Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:14 PM GMT

PDB ID	:	4HLU
Title	:	Structure of the EcfA-A' heterodimer bound to ADP
Authors	:	Wang, D.N.; Karpowich, N.K.
Deposited on	:	2012-10-17
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

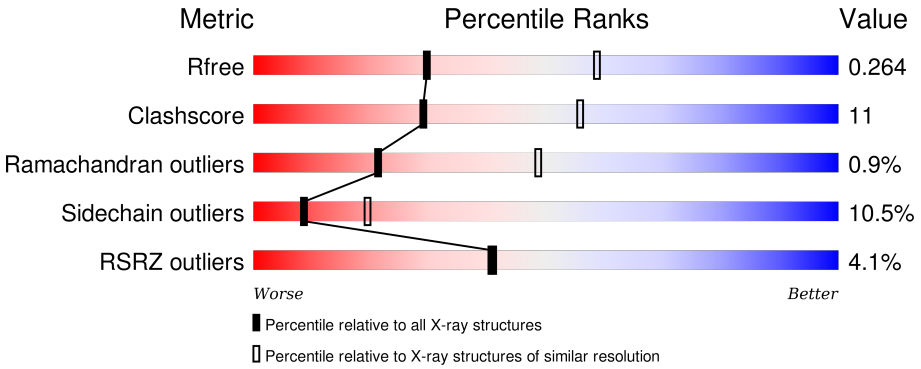
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	268	% 72% 23%
1	B	268	4% 70% 25%
2	C	268	6% 62% 26% 7%
2	D	268	4% 63% 26% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	A	302	-	-	X	X
4	ACT	B	302	-	-	X	X
4	ACT	C	1302	-	-	X	X
4	ACT	C	1303	-	-	X	-
4	ACT	D	1302	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8336 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 Putative ABC transporter ATP-binding protein TM_0222.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2119	1360	361	391	7			
1	B	265	Total	C	N	O	S	0	0	0
			2119	1360	361	391	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q9WY65
A	0	MET	-	EXPRESSION TAG	UNP Q9WY65
A	1	GLY	-	EXPRESSION TAG	UNP Q9WY65
B	-1	GLY	-	EXPRESSION TAG	UNP Q9WY65
B	0	MET	-	EXPRESSION TAG	UNP Q9WY65
B	1	GLY	-	EXPRESSION TAG	UNP Q9WY65

- Molecule 2 is a protein called Energy-coupling factor transporter ATP-binding protein EcfA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	245	Total	C	N	O	S	0	0	0
			1927	1237	318	365	7			
2	C	249	Total	C	N	O	S	0	0	0
			1954	1253	323	371	7			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	992	GLY	-	EXPRESSION TAG	UNP Q9X1Z1
D	993	SER	-	EXPRESSION TAG	UNP Q9X1Z1
D	994	GLY	-	EXPRESSION TAG	UNP Q9X1Z1
D	995	GLY	-	EXPRESSION TAG	UNP Q9X1Z1
D	996	SER	-	EXPRESSION TAG	UNP Q9X1Z1
D	997	HIS	-	EXPRESSION TAG	UNP Q9X1Z1

