



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:11 am GMT

PDB ID : 1AO0
Title : GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE (PRPP) AMIDOTRANSFERASE FROM B. SUBTILIS COMPLEXED WITH ADP AND GMP
Authors : Tomchick, D.R.; Smith, J.L.
Deposited on : 1997-07-15
Resolution : 2.80 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

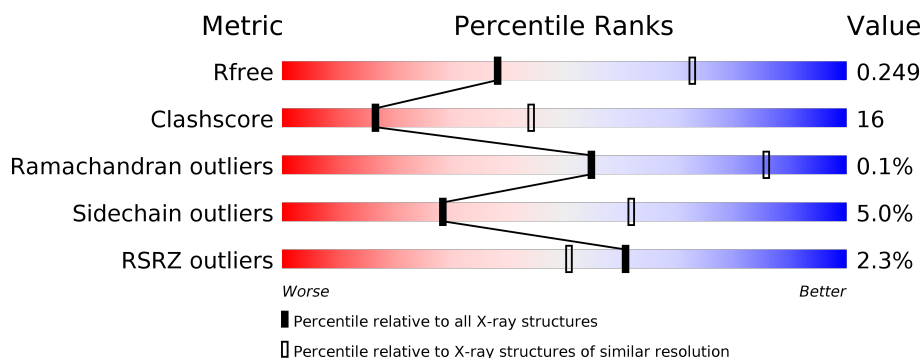
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	459	
1	B	459	
1	C	459	
1	D	459	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14152 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 GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	21	0	0
			3477	2175	609	673	20			
1	B	455	Total	C	N	O	S	44	0	0
			3477	2175	609	673	20			
1	C	455	Total	C	N	O	S	22	0	0
			3477	2175	609	673	20			
1	D	455	Total	C	N	O	S	17	0	0
			3477	2175	609	673	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	402	GLU	GLY	SEQUENCE CORRECTION	UNP P00497
B	402	GLU	GLY	SEQUENCE CORRECTION	UNP P00497
C	402	GLU	GLY	SEQUENCE CORRECTION	UNP P00497
D	402	GLU	GLY	SEQUENCE CORRECTION	UNP P00497

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

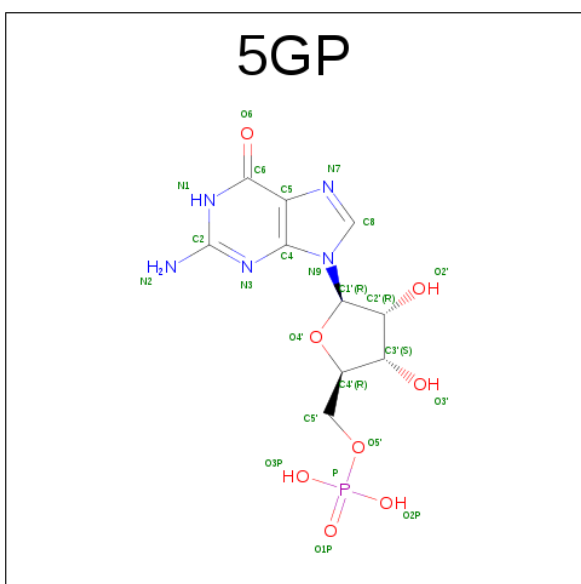
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



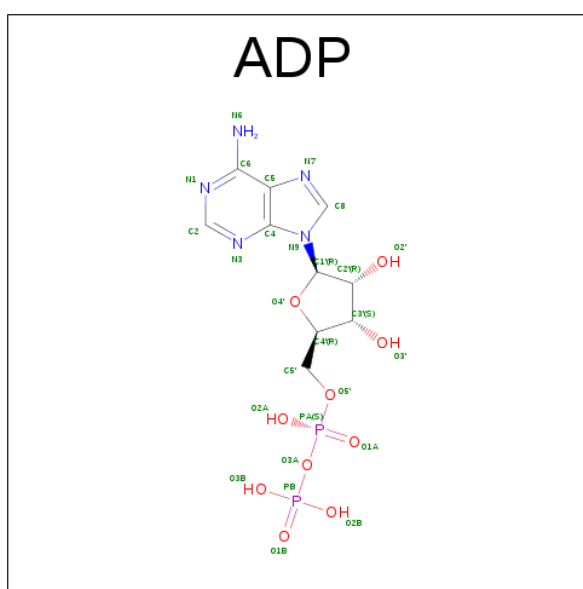
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
4	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
4	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
4	D	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		

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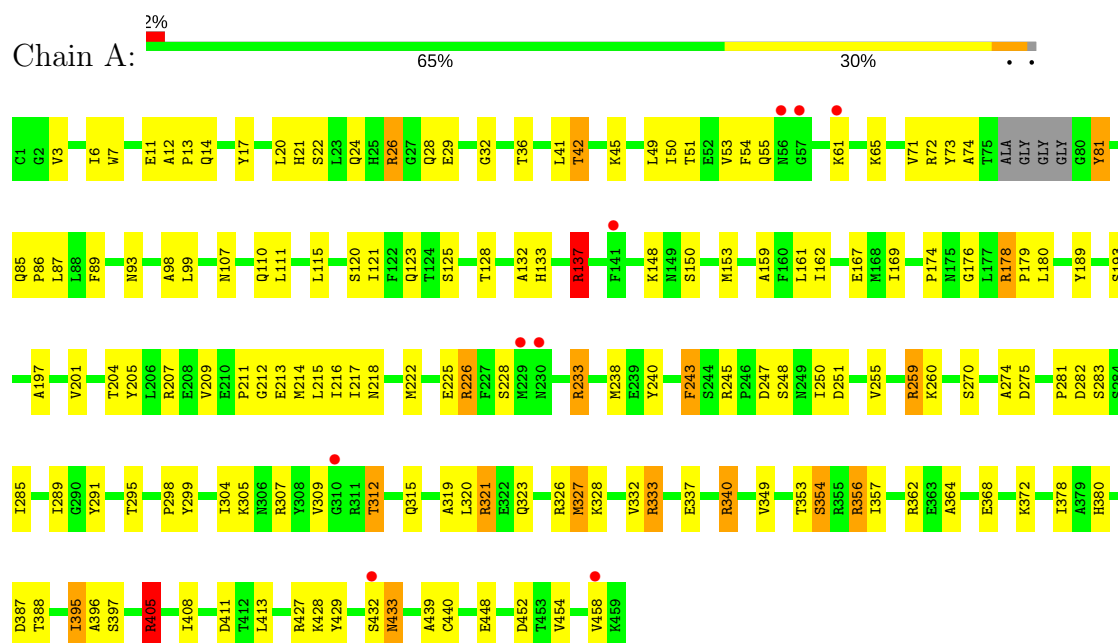
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	O 1	0	0
6	C	1	Total 1	O 1	0	0
6	D	1	Total 1	O 1	0	0

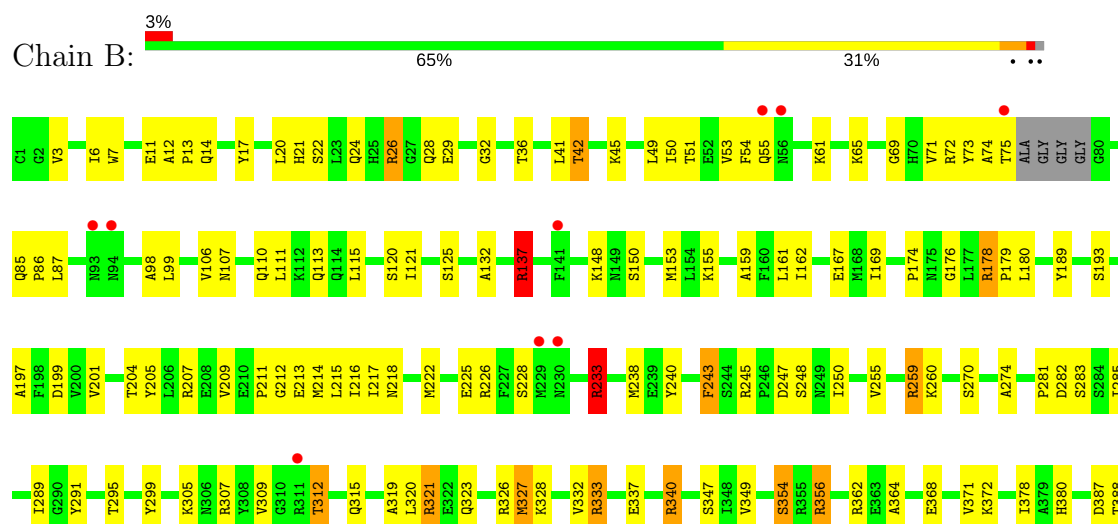
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE

