WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

PDB ID	:	2HHL
Title	:	Crystal structure of the human small CTD phosphatase 3 isoform 1
Authors	:	Malashkevich, V.N.; Toro, R.; Ramagopal, U.; Sauder, J.M.; Schwinn, K.D.; Thompson, D.A.; Rutter, M.E.; Dickey, M.; Groshong, C.; Bain, K.T.; Adams, J.M.; Reyes, C.; Rooney, I.; Powell, A.; Boice, A.; Gheyi, T.; Ozyurt, S.; Atwell, S.; Wasserman, S.R.; Emtage, S.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2006-06-28
Resolution	:	2.10 Å(reported)

The following versions of software and data (see references (i)) 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 2.10 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	Percentile Ranks	Value
Rfree		0.252
Clashscore		7
Ramachandran outliers		0.3%
Sidechain outliers		2.6%
RSRZ outliers		5.5%

Worse ▬▬▬ *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
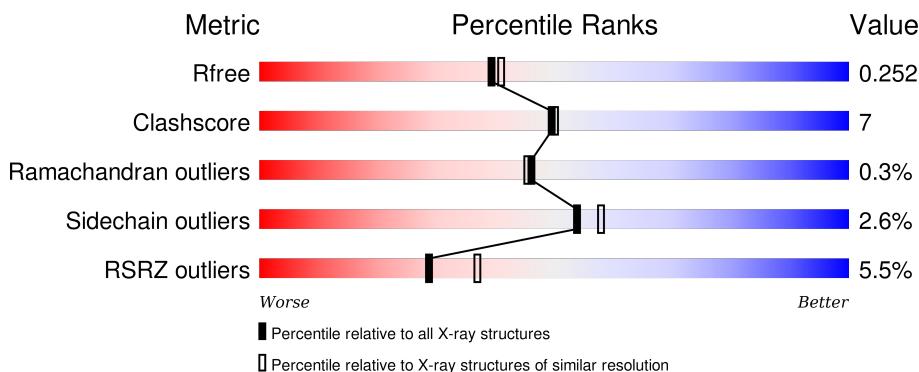
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	195	7% ▬ 83% ... 9% 8%
1	B	195	5% ▬ 80% ... 11% • 8%
1	C	195	5% ▬ 77% ... 14% • 6%
1	D	195	3% ▬ 80% ... 8% • 12%
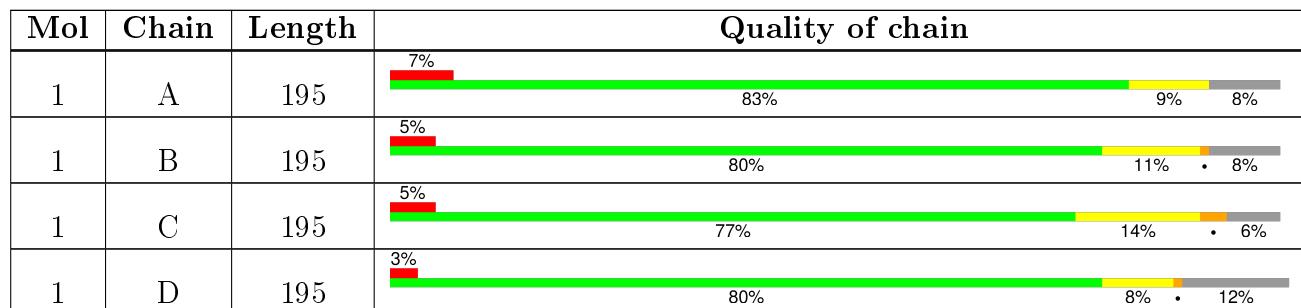
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

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	KEG	A	902	-	-	X	-
2	KEG	D	901	-	-	X	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6472 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 CTD small phosphatase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1451	944	239	263	5			
1	B	179	Total	C	N	O	S	0	0	0
			1442	939	237	261	5			
1	C	184	Total	C	N	O	S	0	0	0
			1487	965	246	271	5			
1	D	172	Total	C	N	O	S	0	0	0
			1394	904	230	255	5			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP O15194
A	2	SER	-	CLONING ARTIFACT	UNP O15194
A	3	LEU	-	CLONING ARTIFACT	UNP O15194
A	188	GLU	-	CLONING ARTIFACT	UNP O15194
A	189	GLY	-	CLONING ARTIFACT	UNP O15194
A	190	HIS	-	EXPRESSION TAG	UNP O15194
A	191	HIS	-	EXPRESSION TAG	UNP O15194
A	192	HIS	-	EXPRESSION TAG	UNP O15194
A	193	HIS	-	EXPRESSION TAG	UNP O15194
A	194	HIS	-	EXPRESSION TAG	UNP O15194
A	195	HIS	-	EXPRESSION TAG	UNP O15194
B	1	MET	-	INITIATING METHIONINE	UNP O15194
B	2	SER	-	CLONING ARTIFACT	UNP O15194
B	3	LEU	-	CLONING ARTIFACT	UNP O15194
B	188	GLU	-	CLONING ARTIFACT	UNP O15194
B	189	GLY	-	CLONING ARTIFACT	UNP O15194
B	190	HIS	-	EXPRESSION TAG	UNP O15194
B	191	HIS	-	EXPRESSION TAG	UNP O15194
B	192	HIS	-	EXPRESSION TAG	UNP O15194
B	193	HIS	-	EXPRESSION TAG	UNP O15194
B	194	HIS	-	EXPRESSION TAG	UNP O15194

