



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:27 AM UTC

PDB ID : 5FAG / pdb_00005fag
Title : Alanine Racemase from Streptomyces coelicolor A3(2) with Bound Propionate Inhibitor
Authors : Tassoni, R.; Pannu, N.S.
Deposited on : 2015-12-11
Resolution : 1.51 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

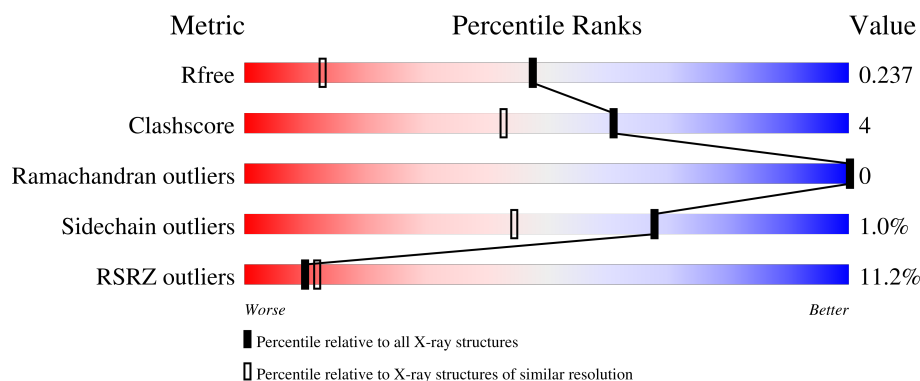
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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	410	3% 86% 9% 5%
1	B	410	2% 87% 7% 7%
1	C	410	9% 85% 8% 7%
1	D	410	28% 85% 7% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12710 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 Alanine racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	22	0
			3047	1915	567	552	13			
1	B	382	Total	C	N	O	S	0	13	0
			2911	1829	536	534	12			
1	C	382	Total	C	N	O	S	0	11	0
			2909	1830	538	529	12			
1	D	382	Total	C	N	O	S	0	14	0
			2926	1842	542	528	14			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP O86786
A	-17	GLY	-	expression tag	UNP O86786
A	-16	SER	-	expression tag	UNP O86786
A	-15	HIS	-	expression tag	UNP O86786
A	-14	HIS	-	expression tag	UNP O86786
A	-13	HIS	-	expression tag	UNP O86786
A	-12	HIS	-	expression tag	UNP O86786
A	-11	HIS	-	expression tag	UNP O86786
A	-10	HIS	-	expression tag	UNP O86786
A	-9	SER	-	expression tag	UNP O86786
A	-8	SER	-	expression tag	UNP O86786
A	-7	GLY	-	expression tag	UNP O86786
A	-6	LEU	-	expression tag	UNP O86786
A	-5	VAL	-	expression tag	UNP O86786
A	-4	PRO	-	expression tag	UNP O86786
A	-3	ARG	-	expression tag	UNP O86786
A	-2	GLY	-	expression tag	UNP O86786
A	-1	SER	-	expression tag	UNP O86786
A	0	HIS	-	expression tag	UNP O86786
B	-18	MET	-	initiating methionine	UNP O86786
B	-17	GLY	-	expression tag	UNP O86786

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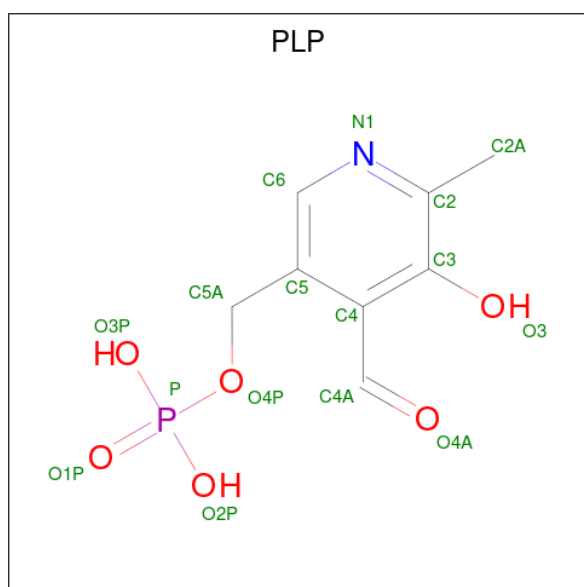
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP O86786
B	-15	HIS	-	expression tag	UNP O86786
B	-14	HIS	-	expression tag	UNP O86786
B	-13	HIS	-	expression tag	UNP O86786
B	-12	HIS	-	expression tag	UNP O86786
B	-11	HIS	-	expression tag	UNP O86786
B	-10	HIS	-	expression tag	UNP O86786
B	-9	SER	-	expression tag	UNP O86786
B	-8	SER	-	expression tag	UNP O86786
B	-7	GLY	-	expression tag	UNP O86786
B	-6	LEU	-	expression tag	UNP O86786
B	-5	VAL	-	expression tag	UNP O86786
B	-4	PRO	-	expression tag	UNP O86786
B	-3	ARG	-	expression tag	UNP O86786
B	-2	GLY	-	expression tag	UNP O86786
B	-1	SER	-	expression tag	UNP O86786
B	0	HIS	-	expression tag	UNP O86786
C	-18	MET	-	initiating methionine	UNP O86786
C	-17	GLY	-	expression tag	UNP O86786
C	-16	SER	-	expression tag	UNP O86786
C	-15	HIS	-	expression tag	UNP O86786
C	-14	HIS	-	expression tag	UNP O86786
C	-13	HIS	-	expression tag	UNP O86786
C	-12	HIS	-	expression tag	UNP O86786
C	-11	HIS	-	expression tag	UNP O86786
C	-10	HIS	-	expression tag	UNP O86786
C	-9	SER	-	expression tag	UNP O86786
C	-8	SER	-	expression tag	UNP O86786
C	-7	GLY	-	expression tag	UNP O86786
C	-6	LEU	-	expression tag	UNP O86786
C	-5	VAL	-	expression tag	UNP O86786
C	-4	PRO	-	expression tag	UNP O86786
C	-3	ARG	-	expression tag	UNP O86786
C	-2	GLY	-	expression tag	UNP O86786
C	-1	SER	-	expression tag	UNP O86786
C	0	HIS	-	expression tag	UNP O86786
D	-18	MET	-	initiating methionine	UNP O86786
D	-17	GLY	-	expression tag	UNP O86786
D	-16	SER	-	expression tag	UNP O86786
D	-15	HIS	-	expression tag	UNP O86786
D	-14	HIS	-	expression tag	UNP O86786
D	-13	HIS	-	expression tag	UNP O86786