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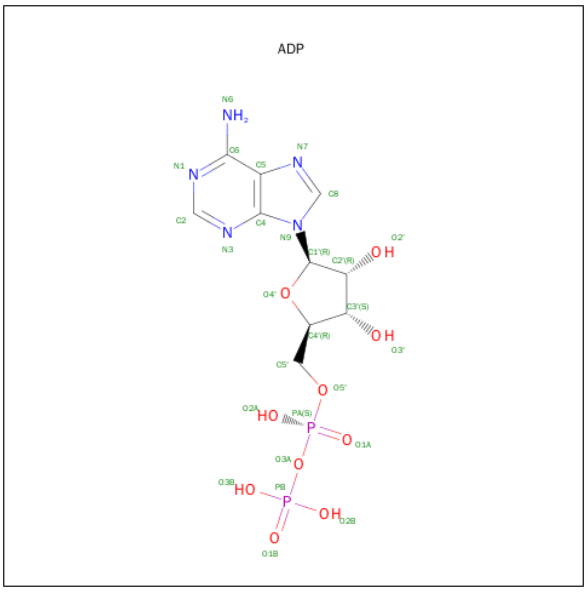
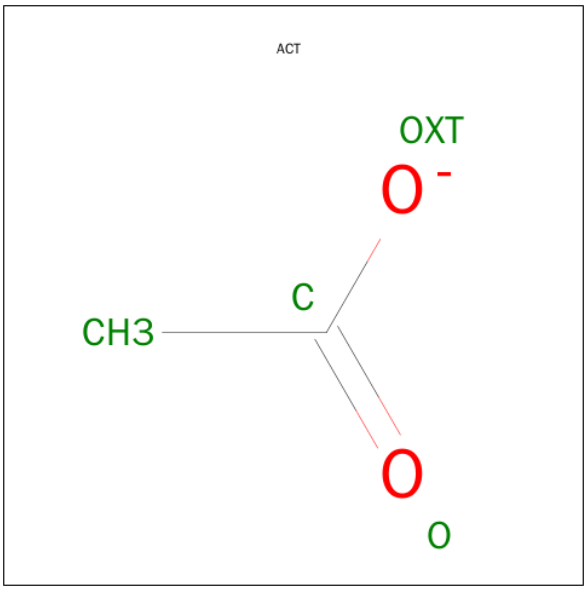
Chain	Residue	Modelled	Actual	Comment	Reference
D	998	MET	-	EXPRESSION TAG	UNP Q9X1Z1
D	999	GLY	-	EXPRESSION TAG	UNP Q9X1Z1
D	1000	SER	-	EXPRESSION TAG	UNP Q9X1Z1
D	1001	GLY	-	EXPRESSION TAG	UNP Q9X1Z1
D	1002	ARG	LYS	ENGINEERED MUTATION	UNP Q9X1Z1
D	1004	GLU	THR	ENGINEERED MUTATION	UNP Q9X1Z1
D	1053	ALA	GLU	ENGINEERED MUTATION	UNP Q9X1Z1
D	1055	ALA	GLU	ENGINEERED MUTATION	UNP Q9X1Z1
D	1125	ALA	GLU	ENGINEERED MUTATION	UNP Q9X1Z1
D	1126	ALA	LYS	ENGINEERED MUTATION	UNP Q9X1Z1
D	1127	ALA	GLU	ENGINEERED MUTATION	UNP Q9X1Z1
C	992	GLY	-	EXPRESSION TAG	UNP Q9X1Z1
C	993	SER	-	EXPRESSION TAG	UNP Q9X1Z1
C	994	GLY	-	EXPRESSION TAG	UNP Q9X1Z1
C	995	GLY	-	EXPRESSION TAG	UNP Q9X1Z1
C	996	SER	-	EXPRESSION TAG	UNP Q9X1Z1
C	997	HIS	-	EXPRESSION TAG	UNP Q9X1Z1
C	998	MET	-	EXPRESSION TAG	UNP Q9X1Z1
C	999	GLY	-	EXPRESSION TAG	UNP Q9X1Z1
C	1000	SER	-	EXPRESSION TAG	UNP Q9X1Z1
C	1001	GLY	-	EXPRESSION TAG	UNP Q9X1Z1
C	1002	ARG	LYS	ENGINEERED MUTATION	UNP Q9X1Z1
C	1004	GLU	THR	ENGINEERED MUTATION	UNP Q9X1Z1
C	1053	ALA	GLU	ENGINEERED MUTATION	UNP Q9X1Z1
C	1055	ALA	GLU	ENGINEERED MUTATION	UNP Q9X1Z1
C	1125	ALA	GLU	ENGINEERED MUTATION	UNP Q9X1Z1
C	1126	ALA	LYS	ENGINEERED MUTATION	UNP Q9X1Z1
C	1127	ALA	GLU	ENGINEERED MUTATION	UNP Q9X1Z1

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is water.

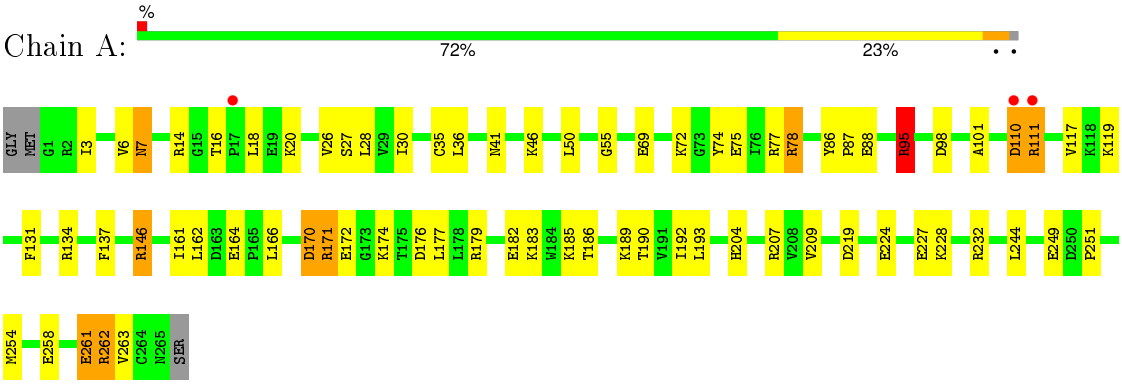
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	21	Total O 21 21	0	0
5	D	23	Total O 23 23	0	0
5	B	21	Total O 21 21	0	0
5	C	24	Total O 24 24	0	0

3 Residue-property plots (i)

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

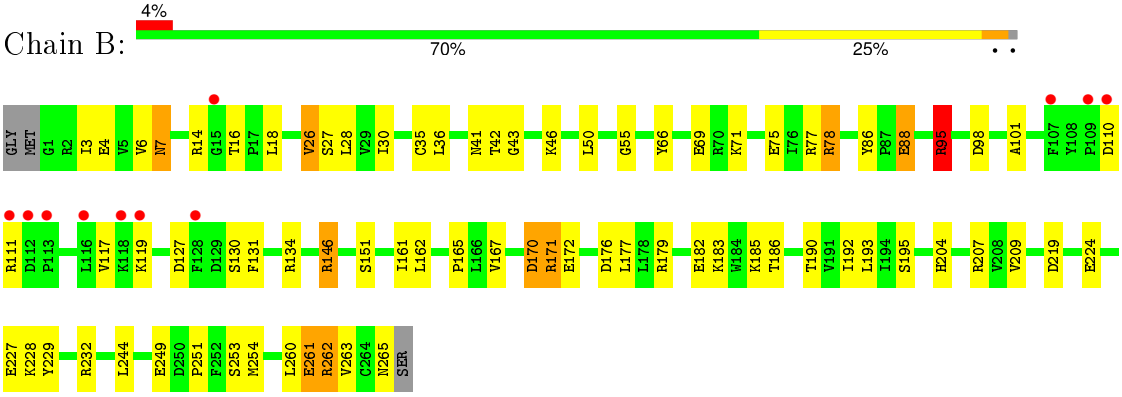
- Molecule 1: Putative ABC transporter ATP-binding protein TM_0222

