:C:368:THR:CG2	2.59	0.44
1:D:277:THR:HG22	1:D:295:VAL:HG22	1.99	0.44
1:E:628:HIS:HD2	3:E:2242:HOH:O	1.99	0.44
1:E:753:LYS:HE3	1:F:287:SER:OG	2.17	0.44
1:D:322:THR:HB	1:D:326:ASN:OD1	2.16	0.44
1:A:700:SER:OG	1:A:702:VAL:HG13	2.17	0.44
1:F:379:HIS:H	1:F:386:ASN:HD22	1.65	0.44
1:D:365:ASP:OD2	1:D:710:LYS:NZ	2.50	0.44
1:D:848:SER:O	1:F:865:ARG:NE	2.51	0.44
1:F:326:ASN:ND2	3:F:2048:HOH:O	2.48	0.44
1:F:910:THR:HB	3:F:2507:HOH:O	2.17	0.44
1:D:712:ASN:H	1:D:712:ASN:ND2	2.14	0.44
1:C:870:ASN:C	1:C:870:ASN:HD22	2.24	0.44
1:D:621:ARG:CD	3:D:2296:HOH:O	2.65	0.44
1:C:689:THR:HG23	1:C:691:GLN:HE22	1.83	0.43
1:F:620:LEU:C	1:F:620:LEU:HD23	2.42	0.43
1:F:609:ARG:HG2	1:F:678:TRP:CZ2	2.50	0.43
1:C:753:LYS:HE2	1:C:755:GLY:O	2.17	0.43
1:D:542:HIS:CD2	1:D:581:GLU:H	2.36	0.43
1:F:609:ARG:HD2	1:F:618:GLU:OE2	2.18	0.43
1:C:305:TYR:CE1	1:C:684:GLU:HG2	2.54	0.43
1:C:322:THR:HB	1:C:326:ASN:OD1	2.18	0.43
1:D:650:ASN:ND2	3:D:2323:HOH:O	2.42	0.43
1:D:754:ILE:HD12	1:D:754:ILE:HA	1.82	0.43
1:A:330:GLN:HA	1:A:331:ASP:HA	1.79	0.43
1:D:679:ASN:HD21	1:D:681:ASP:CG	2.27	0.43
1:E:293:ARG:HD3	1:E:311:PHE:CE2	2.54	0.43
1:E:322:THR:HG21	3:E:2047:HOH:O	2.17	0.43
1:F:503:MET:HG2	1:F:504:GLY:HA3	2.01	0.43
1:B:439:GLN:NE2	1:B:441:TYR:H	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:LEU:HB3	1:B:621:ARG:CZ	2.49	0.43
1:B:903:LEU:HA	1:C:898:PHE:O	2.19	0.43
1:E:743:HIS:HD2	3:E:2182:HOH:O	2.01	0.43
1:C:324:TYR:HB2	1:C:326:ASN:HD21	1.83	0.43
1:C:614:GLY:HA2	1:C:617:TRP:CZ2	2.54	0.43
1:C:735:LYS:O	1:C:743:HIS:HE1	2.02	0.43
1:D:522:SER:HB3	1:D:568:ARG:NH2	2.33	0.43
1:F:753:LYS:HE2	1:F:755:GLY:O	2.19	0.43
1:B:414:THR:CG2	3:B:2109:HOH:O	2.67	0.42
1:C:732:ASN:HD21	1:C:736:ASP:H	1.66	0.42
1:E:596:ARG:HG3	1:E:629:THR:O	2.18	0.42
1:A:486:THR:HB	1:A:487:PRO:CD	2.50	0.42
1:A:759:ARG:HD3	3:C:2339:HOH:O	2.18	0.42
1:D:443:THR:HB	1:D:483:THR:HG22	2.02	0.42
1:D:465:THR:CB	1:D:490:GLN:NE2	2.82	0.42
1:E:784:ARG:HD3	1:F:773:ALA:O	2.19	0.42
1:A:568:ARG:HG2	3:A:2262:HOH:O	2.20	0.42
1:E:330:GLN:HA	1:E:331:ASP:HA	1.79	0.42
1:F:330:GLN:HE21	1:F:527:HIS:HE1	1.64	0.42
1:D:594:ILE:HG12	1:D:607:LEU:HD23	2.01	0.42
1:B:379:HIS:H	1:B:386:ASN:HD22	1.68	0.42
1:D:324:TYR:HB2	1:D:326:ASN:HD21	1.84	0.42
1:D:609:ARG:NH1	1:D:675:VAL:O	2.53	0.42
1:D:330:GLN:HE21	1:D:527:HIS:HE1	1.66	0.42
1:E:897:ARG:NH2	3:E:2451:HOH:O	2.52	0.42
1:F:399:LEU:O	1:F:420:ASP:HA	2.20	0.42
1:E:350:HIS:CE1	1:E:699:ASN:HB3	2.55	0.42
1:B:553:LEU:HD22	1:B:591:LEU:HD21	2.02	0.42
1:A:330:GLN:HB2	1:A:527:HIS:CE1	2.54	0.42
1:B:324:TYR:HB2	1:B:326:ASN:HD21	1.85	0.42
