



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:55 AM GMT

PDB ID : 2JA3
Title : CYTOPLASMIC DOMAIN OF THE HUMAN CHLORIDE TRANSPORTER
CLC-5 IN COMPLEX WITH ADP
Authors : Meyer, S.; Savaresi, S.; Forster, I.C.; Dutzler, R.
Deposited on : 2006-11-21
Resolution : 3.05 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 (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

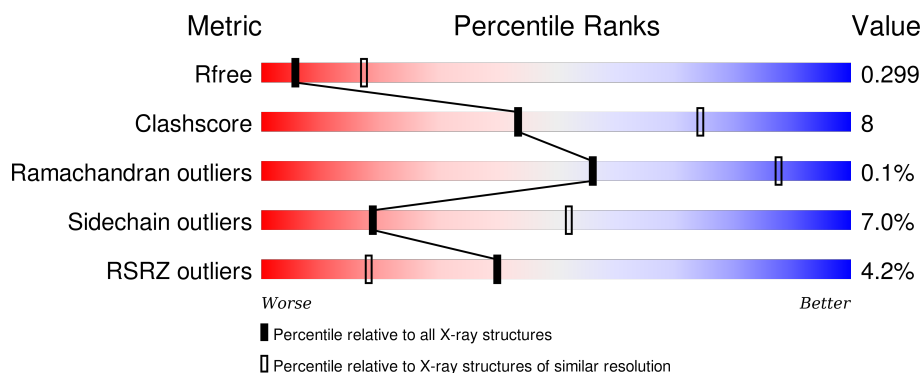
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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	185	<div> <div>4%</div> <div>68% 19% • 10%</div> </div>
1	B	185	<div> <div>3%</div> <div>75% 15% • 8%</div> </div>
1	C	185	<div> <div>%</div> <div>68% 22% • • 7%</div> </div>
1	D	185	<div> <div>2%</div> <div>74% 17% • 8%</div> </div>
1	E	185	<div> <div>4%</div> <div>72% 16% • 10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	185	

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

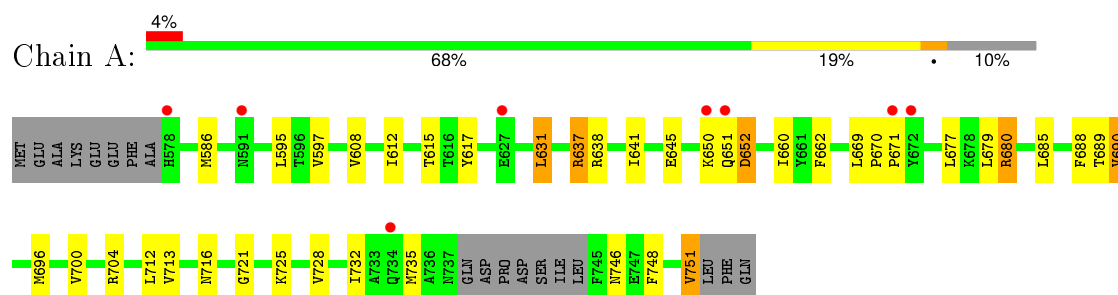
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	D	1753	-	-	-	X

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

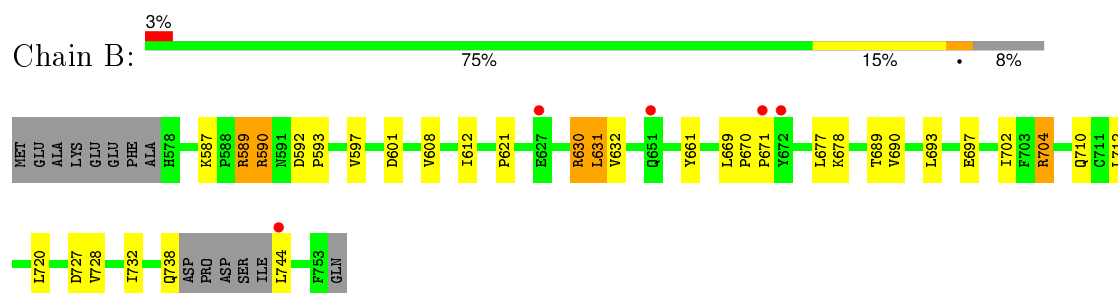
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