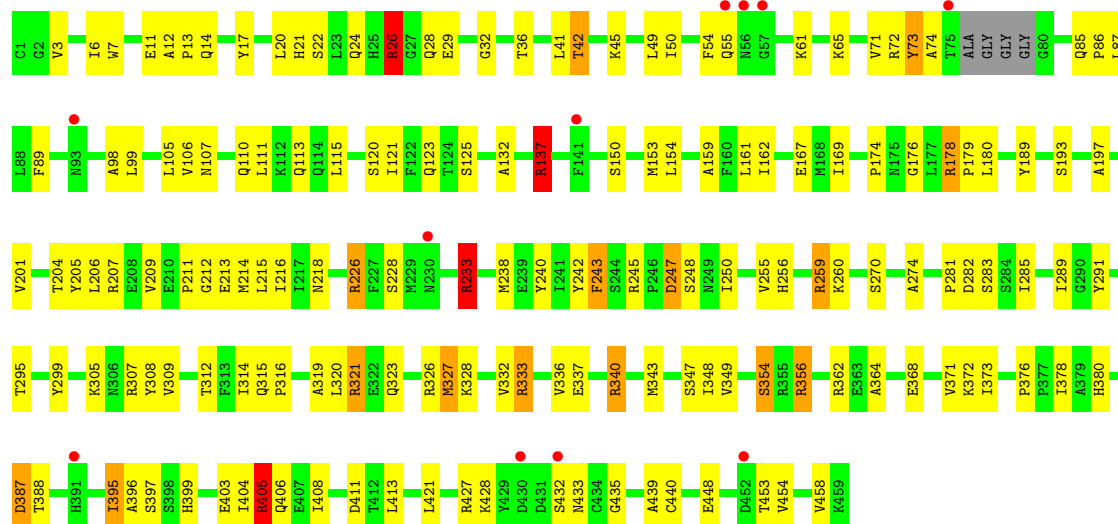


• Molecule 1: GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE

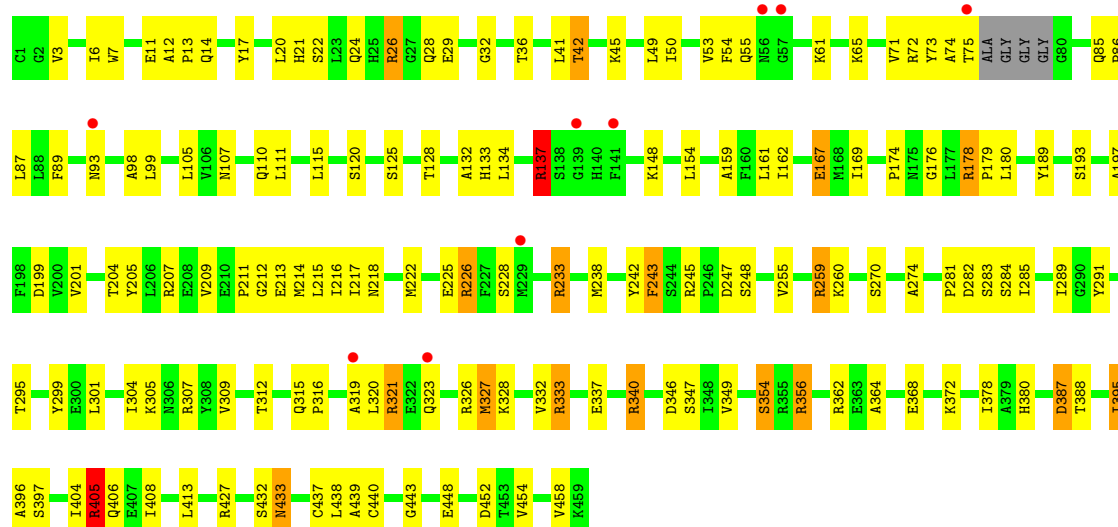




• Molecule 1: GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE



• Molecule 1: GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	160.30Å 70.40Å 182.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 19.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.0 (15.00-2.80) 91.0 (19.97-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.03 (at 2.79Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.214 , 0.264 0.205 , 0.249	Depositor DCC
R_{free} test set	2348 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.821	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14152	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.82% 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: SF4, 5GP, MG, ADP

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	0.70	0/3534	0.74	0/4772
1	B	0.69	0/3534	0.75	0/4772
1	C	0.70	0/3534	0.75	2/4772 (0.0%)
1	D	0.70	0/3534	0.74	0/4772
All	All	0.70	0/14136	0.74	2/19088 (0.0%)

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	A	0	22
1	B	0	22
1	C	0	21
1	D	0	23
All	All	0	88

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	247	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	C	26	ARG	NE-CZ-NH1	-5.30	117.65	120.30

There are no chirality outliers.

All (88) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ARG	Sidechain
1	A	178	ARG	Sidechain
1	A	207	ARG	Sidechain
1	A	226	ARG	Sidechain
1	A	233	ARG	Sidechain
1	A	243	PHE	Sidechain
1	A	245	ARG	Sidechain
1	A	259	ARG	Sidechain
1	A	26	ARG	Sidechain
1	A	299	TYR	Sidechain
1	A	307	ARG	Sidechain
1	A	321	ARG	Sidechain
1	A	326	ARG	Sidechain
1	A	333	ARG	Sidechain
1	A	356	ARG	Sidechain
1	A	362	ARG	Sidechain
1	A	405	ARG	Sidechain
1	A	427	ARG	Sidechain
1	A	429	TYR	Sidechain
1	A	448	GLU	Mainchain
1	A	72	ARG	Sidechain
1	A	73	TYR	Sidechain
1	B	137	ARG	Sidechain
1	B	178	ARG	Sidechain
1	B	207	ARG	Sidechain
1	B	226	ARG	Sidechain
1	B	233	ARG	Sidechain
1	B	243	PHE	Sidechain
1	B	245	ARG	Sidechain
1	B	259	ARG	Sidechain
1	B	26	ARG	Sidechain
1	B	299	TYR	Sidechain
1	B	307	ARG	Sidechain
1	B	321	ARG	Sidechain
1	B	326	ARG	Sidechain
1	B	333	ARG	Sidechain
1	B	356	ARG	Sidechain
1	B	362	ARG	Sidechain
1	B	405	ARG	Sidechain
1	B	427	ARG	Sidechain
1	B	428	LYS	Mainchain
1	B	448	GLU	Mainchain
1	B	72	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	73	TYR	Sidechain
1	C	137	ARG	Sidechain
1	C	178	ARG	Sidechain
1	C	207	ARG	Sidechain
1	C	226	ARG	Sidechain
1	C	233	ARG	Sidechain
1	C	242	TYR	Sidechain
1	C	243	PHE	Sidechain
1	C	245	ARG	Sidechain
1	C	259	ARG	Sidechain
1	C	26	ARG	Sidechain
1	C	299	TYR	Sidechain
1	C	307	ARG	Sidechain
1	C	321	ARG	Sidechain
1	C	326	ARG	Sidechain
1	C	333	ARG	Sidechain
1	C	356	ARG	Sidechain
1	C	362	ARG	Sidechain
1	C	405	ARG	Sidechain
1	C	448	GLU	Mainchain
1	C	72	ARG	Sidechain
1	C	73	TYR	Sidechain
1	D	137	ARG	Sidechain
1	D	167	GLU	Mainchain
1	D	178	ARG	Sidechain
1	D	207	ARG	Sidechain
1	D	226	ARG	Sidechain
1	D	233	ARG	Sidechain
1	D	242	TYR	Sidechain
1	D	243	PHE	Sidechain
1	D	245	ARG	Sidechain
1	D	259	ARG	Sidechain
1	D	26	ARG	Sidechain
1	D	299	TYR	Sidechain
1	D	307	ARG	Sidechain
1	D	321	ARG	Sidechain
1	D	326	ARG	Sidechain
1	D	333	ARG	Sidechain
1	D	356	ARG	Sidechain
1	D	362	ARG	Sidechain
1	D	405	ARG	Sidechain,Mainchain
1	D	448	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	D	72	ARG	Sidechain
1	D	73	TYR	Sidechain

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	3477	0	3459	120	0
1	B	3477	0	3459	110	0
1	C	3477	0	3459	124	0
1	D	3477	0	3459	118	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	8	0	0	1	0
3	B	8	0	0	1	0
3	C	8	0	0	1	0
3	D	8	0	0	1	0
4	A	24	0	11	2	0
4	B	24	0	11	3	0
4	C	24	0	11	3	0
4	D	24	0	11	6	0
5	A	27	0	12	1	0
5	B	27	0	12	2	0
5	C	27	0	12	1	0
5	D	27	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	14152	0	13928	443	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 16.