1:C:620:LEU:HD23	1:C:620:LEU:C	2.44	0.42
1:E:421:ARG:HD2	1:E:512:TRP:CD2	2.54	0.42
1:A:753:LYS:HE2	1:A:755:GLY:O	2.20	0.41
1:D:325:TYR:OH	1:D:350:HIS:CE1	2.73	0.41
1:B:352:VAL:HA	1:B:355:LEU:HD23	2.02	0.41
1:C:607:LEU:HB3	1:C:620:LEU:HD22	2.02	0.41
1:D:330:GLN:HA	1:D:331:ASP:HA	1.80	0.41
1:D:444:ILE:HG22	1:D:446:VAL:HG23	2.02	0.41
1:E:325:TYR:OH	1:E:350:HIS:CE1	2.73	0.41
1:A:439:GLN:HE22	1:A:441:TYR:HB2	1.85	0.41
1:B:716:TYR:O	1:B:749:CYS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:771:ASN:HD22	1:E:771:ASN:HA	1.76	0.41
1:F:325:TYR:OH	1:F:350:HIS:CE1	2.74	0.41
1:A:327:ALA:HB3	1:A:328:TRP:CE3	2.56	0.41
1:A:542:HIS:CD2	1:A:581:GLU:H	2.39	0.41
1:B:549:ARG:HD3	1:B:579:ALA:O	2.21	0.41
1:E:618:GLU:HG2	1:E:678:TRP:NE1	2.36	0.41
1:E:700:SER:OG	1:E:702:VAL:HG13	2.20	0.41
1:F:435:LYS:HZ1	1:F:488:ASN:HD22	1.68	0.41
1:E:542:HIS:HD2	3:E:2202:HOH:O	2.03	0.41
1:F:870:ASN:C	1:F:870:ASN:HD22	2.28	0.41
1:B:661:TYR:CZ	1:B:698:VAL:HB	2.56	0.41
1:D:609:ARG:HD2	1:D:618:GLU:OE1	2.21	0.41
1:B:330:GLN:HA	1:B:331:ASP:HA	1.81	0.41
1:C:379:HIS:H	1:C:386:ASN:ND2	2.19	0.41
1:E:342:ALA:CB	1:E:717:MET:HE2	2.49	0.41
1:C:621:ARG:CD	3:C:2307:HOH:O	2.64	0.41
1:D:465:THR:HB	1:D:490:GLN:NE2	2.36	0.41
1:D:779:ASP:HB2	3:E:2089:HOH:O	2.20	0.41
1:E:379:HIS:HB2	1:E:386:ASN:HA	2.03	0.41
1:F:499:LYS:HA	1:F:499:LYS:HD2	1.63	0.41
1:A:440:ARG:HE	1:A:489:GLN:HE21	1.68	0.41
1:A:882:LYS:HD2	1:C:896:ASN:HB2	2.03	0.41
1:B:287:SER:OG	1:C:753:LYS:HE3	2.21	0.41
1:D:609:ARG:HD2	1:D:618:GLU:HB2	2.03	0.41
1:C:439:GLN:HE22	1:C:441:TYR:HB2	1.85	0.40
1:D:306:TYR:HD1	1:D:687:ASN:HD22	1.68	0.40
1:E:614:GLY:HA2	1:E:617:TRP:CZ2	2.56	0.40
1:C:386:ASN:HD22	1:C:386:ASN:HA	1.71	0.40
1:E:764:PHE:HB3	1:F:316:LEU:HD23	2.02	0.40
1:F:379:HIS:HB2	1:F:386:ASN:HA	2.04	0.40
1:B:331:ASP:HB3	1:B:528:SER:HA	2.02	0.40
1:C:662:LYS:HB3	3:C:2334:HOH:O	2.22	0.40
1:D:614:GLY:HA2	1:D:617:TRP:CZ2	2.56	0.40
1:E:347:SER:HB3	1:E:355:LEU:HB2	2.03	0.40
1:E:553:LEU:HD21	1:E:591:LEU:HD21	2.03	0.40
1:F:614:GLY:HA2	1:F:617:TRP:CZ2	2.56	0.40
1:B:714:ILE:HG22	1:B:754:ILE:HD13	2.04	0.40
1:D:527:HIS:CD2	1:D:582:PRO:O	2.71	0.40
1:F:641:ILE:HG12	1:F:672:ARG:HG2	2.04	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	664/666 (100%)	642 (97%)	21 (3%)	1 (0%)	43	36
1	B	664/666 (100%)	640 (96%)	23 (4%)	1 (0%)	43	36
1	C	664/666 (100%)	642 (97%)	21 (3%)	1 (0%)	43	36
1	D	664/666 (100%)	639 (96%)	24 (4%)	1 (0%)	43	36
1	E	664/666 (100%)	636 (96%)	27 (4%)	1 (0%)	43	36
1	F	664/666 (100%)	639 (96%)	24 (4%)	1 (0%)	43	36
All	All	3984/3996 (100%)	3838 (96%)	140 (4%)	6 (0%)	43	36