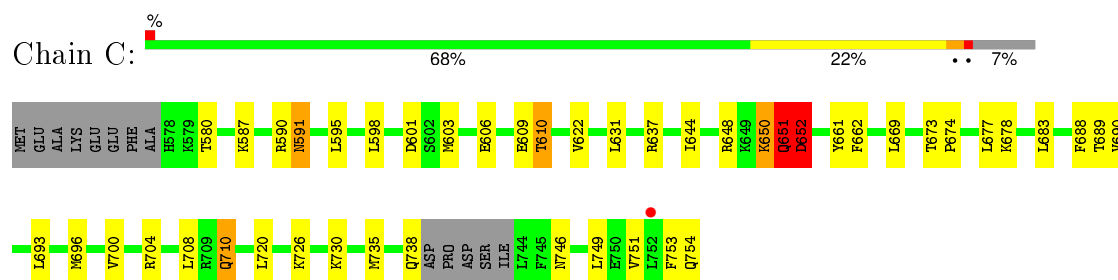
• Molecule 1: CHLORIDE CHANNEL PROTEIN 5



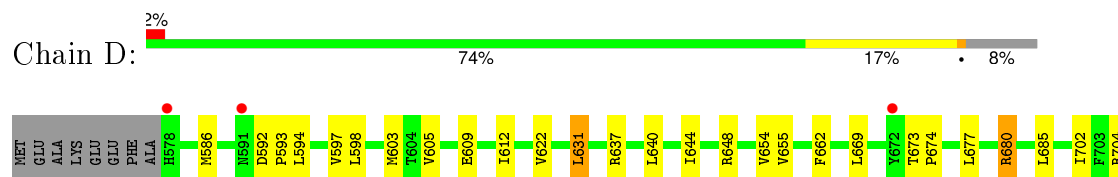
• Molecule 1: CHLORIDE CHANNEL PROTEIN 5

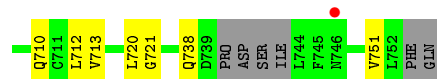


• Molecule 1: CHLORIDE CHANNEL PROTEIN 5

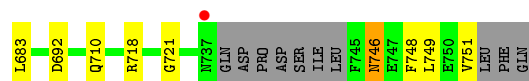


• Molecule 1: CHLORIDE CHANNEL PROTEIN 5

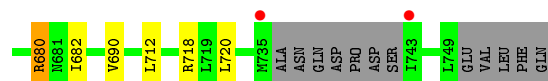
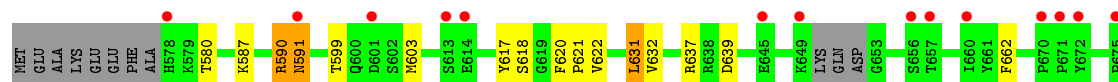
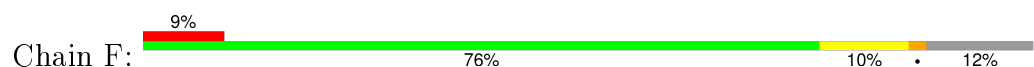




• Molecule 1: CHLORIDE CHANNEL PROTEIN 5



• Molecule 1: CHLORIDE CHANNEL PROTEIN 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.57Å 149.31Å 81.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.83 – 3.05 19.83 – 3.05	Depositor EDS
% Data completeness (in resolution range)	93.8 (19.83-3.05) 93.8 (19.83-3.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.04Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.278 , 0.317 0.259 , 0.299	Depositor DCC
R_{free} test set	1439 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	79.4	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 21.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 27987 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8165	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 4.25% 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, 0.375 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

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	0.32	0/1348	0.50	0/1830
1	B	0.33	0/1385	0.50	0/1880
1	C	0.34	0/1394	0.51	0/1892
1	D	0.31	0/1375	0.51	0/1867
1	E	0.30	0/1348	0.52	0/1830
1	F	0.26	0/1285	0.44	0/1745
All	All	0.31	0/8135	0.50	0/11044