All (443) 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:A:137:ARG:NH2	1:C:137:ARG:HH22	1.49	1.10
1:A:137:ARG:HH22	1:C:137:ARG:NH2	1.50	1.08
1:A:20:LEU:HD22	1:A:71:VAL:HG23	1.52	0.92
1:A:340:ARG:HB2	1:A:368:GLU:HB2	1.52	0.91
1:B:20:LEU:HD22	1:B:71:VAL:HG23	1.54	0.89
1:C:20:LEU:HD22	1:C:71:VAL:HG23	1.55	0.89
1:D:20:LEU:HD22	1:D:71:VAL:HG23	1.54	0.88
1:C:340:ARG:HB2	1:C:368:GLU:HB2	1.58	0.85
1:D:99:LEU:HD23	1:D:162:ILE:HG12	1.59	0.84
1:B:99:LEU:HD23	1:B:162:ILE:HG12	1.57	0.84
1:B:340:ARG:HB2	1:B:368:GLU:HB2	1.60	0.84
1:B:137:ARG:HH22	1:D:137:ARG:HH22	1.25	0.83
1:D:340:ARG:HB2	1:D:368:GLU:HB2	1.59	0.82
1:B:333:ARG:HH11	1:B:337:GLU:HG3	1.46	0.81
1:A:99:LEU:HD23	1:A:162:ILE:HG12	1.63	0.80
1:C:99:LEU:HD23	1:C:162:ILE:HG12	1.61	0.80
1:C:333:ARG:HH21	1:C:337:GLU:HG3	1.47	0.79
1:D:315:GLN:HE22	1:D:327:MET:HG2	1.47	0.79
1:D:36:THR:HB	1:D:41:LEU:HD22	1.64	0.78
1:A:332:VAL:HG22	1:B:247:ASP:HB3	1.64	0.78
1:D:333:ARG:HH21	1:D:337:GLU:HG3	1.47	0.78
1:A:333:ARG:HH21	1:A:337:GLU:HG3	1.48	0.78
1:C:332:VAL:HG22	1:D:247:ASP:HB3	1.66	0.77
1:C:36:THR:HB	1:C:41:LEU:HD22	1.67	0.76
1:B:427:ARG:HB3	1:B:434:CYS:HB3	1.68	0.76
1:B:36:THR:HB	1:B:41:LEU:HD22	1.66	0.75
1:A:36:THR:HB	1:A:41:LEU:HD22	1.66	0.75
1:A:315:GLN:HE22	1:A:327:MET:HG2	1.51	0.75
1:A:26:ARG:NH1	1:A:243:PHE:HD2	1.84	0.75
1:B:315:GLN:HE22	1:B:327:MET:HG2	1.51	0.74
1:D:3:VAL:HB	1:D:161:LEU:HD12	1.69	0.73
1:C:26:ARG:NH1	1:C:243:PHE:HD2	1.87	0.73
1:C:3:VAL:HB	1:C:161:LEU:HD12	1.69	0.73
1:A:93:ASN:HD21	1:C:113:GLN:HG2	1.52	0.73
1:D:26:ARG:NH1	1:D:243:PHE:HD2	1.87	0.73
1:A:137:ARG:HH22	1:C:137:ARG:HH22	0.77	0.72
1:B:29:GLU:HG3	1:B:74:ALA:H	1.54	0.72
1:C:315:GLN:HE22	1:C:327:MET:HG2	1.54	0.72
1:D:29:GLU:HG3	1:D:74:ALA:H	1.56	0.71
1:A:3:VAL:HB	1:A:161:LEU:HD12	1.72	0.71
1:B:3:VAL:HB	1:B:161:LEU:HD12	1.71	0.71
1:B:26:ARG:NH1	1:B:243:PHE:HD2	1.88	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:GLU:HG3	1:D:74:ALA:N	2.05	0.70
1:B:29:GLU:HG3	1:B:74:ALA:N	2.07	0.70
1:A:29:GLU:HG3	1:A:74:ALA:N	2.09	0.68
1:D:178:ARG:HH22	1:D:388:THR:HG21	1.57	0.68
1:D:319:ALA:O	1:D:323:GLN:HG2	1.96	0.66
1:A:178:ARG:HH22	1:A:388:THR:HG21	1.60	0.66
1:B:137:ARG:HH22	1:D:137:ARG:NH2	1.93	0.66
1:A:270:SER:O	1:A:372:LYS:HE3	1.95	0.65
1:B:270:SER:O	1:B:372:LYS:HE3	1.96	0.65
1:B:21:HIS:HA	1:B:50:ILE:HD12	1.78	0.65
1:C:21:HIS:HA	1:C:50:ILE:HD12	1.78	0.65
4:B:467:5GP:H1'	5:B:468:ADP:O1B	1.97	0.65
1:D:270:SER:O	1:D:372:LYS:HE3	1.97	0.65
1:C:270:SER:O	1:C:372:LYS:HE3	1.97	0.64
1:D:378:ILE:O	1:D:396:ALA:HB3	1.97	0.64
1:A:319:ALA:O	1:A:323:GLN:HG2	1.98	0.64
1:B:178:ARG:HH22	1:B:388:THR:HG21	1.63	0.64
1:B:214:MET:HE2	1:B:216:ILE:HD11	1.80	0.64
1:C:332:VAL:HG22	1:D:247:ASP:CB	2.28	0.64
1:C:378:ILE:O	1:C:396:ALA:HB3	1.98	0.64
1:C:178:ARG:HH22	1:C:388:THR:HG21	1.62	0.63
1:C:85:GLN:HB3	1:C:86:PRO:HA	1.80	0.63
1:C:319:ALA:O	1:C:323:GLN:HG2	1.98	0.63
4:A:467:5GP:H1'	5:A:468:ADP:O1B	1.98	0.63
1:A:247:ASP:HB3	1:B:332:VAL:HG22	1.80	0.62
1:B:107:ASN:ND2	1:B:111:LEU:HD11	2.14	0.62
1:A:214:MET:CE	1:A:216:ILE:HD11	2.30	0.62
4:D:467:5GP:H1'	5:D:468:ADP:O3B	1.99	0.62
1:C:214:MET:HE2	1:C:216:ILE:HD11	1.82	0.62
1:A:85:GLN:HB3	1:A:86:PRO:HA	1.81	0.61
1:B:319:ALA:O	1:B:323:GLN:HG2	1.99	0.61
4:C:467:5GP:H1'	5:C:468:ADP:O3B	2.00	0.61
1:C:24:GLN:OE1	1:C:50:ILE:HG13	2.00	0.61
1:D:214:MET:CE	1:D:216:ILE:HD11	2.30	0.61
1:B:85:GLN:HB3	1:B:86:PRO:HA	1.82	0.60
1:B:137:ARG:NH2	1:D:137:ARG:HH22	1.97	0.60
1:B:99:LEU:CD2	1:B:162:ILE:HG12	2.30	0.60
1:A:24:GLN:OE1	1:A:50:ILE:HG13	2.01	0.60
1:A:26:ARG:NH1	1:A:243:PHE:CD2	2.68	0.60
1:D:21:HIS:HA	1:D:50:ILE:HD12	1.84	0.60
1:A:214:MET:HE2	1:A:216:ILE:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:MET:CE	1:B:216:ILE:HD11	2.32	0.60
1:B:169:ILE:HG12	1:B:216:ILE:HG13	1.84	0.59
1:A:21:HIS:HA	1:A:50:ILE:HD12	1.84	0.59
1:A:349:VAL:O	1:A:395:ILE:HG22	2.02	0.59
1:B:305:LYS:HD2	1:B:328:LYS:HE2	1.85	0.59
1:D:85:GLN:HB3	1:D:86:PRO:HA	1.83	0.59
1:A:26:ARG:HH11	1:A:243:PHE:HD2	1.48	0.59
1:D:26:ARG:NH1	1:D:243:PHE:CD2	2.71	0.59
1:C:214:MET:CE	1:C:216:ILE:HD11	2.33	0.59
1:C:179:PRO:HG2	1:C:193:SER:O	2.03	0.59
1:B:179:PRO:HG2	1:B:193:SER:O	2.02	0.59
1:B:24:GLN:OE1	1:B:50:ILE:HG13	2.03	0.59
1:A:29:GLU:HG3	1:A:74:ALA:HB3	1.85	0.58
1:D:333:ARG:NH2	1:D:337:GLU:HG3	2.17	0.58
1:A:378:ILE:O	1:A:396:ALA:HB3	2.03	0.58
1:C:99:LEU:CD2	1:C:162:ILE:HG12	2.33	0.58
1:C:29:GLU:HG3	1:C:74:ALA:N	2.18	0.58
1:D:214:MET:HE2	1:D:216:ILE:HD11	1.85	0.58
1:C:247:ASP:HB3	1:D:332:VAL:HG22	1.84	0.58
1:B:349:VAL:O	1:B:395:ILE:HG22	2.04	0.58
1:A:305:LYS:HD2	1:A:328:LYS:HE2	1.86	0.58
1:A:107:ASN:ND2	1:A:111:LEU:HD11	2.18	0.58
1:D:26:ARG:HH11	1:D:243:PHE:HD2	1.51	0.58
1:B:26:ARG:NH1	1:B:243:PHE:CD2	2.72	0.57
1:D:204:THR:HG22	1:D:205:TYR:O	2.04	0.57
1:B:204:THR:HG22	1:B:205:TYR:O	2.04	0.57
1:C:399:HIS:HA	1:C:403:GLU:OE1	2.04	0.57
1:B:26:ARG:HH11	1:B:243:PHE:HD2	1.50	0.57
1:C:405:ARG:HH12	1:C:406:GLN:HG2	1.70	0.57
1:D:32:GLY:HA3	1:D:45:LYS:HB2	1.86	0.57
1:D:274:ALA:HA	1:D:340:ARG:HG3	1.86	0.57
1:C:428:LYS:HE2	1:C:428:LYS:HA	1.87	0.57
1:C:204:THR:HG22	1:C:205:TYR:O	2.05	0.57
1:D:99:LEU:CD2	1:D:162:ILE:HG12	2.32	0.57
1:C:209:VAL:HG22	1:C:215:LEU:HD11	1.87	0.56
1:A:99:LEU:CD2	1:A:162:ILE:HG12	2.34	0.56
1:C:26:ARG:HH11	1:C:243:PHE:HD2	1.53	0.56
1:C:213:GLU:HG2	1:C:214:MET:N	2.20	0.56
1:C:107:ASN:ND2	1:C:111:LEU:HD11	2.21	0.56
1:D:349:VAL:O	1:D:395:ILE:HG22	2.05	0.56
1:D:347:SER:OG	4:D:467:5GP:H3'	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLU:HG3	1:A:74:ALA:H	1.70	0.56
1:C:349:VAL:O	1:C:395:ILE:HG22	2.06	0.56
1:D:24:GLN:OE1	1:D:50:ILE:HG13	2.06	0.56
1:D:238:MET:CE	4:D:467:5GP:N2	2.69	0.56
1:C:26:ARG:NH1	1:C:243:PHE:CD2	2.72	0.56
1:A:332:VAL:HG22	1:B:247:ASP:CB	2.36	0.55
1:D:179:PRO:HG2	1:D:193:SER:O	2.05	0.55
1:C:305:LYS:HD2	1:C:328:LYS:HE2	1.89	0.55
1:D:107:ASN:ND2	1:D:111:LEU:HD11	2.22	0.55
1:A:333:ARG:HB2	1:A:364:ALA:O	2.06	0.55
1:B:274:ALA:HA	1:B:340:ARG:HG3	1.87	0.55
1:D:291:TYR:CE1	1:D:295:THR:HG21	2.42	0.54
1:A:312:THR:HB	1:B:51:THR:HB	1.89	0.54
1:B:291:TYR:CE1	1:B:295:THR:HG21	2.42	0.54
1:C:333:ARG:CB	1:C:364:ALA:HB1	2.37	0.54
1:C:333:ARG:NH2	1:C:337:GLU:HG3	2.19	0.54
1:A:179:PRO:HG2	1:A:193:SER:O	2.08	0.54
1:B:378:ILE:O	1:B:396:ALA:HB3	2.08	0.54
1:A:333:ARG:NH2	1:A:337:GLU:HG3	2.21	0.54
1:C:274:ALA:HA	1:C:340:ARG:HG3	1.89	0.54
1:D:439:ALA:HB3	3:D:466:SF4:S2	2.47	0.54
1:B:107:ASN:CG	1:B:111:LEU:HD11	2.28	0.54
1:B:11:GLU:HB3	1:B:14:GLN:HE21	1.72	0.54
1:C:333:ARG:HB2	1:C:364:ALA:O	2.08	0.53