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Chain	Residue	Modelled	Actual	Comment	Reference
B	195	HIS	-	EXPRESSION TAG	UNP O15194
C	1	MET	-	INITIATING METHIONINE	UNP O15194
C	2	SER	-	CLONING ARTIFACT	UNP O15194
C	3	LEU	-	CLONING ARTIFACT	UNP O15194
C	188	GLU	-	CLONING ARTIFACT	UNP O15194
C	189	GLY	-	CLONING ARTIFACT	UNP O15194
C	190	HIS	-	EXPRESSION TAG	UNP O15194
C	191	HIS	-	EXPRESSION TAG	UNP O15194
C	192	HIS	-	EXPRESSION TAG	UNP O15194
C	193	HIS	-	EXPRESSION TAG	UNP O15194
C	194	HIS	-	EXPRESSION TAG	UNP O15194
C	195	HIS	-	EXPRESSION TAG	UNP O15194
D	1	MET	-	INITIATING METHIONINE	UNP O15194
D	2	SER	-	CLONING ARTIFACT	UNP O15194
D	3	LEU	-	CLONING ARTIFACT	UNP O15194
D	188	GLU	-	CLONING ARTIFACT	UNP O15194
D	189	GLY	-	CLONING ARTIFACT	UNP O15194
D	190	HIS	-	EXPRESSION TAG	UNP O15194
D	191	HIS	-	EXPRESSION TAG	UNP O15194
D	192	HIS	-	EXPRESSION TAG	UNP O15194
D	193	HIS	-	EXPRESSION TAG	UNP O15194
D	194	HIS	-	EXPRESSION TAG	UNP O15194
D	195	HIS	-	EXPRESSION TAG	UNP O15194