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	1
1	C	0	3
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	651	GLN	Peptide
1	C	650	LYS	Peptide
1	C	651	GLN	Peptide
1	C	652	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1326	0	1384	26	0
1	B	1362	0	1423	26	0
1	C	1371	0	1431	27	0
1	D	1353	0	1407	25	0
1	E	1326	0	1384	24	0
1	F	1265	0	1312	11	0
2	A	27	0	12	1	0
2	B	27	0	12	1	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	1	0
2	F	27	0	12	1	0
All	All	8165	0	8413	134	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (134) 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:B:704:ARG:HH11	1:B:704:ARG:HG2	1.09	1.10
1:C:651:GLN:OE1	1:C:651:GLN:HA	1.46	1.09
1:A:586:MET:HE2	1:A:721:GLY:HA3	1.49	0.93
1:B:630:ARG:HH11	1:B:630:ARG:HG2	1.34	0.89
1:F:590:ARG:O	1:F:591:ASN:HB2	1.77	0.83
1:C:650:LYS:CB	1:C:652:ASP:OD1	2.30	0.80
1:C:651:GLN:OE1	1:C:651:GLN:CA	2.30	0.79
1:E:617:TYR:O	1:E:637:ARG:NH1	2.16	0.78
1:B:704:ARG:NH1	1:B:704:ARG:HG2	1.90	0.77
1:D:612:ILE:O	1:D:637:ARG:NH2	2.22	0.72
1:C:606:GLU:O	1:C:610:THR:HG22	1.89	0.72
1:A:652:ASP:OD1	1:A:652:ASP:N	2.23	0.71
1:B:704:ARG:CG	1:B:704:ARG:HH11	1.94	0.70
1:C:650:LYS:HB2	1:C:652:ASP:OD1	1.90	0.70
2:A:1752:ADP:C8	2:A:1752:ADP:H5'1	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:LEU:HD11	1:A:712:LEU:HD12	1.75	0.68
1:F:639:ASP:HB3	1:F:682:ILE:HD11	1.75	0.68
1:C:746:ASN:HA	1:C:749:LEU:HD12	1.76	0.67
1:B:590:ARG:H	1:B:590:ARG:HD3	1.59	0.66
1:D:586:MET:CE	1:D:713:VAL:HB	2.28	0.64
1:F:617:TYR:O	1:F:637:ARG:HD2	1.98	0.63
1:C:609:GLU:OE1	1:C:648:ARG:NH1	2.31	0.63
1:C:704:ARG:NH2	1:C:751:VAL:HG13	2.15	0.62
1:B:630:ARG:CG	1:B:630:ARG:HH11	2.11	0.61
1:E:652:ASP:OD1	1:E:652:ASP:N	2.32	0.61
1:C:650:LYS:HB3	1:C:652:ASP:OD1	2.00	0.60
1:B:587:LYS:HD3	1:B:589:ARG:HD3	1.83	0.60
1:C:726:LYS:HG2	1:C:730:LYS:HE3	1.82	0.60
1:F:639:ASP:HB3	1:F:682:ILE:CD1	2.31	0.60
1:F:622:VAL:HG23	1:F:632:VAL:HB	1.83	0.60
1:A:662:PHE:O	1:A:680:ARG:HG2	2.03	0.59
1:C:591:ASN:HD22	1:C:591:ASN:C	2.06	0.59
1:C:688:PHE:HE2	1:D:702:ILE:HD11	1.67	0.58
1:B:727:ASP:OD2	2:B:1754:ADP:O2'	2.20	0.57
1:D:586:MET:HE3	1:D:713:VAL:HB	1.86	0.56
1:D:609:GLU:OE1	1:D:648:ARG:NH1	2.38	0.55
1:A:650:LYS:HB3	1:A:652:ASP:OD1	2.06	0.55
1:E:746:ASN:HB3	1:E:749:LEU:HD12	1.89	0.55
1:D:673:THR:HB	1:D:674:PRO:HD2	1.88	0.55