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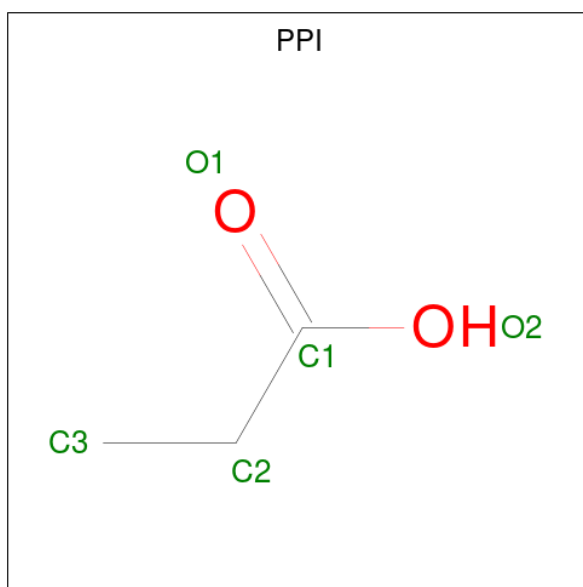
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP O86786
D	-11	HIS	-	expression tag	UNP O86786
D	-10	HIS	-	expression tag	UNP O86786
D	-9	SER	-	expression tag	UNP O86786
D	-8	SER	-	expression tag	UNP O86786
D	-7	GLY	-	expression tag	UNP O86786
D	-6	LEU	-	expression tag	UNP O86786
D	-5	VAL	-	expression tag	UNP O86786
D	-4	PRO	-	expression tag	UNP O86786
D	-3	ARG	-	expression tag	UNP O86786
D	-2	GLY	-	expression tag	UNP O86786
D	-1	SER	-	expression tag	UNP O86786
D	0	HIS	-	expression tag	UNP O86786

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is PROPANOIC ACID (CCD ID: PPI) (formula: $C_3H_6O_2$).

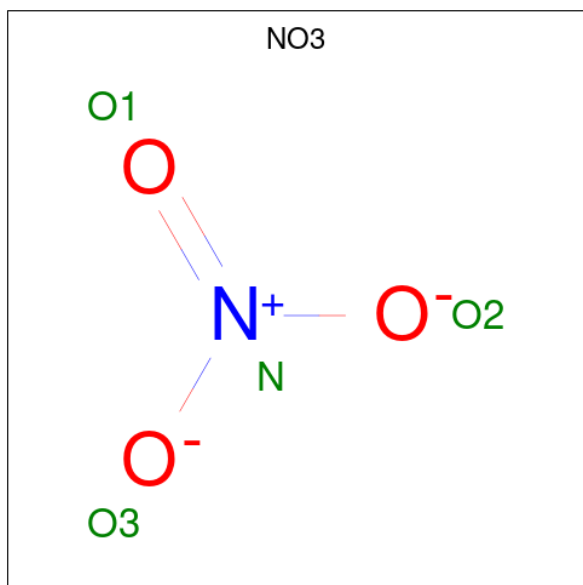


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		
3	C	1	Total	C	O	0	0
			5	3	2		
3	D	1	Total	C	O	0	0
			5	3	2		
3	D	1	Total	C	O	0	0
			5	3	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		
4	B	2	Total	Na	0	0
			2	2		
4	C	1	Total	Na	0	0
			1	1		

- Molecule 5 is NITRATE ION (CCD ID: NO3) (formula: NO₃).