1:C:21:HIS:HA	1:C:50:ILE:CD1	2.38	0.53
1:C:11:GLU:HB3	1:C:14:GLN:HE21	1.73	0.53
1:C:320:LEU:HA	1:C:323:GLN:HG2	1.90	0.53
1:B:333:ARG:NH1	1:B:337:GLU:HG3	2.19	0.53
1:C:256:HIS:CE1	1:D:301:LEU:HG	2.43	0.53
1:B:107:ASN:O	1:B:111:LEU:HD12	2.09	0.53
1:B:333:ARG:HB2	1:B:364:ALA:O	2.09	0.53
1:C:333:ARG:HB3	1:C:364:ALA:HB1	1.90	0.53
1:A:32:GLY:HA3	1:A:45:LYS:HB2	1.91	0.53
1:B:333:ARG:CB	1:B:364:ALA:HB1	2.39	0.53
1:A:87:LEU:O	1:A:98:ALA:HA	2.10	0.52
1:B:213:GLU:HG2	1:B:214:MET:N	2.24	0.52
1:D:213:GLU:HG2	1:D:214:MET:N	2.23	0.52
1:A:169:ILE:HG12	1:A:216:ILE:HG13	1.91	0.52
1:B:87:LEU:O	1:B:98:ALA:HA	2.09	0.52
1:D:169:ILE:HG12	1:D:216:ILE:HG13	1.89	0.52
1:B:197:ALA:O	1:B:201:VAL:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:LEU:HA	1:B:323:GLN:HG2	1.90	0.52
1:D:11:GLU:HB3	1:D:14:GLN:HE21	1.74	0.52
1:C:107:ASN:O	1:C:111:LEU:HD12	2.10	0.52
1:A:439:ALA:HB3	3:A:466:SF4:S2	2.50	0.52
1:B:21:HIS:HA	1:B:50:ILE:CD1	2.39	0.52
1:A:274:ALA:HA	1:A:340:ARG:HG3	1.92	0.52
1:B:427:ARG:HB3	1:B:434:CYS:CB	2.39	0.52
1:D:87:LEU:O	1:D:98:ALA:HA	2.10	0.52
1:A:11:GLU:HB3	1:A:14:GLN:HE21	1.74	0.51
1:B:427:ARG:HD3	1:B:436:GLN:OE1	2.10	0.51
1:D:309:VAL:O	1:D:309:VAL:HG12	2.11	0.51
1:D:320:LEU:HA	1:D:323:GLN:HG2	1.90	0.51
1:D:305:LYS:HD2	1:D:328:LYS:HE2	1.92	0.51
1:A:320:LEU:HA	1:A:323:GLN:HG2	1.92	0.51
1:D:107:ASN:O	1:D:111:LEU:HD12	2.11	0.51
1:A:333:ARG:HB3	1:A:364:ALA:HB1	1.92	0.51
1:B:167:GLU:HG2	1:B:218:ASN:HB3	1.93	0.51
1:D:333:ARG:HB2	1:D:364:ALA:O	2.10	0.51
1:A:243:PHE:CZ	1:A:387:ASP:HB2	2.46	0.51
1:A:327:MET:HE1	1:A:356:ARG:HH11	1.76	0.51
1:B:209:VAL:HG22	1:B:215:LEU:HD11	1.93	0.51
1:A:176:GLY:N	1:A:211:PRO:HB3	2.26	0.50
1:A:29:GLU:CB	1:A:74:ALA:HB3	2.41	0.50
1:A:51:THR:HB	1:B:312:THR:HB	1.93	0.50
1:A:333:ARG:CB	1:A:364:ALA:HB1	2.42	0.50
1:B:333:ARG:HB3	1:B:364:ALA:HB1	1.92	0.50
1:D:167:GLU:HG2	1:D:218:ASN:HB3	1.93	0.50
1:D:255:VAL:HG12	1:D:259:ARG:HD2	1.94	0.50
1:A:204:THR:HG22	1:A:205:TYR:O	2.11	0.50
1:A:260:LYS:HE3	1:A:289:ILE:HG22	1.93	0.50
1:B:32:GLY:HA3	1:B:45:LYS:HB2	1.93	0.50
1:C:169:ILE:HG12	1:C:216:ILE:HG13	1.93	0.50
1:C:347:SER:OG	4:C:467:5GP:H3'	2.12	0.50
1:D:159:ALA:HB1	1:D:180:LEU:HD22	1.93	0.50
1:C:32:GLY:HA3	1:C:45:LYS:HB2	1.94	0.50
1:D:248:SER:O	1:D:255:VAL:HG23	2.12	0.50
1:B:439:ALA:HB3	3:B:466:SF4:S2	2.52	0.49
1:C:6:ILE:HA	1:C:189:TYR:O	2.12	0.49
1:C:107:ASN:CG	1:C:111:LEU:HD11	2.33	0.49
1:D:333:ARG:HB3	1:D:364:ALA:HB1	1.94	0.49
1:B:255:VAL:HG12	1:B:259:ARG:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:MET:HE1	1:C:356:ARG:HH11	1.77	0.49
1:C:87:LEU:O	1:C:98:ALA:HA	2.12	0.49
1:A:213:GLU:HG2	1:A:214:MET:N	2.28	0.49
1:C:22:SER:OG	1:C:197:ALA:HA	2.13	0.49
1:D:243:PHE:CZ	1:D:387:ASP:HB2	2.47	0.49
1:C:14:GLN:NE2	1:C:14:GLN:H	2.10	0.49
1:C:291:TYR:CE1	1:C:295:THR:HG21	2.47	0.49
1:C:314:ILE:HD11	1:D:55:GLN:HE21	1.78	0.49
1:D:6:ILE:HA	1:D:189:TYR:O	2.13	0.49
1:B:6:ILE:HA	1:B:189:TYR:O	2.13	0.49
1:C:12:ALA:N	1:C:13:PRO:HD2	2.28	0.49
1:D:333:ARG:CB	1:D:364:ALA:HB1	2.42	0.49
1:B:248:SER:O	1:B:255:VAL:HG23	2.13	0.48
1:B:243:PHE:CZ	1:B:387:ASP:HB2	2.48	0.48
1:A:6:ILE:HA	1:A:189:TYR:O	2.13	0.48
1:A:89:PHE:CE1	1:C:123:GLN:HG2	2.49	0.48
1:C:243:PHE:CZ	1:C:387:ASP:HB2	2.48	0.48
1:D:107:ASN:CG	1:D:111:LEU:HD11	2.33	0.48
1:D:209:VAL:HG22	1:D:215:LEU:HD11	1.94	0.48
1:A:29:GLU:CG	1:A:74:ALA:HB3	2.43	0.48
1:A:107:ASN:O	1:A:111:LEU:HD12	2.14	0.48
1:A:255:VAL:HG12	1:A:259:ARG:HD2	1.95	0.48
1:D:197:ALA:O	1:D:201:VAL:HG22	2.14	0.48
1:A:14:GLN:H	1:A:14:GLN:NE2	2.11	0.48
1:A:340:ARG:CB	1:A:368:GLU:HB2	2.33	0.48
1:D:29:GLU:CB	1:D:74:ALA:HB3	2.43	0.48
1:D:349:VAL:HB	4:D:467:5GP:O2P	2.13	0.48
1:A:22:SER:OG	1:A:197:ALA:HA	2.13	0.48
1:C:176:GLY:N	1:C:211:PRO:HB3	2.29	0.48
1:C:308:TYR:HB2	1:D:21:HIS:CE1	2.49	0.47
1:A:107:ASN:CG	1:A:111:LEU:HD11	2.34	0.47
1:B:371:VAL:HG21	1:B:408:ILE:HD12	1.96	0.47
1:D:14:GLN:NE2	1:D:14:GLN:H	2.12	0.47
1:D:29:GLU:HG3	1:D:74:ALA:HB3	1.96	0.47
1:A:309:VAL:HG12	1:A:309:VAL:O	2.14	0.47
1:C:167:GLU:HG2	1:C:218:ASN:HB3	1.95	0.47
1:D:21:HIS:HA	1:D:50:ILE:CD1	2.44	0.47
1:B:309:VAL:O	1:B:309:VAL:HG12	2.15	0.47
1:A:353:THR:O	1:A:357:ILE:HG13	2.15	0.47
1:B:354:SER:HB2	1:B:408:ILE:HG21	1.95	0.47
1:A:327:MET:HE1	1:A:356:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:HG2	1:A:218:ASN:HB3	1.96	0.47
1:A:89:PHE:HE1	1:C:123:GLN:HG2	1.80	0.47
1:D:238:MET:HE2	4:D:467:5GP:N2	2.30	0.47
1:C:54:PHE:O	1:C:55:GLN:HB2	2.15	0.47
1:C:247:ASP:CB	1:D:332:VAL:HG22	2.45	0.47
1:A:217:ILE:HG13	1:A:222:MET:HG3	1.95	0.47
1:A:291:TYR:CE1	1:A:295:THR:HG21	2.51	0.47
1:A:21:HIS:HA	1:A:50:ILE:CD1	2.44	0.47
1:B:281:PRO:HA	1:B:282:ASP:HA	1.46	0.47
1:D:226:ARG:HA	1:D:226:ARG:HD2	1.72	0.47
1:A:428:LYS:HE2	1:A:428:LYS:HA	1.97	0.46
1:C:28:GLN:HB3	1:C:49:LEU:HD23	1.97	0.46
1:B:53:VAL:HG12	1:B:54:PHE:CE1	2.50	0.46
1:A:380:HIS:HB2	1:A:440:CYS:HA	1.97	0.46
1:B:12:ALA:N	1:B:13:PRO:HD2	2.30	0.46
1:D:115:LEU:O	1:D:120:SER:HB2	2.15	0.46
1:A:214:MET:HE3	1:A:216:ILE:HD11	1.98	0.46
1:D:36:THR:CB	1:D:41:LEU:HD22	2.39	0.46
1:D:53:VAL:HG12	1:D:54:PHE:CE1	2.51	0.46
1:B:14:GLN:H	1:B:14:GLN:NE2	2.14	0.46
1:C:405:ARG:HG2	1:C:413:LEU:HB2	1.96	0.46
1:D:105:LEU:HD13	1:D:154:LEU:HD22	1.96	0.46
1:B:217:ILE:HG13	1:B:222:MET:HG3	1.97	0.46
1:B:260:LYS:HE3	1:B:289:ILE:HG22	1.96	0.46
1:D:454:VAL:HB	1:D:458:VAL:HB	1.97	0.46
1:B:22:SER:OG	1:B:197:ALA:HA	2.16	0.46
1:C:99:LEU:CD1	1:C:132:ALA:HB2	2.46	0.46
1:D:176:GLY:N	1:D:211:PRO:HB3	2.31	0.46
1:A:209:VAL:HG22	1:A:215:LEU:HD11	1.97	0.46
1:C:260:LYS:HE3	1:C:289:ILE:HG22	1.98	0.46
1:A:81:TYR:CD1	1:A:81:TYR:C	2.89	0.46
1:C:439:ALA:HB3	3:C:466:SF4:S2	2.56	0.46
1:A:304:ILE:HG23	5:B:468:ADP:N1	2.32	0.45
1:C:327:MET:HE1	1:C:356:ARG:NH1	2.31	0.45
1:D:217:ILE:HG13	1:D:222:MET:HG3	1.97	0.45
1:C:332:VAL:CG2	1:D:247:ASP:HB3	2.41	0.45
1:A:197:ALA:O	1:A:201:VAL:HG22	2.16	0.45
1:C:405:ARG:NH1	1:C:406:GLN:HG2	2.31	0.45
1:D:354:SER:HB2	1:D:408:ILE:HG21	1.96	0.45
1:B:233:ARG:O	1:B:435:GLY:HA2	2.16	0.45
1:C:14:GLN:O	1:C:17:TYR:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:SER:HA	1:C:153:MET:HE3	1.99	0.45
1:C:327:MET:HB2	1:C:327:MET:HE2	1.90	0.45
1:C:454:VAL:HB	1:C:458:VAL:HB	1.97	0.45
1:C:281:PRO:HA	1:C:282:ASP:HA	1.46	0.45
1:D:214:MET:HE3	1:D:216:ILE:HD11	1.98	0.45
1:A:148:LYS:HD2	1:A:225:GLU:OE2	2.17	0.45
1:B:327:MET:HE1	1:B:356:ARG:HH11	1.81	0.45
1:C:238:MET:CE	4:C:467:5GP:N2	2.80	0.45
1:A:159:ALA:HB1	1:A:180:LEU:HD22	1.99	0.45
1:B:454:VAL:HB	1:B:458:VAL:HB	1.98	0.45
1:D:327:MET:HE1	1:D:356:ARG:HH11	1.81	0.45
1:B:14:GLN:O	1:B:17:TYR:HB3	2.17	0.45