1:A:696:MET:O	1:A:700:VAL:HG23	2.08	0.54
1:A:617:TYR:O	1:A:637:ARG:NH1	2.41	0.54
1:C:644:ILE:O	1:C:648:ARG:HG3	2.08	0.54
1:E:622:VAL:HG11	1:E:683:LEU:HD11	1.91	0.53
1:A:641:ILE:O	1:A:645:GLU:HB2	2.09	0.53
1:F:662:PHE:O	1:F:680:ARG:HG2	2.08	0.53
1:E:673:THR:CG2	1:E:674:PRO:HD2	2.38	0.53
1:D:640:LEU:O	1:D:644:ILE:HG13	2.09	0.53
1:C:673:THR:HB	1:C:674:PRO:HD2	1.89	0.53
1:D:704:ARG:NH2	1:D:751:VAL:HG13	2.23	0.53
1:A:586:MET:CE	1:A:721:GLY:HA3	2.32	0.52
1:A:615:THR:O	1:A:637:ARG:NH2	2.42	0.52
1:C:590:ARG:O	1:C:591:ASN:ND2	2.42	0.52
1:D:631:LEU:HD11	1:D:712:LEU:CD1	2.40	0.52
1:D:704:ARG:NH2	1:D:751:VAL:CG1	2.72	0.52
1:B:661:TYR:CZ	1:B:678:LYS:HB2	2.44	0.52
1:F:599:THR:OG1	1:F:603:MET:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:ARG:NH1	1:B:630:ARG:HG2	2.14	0.52
1:A:688:PHE:HE2	1:B:702:ILE:HD11	1.74	0.52
1:D:605:VAL:HG21	1:D:654:VAL:HG11	1.92	0.51
1:E:603:MET:HE2	1:E:608:VAL:HG22	1.92	0.51
1:E:622:VAL:HG11	1:E:683:LEU:CD1	2.41	0.51
1:C:598:LEU:HD22	1:C:603:MET:CE	2.40	0.51
1:C:693:LEU:HD13	1:D:685:LEU:HD13	1.92	0.50
1:B:597:VAL:HG23	1:B:621:PRO:HB2	1.94	0.50
1:D:586:MET:HE2	1:D:721:GLY:HA3	1.92	0.50
1:A:586:MET:HE2	1:A:721:GLY:CA	2.32	0.49
1:D:598:LEU:HD22	1:D:603:MET:HE2	1.94	0.49
1:C:704:ARG:HH21	1:C:751:VAL:HG13	1.77	0.49
1:F:618:SER:OG	2:F:1750:ADP:O2B	2.27	0.49
1:A:637:ARG:HH11	1:A:637:ARG:HB2	1.78	0.48
1:D:662:PHE:O	1:D:680:ARG:HG2	2.14	0.48
1:E:662:PHE:HB3	1:E:683:LEU:HD22	1.96	0.47
1:E:650:LYS:HD2	1:E:652:ASP:OD1	2.14	0.47
1:E:650:LYS:HB3	1:E:652:ASP:OD1	2.15	0.46
1:B:689:THR:CG2	1:B:690:VAL:N	2.78	0.46
1:B:608:VAL:O	1:B:612:ILE:HG13	2.15	0.46
1:A:728:VAL:O	1:A:732:ILE:HG13	2.15	0.46
1:F:631:LEU:HD11	1:F:712:LEU:HD13	1.97	0.46
1:E:666:SER:OG	1:E:667:PRO:HD2	2.16	0.46
1:D:704:ARG:HH21	1:D:751:VAL:HG13	1.80	0.45
1:D:631:LEU:HD11	1:D:712:LEU:HD12	1.98	0.45
1:E:622:VAL:CG1	1:E:683:LEU:HD11	2.46	0.45
1:C:696:MET:O	1:C:700:VAL:HG23	2.17	0.45
1:A:650:LYS:HD2	1:A:652:ASP:OD1	2.17	0.45
1:E:615:THR:O	1:E:637:ARG:NH2	2.51	0.44
1:C:753:PHE:O	1:C:754:GLN:HG2	2.17	0.44
1:B:728:VAL:O	1:B:732:ILE:HG13	2.18	0.44
1:A:735:MET:HB3	1:A:748:PHE:HB2	1.99	0.44
1:E:595:LEU:HD11	1:E:721:GLY:HA2	1.99	0.44
1:A:704:ARG:NH2	1:A:751:VAL:HG23	2.33	0.43
1:D:594:LEU:HD22	1:D:594:LEU:H	1.82	0.43