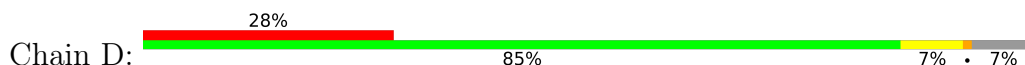


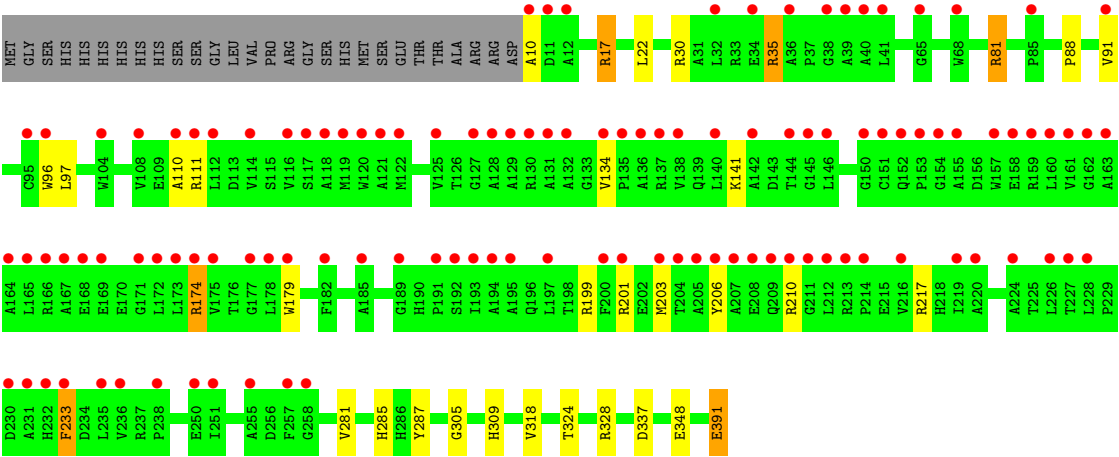
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	N	O	0	0
			4	1	3		
5	B	1	Total	N	O	0	0
			4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	237	Total	O	0	0
			237	237		
6	B	239	Total	O	0	0
			239	239		
6	C	167	Total	O	0	0
			167	167		
6	D	161	Total	O	0	0
			161	161		

- Molecule 1: Alanine racemase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.95Å 88.58Å 108.88Å 90.00° 102.60° 90.00°	Depositor
Resolution (Å)	48.06 – 1.51 48.06 – 1.51	Depositor EDS
% Data completeness (in resolution range)	96.6 (48.06-1.51) 96.6 (48.06-1.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 1.51Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.199 , 0.225 0.212 , 0.237	Depositor DCC
R_{free} test set	11051 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12710	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1838e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: KCX, PLP, PPI, NO3, NA

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	1.33	13/3174 (0.4%)	1.13	7/4321 (0.2%)
1	B	1.33	5/3003 (0.2%)	1.11	5/4098 (0.1%)
1	C	1.23	3/3001 (0.1%)	1.07	7/4093 (0.2%)
1	D	1.23	4/3027 (0.1%)	1.06	3/4127 (0.1%)
All	All	1.28	25/12205 (0.2%)	1.09	22/16639 (0.1%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	233	PHE	C-O	-7.12	1.17	1.24
1	A	217[A]	ARG	CA-C	6.95	1.61	1.52
1	A	217[B]	ARG	CA-C	6.95	1.61	1.52
1	A	196	GLN	CA-C	-6.81	1.44	1.52
1	A	298	VAL	CA-C	6.01	1.57	1.53
1	A	220	ALA	C-O	-5.97	1.16	1.24
1	C	205	ALA	N-CA	5.85	1.53	1.46
1	D	97	LEU	CA-C	-5.79	1.45	1.53
1	B	384	VAL	N-CA	-5.77	1.41	1.46
1	A	39	ALA	C-O	-5.74	1.16	1.23
1	A	202	GLU	CA-CB	-5.65	1.44	1.53
1	B	61	ALA	N-CA	-5.65	1.39	1.46
1	D	305	GLY	C-O	-5.59	1.16	1.24
1	B	209	GLN	N-CA	5.49	1.53	1.46
1	A	221	ASN	N-CA	5.33	1.52	1.45
1	A	171	GLY	N-CA	5.32	1.52	1.45
1	C	268	SER	N-CA	5.27	1.52	1.46
1	B	138	VAL	CA-C	-5.26	1.46	1.52
1	A	179	TRP	CA-C	-5.25	1.46	1.52
1	D	233	PHE	C-O	-5.19	1.17	1.24
1	B	216	VAL	N-CA	-5.17	1.40	1.46
1	D	318	VAL	CA-C	5.13	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	GLN	N-CA	5.10	1.52	1.46
1	A	233	PHE	C-O	-5.09	1.17	1.24
1	A	241	ALA	CA-C	-5.00	1.46	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	GLY	N-CA-C	8.96	127.06	115.32
1	A	220	ALA	N-CA-C	8.22	121.83	109.25
1	A	39	ALA	N-CA-C	7.43	121.59	109.85
1	C	213	ARG	NE-CZ-NH2	6.78	125.30	119.20
1	B	213	ARG	NE-CZ-NH2	6.31	124.88	119.20
1	A	149	GLY	CA-C-N	-6.26	114.45	121.83
1	A	149	GLY	C-N-CA	-6.26	114.45	121.83
1	A	329	ILE	N-CA-C	-6.21	100.70	108.89
1	D	328	ARG	N-CA-C	6.11	119.33	110.28
1	A	150	GLY	N-CA-C	6.02	121.82	112.60
1	C	54	ALA	N-CA-C	5.80	117.28	111.07
1	C	329	ILE	N-CA-C	-5.71	101.44	109.21
1	D	201	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	C	149	GLY	N-CA-C	-5.59	103.61	112.66
1	B	213	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	B	134	VAL	CB-CA-C	-5.40	101.53	111.36
1	B	111	ARG	CB-CG-CD	-5.31	99.09	111.30
1	B	374	TYR	CB-CA-C	-5.12	102.62	110.81
1	C	87	LEU	CA-C-N	-5.11	114.50	119.76
1	C	87	LEU	C-N-CA	-5.11	114.50	119.76
1	C	213	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	D	96	TRP	N-CA-C	5.01	121.66	114.39

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	3047	0	3086	21	0
1	B	2911	0	2904	15	0
1	C	2909	0	2913	21	0
1	D	2926	0	2943	37	0
2	A	15	0	6	5	0
2	B	15	0	6	2	0
2	C	15	0	7	5	0
2	D	15	0	6	3	0
3	A	5	0	5	2	0
3	B	20	0	20	2	0
3	C	5	0	5	2	0
3	D	10	0	10	5	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	237	0	0	5	0
6	B	239	0	0	9	0
6	C	167	0	0	5	0
6	D	161	0	0	6	0
All	All	12710	0	11911	100	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 4.