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	678	TRP
1	A	704	VAL
1	C	704	VAL
1	E	704	VAL
1	D	704	VAL
1	F	704	VAL

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	564/564 (100%)	533 (94%)	31 (6%)	19	11
1	B	564/564 (100%)	529 (94%)	35 (6%)	16	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	564/564 (100%)	532 (94%)	32 (6%)	18	11
1	D	564/564 (100%)	526 (93%)	38 (7%)	15	7
1	E	564/564 (100%)	534 (95%)	30 (5%)	20	12
1	F	564/564 (100%)	532 (94%)	32 (6%)	18	11
All	All	3384/3384 (100%)	3186 (94%)	198 (6%)	18	10

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	SER
1	A	251	VAL
1	A	258	LEU
1	A	270	LYS
1	A	295	VAL
1	A	312	VAL
1	A	335	VAL
1	A	355	LEU
1	A	414	THR
1	A	425	ARG
1	A	439	GLN
1	A	457	VAL
1	A	476	VAL
1	A	488	ASN
1	A	490	GLN
1	A	493	ASP
1	A	499	LYS
1	A	585	LYS
1	A	603	LEU
1	A	607	LEU
1	A	609	ARG
1	A	621	ARG
1	A	640	LEU
1	A	702	VAL
1	A	717	MET
1	A	754	ILE
1	A	771	ASN
1	A	796	LEU
1	A	816	LEU
1	A	888	VAL
1	A	909	VAL
1	B	258	LEU

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Mol	Chain	Res	Type
1	B	260	SER
1	B	265	THR
1	B	295	VAL
1	B	312	VAL
1	B	335	VAL
1	B	355	LEU
1	B	368	THR
1	B	414	THR
1	B	439	GLN
1	B	443	THR
1	B	488	ASN
1	B	522	SER
1	B	585	LYS
1	B	596	ARG
1	B	603	LEU
1	B	607	LEU
1	B	609	ARG
1	B	613	ILE
1	B	620	LEU
1	B	621	ARG
1	B	640	LEU
1	B	683	ILE
1	B	688	ILE
1	B	702	VAL
1	B	717	MET
1	B	754	ILE
1	B	760	VAL
1	B	771	ASN
1	B	796	LEU
1	B	816	LEU
1	B	849	THR
1	B	888	VAL
1	B	909	VAL
1	B	910	THR
1	C	258	LEU
1	C	282	SER
1	C	295	VAL
1	C	322	THR
1	C	335	VAL
1	C	355	LEU
1	C	368	THR
1	C	414	THR

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Mol	Chain	Res	Type
1	C	439	GLN
1	C	443	THR
1	C	457	VAL
1	C	476	VAL
1	C	488	ASN
1	C	546	VAL
1	C	585	LYS
1	C	596	ARG
1	C	603	LEU
1	C	607	LEU
1	C	609	ARG
1	C	619	SER
1	C	620	LEU
1	C	621	ARG
1	C	640	LEU
1	C	702	VAL
1	C	717	MET
1	C	754	ILE
1	C	760	VAL
1	C	771	ASN
1	C	796	LEU
1	C	816	LEU
1	C	909	VAL
1	C	910	THR
1	D	258	LEU
1	D	270	LYS
1	D	279	LYS
1	D	282	SER
1	D	295	VAL
1	D	312	VAL
1	D	355	LEU
1	D	368	THR
1	D	414	THR
1	D	439	GLN
1	D	443	THR
1	D	457	VAL
1	D	476	VAL
1	D	488	ASN
1	D	499	LYS
1	D	522	SER
1	D	568	ARG
1	D	585	LYS