1:C:255:VAL:HG12	1:C:259:ARG:HD2	1.98	0.45
1:D:22:SER:OG	1:D:197:ALA:HA	2.16	0.45
1:A:14:GLN:O	1:A:17:TYR:HB3	2.17	0.45
1:A:54:PHE:O	1:A:55:GLN:HB2	2.17	0.45
1:C:309:VAL:HG12	1:C:309:VAL:O	2.17	0.45
1:D:28:GLN:HB3	1:D:49:LEU:HD23	2.00	0.45
1:A:99:LEU:HD23	1:A:162:ILE:HG23	1.99	0.44
1:B:113:GLN:HG2	1:D:93:ASN:HD21	1.82	0.44
1:A:354:SER:HB2	1:A:408:ILE:HG21	1.99	0.44
1:A:99:LEU:HB2	1:A:128:THR:CG2	2.47	0.44
1:B:176:GLY:N	1:B:211:PRO:HB3	2.32	0.44
1:B:327:MET:HE1	1:B:356:ARG:NH1	2.33	0.44
1:B:53:VAL:HG12	1:B:54:PHE:CD1	2.52	0.44
1:C:206:LEU:HA	1:C:206:LEU:HD12	1.82	0.44
1:D:107:ASN:O	1:D:110:GLN:HB2	2.17	0.44
1:D:42:THR:HG21	1:D:61:LYS:O	2.17	0.44
1:A:275:ASP:O	1:A:298:PRO:HD2	2.17	0.44
1:D:115:LEU:HD11	1:D:134:LEU:HD23	1.99	0.44
1:D:284:SER:HB3	1:D:346:ASP:H	1.82	0.44
1:B:99:LEU:HD23	1:B:162:ILE:HG23	2.00	0.44
1:A:12:ALA:N	1:A:13:PRO:HD2	2.31	0.44
1:A:281:PRO:HA	1:A:282:ASP:HA	1.49	0.44
1:D:54:PHE:O	1:D:55:GLN:HB2	2.18	0.44
1:D:327:MET:HB2	1:D:327:MET:HE2	1.90	0.44
1:A:454:VAL:HB	1:A:458:VAL:HB	2.00	0.44
1:B:405:ARG:HD3	1:B:412:THR:HA	1.99	0.44
1:B:148:LYS:HD2	1:B:225:GLU:OE2	2.18	0.43
1:B:240:TYR:CE1	1:B:250:ILE:HB	2.53	0.43
1:A:247:ASP:CB	1:B:332:VAL:HG22	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:HIS:HB2	1:B:440:CYS:HA	1.99	0.43
1:C:368:GLU:HA	1:C:411:ASP:OD2	2.18	0.43
1:C:7:TRP:CZ2	1:C:65:LYS:HE3	2.53	0.43
1:B:347:SER:OG	4:B:467:5GP:H3'	2.18	0.43
1:C:233:ARG:O	1:C:435:GLY:HA2	2.18	0.43
1:C:248:SER:O	1:C:255:VAL:HG23	2.18	0.43
1:C:380:HIS:HB2	1:C:440:CYS:HA	1.99	0.43
1:C:42:THR:HG21	1:C:61:LYS:O	2.17	0.43
1:A:123:GLN:HG2	1:C:89:PHE:CE1	2.53	0.43
1:C:399:HIS:HB3	1:C:403:GLU:HB2	2.01	0.43
1:D:148:LYS:HD2	1:D:225:GLU:OE2	2.18	0.43
1:D:340:ARG:CB	1:D:368:GLU:HB2	2.40	0.43
1:A:174:PRO:HA	1:A:212:GLY:N	2.33	0.43
1:C:340:ARG:CB	1:C:368:GLU:HB2	2.38	0.43
1:D:380:HIS:HB2	1:D:440:CYS:HA	1.99	0.43
1:A:110:GLN:HG3	1:A:452:ASP:OD2	2.18	0.43
1:A:29:GLU:HG3	1:A:74:ALA:CA	2.48	0.43
1:C:395:ILE:HG12	1:C:404:ILE:HG12	1.99	0.43
1:C:115:LEU:O	1:C:120:SER:HB2	2.19	0.43
1:A:133:HIS:CD2	1:C:121:ILE:HG13	2.54	0.43
1:D:99:LEU:CD1	1:D:132:ALA:HB2	2.48	0.43
1:A:238:MET:CE	4:A:467:5GP:N2	2.82	0.43
1:B:238:MET:CE	4:B:467:5GP:N2	2.81	0.43
1:D:99:LEU:HD23	1:D:162:ILE:HG23	2.01	0.43
1:B:20:LEU:HD11	1:B:69:GLY:HA3	2.00	0.43
1:C:29:GLU:HG3	1:C:74:ALA:H	1.81	0.43
1:D:238:MET:HE2	4:D:467:5GP:HN21	1.84	0.43
1:C:320:LEU:HA	1:C:323:GLN:CG	2.49	0.43
1:D:260:LYS:HE3	1:D:289:ILE:HG22	2.01	0.43
1:D:405:ARG:HH21	1:D:406:GLN:HG2	1.84	0.43
1:A:24:GLN:O	1:A:24:GLN:HG3	2.19	0.42
1:A:29:GLU:HG3	1:A:74:ALA:CB	2.47	0.42
1:B:115:LEU:O	1:B:120:SER:HB2	2.18	0.42
1:B:320:LEU:HA	1:B:323:GLN:CG	2.49	0.42
1:B:327:MET:HB2	1:B:327:MET:HE2	1.88	0.42
1:C:197:ALA:O	1:C:201:VAL:HG22	2.19	0.42
1:D:404:ILE:HG22	1:D:413:LEU:CD2	2.49	0.42
1:A:85:GLN:HB3	1:A:86:PRO:CA	2.48	0.42
1:B:42:THR:HG21	1:B:61:LYS:O	2.18	0.42
1:C:247:ASP:HB3	1:D:304:ILE:HG13	2.01	0.42
1:D:281:PRO:HA	1:D:282:ASP:HA	1.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:MET:HE1	1:D:356:ARG:NH1	2.33	0.42
1:A:107:ASN:O	1:A:110:GLN:HB2	2.20	0.42
1:A:81:TYR:CD1	1:A:81:TYR:O	2.72	0.42
1:B:121:ILE:CD1	1:D:133:HIS:HD2	2.32	0.42
1:C:226:ARG:HA	1:C:226:ARG:HD2	1.73	0.42
1:D:110:GLN:HG3	1:D:452:ASP:OD2	2.19	0.42
1:A:368:GLU:HA	1:A:411:ASP:OD2	2.20	0.42
1:B:159:ALA:HB1	1:B:180:LEU:HD22	2.01	0.42
1:A:226:ARG:HD2	1:A:226:ARG:HA	1.72	0.42
1:B:110:GLN:HG3	1:B:452:ASP:OD2	2.20	0.42
1:B:99:LEU:CD1	1:B:132:ALA:HB2	2.50	0.42
1:C:333:ARG:HA	1:C:336:VAL:HG22	2.01	0.42
1:D:433:ASN:HD22	1:D:433:ASN:C	2.23	0.42
1:A:28:GLN:HB3	1:A:49:LEU:HD23	2.02	0.42
1:D:99:LEU:HB2	1:D:128:THR:CG2	2.50	0.42
1:D:12:ALA:N	1:D:13:PRO:HD2	2.34	0.42
1:A:248:SER:O	1:A:255:VAL:HG23	2.20	0.42
1:B:11:GLU:HB3	1:B:14:GLN:NE2	2.35	0.42
1:B:150:SER:HA	1:B:153:MET:HE3	2.02	0.42
1:C:174:PRO:HA	1:C:212:GLY:N	2.35	0.42
1:C:376:PRO:HD3	1:C:421:LEU:HD22	2.02	0.42
1:C:99:LEU:HD23	1:C:162:ILE:HG23	2.02	0.42
1:C:321:ARG:HD2	1:C:327:MET:SD	2.59	0.42
1:B:28:GLN:HB3	1:B:49:LEU:HD23	2.02	0.41
1:A:123:GLN:HG2	1:C:89:PHE:HE1	1.85	0.41
1:A:240:TYR:CE1	1:A:250:ILE:HB	2.55	0.41
1:C:107:ASN:O	1:C:110:GLN:HB2	2.19	0.41
1:C:73:TYR:CD1	1:C:74:ALA:N	2.87	0.41
1:D:315:GLN:HA	1:D:316:PRO:HD2	1.95	0.41
1:A:137:ARG:NH2	1:C:137:ARG:NH2	2.30	0.41
1:A:53:VAL:HG12	1:A:54:PHE:CE1	2.55	0.41
1:B:368:GLU:HA	1:B:411:ASP:OD2	2.21	0.41
1:B:54:PHE:O	1:B:55:GLN:HB2	2.21	0.41
1:C:106:VAL:HG22	1:C:453:THR:HG21	2.02	0.41
1:A:89:PHE:CD1	1:C:121:ILE:CG2	3.03	0.41
1:C:105:LEU:HD13	1:C:154:LEU:HD22	2.01	0.41
1:A:115:LEU:O	1:A:120:SER:HB2	2.20	0.41
1:A:405:ARG:HE	1:A:405:ARG:HB3	1.74	0.41
1:B:121:ILE:HG13	1:D:133:HIS:CD2	2.55	0.41
1:A:150:SER:HA	1:A:153:MET:CE	2.50	0.41
1:B:85:GLN:HB3	1:B:86:PRO:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:ARG:HD2	1:D:327:MET:SD	2.60	0.41
1:A:321:ARG:HD2	1:A:327:MET:SD	2.61	0.41
1:C:85:GLN:HA	1:C:86:PRO:C	2.41	0.41
1:D:174:PRO:HA	1:D:212:GLY:N	2.35	0.41
1:B:321:ARG:HD2	1:B:327:MET:SD	2.61	0.41
1:B:405:ARG:HG3	1:B:413:LEU:CB	2.51	0.41
1:C:343:MET:HE3	1:C:371:VAL:HG13	2.03	0.41
1:C:348:ILE:HG13	1:C:373:ILE:HD12	2.02	0.41
1:A:42:THR:HG21	1:A:61:LYS:O	2.20	0.41
1:D:115:LEU:HD11	1:D:134:LEU:CD2	2.50	0.41
1:D:53:VAL:HG12	1:D:54:PHE:CD1	2.55	0.41
1:A:405:ARG:HG3	1:A:413:LEU:HB3	2.03	0.41
1:A:433:ASN:HD22	1:A:433:ASN:C	2.24	0.41
1:B:106:VAL:HG22	1:B:453:THR:HG21	2.03	0.41
1:C:50:ILE:HG13	1:C:50:ILE:H	1.68	0.41
1:A:327:MET:HE2	1:A:327:MET:HB2	1.93	0.40
1:B:174:PRO:HA	1:B:212:GLY:N	2.36	0.40
1:C:11:GLU:HB3	1:C:14:GLN:NE2	2.36	0.40
1:C:316:PRO:HG2	1:C:321:ARG:HD3	2.02	0.40
1:D:380:HIS:CD2	1:D:443:GLY:N	2.89	0.40
1:B:121:ILE:CG2	1:D:89:PHE:CD1	3.04	0.40
1:A:99:LEU:CD1	1:A:132:ALA:HB2	2.51	0.40
1:C:159:ALA:HB1	1:C:180:LEU:HD22	2.04	0.40
1:C:240:TYR:CE1	1:C:250:ILE:HB	2.56	0.40
1:D:7:TRP:CZ2	1:D:65:LYS:HE3	2.56	0.40
1:A:7:TRP:CZ2	1:A:65:LYS:HE3	2.57	0.40
1:B:106:VAL:N	1:B:155:LYS:O	2.53	0.40
1:B:7:TRP:CZ2	1:B:65:LYS:HE3	2.56	0.40
1:C:213:GLU:CG	1:C:214:MET:N	2.85	0.40
1:C:354:SER:HB2	1:C:408:ILE:HG21	2.03	0.40
1:D:14:GLN:O	1:D:17:TYR:HB3	2.21	0.40
1:D:437:CYS:O	1:D:438:LEU:HD23	2.22	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	451/459 (98%)	429 (95%)	22 (5%)	0	100	100
1	B	451/459 (98%)	429 (95%)	21 (5%)	1 (0%)	51	83
1	C	451/459 (98%)	427 (95%)	24 (5%)	0	100	100
1	D	451/459 (98%)	428 (95%)	23 (5%)	0	100	100
All	All	1804/1836 (98%)	1713 (95%)	90 (5%)	1 (0%)	55	86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	430	ASP