All (100) 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)
3:C:402:PPI:O1	6:C:501:HOH:O	1.60	1.19
1:B:137:ARG:HD3	6:B:601:HOH:O	1.40	1.17
1:D:35[A]:ARG:HH11	1:D:35[A]:ARG:HG3	1.15	1.07
1:B:92:ARG:NH1	6:B:601:HOH:O	1.88	1.05
6:A:586:HOH:O	1:B:383[B]:ARG:HD3	1.58	1.00
1:C:281:VAL:CG1	1:C:335:VAL:HG21	1.95	0.96
1:D:111[B]:ARG:HH11	1:D:111[B]:ARG:CG	1.79	0.93
1:B:92:ARG:CZ	6:B:601:HOH:O	2.18	0.92
1:C:17[B]:ARG:NH1	1:C:348:GLU:OE1	2.04	0.89
1:D:111[B]:ARG:HH11	1:D:111[B]:ARG:HG3	1.39	0.87
1:D:35[A]:ARG:HH11	1:D:35[A]:ARG:CG	1.86	0.86
1:D:174:ARG:HG2	1:D:174:ARG:HH11	1.41	0.85
1:D:337:ASP:H	3:D:503:PPI:H31	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ASP:OD1	1:B:159[B]:ARG:NH1	2.12	0.82
1:D:111[B]:ARG:HG3	1:D:111[B]:ARG:NH1	1.94	0.81
1:D:324:THR:O	3:D:503:PPI:H32	1.81	0.80
1:D:35[A]:ARG:HG3	1:D:35[A]:ARG:NH1	1.96	0.79
1:A:159[C]:ARG:HA	1:A:159[C]:ARG:HE	1.51	0.73
1:A:179:TRP:HZ3	2:A:401:PLP:H2A1	1.51	0.72
1:C:281:VAL:HG11	1:C:335:VAL:HG21	1.72	0.72
1:D:199[B]:ARG:HG2	1:D:203[B]:MET:CE	2.21	0.69
3:B:505:PPI:H32	6:B:812:HOH:O	1.93	0.68
1:D:10:ALA:N	6:D:602:HOH:O	2.25	0.68
1:A:159[C]:ARG:HE	1:A:159[C]:ARG:CA	2.08	0.67
1:A:12:ALA:O	6:A:501:HOH:O	2.14	0.66
1:D:30[A]:ARG:NH2	6:D:601:HOH:O	2.15	0.66
1:D:35[A]:ARG:CG	1:D:35[A]:ARG:NH1	2.49	0.65
1:A:174:ARG:HH21	1:A:213:ARG:HB2	1.63	0.64
1:C:335:VAL:HG22	6:C:547:HOH:O	1.98	0.64
1:C:326:ALA:HB3	1:C:335:VAL:HG23	1.80	0.62
1:C:179:TRP:HZ3	2:C:401:PLP:H2A1	1.65	0.61
1:B:174:ARG:NH2	6:B:603:HOH:O	2.33	0.61
1:D:111[B]:ARG:HH11	1:D:111[B]:ARG:HG2	1.65	0.61
1:A:208:GLU:O	1:A:213:ARG:NH2	2.35	0.60
1:A:285:HIS:HD2	6:A:718:HOH:O	1.84	0.60
1:C:281:VAL:HG12	1:C:335:VAL:HG21	1.82	0.60
1:D:88:PRO:O	1:D:91[A]:VAL:HG22	2.01	0.59
1:C:88:PRO:O	1:C:91[B]:VAL:HG22	2.03	0.58
1:D:179:TRP:HZ3	2:D:502:PLP:H2A1	1.67	0.58
1:D:206:TYR:OH	1:D:210:ARG:NH2	2.33	0.58
1:B:309:HIS:HD2	6:B:782:HOH:O	1.86	0.58
1:C:34:GLU:HG3	6:C:589:HOH:O	2.03	0.57
1:D:174:ARG:HG2	1:D:174:ARG:NH1	2.14	0.57
1:A:309:HIS:HD2	6:B:765:HOH:O	1.88	0.56
1:A:22[A]:LEU:HD21	1:A:388:TYR:HD1	1.70	0.56
1:C:22[A]:LEU:HD21	1:C:388:TYR:HD1	1.70	0.56
1:A:179:TRP:CZ3	2:A:401:PLP:H2A1	2.37	0.55
1:A:283:TYR:OH	3:A:402:PPI:C1	2.54	0.55
1:D:285:HIS:HD2	6:D:749:HOH:O	1.90	0.55
1:B:159[B]:ARG:NH2	6:B:607:HOH:O	2.40	0.54
6:C:584:HOH:O	1:D:309:HIS:HD2	1.90	0.54
1:D:199[B]:ARG:HG2	1:D:203[B]:MET:HE1	1.89	0.53
1:C:248:SER:OG	1:C:250[A]:GLU:HG2	2.07	0.53
1:D:217:ARG:NH1	1:D:233:PHE:HE1	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199[B]:ARG:CG	1:D:203[B]:MET:CE	2.86	0.53