- Molecule 2 is 12-TUNGSTOPHOSPHATE (three-letter code: KEG) (formula: $O_{40}PW_{12}$).
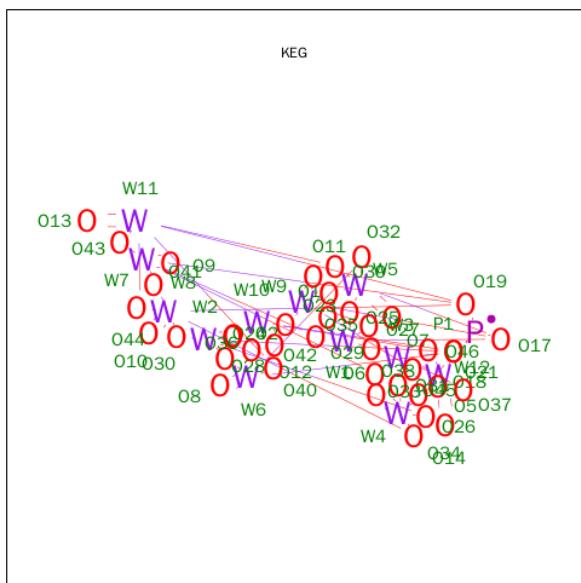
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 53	O 40	P 1	W 12	0	0
2	C	1	Total 52	O 40		W 12	0	0
2	D	1	Total 53	O 40	P 1	W 12	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total 102	O 102	0	0
3	B	141	Total 141	O 141	0	0
3	C	138	Total 138	O 138	0	0
3	D	159	Total 159	O 159	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: CTD small phosphatase-like protein
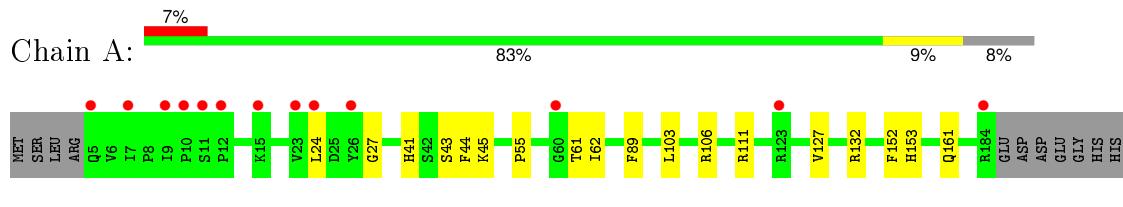
- Molecule 1: CTD small phosphatase-like protein
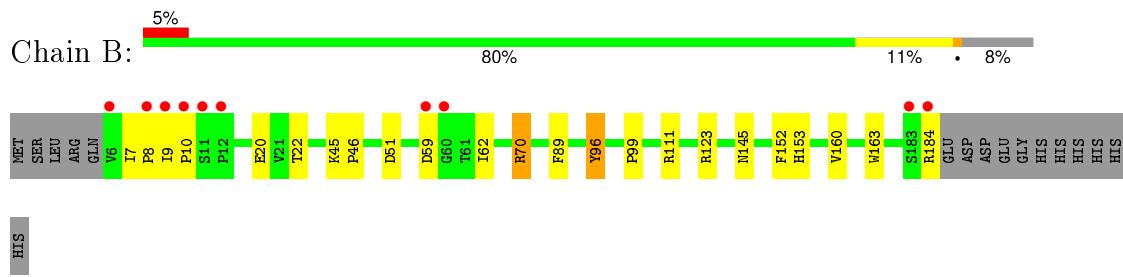
- Molecule 1: CTD small phosphatase-like protein
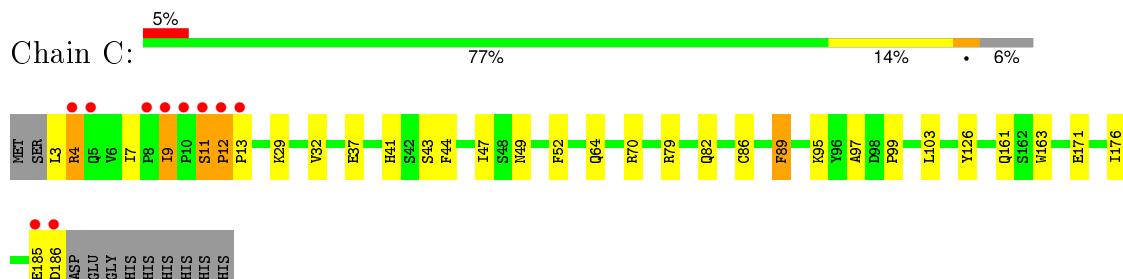
- Molecule 1: CTD small phosphatase-like protein
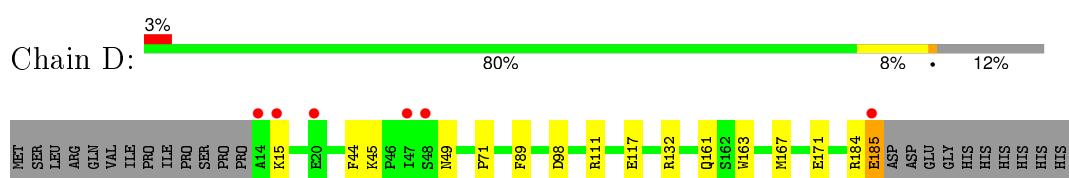
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	47.42Å 49.86Å 179.75Å 90.00° 96.90° 90.00°	Depositor
Resolution (Å)	19.86 – 2.10 19.86 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.4 (19.86-2.10) 96.4 (19.86-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.188 , 0.252 0.189 , 0.252	Depositor DCC
R_{free} test set	2386 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.8	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 47398 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6472	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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 44.14 % 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 1.5944e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.96	0/1490	0.86	0/2030
1	B	1.00	2/1481 (0.1%)	0.88	3/2018 (0.1%)
1	C	1.00	3/1526 (0.2%)	0.86	1/2078 (0.0%)
1	D	1.03	1/1429 (0.1%)	0.88	1/1942 (0.1%)
All	All	1.00	6/5926 (0.1%)	0.87	5/8068 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	96	TYR	CE2-CZ	5.96	1.46	1.38
1	C	126	TYR	CD2-CE2	5.69	1.47	1.39
1	D	117	GLU	CG-CD	5.65	1.60	1.51
1	C	97	ALA	CA-CB	5.40	1.63	1.52
1	C	86	CYS	CB-SG	-5.22	1.73	1.81
1	B	160	VAL	CB-CG2	5.11	1.63	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	111	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	D	111	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	C	95	LYS	CD-CE-NZ	-5.40	99.27	111.70
1	B	70	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	51	ASP	CB-CG-OD2	5.09	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1451	0	1447	15	1
1	B	1442	0	1439	10	0
1	C	1487	0	1481	26	0
1	D	1394	0	1381	19	0
2	A	53	0	0	12	1
2	C	52	0	0	8	0
2	D	53	0	0	9	0
3	A	102	0	0	4	0
3	B	141	0	0	3	0
3	C	138	0	0	2	0
3	D	159	0	0	0	0
All	All	6472	0	5748	83	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 7.