1:D:654:VAL:CG1	1:D:655:VAL:N	2.81	0.43
1:D:598:LEU:HD22	1:D:603:MET:CE	2.48	0.43
1:E:630:ARG:NH1	1:F:718:ARG:NE	2.66	0.43
1:B:697:GLU:N	1:B:697:GLU:CD	2.70	0.43
1:B:720:LEU:HA	1:B:720:LEU:HD23	1.87	0.43
1:B:704:ARG:NH1	1:B:704:ARG:CG	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:MET:HE3	1:A:713:VAL:HB	2.00	0.43
1:C:650:LYS:HB3	1:C:652:ASP:H	1.83	0.43
1:C:688:PHE:CD1	1:C:708:LEU:HD22	2.54	0.43
1:E:746:ASN:H	1:E:746:ASN:ND2	2.16	0.43
1:D:605:VAL:HG21	1:D:654:VAL:CG1	2.49	0.42
1:B:630:ARG:CG	1:B:630:ARG:NH1	2.75	0.42
1:D:592:ASP:HB3	1:D:593:PRO:HD2	2.01	0.42
1:A:716:ASN:OD1	1:B:632:VAL:HG22	2.19	0.42
1:E:748:PHE:O	1:E:751:VAL:HG22	2.19	0.42
1:B:590:ARG:H	1:B:590:ARG:CD	2.21	0.42
1:A:725:LYS:HE3	1:C:753:PHE:CE2	2.55	0.42
1:B:738:GLN:HG2	1:B:744:LEU:HD23	2.02	0.42
1:D:586:MET:HE1	1:D:713:VAL:HB	1.98	0.42
1:E:639:ASP:O	1:E:643:SER:HB2	2.20	0.42
1:C:710:GLN:HB3	1:C:710:GLN:HE21	1.62	0.42
1:A:689:THR:HG22	1:A:690:VAL:N	2.34	0.42
1:A:608:VAL:O	1:A:612:ILE:HG13	2.20	0.41
1:E:597:VAL:HG22	1:E:598:LEU:H	1.85	0.41
1:E:637:ARG:HH11	1:E:637:ARG:HB2	1.85	0.41
1:B:592:ASP:HB3	1:B:593:PRO:HD2	2.03	0.41
1:B:631:LEU:HD11	1:B:712:LEU:HD13	2.02	0.41
1:E:673:THR:HG22	1:E:674:PRO:HD2	2.02	0.41
1:A:660:ILE:HG21	1:A:679:LEU:HD12	2.02	0.41
1:F:620:PHE:HA	1:F:621:PRO:HD3	1.89	0.41
1:E:592:ASP:HB3	1:E:593:PRO:HD2	2.02	0.41
1:C:662:PHE:HB3	1:C:683:LEU:HD22	2.03	0.41
1:C:661:TYR:CZ	1:C:678:LYS:HB2	2.55	0.41
1:A:685:LEU:HD13	1:B:693:LEU:HD13	2.02	0.41
1:E:583:MET:HB3	1:E:692:ASP:HB2	2.03	0.41
1:B:670:PRO:HB3	1:B:671:PRO:HD2	2.03	0.41
2:E:1752:ADP:O1A	2:E:1752:ADP:H3'	2.21	0.41
1:A:689:THR:CG2	1:A:690:VAL:N	2.83	0.41
1:A:670:PRO:HB3	1:A:671:PRO:HD2	2.03	0.40
1:D:654:VAL:HG13	1:D:655:VAL:N	2.36	0.40
1:C:704:ARG:HH22	1:C:751:VAL:HA	1.86	0.40
1:D:631:LEU:HD11	1:D:712:LEU:HD13	2.03	0.40
1:E:597:VAL:HG22	1:E:598:LEU:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	163/185 (88%)	155 (95%)	8 (5%)	0	100	100
1	B	167/185 (90%)	161 (96%)	6 (4%)	0	100	100
1	C	168/185 (91%)	163 (97%)	5 (3%)	0	100	100
1	D	167/185 (90%)	163 (98%)	4 (2%)	0	100	100
1	E	163/185 (88%)	159 (98%)	4 (2%)	0	100	100
1	F	156/185 (84%)	142 (91%)	13 (8%)	1 (1%)	30	66
All	All	984/1110 (89%)	943 (96%)	40 (4%)	1 (0%)	56	88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	591	ASN