Chain A:



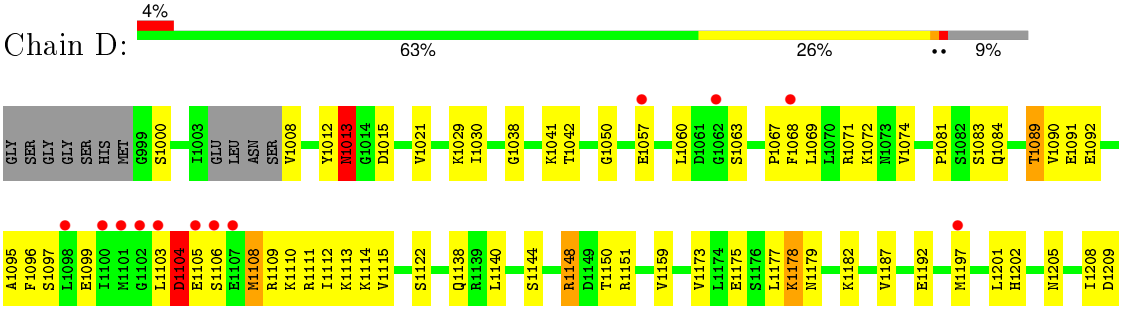
- Molecule 1: Putative ABC transporter ATP-binding protein TM_0222

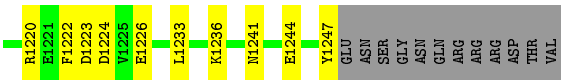
Chain B:



- Molecule 2: Energy-coupling factor transporter ATP-binding protein EcfA

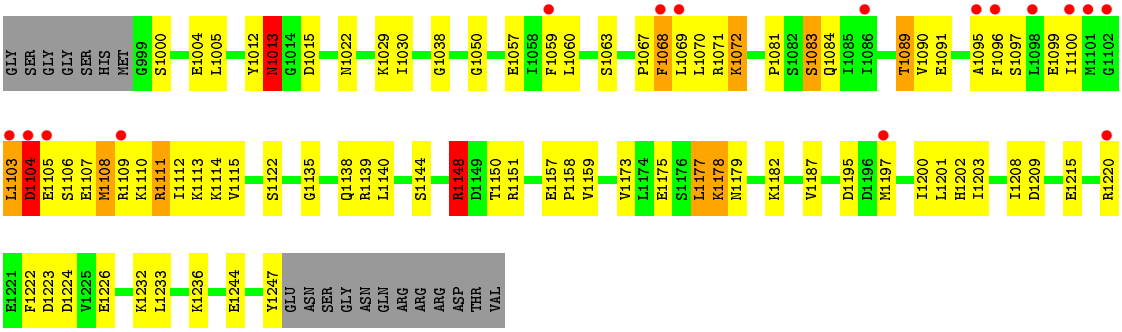
Chain D:





• Molecule 2: Energy-coupling factor transporter ATP-binding protein EcfA

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	67.78Å 67.78Å 252.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.15 – 2.70 48.15 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.15-2.70) 97.6 (48.15-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.51 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.213 , 0.258 0.224 , 0.264	Depositor DCC
R_{free} test set	1718 reflections (4.94%)	DCC
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 56.6	EDS
Estimated twinning fraction	0.011 for -h,-k,l 0.049 for h,-h-k,-l 0.037 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 35687 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8336	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.38	1/2158 (0.0%)	0.77	11/2909 (0.4%)
1	B	0.36	0/2158	0.64	4/2909 (0.1%)
2	C	0.40	0/1990	0.78	5/2685 (0.2%)
2	D	0.43	0/1962	0.76	4/2645 (0.2%)
All	All	0.39	1/8268 (0.0%)	0.74	24/11148 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	261	GLU	CB-CG	-5.59	1.41	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1148	ARG	NE-CZ-NH2	15.11	127.85	120.30
2	C	1148	ARG	NE-CZ-NH1	14.89	127.74	120.30
2	C	1148	ARG	NE-CZ-NH2	-14.52	113.04	120.30
2	D	1148	ARG	NE-CZ-NH1	-12.33	114.14	120.30
1	A	170	ASP	CB-CG-OD2	-12.18	107.33	118.30
1	B	110	ASP	CB-CG-OD1	-12.06	107.44	118.30
1	A	170	ASP	CB-CG-OD1	11.09	128.28	118.30
1	A	110	ASP	CB-CG-OD1	-9.64	109.62	118.30
1	B	110	ASP	CB-CG-OD2	9.61	126.95	118.30
1	A	110	ASP	CB-CA-C	-9.16	92.09	110.40
1	A	170	ASP	CB-CA-C	-8.49	93.41	110.40
2	D	1013	ASN	N-CA-CB	-7.94	96.31	110.60
1	A	110	ASP	CB-CG-OD2	7.27	124.84	118.30
1	A	111	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	95	ARG	CG-CD-NE	7.03	126.56	111.80
1	A	95	ARG	NE-CZ-NH1	6.97	123.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1148	ARG	CD-NE-CZ	6.70	132.98	123.60
2	D	1148	ARG	CD-NE-CZ	6.40	132.56	123.60
1	B	170	ASP	N-CA-CB	6.29	121.92	110.60
1	A	261	GLU	CA-CB-CG	6.00	126.59	113.40
1	B	95	ARG	CG-CD-NE	5.75	123.87	111.80
1	A	111	ARG	CG-CD-NE	-5.71	99.80	111.80
2	C	1068	PHE	CB-CG-CD2	-5.64	116.85	120.80
2	C	1013	ASN	CB-CA-C	5.38	121.16	110.40