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	377/377 (100%)	358 (95%)	19 (5%)	28	62
1	B	377/377 (100%)	358 (95%)	19 (5%)	28	62
1	C	377/377 (100%)	359 (95%)	18 (5%)	30	63
1	D	377/377 (100%)	357 (95%)	20 (5%)	26	59
All	All	1508/1508 (100%)	1432 (95%)	76 (5%)	28	62

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	THR
1	A	81	TYR
1	A	121	ILE
1	A	125	SER
1	A	137	ARG

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Mol	Chain	Res	Type
1	A	228	SER
1	A	233	ARG
1	A	251	ASP
1	A	283	SER
1	A	285	ILE
1	A	312	THR
1	A	327	MET
1	A	340	ARG
1	A	354	SER
1	A	395	ILE
1	A	397	SER
1	A	405	ARG
1	A	432	SER
1	A	433	ASN
1	B	42	THR
1	B	75	THR
1	B	125	SER
1	B	137	ARG
1	B	199	ASP
1	B	228	SER
1	B	233	ARG
1	B	283	SER
1	B	285	ILE
1	B	312	THR
1	B	327	MET
1	B	340	ARG
1	B	354	SER
1	B	395	ILE
1	B	397	SER
1	B	405	ARG
1	B	427	ARG
1	B	432	SER
1	B	433	ASN
1	C	42	THR
1	C	125	SER
1	C	137	ARG
1	C	228	SER
1	C	233	ARG
1	C	283	SER
1	C	285	ILE
1	C	312	THR
1	C	327	MET