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	156/173 (90%)	144 (92%)	12 (8%)	16	48
1	B	160/173 (92%)	151 (94%)	9 (6%)	26	61
1	C	161/173 (93%)	142 (88%)	19 (12%)	6	24
1	D	158/173 (91%)	149 (94%)	9 (6%)	25	60
1	E	156/173 (90%)	146 (94%)	10 (6%)	22	55
1	F	146/173 (84%)	139 (95%)	7 (5%)	31	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	937/1038 (90%)	871 (93%)	66 (7%)	19	52

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	595	LEU
1	A	597	VAL
1	A	631	LEU
1	A	637	ARG
1	A	638	ARG
1	A	652	ASP
1	A	669	LEU
1	A	677	LEU
1	A	680	ARG
1	A	690	VAL
1	A	746	ASN
1	A	751	VAL
1	B	589	ARG
1	B	590	ARG
1	B	601	ASP
1	B	630	ARG
1	B	631	LEU
1	B	669	LEU
1	B	677	LEU
1	B	704	ARG
1	B	710	GLN
1	C	580	THR
1	C	587	LYS
1	C	591	ASN
1	C	595	LEU
1	C	601	ASP
1	C	610	THR
1	C	622	VAL
1	C	631	LEU
1	C	637	ARG
1	C	651	GLN
1	C	652	ASP
1	C	669	LEU
1	C	677	LEU
1	C	689	THR
1	C	690	VAL
1	C	710	GLN