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	2119	0	2160	46	1
1	B	2119	0	2160	54	1
2	C	1954	0	1958	54	0
2	D	1927	0	1933	44	0
3	A	27	0	12	1	0
3	B	27	0	12	2	0
3	C	27	0	12	1	0
3	D	27	0	12	3	0
4	A	4	0	3	2	0
4	B	4	0	3	5	0
4	C	8	0	6	7	0
4	D	4	0	3	1	0
5	A	21	0	0	2	0
5	B	21	0	0	6	0
5	C	24	0	0	7	0
5	D	23	0	0	9	0
All	All	8336	0	8274	188	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (188) 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:189:LYS:NZ	5:A:408:HOH:O	1.83	1.10
2:C:1157:GLU:OE2	5:C:1416:HOH:O	1.86	0.94
2:C:1173:VAL:O	2:C:1177:LEU:HD12	1.69	0.93
2:C:1105:GLU:HA	2:C:1108:MET:HG3	1.50	0.91
2:D:1105:GLU:HA	2:D:1108:MET:HG3	1.52	0.90
2:D:1074:VAL:O	5:D:1409:HOH:O	1.90	0.88
1:A:164:GLU:OE2	5:A:412:HOH:O	1.91	0.88
1:B:151:SER:O	5:B:409:HOH:O	1.92	0.86
1:A:249:GLU:OE2	1:A:262:ARG:NH1	2.09	0.85
1:B:249:GLU:OE2	1:B:262:ARG:NH1	2.11	0.83
2:D:1042:THR:OG1	5:D:1419:HOH:O	1.92	0.81
2:C:1097:SER:O	5:C:1418:HOH:O	1.98	0.80
3:D:1301:ADP:O2B	5:D:1419:HOH:O	2.00	0.80
1:B:165:PRO:HD2	4:B:302:ACT:H2	1.64	0.80
1:A:95:ARG:HH11	1:A:95:ARG:HB2	1.50	0.76
1:A:146:ARG:NH2	1:A:176:ASP:OD2	2.20	0.75
1:A:166:LEU:H	4:A:302:ACT:H2	1.52	0.74
2:D:1013:ASN:OD1	1:B:261:GLU:OE2	2.08	0.71
1:B:232:ARG:HD2	2:C:1247:TYR:HE2	1.54	0.71
1:B:14:ARG:HG2	1:B:14:ARG:HH11	1.56	0.70
1:B:4:GLU:OE1	5:B:412:HOH:O	2.07	0.70
2:C:1203:ILE:O	5:C:1406:HOH:O	2.10	0.70
1:B:146:ARG:NH2	1:B:176:ASP:OD2	2.24	0.69
2:D:1099:GLU:HA	2:D:1103:LEU:HD13	1.73	0.69
2:D:1205:ASN:OD1	5:D:1417:HOH:O	2.11	0.69
1:A:185:LYS:NZ	1:A:204:HIS:O	2.26	0.68
1:B:185:LYS:NZ	1:B:204:HIS:O	2.27	0.68
2:C:1148:ARG:HH21	2:C:1150:THR:HG21	1.59	0.67
1:B:7:ASN:H	1:B:27:SER:HB3	1.61	0.65
1:A:75:GLU:HA	1:A:78:ARG:HD3	1.77	0.65
1:B:95:ARG:HB2	1:B:95:ARG:HH11	1.62	0.64
1:B:75:GLU:HA	1:B:78:ARG:HD3	1.80	0.64
2:C:1159:VAL:H	4:C:1302:ACT:H1	1.63	0.64
1:B:95:ARG:CB	1:B:95:ARG:HH11	2.12	0.63
1:B:86:TYR:HB3	1:B:88:GLU:OE2	1.99	0.62
1:A:263:VAL:O	2:D:1236:LYS:NZ	2.32	0.62
2:D:1041:LYS:N	3:D:1301:ADP:O1B	2.33	0.61
2:D:1103:LEU:N	2:D:1104:ASP:OD2	2.25	0.61
2:C:1201:LEU:HD23	2:C:1208:ILE:HD13	1.82	0.61
2:D:1000:SER:O	2:D:1151:ARG:NH1	2.31	0.60
1:B:232:ARG:HD2	2:C:1247:TYR:CE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1201:LEU:HD23	2:D:1208:ILE:HD13	1.82	0.60
2:C:1012:TYR:O	2:C:1013:ASN:HB3	2.01	0.59
2:C:1000:SER:O	2:C:1151:ARG:NH1	2.32	0.59
1:A:95:ARG:HH11	1:A:95:ARG:CB	2.16	0.59
2:D:1038:GLY:N	3:D:1301:ADP:O3B	2.30	0.58
2:C:1103:LEU:HA	2:C:1104:ASP:O	2.04	0.57
2:C:1195:ASP:OD2	5:C:1420:HOH:O	2.17	0.57
2:D:1241:ASN:N	5:D:1408:HOH:O	2.10	0.57
1:A:7:ASN:H	1:A:27:SER:HB3	1.70	0.56
2:C:1175:GLU:O	2:C:1179:ASN:OD1	2.23	0.56
2:C:1139:ARG:NH2	4:C:1303:ACT:O	2.34	0.56
1:A:162:LEU:HB2	1:A:193:LEU:HD23	1.87	0.56
2:C:1177:LEU:HB3	2:C:1182:LYS:HG3	1.88	0.56
1:B:229:TYR:O	5:B:420:HOH:O	2.17	0.56
2:C:1004:GLU:HB2	2:C:1059:PHE:HB2	1.87	0.56
1:A:224:GLU:HB3	1:A:228:LYS:HE3	1.88	0.55