1:C:235[B]:LEU:HD23	1:C:236:VAL:N	2.23	0.53
1:D:199[B]:ARG:CG	1:D:203[B]:MET:HE2	2.39	0.52
3:A:402:PPI:H33	2:B:502:PLP:C4A	2.38	0.52
1:C:309:HIS:HD2	6:D:714:HOH:O	1.93	0.52
1:B:285:HIS:HD2	6:B:815:HOH:O	1.93	0.52
1:A:35[B]:ARG:NH2	6:A:506:HOH:O	2.44	0.51
1:B:179:TRP:HZ3	2:B:502:PLP:H2A1	1.76	0.50
1:D:17[B]:ARG:NH2	1:D:348:GLU:OE1	2.40	0.50
2:A:401:PLP:C4A	3:B:501:PPI:H22	2.42	0.49
1:D:206:TYR:HH	1:D:210:ARG:HH21	1.58	0.49
1:D:281[A]:VAL:CG1	1:D:287:TYR:HB3	2.44	0.48
1:A:35[B]:ARG:NH2	1:A:257:PHE:O	2.48	0.46
1:A:22[B]:LEU:HD12	1:A:391:GLU:HG3	1.97	0.46
1:D:391:GLU:HB2	6:D:671:HOH:O	2.14	0.46
1:C:42:MET:HB2	1:C:235[B]:LEU:HD21	1.98	0.46
1:B:84:GLU:HA	1:B:85:PRO:C	2.39	0.46
1:D:199[B]:ARG:HG2	1:D:203[B]:MET:HE2	1.95	0.46
1:C:162:GLY:O	1:C:166[A]:ARG:HD3	2.15	0.46
1:C:84:GLU:HA	1:C:85:PRO:C	2.40	0.45
1:D:199[B]:ARG:HE	1:D:199[B]:ARG:HB2	1.53	0.45
1:D:179:TRP:CZ3	2:D:502:PLP:H2A1	2.51	0.44
1:D:22:LEU:HD12	1:D:391:GLU:HG3	1.99	0.44
1:D:217:ARG:NH1	1:D:233:PHE:CE1	2.86	0.44
2:C:401:PLP:C4A	3:D:501:PPI:H22	2.48	0.43
1:C:179:TRP:CZ3	2:C:401:PLP:H2A1	2.48	0.43
1:B:43:ALA:HB3	1:B:69:LEU:HD23	2.00	0.43
3:D:503:PPI:H33	6:D:709:HOH:O	2.18	0.42
1:A:84:GLU:HA	1:A:85:PRO:C	2.44	0.42
1:A:11[B]:ASP:OD1	1:B:103:PRO:HD3	2.20	0.42
3:C:402:PPI:H22	2:D:502:PLP:C4A	2.49	0.42
1:D:81:ARG:HD2	1:D:110:ALA:O	2.20	0.42
1:D:199[B]:ARG:HG3	1:D:203[B]:MET:HE2	2.01	0.42
1:C:43:ALA:HB3	1:C:69:LEU:HD23	2.02	0.42
1:B:206:TYR:HH	1:B:210:ARG:HH11	1.64	0.42
1:A:179:TRP:CZ3	2:A:401:PLP:C2A	3.03	0.41
1:A:146:LEU:HD13	1:A:183:ALA:HA	2.01	0.41
1:C:285:HIS:HD2	6:C:656:HOH:O	2.02	0.41
1:C:46:LYS:NZ	2:C:401:PLP:O3	2.54	0.41
1:C:147:GLY:O	1:D:281[A]:VAL:HG23	2.21	0.41
1:A:46:LYS:NZ	2:A:401:PLP:O3	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22[A]:LEU:HD21	1:A:388:TYR:CD1	2.54	0.40
6:A:586:HOH:O	1:B:383[B]:ARG:CD	2.38	0.40
2:C:401:PLP:C4A	3:D:501:PPI:H32	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/410 (100%)	400 (97%)	11 (3%)	0	100	100
1	B	392/410 (96%)	381 (97%)	11 (3%)	0	100	100
1	C	391/410 (95%)	377 (96%)	14 (4%)	0	100	100
1	D	394/410 (96%)	382 (97%)	12 (3%)	0	100	100
All	All	1588/1640 (97%)	1540 (97%)	48 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	304/297 (102%)	300 (99%)	4 (1%)	61	34
1	B	286/297 (96%)	284 (99%)	2 (1%)	76	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	285/297 (96%)	283 (99%)	2 (1%)	76	57
1	D	288/297 (97%)	279 (97%)	9 (3%)	35	8
All	All	1163/1188 (98%)	1146 (98%)	17 (2%)	68	29