All (83) 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:62:ILE:HG13	2:C:900:KEG:O41	1.51	1.09
2:A:902:KEG:O33	2:A:902:KEG:O32	1.71	1.09
1:D:163:TRP:HZ2	1:D:167:MET:CE	1.72	1.03
1:D:163:TRP:HZ2	1:D:167:MET:HE3	1.24	1.00
2:A:902:KEG:O13	2:A:902:KEG:P1	2.23	0.97
2:A:902:KEG:O40	2:A:902:KEG:O28	1.84	0.94
1:C:4:ARG:HH11	1:C:4:ARG:HG3	1.27	0.94
1:D:167:MET:HA	1:D:167:MET:HE2	1.50	0.91
2:C:900:KEG:O6	2:C:900:KEG:O18	1.90	0.90
1:D:163:TRP:CZ2	1:D:167:MET:CE	2.56	0.89
1:C:4:ARG:NH2	1:C:11:SER:HB2	1.89	0.87
1:C:47:ILE:HG22	1:C:49:ASN:OD1	1.75	0.87
1:D:15:LYS:O	1:D:132:ARG:NH2	2.07	0.86
1:B:59:ASP:HB3	3:B:288:HOH:O	1.75	0.86
1:D:163:TRP:CZ2	1:D:167:MET:HE3	2.14	0.81
1:D:44:PHE:N	2:D:901:KEG:O37	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:PHE:HD2	2:A:902:KEG:O1	1.64	0.80
1:D:184:ARG:O	1:D:185:GLU:HB2	1.81	0.80
1:C:82:GLN:HG2	3:C:1007:HOH:O	1.85	0.76
1:A:62:ILE:CG1	2:C:900:KEG:O41	2.32	0.76
1:D:163:TRP:CZ2	1:D:167:MET:HE1	2.23	0.74
1:D:49:ASN:N	1:D:49:ASN:OD1	2.19	0.70
2:D:901:KEG:O18	2:D:901:KEG:O6	2.09	0.70
1:D:44:PHE:CD2	2:D:901:KEG:O41	2.45	0.69
1:C:37:GLU:OE2	1:C:41:HIS:HD2	1.76	0.69
2:A:902:KEG:P1	2:A:902:KEG:O34	2.52	0.68
2:A:902:KEG:O44	2:A:902:KEG:O11	2.12	0.67
1:C:44:PHE:HB2	2:C:900:KEG:O8	1.95	0.67
2:C:900:KEG:O45	2:C:900:KEG:O42	2.13	0.67
1:C:4:ARG:HH22	1:C:11:SER:HB2	1.60	0.66
2:D:901:KEG:O45	2:D:901:KEG:O42	2.18	0.62
1:C:64:GLN:HG3	3:C:1003:HOH:O	1.99	0.62
1:C:3:LEU:HD11	1:C:7:ILE:HD12	1.81	0.62
2:D:901:KEG:P1	2:D:901:KEG:O13	2.58	0.61
1:C:4:ARG:CG	1:C:4:ARG:HH11	2.07	0.61
1:D:44:PHE:HD2	2:D:901:KEG:O41	1.83	0.61
1:C:11:SER:N	1:C:12:PRO:HD3	2.16	0.60
1:D:71:PRO:HD3	1:D:167:MET:HE1	1.85	0.59
1:C:4:ARG:NH1	1:C:4:ARG:HG3	2.07	0.59
1:D:167:MET:CE	1:D:167:MET:HA	2.29	0.58
1:B:7:ILE:HG22	1:B:8:PRO:HD2	1.87	0.57
1:A:161:GLN:HG3	3:A:988:HOH:O	2.04	0.56
1:A:103:LEU:HD21	1:C:64:GLN:HG2	1.88	0.56
1:A:44:PHE:CD2	2:A:902:KEG:O1	2.52	0.56
1:B:153:HIS:HD2	3:B:200:HOH:O	1.91	0.54
1:A:45:LYS:HB2	2:A:902:KEG:O7	2.07	0.53
1:D:44:PHE:CE2	2:D:901:KEG:O41	2.62	0.53
1:A:55:PRO:HB3	2:C:900:KEG:O21	2.10	0.52
2:A:902:KEG:O18	2:A:902:KEG:O6	2.28	0.51
1:A:132:ARG:NH2	3:A:960:HOH:O	2.39	0.51
1:D:71:PRO:HD3	1:D:167:MET:CE	2.41	0.51
1:B:145:ASN:H	1:B:145:ASN:HD22	1.58	0.51
1:C:43:SER:HA	2:C:900:KEG:O1	2.11	0.50
1:C:185:GLU:O	1:C:186:ASP:HB2	2.12	0.50
1:C:4:ARG:HH12	1:C:9:ILE:HG12	1.75	0.50
1:A:153:HIS:HD2	3:A:918:HOH:O	1.97	0.47
1:D:161:GLN:NE2	1:D:171:GLU:OE2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:ARG:NH1	1:C:9:ILE:HG12	2.30	0.47
1:C:4:ARG:HH21	1:C:11:SER:HB2	1.75	0.46
1:A:43:SER:HB3	2:A:902:KEG:O8	2.15	0.46
1:B:45:LYS:HA	1:B:46:PRO:HD3	1.84	0.46
1:C:11:SER:N	1:C:12:PRO:CD	2.79	0.46
1:A:41:HIS:NE2	2:A:902:KEG:O21	2.46	0.45
1:C:70:ARG:CZ	1:C:163:TRP:HB2	2.46	0.45
1:A:106:ARG:HD3	3:A:980:HOH:O	2.16	0.45
1:B:22:THR:HB	3:B:262:HOH:O	2.16	0.45
1:C:32:VAL:HG13	1:C:89:PHE:CB	2.47	0.44
1:B:152:PHE:HB2	1:B:153:HIS:CD2	2.53	0.44
1:C:4:ARG:CG	1:C:4:ARG:NH1	2.72	0.44
2:C:900:KEG:O28	2:C:900:KEG:O40	2.37	0.43
1:C:161:GLN:NE2	1:C:171:GLU:OE2	2.49	0.43
1:A:152:PHE:HB2	1:A:153:HIS:CD2	2.54	0.42
1:B:9:ILE:HA	1:B:10:PRO:HD3	1.77	0.42
1:B:70:ARG:CZ	1:B:163:TRP:HB2	2.50	0.42
1:B:96:TYR:O	1:B:99:PRO:HD2	2.20	0.42
1:D:45:LYS:NZ	2:D:901:KEG:O28	2.50	0.41
1:C:52:PHE:HB3	1:C:103:LEU:HD13	2.02	0.41
2:D:901:KEG:O44	2:D:901:KEG:P1	2.79	0.41
2:A:902:KEG:O14	2:A:902:KEG:P1	2.79	0.40
1:C:79:ARG:HG2	1:C:176:ILE:HG23	2.02	0.40
1:C:11:SER:C	1:C:13:PRO:HD3	2.41	0.40
1:D:184:ARG:O	1:D:185:GLU:CB	2.61	0.40
1:A:127:VAL:HG11	1:A:152:PHE:CE2	2.57	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:27:GLY:CA	2:A:902:KEG:O27[1_655]	2.06	0.14