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Mol	Chain	Res	Type
1	D	596	ARG
1	D	599	ARG
1	D	603	LEU
1	D	607	LEU
1	D	609	ARG
1	D	620	LEU
1	D	621	ARG
1	D	640	LEU
1	D	662	LYS
1	D	702	VAL
1	D	712	ASN
1	D	717	MET
1	D	754	ILE
1	D	771	ASN
1	D	796	LEU
1	D	816	LEU
1	D	849	THR
1	D	882	LYS
1	D	909	VAL
1	D	910	THR
1	E	247	LYS
1	E	258	LEU
1	E	295	VAL
1	E	335	VAL
1	E	355	LEU
1	E	368	THR
1	E	425	ARG
1	E	439	GLN
1	E	443	THR
1	E	457	VAL
1	E	488	ASN
1	E	499	LYS
1	E	568	ARG
1	E	585	LYS
1	E	596	ARG
1	E	602	ARG
1	E	603	LEU
1	E	607	LEU
1	E	609	ARG
1	E	620	LEU
1	E	621	ARG
1	E	640	LEU

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Mol	Chain	Res	Type
1	E	702	VAL
1	E	717	MET
1	E	754	ILE
1	E	771	ASN
1	E	796	LEU
1	E	816	LEU
1	E	849	THR
1	E	909	VAL
1	F	258	LEU
1	F	295	VAL
1	F	312	VAL
1	F	335	VAL
1	F	355	LEU
1	F	414	THR
1	F	439	GLN
1	F	443	THR
1	F	476	VAL
1	F	488	ASN
1	F	499	LYS
1	F	568	ARG
1	F	585	LYS
1	F	596	ARG
1	F	603	LEU
1	F	607	LEU
1	F	609	ARG
1	F	620	LEU
1	F	621	ARG
1	F	625	ASN
1	F	640	LEU
1	F	673	LEU
1	F	702	VAL
1	F	717	MET
1	F	754	ILE
1	F	760	VAL
1	F	765	ARG
1	F	771	ASN
1	F	796	LEU
1	F	816	LEU
1	F	849	THR
1	F	910	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (180) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
1	A	350	HIS
1	A	367	GLN
1	A	386	ASN
1	A	438	ASN
1	A	439	GLN
1	A	445	HIS
1	A	449	HIS
1	A	461	ASN
1	A	488	ASN
1	A	489	GLN
1	A	490	GLN
1	A	500	ASN
1	A	502	HIS
1	A	508	HIS
1	A	527	HIS
1	A	534	ASN
1	A	535	ASN
1	A	542	HIS
1	A	561	ASN
1	A	624	HIS
1	A	625	ASN
1	A	628	HIS
1	A	650	ASN
1	A	687	ASN
1	A	691	GLN
1	A	699	ASN
1	A	732	ASN
1	A	743	HIS
1	A	771	ASN
1	A	870	ASN
1	A	877	GLN
1	B	263	ASN
1	B	338	ASN
1	B	350	HIS
1	B	367	GLN
1	B	386	ASN
1	B	397	ASN
1	B	438	ASN
1	B	439	GLN
1	B	449	HIS
1	B	461	ASN
1	B	481	ASN

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Mol	Chain	Res	Type
1	B	488	ASN
1	B	489	GLN
1	B	502	HIS
1	B	508	HIS
1	B	527	HIS
1	B	542	HIS
1	B	624	HIS
1	B	628	HIS
1	B	650	ASN
1	B	676	ASN
1	B	679	ASN
1	B	687	ASN
1	B	691	GLN
1	B	732	ASN
1	B	743	HIS
1	B	771	ASN
1	B	832	ASN
1	B	853	GLN
1	B	870	ASN
1	B	877	GLN
1	C	263	ASN
1	C	350	HIS
1	C	367	GLN
1	C	386	ASN
1	C	438	ASN
1	C	439	GLN
1	C	445	HIS
1	C	449	HIS
1	C	481	ASN
1	C	488	ASN
1	C	489	GLN
1	C	502	HIS
1	C	508	HIS
1	C	527	HIS
1	C	534	ASN
1	C	535	ASN
1	C	542	HIS
1	C	625	ASN
1	C	628	HIS
1	C	676	ASN
1	C	687	ASN
1	C	691	GLN