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17[A]	ARG
1	A	17[B]	ARG
1	A	134	VAL
1	A	209	GLN
1	B	17[A]	ARG
1	B	17[B]	ARG
1	C	17[A]	ARG
1	C	17[B]	ARG
1	D	17[A]	ARG
1	D	17[B]	ARG
1	D	35[A]	ARG
1	D	35[C]	ARG
1	D	35[D]	ARG
1	D	81	ARG
1	D	134	VAL
1	D	174	ARG
1	D	391	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	HIS
1	A	286	HIS
1	A	309	HIS
1	B	285	HIS
1	B	309	HIS
1	B	390	ASN
1	C	309	HIS
1	C	390	ASN
1	D	152	GLN
1	D	285	HIS
1	D	286	HIS
1	D	309	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	KCX	B	141	1	10,11,12	2.67	2 (20%)	6,12,14	2.03	2 (33%)
1	KCX	A	141	1	10,11,12	1.35	2 (20%)	6,12,14	1.30	1 (16%)
1	KCX	C	141	1	10,11,12	2.80	2 (20%)	6,12,14	2.10	2 (33%)
1	KCX	D	141	1	10,11,12	0.84	0	6,12,14	1.33	1 (16%)

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
1	KCX	B	141	1	-	1/9/10/12	-
1	KCX	A	141	1	-	1/9/10/12	-
1	KCX	C	141	1	-	1/9/10/12	-
1	KCX	D	141	1	-	1/9/10/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	KCX	OQ1-CX	7.86	1.36	1.21
1	C	141	KCX	OQ1-CX	7.85	1.36	1.21
1	A	141	KCX	CB-CA	2.80	1.57	1.53
1	C	141	KCX	CB-CA	2.70	1.57	1.53
1	A	141	KCX	CA-N	-2.56	1.40	1.48
1	B	141	KCX	CB-CA	2.35	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	141	KCX	OQ1-CX-NZ	-3.70	119.30	124.92
1	B	141	KCX	OQ1-CX-NZ	-3.62	119.42	124.92
1	C	141	KCX	CE-NZ-CX	3.42	127.78	121.98
1	B	141	KCX	CE-NZ-CX	3.26	127.51	121.98
1	D	141	KCX	CE-NZ-CX	2.98	127.03	121.98
1	A	141	KCX	CE-NZ-CX	2.85	126.81	121.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	141	KCX	CG-CD-CE-NZ
1	D	141	KCX	CG-CD-CE-NZ
1	C	141	KCX	CG-CD-CE-NZ
1	B	141	KCX	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 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	PPI	B	506	-	4,4,4	0.95	0	4,4,4	0.97	0
3	PPI	B	507	-	4,4,4	0.86	0	4,4,4	1.52	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	A	401	1	15,15,16	3.02	4 (26%)	21,22,23	2.21	7 (33%)
2	PLP	C	401	1	15,15,16	2.63	3 (20%)	21,22,23	2.70	8 (38%)
3	PPI	B	501	-	4,4,4	1.60	1 (25%)	4,4,4	0.96	0
3	PPI	B	505	-	4,4,4	1.12	0	4,4,4	0.90	0
3	PPI	C	402	-	4,4,4	1.21	1 (25%)	4,4,4	1.17	0
3	PPI	D	501	-	4,4,4	1.56	1 (25%)	4,4,4	1.05	0
5	NO3	A	405	-	1,3,3	0.68	0	0,3,3	-	-
5	NO3	B	508	-	1,3,3	0.70	0	0,3,3	-	-
3	PPI	A	402	-	4,4,4	0.62	0	4,4,4	1.64	1 (25%)
2	PLP	B	502	1	15,15,16	3.43	7 (46%)	21,22,23	3.32	10 (47%)
2	PLP	D	502	1	15,15,16	3.06	5 (33%)	21,22,23	2.40	8 (38%)
3	PPI	D	503	-	4,4,4	1.11	0	4,4,4	1.20	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
3	PPI	B	506	-	-	2/2/2/2	-
3	PPI	B	507	-	-	0/2/2/2	-
2	PLP	A	401	1	-	0/6/6/8	0/1/1/1
2	PLP	C	401	1	-	0/6/6/8	0/1/1/1
3	PPI	B	501	-	-	2/2/2/2	-
3	PPI	B	505	-	-	2/2/2/2	-
3	PPI	C	402	-	-	2/2/2/2	-
3	PPI	D	501	-	-	1/2/2/2	-
3	PPI	A	402	-	-	1/2/2/2	-
2	PLP	B	502	1	-	0/6/6/8	0/1/1/1
2	PLP	D	502	1	-	0/6/6/8	0/1/1/1
3	PPI	D	503	-	-	2/2/2/2	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	PLP	C5-C4	10.88	1.52	1.40
2	A	401	PLP	C5-C4	10.25	1.52	1.40
2	C	401	PLP	C5-C4	8.44	1.50	1.40
2	D	502	PLP	C5-C4	8.22	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	502	PLP	C3-C2	5.72	1.46	1.41
2	D	502	PLP	C3-C4	4.48	1.48	1.40
2	B	502	PLP	P-O1P	3.77	1.62	1.50
2	C	401	PLP	C3-C4	3.68	1.47	1.40
2	A	401	PLP	C3-C4	3.44	1.46	1.40
2	B	502	PLP	C3-C4	3.43	1.46	1.40
2	B	502	PLP	C3-C2	3.42	1.44	1.41
3	B	501	PPI	O2-C1	-3.04	1.20	1.30
2	C	401	PLP	C3-C2	2.64	1.43	1.41
2	A	401	PLP	C3-C2	2.60	1.43	1.41
3	D	501	PPI	O2-C1	-2.56	1.22	1.30
2	D	502	PLP	P-O3P	-2.54	1.45	1.54
2	B	502	PLP	C6-C5	2.42	1.42	1.37
2	B	502	PLP	P-O2P	-2.30	1.46	1.54
3	C	402	PPI	O2-C1	-2.30	1.23	1.30
2	D	502	PLP	C2-N1	2.29	1.37	1.33
2	A	401	PLP	C4A-C4	-2.11	1.47	1.51
2	B	502	PLP	C2-N1	2.08	1.37	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	PLP	C4A-C4-C5	10.21	131.46	120.94
2	C	401	PLP	C2A-C2-C3	-6.75	112.90	120.80
2	B	502	PLP	C2A-C2-C3	-5.87	113.93	120.80
2	C	401	PLP	C4A-C4-C5	5.64	126.75	120.94
2	A	401	PLP	C4A-C4-C5	5.61	126.72	120.94
2	D	502	PLP	C2A-C2-C3	-5.58	114.27	120.80
2	B	502	PLP	C4A-C4-C3	-5.29	111.71	120.52
2	C	401	PLP	C2A-C2-N1	4.08	125.32	117.64
2	D	502	PLP	C6-C5-C4	3.97	121.35	118.10
2	C	401	PLP	C4A-C4-C3	-3.87	114.07	120.52
2	A	401	PLP	C6-N1-C2	3.73	125.97	119.20
2	D	502	PLP	C2A-C2-N1	3.61	124.44	117.64
2	D	502	PLP	C4A-C4-C5	3.58	124.63	120.94
2	D	502	PLP	O3P-P-O4P	3.48	115.74	106.67
2	B	502	PLP	C2A-C2-N1	3.47	124.17	117.64
2	C	401	PLP	C6-N1-C2	3.30	125.19	119.20
2	A	401	PLP	C4A-C4-C3	-3.05	115.44	120.52
2	B	502	PLP	C6-N1-C2	2.96	124.57	119.20
2	B	502	PLP	O3P-P-O2P	2.80	118.30	107.80
2	B	502	PLP	C5-C6-N1	-2.76	119.34	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PLP	O2P-P-O1P	2.76	121.60	110.83
2	D	502	PLP	C6-N1-C2	2.76	124.20	119.20
2	C	401	PLP	C4-C3-C2	-2.73	115.81	119.89
2	C	401	PLP	C5-C6-N1	-2.69	119.45	123.83
2	A	401	PLP	C5-C6-N1	-2.63	119.55	123.83
2	B	502	PLP	C5A-C5-C6	-2.63	115.07	119.36
2	A	401	PLP	C2A-C2-C3	-2.60	117.75	120.80
2	D	502	PLP	C5-C6-N1	-2.55	119.69	123.83
3	B	507	PPI	O2-C1-O1	-2.53	116.82	123.33
2	C	401	PLP	O4P-P-O1P	-2.52	99.62	106.44
2	A	401	PLP	C4-C3-C2	-2.21	116.58	119.89
2	B	502	PLP	C6-C5-C4	2.17	119.88	118.10
2	B	502	PLP	O3-C3-C2	2.13	121.99	117.58
3	A	402	PPI	O2-C1-C2	2.03	122.00	113.49
2	D	502	PLP	C4-C3-C2	-2.02	116.86	119.89