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Mol	Chain	Res	Type
1	C	340	ARG
1	C	354	SER
1	C	387	ASP
1	C	395	ILE
1	C	397	SER
1	C	405	ARG
1	C	427	ARG
1	C	432	SER
1	C	433	ASN
1	D	42	THR
1	D	75	THR
1	D	125	SER
1	D	137	ARG
1	D	199	ASP
1	D	228	SER
1	D	233	ARG
1	D	283	SER
1	D	285	ILE
1	D	312	THR
1	D	327	MET
1	D	340	ARG
1	D	354	SER
1	D	387	ASP
1	D	395	ILE
1	D	397	SER
1	D	405	ARG
1	D	427	ARG
1	D	432	SER
1	D	433	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	44	HIS
1	A	92	GLN
1	A	93	ASN
1	A	315	GLN
1	A	380	HIS
1	A	433	ASN
1	B	14	GLN
1	B	44	HIS

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Mol	Chain	Res	Type
1	B	113	GLN
1	B	315	GLN
1	B	380	HIS
1	B	433	ASN
1	C	14	GLN
1	C	21	HIS
1	C	44	HIS
1	C	315	GLN
1	C	380	HIS
1	C	433	ASN
1	D	14	GLN
1	D	44	HIS
1	D	55	GLN
1	D	93	ASN
1	D	315	GLN
1	D	380	HIS
1	D	433	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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	SF4	A	466	1	0,12,12	0.00	-	0,24,24	0.00	-
4	5GP	A	467	2,5	22,26,26	1.18	1 (4%)	26,40,40	2.67	6 (23%)
5	ADP	A	468	4	25,29,29	0.84	0	24,45,45	1.13	3 (12%)
3	SF4	B	466	1	0,12,12	0.00	-	0,24,24	0.00	-
4	5GP	B	467	2,5	22,26,26	1.21	2 (9%)	26,40,40	2.58	8 (30%)
5	ADP	B	468	4	25,29,29	0.83	0	24,45,45	1.06	3 (12%)
3	SF4	C	466	1	0,12,12	0.00	-	0,24,24	0.00	-
4	5GP	C	467	2,5	22,26,26	1.34	3 (13%)	26,40,40	2.63	6 (23%)
5	ADP	C	468	4	25,29,29	0.85	0	24,45,45	1.07	2 (8%)
3	SF4	D	466	1	0,12,12	0.00	-	0,24,24	0.00	-
4	5GP	D	467	2,5	22,26,26	1.23	1 (4%)	26,40,40	2.57	6 (23%)
5	ADP	D	468	4	25,29,29	0.88	1 (4%)	24,45,45	1.06	2 (8%)