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	178/195 (91%)	173 (97%)	5 (3%)	0	100	100
1	B	177/195 (91%)	169 (96%)	8 (4%)	0	100	100
1	C	182/195 (93%)	176 (97%)	4 (2%)	2 (1%)	17	11
1	D	170/195 (87%)	162 (95%)	8 (5%)	0	100	100
All	All	707/780 (91%)	680 (96%)	25 (4%)	2 (0%)	46	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	12	PRO
1	C	11	SER

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	164/178 (92%)	160 (98%)	4 (2%)	57	61
1	B	163/178 (92%)	158 (97%)	5 (3%)	47	50
1	C	168/178 (94%)	163 (97%)	5 (3%)	48	51
1	D	156/178 (88%)	153 (98%)	3 (2%)	65	70
All	All	651/712 (91%)	634 (97%)	17 (3%)	54	58

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

Mol	Chain	Res	Type
1	A	24	LEU
1	A	61	THR
1	A	89	PHE
1	A	111	ARG
1	B	20	GLU
1	B	62	ILE

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Mol	Chain	Res	Type
1	B	89	PHE
1	B	123	ARG
1	B	184	ARG
1	C	4	ARG
1	C	9	ILE
1	C	29	LYS
1	C	89	PHE
1	C	99	PRO
1	D	89	PHE
1	D	98	ASP
1	D	185	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	B	63	HIS
1	B	145	ASN
1	B	153	HIS
1	C	41	HIS
1	C	145	ASN
1	C	153	HIS
1	D	145	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)

3 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	KEG	A	902	-	76,76,76	91.48	75 (98%)	6,234,234	32.66	6 (100%)
2	KEG	C	900	-	72,72,76	98.88	70 (97%)	0,216,234	0.00	-
2	KEG	D	901	-	76,76,76	96.19	76 (100%)	6,234,234	35.57	5 (83%)

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	KEG	A	902	-	-	0/0/456/456	0/0/24/24
2	KEG	C	900	-	-	0/0/360/456	0/0/17/24
2	KEG	D	901	-	-	0/0/456/456	0/0/24/24