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Mol	Chain	Res	Type
1	C	732	ASN
1	C	743	HIS
1	C	771	ASN
1	C	781	ASN
1	C	832	ASN
1	C	853	GLN
1	C	860	ASN
1	C	870	ASN
1	D	338	ASN
1	D	350	HIS
1	D	367	GLN
1	D	386	ASN
1	D	438	ASN
1	D	439	GLN
1	D	445	HIS
1	D	449	HIS
1	D	481	ASN
1	D	489	GLN
1	D	502	HIS
1	D	508	HIS
1	D	527	HIS
1	D	534	ASN
1	D	542	HIS
1	D	625	ASN
1	D	628	HIS
1	D	650	ASN
1	D	679	ASN
1	D	687	ASN
1	D	691	GLN
1	D	699	ASN
1	D	712	ASN
1	D	732	ASN
1	D	743	HIS
1	D	771	ASN
1	D	832	ASN
1	D	853	GLN
1	D	860	ASN
1	D	870	ASN
1	E	263	ASN
1	E	350	HIS
1	E	367	GLN
1	E	386	ASN

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Mol	Chain	Res	Type
1	E	439	GLN
1	E	445	HIS
1	E	449	HIS
1	E	481	ASN
1	E	488	ASN
1	E	502	HIS
1	E	508	HIS
1	E	527	HIS
1	E	534	ASN
1	E	535	ASN
1	E	542	HIS
1	E	625	ASN
1	E	628	HIS
1	E	650	ASN
1	E	691	GLN
1	E	732	ASN
1	E	743	HIS
1	E	771	ASN
1	E	832	ASN
1	E	853	GLN
1	E	870	ASN
1	E	877	GLN
1	F	263	ASN
1	F	338	ASN
1	F	350	HIS
1	F	367	GLN
1	F	386	ASN
1	F	415	ASN
1	F	438	ASN
1	F	439	GLN
1	F	449	HIS
1	F	461	ASN
1	F	488	ASN
1	F	489	GLN
1	F	502	HIS
1	F	508	HIS
1	F	527	HIS
1	F	542	HIS
1	F	570	GLN
1	F	625	ASN
1	F	628	HIS
1	F	650	ASN

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Mol	Chain	Res	Type
1	F	676	ASN
1	F	691	GLN
1	F	732	ASN
1	F	743	HIS
1	F	771	ASN
1	F	781	ASN
1	F	832	ASN
1	F	853	GLN
1	F	860	ASN
1	F	870	ASN
1	F	877	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	F	1686	-	4,4,4	1.07	0	6,6,6	0.59	0
2	PO4	C	1685	-	4,4,4	1.05	0	6,6,6	0.51	0
2	PO4	C	1686	-	4,4,4	1.33	0	6,6,6	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	F	1685	-	4,4,4	1.04	0	6,6,6	0.36	0
2	PO4	B	1685	-	4,4,4	1.25	0	6,6,6	0.71	0
2	PO4	D	1685	-	4,4,4	1.26	0	6,6,6	0.46	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1685	PO4	1	0
2	B	1685	PO4	1	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	666/666 (100%)	-0.20	16 (2%) 59 63	8, 14, 21, 28	0
1	B	666/666 (100%)	-0.33	2 (0%) 90 91	9, 13, 20, 29	0
1	C	666/666 (100%)	-0.27	1 (0%) 91 92	9, 13, 21, 28	0
1	D	666/666 (100%)	-0.38	0 100 100	9, 13, 20, 28	0
1	E	666/666 (100%)	-0.22	2 (0%) 90 91	9, 14, 20, 29	0
1	F	666/666 (100%)	-0.29	1 (0%) 91 92	9, 14, 20, 28	0
All	All	3996/3996 (100%)	-0.28	22 (0%) 85 87	8, 13, 20, 29	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	492	SER	4.1
1	A	436	ALA	4.0
1	A	491	THR	3.0
1	A	437	ALA	2.9
1	A	465	THR	2.9
1	F	491	THR	2.8
1	A	494	LEU	2.8
1	A	490	GLN	2.6
1	A	493	ASP	2.6
1	A	488	ASN	2.4
1	B	245	SER	2.4
1	A	504	GLY	2.3
1	A	430	THR	2.3
1	A	499	LYS	2.3
1	B	264	ASP	2.3
1	E	910	THR	2.3
1	C	682	ASP	2.2
1	A	264	ASP	2.1
1	A	497	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	504	GLY	2.1
1	A	245	SER	2.0
1	A	440	ARG	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 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($\text{\AA}^2$)	Q<0.9
2	PO4	B	1685	5/5	0.95	0.13	32,33,34,36	0
2	PO4	D	1685	5/5	0.95	0.11	36,36,39,39	0
2	PO4	F	1685	5/5	0.95	0.11	38,38,39,40	0
2	PO4	F	1686	5/5	0.95	0.12	39,40,40,42	0
2	PO4	C	1686	5/5	0.96	0.10	32,34,35,36	0
2	PO4	C	1685	5/5	0.96	0.09	32,33,36,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.