1:B:263:VAL:O	2:C:1236:LYS:NZ	2.38	0.55
1:B:162:LEU:HB2	1:B:193:LEU:HD23	1.86	0.55
2:C:1089:THR:OG1	2:C:1091:GLU:HG2	2.07	0.55
2:C:1159:VAL:HG22	4:C:1302:ACT:H1	1.89	0.54
1:A:35:CYS:SG	1:A:185:LYS:HD2	2.48	0.54
2:D:1008:VAL:N	5:D:1423:HOH:O	2.40	0.54
2:D:1089:THR:OG1	2:D:1091:GLU:HG2	2.06	0.54
2:C:1148:ARG:HH21	2:C:1150:THR:CG2	2.20	0.54
2:D:1103:LEU:HA	2:D:1104:ASP:O	2.08	0.54
1:B:224:GLU:HB3	1:B:228:LYS:HE3	1.90	0.53
2:D:1008:VAL:N	5:D:1412:HOH:O	2.41	0.53
2:C:1247:TYR:HB2	5:C:1422:HOH:O	2.08	0.53
1:B:55:GLY:O	1:B:77:ARG:NH1	2.42	0.53
1:B:35:CYS:SG	1:B:185:LYS:HD2	2.49	0.52
2:C:1050:GLY:O	2:C:1071:ARG:NE	2.42	0.52
1:B:171:ARG:HD2	2:C:1226:GLU:HB2	1.92	0.52
1:A:55:GLY:O	1:A:77:ARG:NH1	2.42	0.52
1:B:195:SER:OG	4:B:302:ACT:H1	2.10	0.51
2:D:1050:GLY:O	2:D:1071:ARG:NE	2.43	0.51
1:A:14:ARG:HH11	1:A:14:ARG:HG2	1.76	0.51
2:D:1148:ARG:HH21	2:D:1150:THR:HG21	1.75	0.51
1:A:95:ARG:NH1	1:A:98:ASP:OD2	2.45	0.50
1:A:74:TYR:O	1:A:78:ARG:HG3	2.12	0.50
2:C:1050:GLY:HA3	2:C:1067:PRO:O	2.12	0.50
1:A:232:ARG:HD2	2:D:1247:TYR:HE2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ARG:NH1	5:B:417:HOH:O	2.44	0.49
2:C:1090:VAL:HG13	2:C:1140:LEU:HD13	1.94	0.49
2:D:1150:THR:O	2:D:1182:LYS:NZ	2.31	0.49
1:A:137:PHE:CD2	2:C:1215:GLU:HB3	2.48	0.49
1:B:179:ARG:NH1	1:B:183:LYS:NZ	2.60	0.48
2:C:1038:GLY:HA2	3:C:1301:ADP:H5'2	1.95	0.48
2:D:1050:GLY:HA3	2:D:1067:PRO:O	2.13	0.48
2:D:1148:ARG:HH21	2:D:1150:THR:CG2	2.26	0.48
2:D:1202:HIS:NE2	2:D:1224:ASP:OD2	2.45	0.48
1:B:7:ASN:O	5:B:405:HOH:O	2.20	0.48
2:C:1159:VAL:HG22	4:C:1302:ACT:CH3	2.43	0.48
2:C:1202:HIS:NE2	2:C:1224:ASP:OD2	2.44	0.48
1:B:95:ARG:NH1	1:B:98:ASP:OD2	2.47	0.47
1:A:111:ARG:HD3	1:A:111:ARG:HA	1.43	0.47
2:D:1090:VAL:HG13	2:D:1140:LEU:HD13	1.95	0.47
1:A:50:LEU:HD11	1:A:192:ILE:HG21	1.96	0.47
2:C:1097:SER:HB3	2:C:1148:ARG:HG2	1.96	0.47
1:A:182:GLU:OE1	1:A:204:HIS:ND1	2.33	0.47
2:D:1159:VAL:N	4:D:1302:ACT:OXT	2.45	0.47
1:B:260:LEU:HD11	2:C:1232:LYS:HB2	1.95	0.47
2:C:1030:ILE:HG13	2:C:1178:LYS:HG3	1.97	0.47
2:C:1081:PRO:HG3	2:C:1138:GLN:HG3	1.97	0.47
2:D:1069:LEU:O	2:D:1072:LYS:HB2	2.15	0.47
2:C:1012:TYR:N	5:C:1417:HOH:O	2.34	0.46
2:D:1081:PRO:HG3	2:D:1138:GLN:HG3	1.96	0.46
1:A:119:LYS:HE2	1:A:119:LYS:HB3	1.77	0.46
1:A:131:PHE:HA	1:A:134:ARG:HG3	1.97	0.46
1:A:179:ARG:NH1	1:A:183:LYS:NZ	2.63	0.46
1:A:50:LEU:HD12	1:A:161:ILE:HD13	1.98	0.46
1:A:207:ARG:NH1	1:A:219:ASP:OD1	2.49	0.46
2:C:1220:ARG:HG2	2:C:1222:PHE:CE2	2.51	0.46
2:C:1158:PRO:HD2	4:C:1302:ACT:H3	1.98	0.46
1:B:50:LEU:HD11	1:B:192:ILE:HG21	1.96	0.46
2:C:1209:ASP:OD1	2:C:1209:ASP:N	2.44	0.46
1:B:195:SER:CB	4:B:302:ACT:H1	2.45	0.46
2:C:1103:LEU:N	2:C:1104:ASP:OD2	2.47	0.46
1:B:182:GLU:OE1	1:B:204:HIS:ND1	2.33	0.46
2:D:1177:LEU:HB3	2:D:1182:LYS:HG3	1.98	0.45
1:B:265:ASN:OD1	2:C:1236:LYS:NZ	2.48	0.45
1:B:50:LEU:HD12	1:B:161:ILE:HD13	1.99	0.45