All (221) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	KEG	W5-O17	-4.79	2.17	2.43
2	A	902	KEG	W5-O17	-2.41	2.30	2.43
2	D	901	KEG	W8-O44	2.01	2.02	1.93
2	C	900	KEG	W8-O44	2.33	2.01	1.92
2	A	902	KEG	W10-O36	2.52	2.05	1.93
2	D	901	KEG	W10-O36	2.65	2.05	1.93
2	D	901	KEG	W11-O40	2.93	2.03	1.91
2	A	902	KEG	W11-O40	3.17	2.04	1.91
2	C	900	KEG	W10-O36	3.75	2.06	1.92
2	C	900	KEG	W9-O42	4.57	2.23	1.93
2	A	902	KEG	W10-O28	5.13	2.17	1.93
2	D	901	KEG	W10-O28	5.57	2.19	1.93
2	A	902	KEG	W9-O42	5.79	2.16	1.91
2	A	902	KEG	W9-O27	6.38	2.23	1.93
2	A	902	KEG	W12-O38	6.56	2.24	1.93
2	D	901	KEG	W9-O27	6.56	2.24	1.93
2	D	901	KEG	W12-O38	6.97	2.26	1.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	KEG	W9-O42	7.06	2.21	1.91
2	C	900	KEG	W10-O28	7.64	2.19	1.92
2	C	900	KEG	W12-O38	8.61	2.23	1.92
2	C	900	KEG	W9-O27	8.74	2.23	1.92
2	A	902	KEG	W1-O1	18.71	2.22	1.71
2	A	902	KEG	W2-O2	19.03	2.23	1.71
2	D	901	KEG	W1-O1	19.23	2.23	1.71
2	D	901	KEG	W2-O2	19.25	2.24	1.71
2	C	900	KEG	W1-O1	20.11	2.22	1.71
2	C	900	KEG	W2-O2	20.79	2.24	1.71
2	A	902	KEG	W9-O45	21.29	2.83	1.91
2	C	900	KEG	W2-O18	21.79	3.43	2.25
2	D	901	KEG	W2-O18	21.95	3.61	2.43
2	D	901	KEG	W1-O17	23.09	3.67	2.43
2	A	902	KEG	W2-O18	24.63	3.75	2.43
2	C	900	KEG	W9-O45	24.64	3.52	1.93
2	C	900	KEG	W1-O17	33.03	4.04	2.25
2	C	900	KEG	W10-O42	37.09	4.33	1.93
2	D	901	KEG	W9-O45	38.33	3.57	1.91
2	A	902	KEG	W1-O17	42.71	4.73	2.43
2	C	900	KEG	W4-O34	45.58	4.87	1.93
2	A	902	KEG	W9-O35	45.75	4.06	1.93
2	C	900	KEG	W8-O34	46.69	4.94	1.93
2	D	901	KEG	P1-O18	46.89	3.17	1.54
2	C	900	KEG	W6-O18	47.35	4.81	2.25
2	D	901	KEG	W6-O18	48.42	5.04	2.43
2	C	900	KEG	W2-O30	49.08	5.10	1.93
2	C	900	KEG	W6-O40	49.16	5.10	1.93
2	C	900	KEG	W3-O33	49.52	5.13	1.93
2	A	902	KEG	W6-O18	50.16	5.13	2.43
2	A	902	KEG	W10-O42	50.24	4.08	1.91
2	A	902	KEG	W4-O21	50.28	5.14	2.43
2	C	900	KEG	W1-O29	50.28	5.18	1.93
2	C	900	KEG	W11-O39	53.17	5.36	1.93
2	C	900	KEG	W3-O25	53.33	5.37	1.93
2	A	902	KEG	P1-O17	55.90	3.49	1.54
2	D	901	KEG	W10-O42	56.65	4.36	1.91
2	D	901	KEG	W4-O21	57.05	5.50	2.43
2	C	900	KEG	W4-O21	59.71	5.48	2.25
2	D	901	KEG	W11-O43	63.22	4.88	1.93
2	A	902	KEG	W3-O33	63.39	4.65	1.91
2	C	900	KEG	W10-O18	64.88	5.76	2.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	KEG	W4-O26	65.57	6.16	1.93
2	D	901	KEG	W6-O40	65.73	4.75	1.91
2	A	902	KEG	W11-O43	66.25	5.02	1.93
2	A	902	KEG	W6-O40	66.40	4.78	1.91
2	A	902	KEG	W4-O34	67.17	4.81	1.91
2	A	902	KEG	W8-O34	67.70	4.84	1.91
2	C	900	KEG	W8-O30	67.71	6.30	1.93
2	C	900	KEG	W12-O45	68.51	6.35	1.93
2	D	901	KEG	W10-O18	68.81	6.14	2.43
2	D	901	KEG	W9-O35	68.84	5.14	1.93