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Mol	Chain	Res	Type
1	C	720	LEU
1	C	735	MET
1	C	738	GLN
1	D	597	VAL
1	D	622	VAL
1	D	631	LEU
1	D	669	LEU
1	D	677	LEU
1	D	680	ARG
1	D	710	GLN
1	D	720	LEU
1	D	738	GLN
1	E	590	ARG
1	E	622	VAL
1	E	637	ARG
1	E	643	SER
1	E	652	ASP
1	E	669	LEU
1	E	677	LEU
1	E	710	GLN
1	E	718	ARG
1	E	746	ASN
1	F	580	THR
1	F	587	LYS
1	F	590	ARG
1	F	631	LEU
1	F	680	ARG
1	F	690	VAL
1	F	720	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	600	GLN
1	A	746	ASN
1	B	600	GLN
1	B	710	GLN
1	B	734	GLN
1	B	738	GLN
1	C	591	ASN
1	C	600	GLN
1	C	646	ASN

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Mol	Chain	Res	Type
1	C	710	GLN
1	C	734	GLN
1	C	738	GLN
1	C	746	ASN
1	D	591	ASN
1	D	600	GLN
1	D	738	GLN
1	E	591	ASN
1	E	600	GLN
1	E	737	ASN
1	E	746	ASN
1	F	600	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	1752	-	22,29,29	1.50	3 (13%)	27,45,45	2.23	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	B	1754	-	22,29,29	1.39	3 (13%)	27,45,45	2.22	5 (18%)
2	ADP	C	1755	-	22,29,29	1.34	3 (13%)	27,45,45	2.22	4 (14%)
2	ADP	D	1753	-	22,29,29	1.45	2 (9%)	27,45,45	2.23	3 (11%)
2	ADP	E	1752	-	22,29,29	1.46	3 (13%)	27,45,45	2.25	3 (11%)
2	ADP	F	1750	-	22,29,29	1.39	3 (13%)	27,45,45	2.29	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	1752	-	-	0/12/32/32	0/3/3/3
2	ADP	B	1754	-	-	0/12/32/32	0/3/3/3
2	ADP	C	1755	-	-	0/12/32/32	0/3/3/3
2	ADP	D	1753	-	-	0/12/32/32	0/3/3/3
2	ADP	E	1752	-	-	0/12/32/32	0/3/3/3
2	ADP	F	1750	-	-	0/12/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1754	ADP	PB-O2B	2.08	1.62	1.54
2	E	1752	ADP	PB-O2B	2.11	1.62	1.54
2	C	1755	ADP	PB-O2B	2.13	1.62	1.54
2	A	1752	ADP	PB-O2B	2.17	1.62	1.54
2	F	1750	ADP	PB-O2B	2.23	1.62	1.54
2	B	1754	ADP	PB-O1B	2.88	1.60	1.51
2	C	1755	ADP	PB-O1B	3.01	1.61	1.51
2	D	1753	ADP	PB-O1B	3.25	1.61	1.51
2	C	1755	ADP	O4'-C1'	3.32	1.45	1.41
2	A	1752	ADP	PB-O1B	3.34	1.62	1.51
2	E	1752	ADP	PB-O1B	3.37	1.62	1.51
2	F	1750	ADP	PB-O1B	3.47	1.62	1.51
2	F	1750	ADP	O4'-C1'	3.56	1.45	1.41
2	B	1754	ADP	O4'-C1'	3.91	1.46	1.41
2	D	1753	ADP	O4'-C1'	4.11	1.46	1.41
2	E	1752	ADP	O4'-C1'	4.14	1.46	1.41
2	A	1752	ADP	O4'-C1'	4.51	1.46	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1754	ADP	N3-C2-N1	-9.91	121.31	128.89
2	A	1752	ADP	N3-C2-N1	-9.68	121.48	128.89
2	F	1750	ADP	N3-C2-N1	-9.51	121.61	128.89
2	E	1752	ADP	N3-C2-N1	-9.49	121.63	128.89
2	C	1755	ADP	N3-C2-N1	-9.41	121.69	128.89
2	D	1753	ADP	N3-C2-N1	-9.37	121.72	128.89
2	E	1752	ADP	PA-O3A-PB	-4.55	117.41	132.67
2	F	1750	ADP	PA-O3A-PB	-4.35	118.07	132.67
2	D	1753	ADP	PA-O3A-PB	-3.98	119.34	132.67
2	C	1755	ADP	PA-O3A-PB	-3.86	119.72	132.67
2	D	1753	ADP	C2'-C1'-N9	-3.09	109.58	114.29
2	B	1754	ADP	PA-O3A-PB	-2.96	122.74	132.67
2	A	1752	ADP	PA-O3A-PB	-2.70	123.60	132.67
2	C	1755	ADP	C2'-C1'-N9	-2.55	110.40	114.29
2	C	1755	ADP	C4-C5-N7	-2.44	107.23	109.48
2	E	1752	ADP	C4-C5-N7	-2.08	107.56	109.48
2	B	1754	ADP	O2B-PB-O1B	-2.06	103.96	110.58
2	A	1752	ADP	C4'-O4'-C1'	-2.04	107.48	109.72
2	B	1754	ADP	C2'-C1'-N9	-2.03	111.19	114.29
2	B	1754	ADP	O3B-PB-O3A	2.24	115.24	105.09
2	A	1752	ADP	O4'-C1'-N9	2.64	113.62	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1752	ADP	1	0
2	B	1754	ADP	1	0
2	E	1752	ADP	1	0
2	F	1750	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	167/185 (90%)	-0.00	8 (4%)	34 15	42, 54, 79, 124	0
1	B	171/185 (92%)	-0.06	5 (2%)	55 29	34, 50, 69, 75	0
1	C	172/185 (92%)	-0.16	1 (0%)	90 78	38, 46, 73, 76	0
1	D	171/185 (92%)	-0.13	4 (2%)	64 38	36, 49, 69, 103	0
1	E	167/185 (90%)	0.04	8 (4%)	34 15	48, 58, 83, 95	0
1	F	162/185 (87%)	0.56	16 (9%)	9 3	62, 103, 157, 165	0
All	All	1010/1110 (90%)	0.04	42 (4%)	40 18	34, 55, 124, 165	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	671	PRO	4.5
1	F	672	TYR	4.2
1	A	591	ASN	3.9
1	D	591	ASN	3.7
1	F	670	PRO	3.5
1	F	656	SER	3.5
1	E	651	GLN	3.5
1	E	591	ASN	3.5
1	B	672	TYR	3.3
1	B	744	LEU	3.3
1	A	650	LYS	3.1
1	D	746	ASN	3.1
1	A	627	GLU	3.1
1	E	649	LYS	2.9
1	E	737	ASN	2.9
1	F	578	HIS	2.8
1	F	735	MET	2.7
1	D	578	HIS	2.7
1	F	743	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	734	GLN	2.6
1	C	752	LEU	2.6
1	A	651	GLN	2.5
1	F	675	PRO	2.5
1	F	660	ILE	2.4
1	F	613	SER	2.4
1	B	671	PRO	2.4
1	F	645	GLU	2.4
1	F	591	ASN	2.4
1	B	627	GLU	2.4
1	B	651	GLN	2.4
1	E	613	SER	2.3
1	E	652	ASP	2.3
1	A	578	HIS	2.3
1	E	653	GLY	2.3
1	A	672	TYR	2.2
1	D	672	TYR	2.2
1	F	649	LYS	2.1
1	E	650	LYS	2.1
1	F	601	ASP	2.1
1	F	657	THR	2.1
1	A	671	PRO	2.0
1	F	614	GLU	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(\AA^2)	Q<0.9
2	ADP	D	1753	27/27	0.80	0.33	2.33	95,97,97,97	0
2	ADP	F	1750	27/27	0.55	0.39	1.90	160,160,161,161	0
2	ADP	B	1754	27/27	0.87	0.26	1.65	58,59,61,61	0
2	ADP	E	1752	27/27	0.75	0.30	1.48	121,121,121,122	0
2	ADP	C	1755	27/27	0.92	0.23	0.51	69,69,70,70	0
2	ADP	A	1752	27/27	0.91	0.23	0.00	68,69,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.