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	506	PPI	O1-C1-C2-C3
3	C	402	PPI	O1-C1-C2-C3
3	C	402	PPI	O2-C1-C2-C3
3	D	503	PPI	O1-C1-C2-C3
3	D	503	PPI	O2-C1-C2-C3
3	B	506	PPI	O2-C1-C2-C3
3	A	402	PPI	O1-C1-C2-C3
3	B	501	PPI	O1-C1-C2-C3
3	B	501	PPI	O2-C1-C2-C3
3	B	505	PPI	O1-C1-C2-C3
3	B	505	PPI	O2-C1-C2-C3
3	D	501	PPI	O1-C1-C2-C3

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PLP	5	0
2	C	401	PLP	5	0
3	B	501	PPI	1	0
3	B	505	PPI	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	PPI	2	0
3	D	501	PPI	2	0
3	A	402	PPI	2	0
2	B	502	PLP	2	0
2	D	502	PLP	3	0
3	D	503	PPI	3	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	389/410 (94%)	0.46	14 (3%)	46	53	12, 26, 44, 83	22 (5%)
1	B	381/410 (92%)	0.28	7 (1%)	67	73	11, 25, 38, 71	13 (3%)
1	C	381/410 (92%)	0.83	35 (9%)	14	17	14, 31, 54, 74	11 (2%)
1	D	381/410 (92%)	1.34	115 (30%)	1	1	13, 34, 66, 90	14 (3%)
All	All	1532/1640 (93%)	0.73	171 (11%)	10	12	11, 28, 54, 90	60 (3%)