2	D	901	KEG	W4-O34	69.06	4.90	1.91
2	C	900	KEG	W6-O32	69.44	6.41	1.93
2	C	900	KEG	W7-O29	69.78	6.43	1.93
2	C	900	KEG	W7-O33	70.09	6.45	1.93
2	A	902	KEG	W7-O41	70.39	5.21	1.93
2	A	902	KEG	W7-O33	70.52	4.96	1.91
2	A	902	KEG	W6-O24	70.73	5.23	1.93
2	A	902	KEG	W10-O18	71.93	6.30	2.43
2	D	901	KEG	W8-O34	72.00	5.02	1.91
2	D	901	KEG	W2-O24	72.82	5.32	1.93
2	A	902	KEG	W2-O30	73.45	5.08	1.91
2	A	902	KEG	W2-O24	73.47	5.35	1.93
2	D	901	KEG	W7-O41	73.98	5.38	1.93
2	A	902	KEG	W12-O37	74.13	5.39	1.93
2	D	901	KEG	W2-O30	74.44	5.13	1.91
2	A	902	KEG	W9-O11	74.64	3.75	1.71
2	D	901	KEG	W12-O37	74.77	5.41	1.93
2	A	902	KEG	P1-O18	74.82	4.15	1.54
2	A	902	KEG	W1-O29	75.09	5.16	1.91
2	D	901	KEG	W6-O24	75.13	5.43	1.93
2	A	902	KEG	W6-O36	75.87	5.47	1.93
2	D	901	KEG	W1-O29	75.92	5.19	1.91
2	C	900	KEG	W5-O32	75.96	6.83	1.93
2	D	901	KEG	W6-O36	76.15	5.48	1.93
2	D	901	KEG	P1-O17	76.15	4.19	1.54
2	D	901	KEG	W3-O33	76.30	5.21	1.91
2	D	901	KEG	W7-O9	79.18	3.87	1.71
2	A	902	KEG	W11-O39	80.27	5.38	1.91
2	C	900	KEG	W2-O26	80.32	7.11	1.93
2	A	902	KEG	W3-O25	81.19	5.42	1.91
2	D	901	KEG	W3-O25	81.20	5.42	1.91
2	C	900	KEG	W11-O43	81.84	4.82	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	KEG	W7-O9	82.29	3.96	1.71
2	D	901	KEG	W11-O39	83.25	5.51	1.91
2	A	902	KEG	W11-O19	84.25	6.97	2.43
2	A	902	KEG	W9-O17	84.52	6.98	2.43
2	D	901	KEG	W9-O11	84.94	4.03	1.71
2	C	900	KEG	W7-O9	86.72	3.90	1.71
2	D	901	KEG	W5-O23	88.11	6.04	1.93
2	C	900	KEG	W9-O35	88.48	5.06	1.92
2	D	901	KEG	W11-O19	89.32	7.24	2.43
2	C	900	KEG	W9-O11	89.93	3.98	1.71
2	A	902	KEG	W5-O7	90.31	4.18	1.71
2	D	901	KEG	W5-O7	90.34	4.18	1.71
2	D	901	KEG	W3-O31	90.79	6.16	1.93
2	D	901	KEG	W9-O17	90.89	7.33	2.43
2	C	900	KEG	W11-O19	91.23	7.19	2.25
2	A	902	KEG	W4-O26	91.23	5.85	1.91
2	D	901	KEG	W11-O13	91.93	4.22	1.71
2	A	902	KEG	W6-O32	92.80	5.92	1.91
2	A	902	KEG	W5-O23	93.72	6.30	1.93
2	A	902	KEG	W3-O5	93.75	4.27	1.71
2	A	902	KEG	W11-O44	94.08	6.31	1.93
2	A	902	KEG	W1-O27	95.36	6.37	1.93
2	C	900	KEG	W12-O37	95.88	5.32	1.92
2	A	902	KEG	W11-O13	96.01	4.34	1.71
2	A	902	KEG	W5-O35	96.13	6.41	1.93
2	C	900	KEG	W11-O13	96.36	4.15	1.71
2	A	902	KEG	W3-O31	96.65	6.43	1.93
2	C	900	KEG	W2-O24	96.83	5.35	1.92
2	C	900	KEG	W7-O41	96.93	5.36	1.92
2	A	902	KEG	W8-O30	97.21	6.11	1.91
2	A	902	KEG	W12-O45	98.06	6.15	1.91
2	D	901	KEG	W4-O26	98.18	6.15	1.91
2	D	901	KEG	W11-O44	99.03	6.55	1.93
2	C	900	KEG	W9-O17	99.25	7.62	2.25
2	D	901	KEG	W7-O29	99.89	6.23	1.91
2	A	902	KEG	W2-O28	100.00	6.59	1.93
2	C	900	KEG	W5-O7	100.07	4.24	1.71
2	A	902	KEG	W8-O19	100.29	7.83	2.43
2	C	900	KEG	W6-O24	100.62	5.49	1.92