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
3	SF4	A	466	1	-	0/0/48/48	0/6/5/5
4	5GP	A	467	2,5	-	0/6/26/26	0/3/3/3
5	ADP	A	468	4	-	0/12/32/32	0/3/3/3
3	SF4	B	466	1	-	0/0/48/48	0/6/5/5
4	5GP	B	467	2,5	-	0/6/26/26	0/3/3/3
5	ADP	B	468	4	-	0/12/32/32	0/3/3/3
3	SF4	C	466	1	-	0/0/48/48	0/6/5/5
4	5GP	C	467	2,5	-	0/6/26/26	0/3/3/3
5	ADP	C	468	4	-	0/12/32/32	0/3/3/3
3	SF4	D	466	1	-	0/0/48/48	0/6/5/5
4	5GP	D	467	2,5	-	0/6/26/26	0/3/3/3
5	ADP	D	468	4	-	0/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	467	5GP	C8-N7	-2.23	1.30	1.34
4	B	467	5GP	C8-N7	-2.14	1.30	1.34
5	D	468	ADP	C8-N7	-2.00	1.30	1.34
4	C	467	5GP	C2-N1	2.14	1.39	1.35
4	A	467	5GP	C6-N1	3.82	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	467	5GP	C6-N1	3.94	1.40	1.33
4	D	467	5GP	C6-N1	4.02	1.40	1.33
4	C	467	5GP	C6-N1	4.33	1.40	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	467	5GP	C5-C6-N1	-9.08	110.56	123.48
4	D	467	5GP	C5-C6-N1	-8.96	110.73	123.48
4	B	467	5GP	C5-C6-N1	-8.85	110.88	123.48
4	A	467	5GP	C5-C6-N1	-8.64	111.18	123.48
4	C	467	5GP	C2-N3-C4	-4.82	109.53	115.16
4	A	467	5GP	C2-N3-C4	-4.28	110.16	115.16
4	B	467	5GP	C2-N3-C4	-3.84	110.68	115.16
4	D	467	5GP	C2-N3-C4	-3.75	110.78	115.16
4	A	467	5GP	C6-C5-C4	-3.42	117.44	120.84
4	D	467	5GP	O3'-C3'-C2'	-3.35	101.11	111.83
4	A	467	5GP	O3'-C3'-C2'	-3.16	101.70	111.83
4	C	467	5GP	O3'-C3'-C2'	-2.99	102.25	111.83
5	A	468	ADP	C4'-O4'-C1'	-2.93	106.65	109.77
5	C	468	ADP	C4'-O4'-C1'	-2.84	106.75	109.77
4	B	467	5GP	O3'-C3'-C2'	-2.72	103.12	111.83
4	B	467	5GP	C6-C5-C4	-2.65	118.21	120.84
4	D	467	5GP	O3'-C3'-C4'	-2.53	103.69	111.09
4	C	467	5GP	O3'-C3'-C4'	-2.53	103.71	111.09
5	D	468	ADP	C4'-O4'-C1'	-2.47	107.14	109.77
5	C	468	ADP	C1'-N9-C4	-2.46	122.38	126.64
5	B	468	ADP	C4'-O4'-C1'	-2.42	107.19	109.77
4	B	467	5GP	O3'-C3'-C4'	-2.36	104.19	111.09
5	A	468	ADP	C1'-N9-C4	-2.34	122.59	126.64
5	B	468	ADP	C1'-N9-C4	-2.17	122.88	126.64
4	B	467	5GP	N3-C2-N1	-2.05	124.46	127.46
5	A	468	ADP	O2'-C2'-C3'	2.00	118.24	111.83
4	C	467	5GP	C4-C5-N7	2.10	111.44	109.41
5	B	468	ADP	O2'-C2'-C3'	2.10	118.55	111.83
4	D	467	5GP	C4-C5-N7	2.18	111.51	109.41
5	D	468	ADP	O2'-C2'-C3'	2.24	119.02	111.83
4	B	467	5GP	C4-C5-N7	2.59	111.92	109.41
4	A	467	5GP	C4-C5-N7	3.69	112.97	109.41
4	D	467	5GP	C6-N1-C2	5.99	124.67	116.06
4	A	467	5GP	C6-N1-C2	6.09	124.82	116.06
4	C	467	5GP	C6-N1-C2	6.17	124.94	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	467	5GP	C6-N1-C2	6.21	125.00	116.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	466	SF4	1	0
4	A	467	5GP	2	0
5	A	468	ADP	1	0
3	B	466	SF4	1	0
4	B	467	5GP	3	0
5	B	468	ADP	2	0
3	C	466	SF4	1	0
4	C	467	5GP	3	0
5	C	468	ADP	1	0
3	D	466	SF4	1	0
4	D	467	5GP	6	0
5	D	468	ADP	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	455/459 (99%)	-0.45	9 (1%) 65 56	10, 24, 65, 96	7 (1%)
1	B	454/459 (98%)	-0.16	13 (2%) 52 41	11, 31, 69, 99	8 (1%)
1	C	455/459 (99%)	-0.30	11 (2%) 59 49	11, 29, 69, 98	9 (1%)
1	D	455/459 (99%)	-0.37	9 (1%) 65 56	11, 28, 65, 96	6 (1%)
All	All	1819/1836 (99%)	-0.32	42 (2%) 61 51	10, 28, 67, 99	30 (1%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	56	ASN	10.2
1	B	429	TYR	6.6
1	A	229	MET	4.8
1	D	56	ASN	4.8
1	B	93	ASN	4.4
1	B	230	ASN	4.3
1	B	141	PHE	4.1
1	B	75	THR	4.0
1	C	432	SER	3.7
1	B	94	ASN	3.4
1	C	93	ASN	3.4
1	A	230	ASN	3.3
1	C	75	THR	3.3
1	C	56	ASN	3.2
1	A	458	VAL	3.1
1	D	57	GLY	3.0
1	D	323	GLN	3.0
1	D	93	ASN	2.9
1	A	56	ASN	2.9
1	B	431	ASP	2.8
1	D	139	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	432	SER	2.6
1	D	141	PHE	2.6
1	C	141	PHE	2.6
1	B	434	CYS	2.5
1	A	61	LYS	2.5
1	A	141	PHE	2.5
1	C	55	GLN	2.5
1	D	319	ALA	2.5
1	D	75	THR	2.4
1	B	229	MET	2.4
1	D	229	MET	2.4
1	C	230	ASN	2.3
1	B	55	GLN	2.2
1	A	57	GLY	2.2
1	C	391	HIS	2.2
1	A	310	GLY	2.2
1	C	430	ASP	2.1
1	C	452	ASP	2.1
1	C	57	GLY	2.1
1	B	433	ASN	2.1
1	B	311	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	ADP	D	468	27/27	0.97	0.16	0.44	10,20,59,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	ADP	B	468	27/27	0.97	0.15	-0.10	10,22,53,67	0
5	ADP	A	468	27/27	0.96	0.13	-0.53	12,24,58,67	0
4	5GP	D	467	24/24	0.97	0.14	-0.58	10,19,46,53	0
5	ADP	C	468	27/27	0.97	0.13	-0.58	10,19,65,73	0
4	5GP	B	467	24/24	0.96	0.13	-0.60	12,28,50,58	0
4	5GP	A	467	24/24	0.97	0.12	-0.65	10,20,52,59	0
4	5GP	C	467	24/24	0.97	0.12	-0.81	10,26,47,53	0
3	SF4	D	466	8/8	0.99	0.07	-1.94	15,18,24,26	0
2	MG	B	469	1/1	0.94	0.07	-2.05	22,22,22,22	0
3	SF4	C	466	8/8	0.99	0.07	-2.12	20,22,24,28	0
3	SF4	A	466	8/8	0.99	0.07	-2.12	12,15,15,15	0
3	SF4	B	466	8/8	0.99	0.08	-2.71	12,21,25,29	0
2	MG	A	469	1/1	0.95	0.06	-3.68	10,10,10,10	0
2	MG	C	469	1/1	0.98	0.05	-4.35	12,12,12,12	0
2	MG	D	469	1/1	0.99	0.04	-4.89	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.