1:B:127:ASP:OD2	1:B:130:SER:OG	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1030:ILE:HG13	2:D:1178:LYS:HG3	1.97	0.45
1:A:176:ASP:OD1	1:A:179:ARG:NE	2.47	0.45
1:B:131:PHE:HA	1:B:134:ARG:HG3	1.96	0.45
2:C:1200:ILE:N	2:C:1200:ILE:HD12	2.31	0.45
2:C:1069:LEU:O	2:C:1072:LYS:HB2	2.16	0.45
2:D:1220:ARG:HA	2:D:1220:ARG:HD3	1.65	0.45
2:C:1220:ARG:HA	2:C:1220:ARG:HD3	1.72	0.45
1:B:207:ARG:NH1	1:B:219:ASP:OD1	2.50	0.44
1:A:78:ARG:HG3	1:A:78:ARG:H	1.69	0.44
2:C:1226:GLU:O	5:C:1424:HOH:O	2.21	0.44
1:B:176:ASP:OD1	1:B:179:ARG:NE	2.48	0.44
2:C:1067:PRO:O	2:C:1070:LEU:HB2	2.18	0.44
1:B:101:ALA:HB2	1:B:117:VAL:HG21	2.00	0.44
1:B:14:ARG:HG2	1:B:14:ARG:NH1	2.25	0.44
1:A:101:ALA:HB2	1:A:117:VAL:HG21	2.00	0.44
2:C:1067:PRO:O	2:C:1071:ARG:HG3	2.18	0.44
2:D:1097:SER:HB3	2:D:1148:ARG:HG3	2.00	0.44
1:B:111:ARG:HA	1:B:111:ARG:HD3	1.40	0.44
1:A:41:ASN:O	1:A:46:LYS:NZ	2.51	0.44
1:B:26:VAL:HA	5:B:406:HOH:O	2.18	0.43
2:D:1220:ARG:HG2	2:D:1222:PHE:CE2	2.53	0.43
1:B:167:VAL:HG23	4:B:302:ACT:O	2.18	0.43
1:B:251:PRO:O	1:B:254:MET:HB3	2.19	0.43
2:D:1148:ARG:NH2	2:D:1150:THR:HG21	2.34	0.43
1:A:36:LEU:HD11	1:A:209:VAL:HG23	2.01	0.43
2:D:1067:PRO:O	2:D:1071:ARG:HG3	2.19	0.43
1:A:86:TYR:HB3	1:A:88:GLU:OE2	2.19	0.43
1:B:36:LEU:HD11	1:B:209:VAL:HG23	2.00	0.43
2:C:1135:GLY:HA3	4:C:1303:ACT:H2	2.02	0.42
1:A:74:TYR:CE2	1:A:78:ARG:HD2	2.54	0.42
2:C:1072:LYS:HD3	2:C:1072:LYS:HA	1.89	0.42
2:D:1173:VAL:O	2:D:1177:LEU:CD1	2.67	0.42
1:A:3:ILE:HB	1:A:30:ILE:HB	2.00	0.42
1:B:42:THR:HG21	4:C:1303:ACT:H3	2.01	0.42
1:B:41:ASN:O	1:B:46:LYS:NZ	2.52	0.42
1:B:43:GLY:N	3:B:301:ADP:O1B	2.40	0.42
1:A:86:TYR:HA	1:A:87:PRO:HD2	1.92	0.42
2:C:1095:ALA:HB2	2:C:1112:ILE:HD11	2.01	0.42
1:B:3:ILE:HB	1:B:30:ILE:HB	2.00	0.42
1:A:170:ASP:O	1:A:174:LYS:HG3	2.20	0.42
1:A:182:GLU:OE2	1:A:185:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LYS:HB2	1:A:46:LYS:HE2	1.87	0.42
2:C:1005:LEU:O	2:C:1022:ASN:HA	2.21	0.41
1:A:20:LYS:HG2	3:A:301:ADP:H1'	2.02	0.41
2:D:1209:ASP:OD1	2:D:1209:ASP:N	2.44	0.41
1:A:251:PRO:O	1:A:254:MET:HB3	2.20	0.41
2:D:1012:TYR:O	2:D:1013:ASN:HB2	2.15	0.41
2:D:1021:VAL:HA	5:D:1404:HOH:O	2.19	0.41
1:A:164:GLU:HA	4:A:302:ACT:H1	2.02	0.41
1:A:179:ARG:NH1	1:A:183:LYS:HZ3	2.18	0.41
1:B:182:GLU:OE2	1:B:185:LYS:HE2	2.20	0.41
1:B:119:LYS:HE2	1:B:119:LYS:HB3	1.78	0.41
2:C:1107:GLU:O	2:C:1111:ARG:N	2.53	0.41
1:B:263:VAL:O	1:B:265:ASN:OD1	2.38	0.41
2:D:1175:GLU:O	2:D:1179:ASN:OD1	2.38	0.41
1:A:171:ARG:HD2	2:D:1226:GLU:HB2	2.03	0.41
1:B:66:TYR:HB2	1:B:71:LYS:HD3	2.04	0.41
2:D:1192:GLU:OE2	5:D:1418:HOH:O	2.22	0.41
2:D:1110:LYS:O	2:D:1113:LYS:HB3	2.21	0.41
1:B:43:GLY:HA2	3:B:301:ADP:H5'2	2.03	0.40
1:A:258:GLU:O	1:A:262:ARG:HG3	2.21	0.40
2:C:1110:LYS:O	2:C:1113:LYS:HB3	2.22	0.40
2:C:1099:GLU:HG2	2:C:1100:ILE:HD12	2.03	0.40
2:D:1095:ALA:HB2	2:D:1112:ILE:HD11	2.03	0.40
1:B:195:SER:HB2	4:B:302:ACT:H1	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LYS:NZ	1:B:253:SER:O[1_455]	1.93	0.27