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	167	ALA	6.0
1	C	10	ALA	5.9
1	D	157	TRP	5.5
1	B	10	ALA	5.4
1	D	160	LEU	5.3
1	D	164	ALA	5.2
1	D	10	ALA	5.1
1	D	197	LEU	4.8
1	D	207	ALA	4.8
1	D	175	VAL	4.7
1	D	134	VAL	4.6
1	D	228	LEU	4.4
1	D	205	ALA	4.4
1	D	173	LEU	4.3
1	D	235	LEU	4.3
1	D	206	TYR	4.3
1	D	172	LEU	4.2
1	D	131	ALA	4.2
1	D	216	VAL	4.2
1	D	125	VAL	4.1
1	C	14	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	214	PRO	4.1
1	D	150	GLY	4.0
1	C	272	VAL	3.9
1	D	212	LEU	3.9
1	D	138	VAL	3.9
1	D	165	LEU	3.9
1	D	162	GLY	3.9
1	D	233	PHE	3.9
1	D	182	PHE	3.8
1	D	169	GLU	3.8
1	A	6	ALA	3.8
1	D	96	TRP	3.7
1	D	140	LEU	3.7
1	C	271	LEU	3.6
1	C	322	TRP	3.6
1	B	356[A]	ASP	3.6
1	D	208	GLU	3.6
1	D	194	ALA	3.5
1	D	120	TRP	3.5
1	D	219	ILE	3.5
1	D	129	ALA	3.5
1	A	4	THR	3.5
1	A	7[A]	ARG	3.4
1	D	163	ALA	3.4
1	D	200	PHE	3.4
1	D	12	ALA	3.4
1	D	91[A]	VAL	3.4
1	D	185	ALA	3.4
1	D	211	GLY	3.3
1	D	118	ALA	3.3
1	D	155	ALA	3.3
1	D	220	ALA	3.3
1	A	134	VAL	3.3
1	D	236	VAL	3.3
1	D	95	CYS	3.3
1	D	68	TRP	3.3
1	D	177	GLY	3.3
1	D	161	VAL	3.3
1	C	131	ALA	3.2
1	D	121	ALA	3.2
1	D	142	ALA	3.2
1	C	290	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	111[A]	ARG	3.1
1	D	174	ARG	3.1
1	C	270	ALA	3.1
1	A	5	THR	3.0
1	D	195	ALA	3.0
1	C	279	HIS	3.0
1	A	356[A]	ASP	2.9
1	D	178	LEU	2.9
1	C	293	THR	2.9
1	D	231	ALA	2.9
1	D	166	ARG	2.9
1	D	130	ARG	2.9
1	D	116	VAL	2.9
1	D	40	ALA	2.8
1	D	213	ARG	2.8
1	C	166[A]	ARG	2.8
1	D	112	LEU	2.8
1	D	36	ALA	2.8
1	D	193	ILE	2.8
1	D	191	PRO	2.8
1	D	189	GLY	2.7
1	D	110	ALA	2.7
1	D	179	TRP	2.7
1	D	224	ALA	2.7
1	C	134	VAL	2.7
1	C	336	VAL	2.7
1	D	151	CYS	2.7
1	D	136	ALA	2.6
1	C	287	TYR	2.6
1	D	114	VAL	2.6
1	D	158	GLU	2.6
1	D	209	GLN	2.6
1	D	117	SER	2.6
1	D	153	PRO	2.6
1	D	251	ILE	2.6
1	C	128	ALA	2.6
1	D	227	THR	2.6
1	D	203[A]	MET	2.6
1	D	104	TRP	2.6
1	D	230	ASP	2.6
1	C	389	VAL	2.6
1	A	131	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	167	ALA	2.5
1	D	226	LEU	2.5
1	A	286	HIS	2.5
1	D	38	GLY	2.5
1	D	108	VAL	2.5
1	C	294	THR	2.5
1	D	204	THR	2.5
1	C	35[A]	ARG	2.5
1	B	12	ALA	2.5
1	D	39	ALA	2.5
1	D	154	GLY	2.5
1	D	41	LEU	2.5
1	D	122	MET	2.5
1	C	12	ALA	2.4
1	D	192	SER	2.4
1	D	201	ARG	2.4
1	C	339	GLY	2.4
1	C	30[A]	ARG	2.4
1	C	165	LEU	2.4
1	A	12	ALA	2.3
1	C	347	ALA	2.3
1	B	11[A]	ASP	2.3
1	D	128	ALA	2.3
1	D	232	HIS	2.3
1	D	137	ARG	2.3
1	B	134	VAL	2.3
1	D	238	PRO	2.3
1	A	8[A]	ARG	2.3
1	D	210	ARG	2.3
1	D	168	GLU	2.2
1	C	96	TRP	2.2
1	C	338	LEU	2.2
1	A	155	ALA	2.2
1	D	11	ASP	2.2
1	D	171	GLY	2.2
1	D	152	GLN	2.2
1	D	146	LEU	2.2
1	D	255	ALA	2.2
1	C	11	ASP	2.2
1	D	34	GLU	2.2
1	D	250	GLU	2.1
1	D	257	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	91	VAL	2.1
1	D	159	ARG	2.1
1	C	340	GLY	2.1
1	D	132	ALA	2.1
1	C	324	THR	2.1
1	A	96	TRP	2.1
1	C	280	GLY	2.1
1	D	65	GLY	2.1
1	D	127	GLY	2.1
1	D	144	THR	2.1
1	D	119[A]	MET	2.1
1	D	145	GLY	2.1
1	A	85	PRO	2.1
1	D	135	PRO	2.1
1	C	295	LEU	2.0
1	C	283	TYR	2.0
1	D	258	GLY	2.0
1	B	111	ARG	2.0
1	D	85	PRO	2.0
1	A	3	GLU	2.0
1	C	274	GLN	2.0
1	C	132	ALA	2.0
1	C	275	VAL	2.0
1	D	32	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KCX	D	141	12/13	0.82	0.17	42,44,79,91	0
1	KCX	A	141	12/13	0.92	0.12	21,24,65,67	0
1	KCX	B	141	12/13	0.93	0.12	19,29,71,71	0
1	KCX	C	141	12/13	0.94	0.10	23,28,64,64	0

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	PPI	B	507	5/5	0.57	0.27	47,47,57,68	0
3	PPI	B	505	5/5	0.76	0.14	40,48,59,62	0
3	PPI	B	501	5/5	0.76	0.19	30,49,51,55	0
3	PPI	B	506	5/5	0.77	0.18	56,61,64,67	0
3	PPI	A	402	5/5	0.77	0.18	33,46,51,54	0
3	PPI	C	402	5/5	0.82	0.14	44,53,59,69	0
3	PPI	D	501	5/5	0.82	0.17	31,50,54,58	0
3	PPI	D	503	5/5	0.82	0.13	28,38,40,43	0
5	NO3	A	405	4/4	0.89	0.10	43,46,47,49	0
5	NO3	B	508	4/4	0.91	0.09	32,38,39,45	0
2	PLP	D	502	15/16	0.93	0.12	30,48,58,62	0
4	NA	A	404	1/1	0.96	0.10	31,31,31,31	0
4	NA	B	504	1/1	0.96	0.12	29,29,29,29	0
2	PLP	B	502	15/16	0.96	0.10	21,31,46,51	0
2	PLP	A	401	15/16	0.96	0.11	21,36,47,51	0
4	NA	A	403	1/1	0.97	0.11	31,31,31,31	0
2	PLP	C	401	15/16	0.97	0.09	22,38,50,56	0
4	NA	B	503	1/1	0.97	0.08	33,33,33,33	0
4	NA	C	403	1/1	0.98	0.05	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.