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	263/268 (98%)	253 (96%)	9 (3%)	1 (0%)	39	69
1	B	263/268 (98%)	253 (96%)	9 (3%)	1 (0%)	39	69
2	C	247/268 (92%)	229 (93%)	14 (6%)	4 (2%)	12	30
2	D	241/268 (90%)	225 (93%)	13 (5%)	3 (1%)	16	39
All	All	1014/1072 (95%)	960 (95%)	45 (4%)	9 (1%)	21	49

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	1013	ASN
1	A	7	ASN
2	C	1104	ASP
2	D	1104	ASP
1	B	7	ASN
2	C	1013	ASN
2	D	1084	GLN
2	C	1084	GLN
2	C	1083	SER

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	235/237 (99%)	216 (92%)	19 (8%)	15	33
1	B	235/237 (99%)	215 (92%)	20 (8%)	13	30
2	C	211/227 (93%)	182 (86%)	29 (14%)	4	11
2	D	208/227 (92%)	183 (88%)	25 (12%)	6	14
All	All	889/928 (96%)	796 (90%)	93 (10%)	8	19

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	16	THR
1	A	18	LEU
1	A	26	VAL
1	A	28	LEU
1	A	69	GLU
1	A	78	ARG
1	A	95	ARG
1	A	110	ASP
1	A	146	ARG
1	A	171	ARG
1	A	172	GLU
1	A	177	LEU
1	A	186	THR
1	A	190	THR
1	A	227	GLU
1	A	244	LEU
1	A	261	GLU
1	A	262	ARG
2	D	1015	ASP
2	D	1029	LYS
2	D	1057	GLU
2	D	1060	LEU
2	D	1063	SER
2	D	1068	PHE
2	D	1083	SER
2	D	1089	THR
2	D	1092	GLU
2	D	1096	PHE
2	D	1104	ASP
2	D	1106	SER
2	D	1108	MET
2	D	1109	ARG
2	D	1111	ARG
2	D	1114	LYS
2	D	1115	VAL
2	D	1122	SER
2	D	1144	SER
2	D	1178	LYS
2	D	1187	VAL
2	D	1197	MET
2	D	1223	ASP
2	D	1233	LEU

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Mol	Chain	Res	Type
2	D	1244	GLU
1	B	6	VAL
1	B	16	THR
1	B	18	LEU
1	B	26	VAL
1	B	28	LEU
1	B	69	GLU
1	B	78	ARG
1	B	88	GLU
1	B	95	ARG
1	B	146	ARG
1	B	170	ASP
1	B	171	ARG
1	B	172	GLU
1	B	177	LEU
1	B	186	THR
1	B	190	THR
1	B	227	GLU
1	B	244	LEU
1	B	261	GLU
1	B	262	ARG
2	C	1013	ASN
2	C	1015	ASP
2	C	1029	LYS
2	C	1057	GLU
2	C	1060	LEU
2	C	1063	SER
2	C	1068	PHE
2	C	1072	LYS
2	C	1083	SER
2	C	1089	THR
2	C	1096	PHE
2	C	1103	LEU
2	C	1104	ASP
2	C	1106	SER
2	C	1108	MET
2	C	1109	ARG
2	C	1111	ARG
2	C	1114	LYS
2	C	1115	VAL
2	C	1122	SER
2	C	1144	SER

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Mol	Chain	Res	Type
2	C	1148	ARG
2	C	1177	LEU
2	C	1178	LYS
2	C	1187	VAL
2	C	1197	MET
2	C	1223	ASP
2	C	1233	LEU
2	C	1244	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	HIS
2	D	1013	ASN
2	C	1179	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)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ADP	A	301	-	22,29,29	1.02	1 (4%)	27,45,45	1.80	3 (11%)
4	ACT	A	302	-	1,3,3	0.63	0	0,3,3	0.00	-
3	ADP	B	301	-	22,29,29	0.98	1 (4%)	27,45,45	1.81	3 (11%)
4	ACT	B	302	-	1,3,3	0.52	0	0,3,3	0.00	-
3	ADP	C	1301	-	22,29,29	1.01	1 (4%)	27,45,45	1.76	3 (11%)
4	ACT	C	1302	-	1,3,3	0.44	0	0,3,3	0.00	-
4	ACT	C	1303	-	1,3,3	1.26	0	0,3,3	0.00	-
3	ADP	D	1301	-	22,29,29	0.97	1 (4%)	27,45,45	1.86	3 (11%)
4	ACT	D	1302	-	1,3,3	1.54	0	0,3,3	0.00	-

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	ADP	A	301	-	-	0/12/32/32	0/3/3/3
4	ACT	A	302	-	-	0/0/0/0	0/0/0/0
3	ADP	B	301	-	-	0/12/32/32	0/3/3/3
4	ACT	B	302	-	-	0/0/0/0	0/0/0/0
3	ADP	C	1301	-	-	0/12/32/32	0/3/3/3
4	ACT	C	1302	-	-	0/0/0/0	0/0/0/0
4	ACT	C	1303	-	-	0/0/0/0	0/0/0/0
3	ADP	D	1301	-	-	0/12/32/32	0/3/3/3
4	ACT	D	1302	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	ADP	C5-C4	3.11	1.47	1.40
3	D	1301	ADP	C5-C4	3.12	1.47	1.40
3	A	301	ADP	C5-C4	3.20	1.47	1.40
3	C	1301	ADP	C5-C4	3.22	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	ADP	N3-C2-N1	-7.08	123.47	128.89
3	D	1301	ADP	N3-C2-N1	-7.06	123.49	128.89
3	B	301	ADP	N3-C2-N1	-7.02	123.52	128.89
3	C	1301	ADP	N3-C2-N1	-6.77	123.71	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1301	ADP	C4-C5-N7	-3.26	106.48	109.48
3	A	301	ADP	C4-C5-N7	-3.23	106.51	109.48
3	B	301	ADP	C4-C5-N7	-3.19	106.55	109.48
3	C	1301	ADP	C4-C5-N7	-3.06	106.66	109.48
3	D	1301	ADP	PA-O3A-PB	-2.86	123.09	132.67
3	B	301	ADP	PA-O3A-PB	-2.58	124.01	132.67
3	A	301	ADP	PA-O3A-PB	-2.54	124.15	132.67
3	C	1301	ADP	PA-O3A-PB	-2.22	125.21	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	ADP	1	0
4	A	302	ACT	2	0
3	B	301	ADP	2	0
4	B	302	ACT	5	0
3	C	1301	ADP	1	0
4	C	1302	ACT	4	0
4	C	1303	ACT	3	0
3	D	1301	ADP	3	0
4	D	1302	ACT	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	265/268 (98%)	0.14	3 (1%)	82	83	31, 60, 103, 149	0
1	B	265/268 (98%)	0.22	11 (4%)	40	39	31, 61, 103, 149	0
2	C	249/268 (92%)	0.28	16 (6%)	23	21	28, 57, 116, 165	0
2	D	245/268 (91%)	0.22	12 (4%)	33	32	28, 57, 115, 165	0
All	All	1024/1072 (95%)	0.21	42 (4%)	41	41	28, 59, 111, 165	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1103	LEU	9.5
2	C	1103	LEU	8.2
2	D	1101	MET	6.4
2	C	1101	MET	5.6
1	B	109	PRO	5.5
1	A	110	ASP	4.1
2	D	1102	GLY	4.0
1	B	110	ASP	3.9
2	C	1098	LEU	3.8
1	B	116	LEU	3.4
2	C	1069	LEU	3.4
2	C	1105	GLU	3.4
2	C	1109	ARG	3.3
2	C	1104	ASP	3.2
1	A	111	ARG	3.2
2	C	1100	ILE	3.0
2	D	1062	GLY	3.0
1	B	111	ARG	2.9
1	A	17	PRO	2.8
2	D	1107	GLU	2.7
2	D	1098	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	1059	PHE	2.6
2	C	1197	MET	2.6
1	B	112	ASP	2.5
1	B	15	GLY	2.5
2	D	1197	MET	2.4
2	D	1068	PHE	2.4
1	B	128	PHE	2.3
2	D	1105	GLU	2.3
2	D	1100	ILE	2.3
2	C	1220	ARG	2.3
1	B	107	PHE	2.3
2	C	1086	ILE	2.3
2	C	1102	GLY	2.2
1	B	119	LYS	2.2
2	D	1057	GLU	2.1
1	B	118	LYS	2.1
1	B	113	PRO	2.1
2	C	1068	PHE	2.1
2	C	1095	ALA	2.1
2	D	1106	SER	2.1
2	C	1096	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	ACT	B	302	4/4	0.93	0.31	7.09	30,40,54,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	ACT	A	302	4/4	0.93	0.30	5.68	6,53,61,64	0
4	ACT	C	1302	4/4	0.96	0.24	3.27	37,43,55,56	0
4	ACT	D	1302	4/4	0.94	0.21	2.40	41,41,44,44	0
4	ACT	C	1303	4/4	0.93	0.21	1.92	43,43,46,59	0
3	ADP	B	301	27/27	0.96	0.15	-0.19	19,50,61,69	0
3	ADP	D	1301	27/27	0.96	0.16	-0.35	35,54,64,70	0
3	ADP	A	301	27/27	0.95	0.14	-0.52	24,41,51,59	0
3	ADP	C	1301	27/27	0.94	0.13	-0.94	45,55,62,74	0

6.5 Other polymers

There are no such residues in this entry.