2	D	901	KEG	W3-O5	101.14	4.48	1.71
2	D	901	KEG	W5-O35	101.18	6.65	1.93
2	A	902	KEG	W7-O29	101.23	6.29	1.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	KEG	W5-O39	101.97	8.51	1.93
2	C	900	KEG	W10-O46	102.55	8.55	1.93
2	D	901	KEG	W7-O33	102.89	6.36	1.91
2	C	900	KEG	W12-O46	102.94	8.57	1.93
2	A	902	KEG	W12-O14	104.31	4.56	1.71
2	C	900	KEG	W1-O25	104.37	8.67	1.93
2	A	902	KEG	W8-O10	104.56	4.57	1.71
2	D	901	KEG	W1-O23	105.00	6.82	1.93
2	D	901	KEG	W6-O32	105.31	6.46	1.91
2	D	901	KEG	W8-O30	105.34	6.46	1.91
2	A	902	KEG	W1-O23	105.80	6.86	1.93
2	D	901	KEG	W4-O38	105.94	6.87	1.93
2	A	902	KEG	W4-O38	106.13	6.88	1.93
2	D	901	KEG	W12-O45	106.20	6.50	1.91
2	A	902	KEG	W12-O21	107.55	8.22	2.43
2	C	900	KEG	W12-O21	107.68	8.08	2.25
2	D	901	KEG	W12-O21	107.81	8.24	2.43
2	D	901	KEG	W8-O19	108.32	8.27	2.43
2	C	900	KEG	W8-O19	108.44	8.12	2.25
2	C	900	KEG	W6-O36	108.66	5.77	1.92
2	C	900	KEG	W3-O5	108.75	4.46	1.71
2	A	902	KEG	W2-O26	109.14	6.63	1.91
2	D	901	KEG	W1-O27	109.51	7.03	1.93
2	D	901	KEG	W4-O31	110.19	7.07	1.93
2	A	902	KEG	W3-O21	112.49	8.49	2.43
2	A	902	KEG	W5-O32	115.50	6.90	1.91
2	D	901	KEG	W5-O32	117.35	6.98	1.91
2	A	902	KEG	W4-O31	117.69	7.42	1.93
2	A	902	KEG	P1-O21	118.00	5.65	1.54
2	D	901	KEG	W8-O10	118.16	4.94	1.71
2	D	901	KEG	W2-O26	118.78	7.05	1.91
2	D	901	KEG	W3-O21	119.23	8.85	2.43
2	D	901	KEG	W2-O28	119.38	7.49	1.93
2	D	901	KEG	W6-O8	121.01	5.02	1.71
2	C	900	KEG	W3-O31	121.12	6.21	1.92
2	C	900	KEG	W3-O21	121.98	8.85	2.25
2	A	902	KEG	P1-O19	122.12	5.79	1.54
2	D	901	KEG	W12-O14	122.85	5.07	1.71
2	C	900	KEG	W5-O23	122.90	6.27	1.92
2	A	902	KEG	W6-O8	123.14	5.08	1.71
2	A	902	KEG	W7-O19	126.63	9.25	2.43
2	C	900	KEG	W8-O10	126.92	4.92	1.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	KEG	W7-O43	127.53	7.87	1.93
2	A	902	KEG	W7-O43	128.08	7.90	1.93
2	D	901	KEG	P1-O19	128.55	6.02	1.54
2	C	900	KEG	W12-O14	131.23	5.03	1.71
2	C	900	KEG	W11-O44	131.28	6.57	1.92
2	D	901	KEG	W7-O19	133.75	9.64	2.43
2	C	900	KEG	W5-O35	133.88	6.66	1.92
2	C	900	KEG	W6-O8	134.72	5.12	1.71
2	C	900	KEG	W7-O19	137.76	9.71	2.25
2	A	902	KEG	W8-O41	137.78	8.35	1.93
2	D	901	KEG	P1-O21	139.29	6.39	1.54
2	C	900	KEG	W4-O38	141.67	6.94	1.92
2	C	900	KEG	W1-O23	142.60	6.97	1.92
2	A	902	KEG	W10-O12	144.73	5.67	1.71
2	A	902	KEG	W10-O46	145.67	8.21	1.91
2	C	900	KEG	W4-O31	146.52	7.11	1.92
2	C	900	KEG	W1-O27	146.95	7.13	1.92
2	D	901	KEG	W8-O41	148.99	8.87	1.93
2	A	902	KEG	W1-O25	150.89	8.44	1.91
2	D	901	KEG	W12-O46	153.39	8.54	1.91
2	A	902	KEG	W4-O6	154.38	5.93	1.71
2	D	901	KEG	W10-O46	155.17	8.62	1.91
2	A	902	KEG	W12-O46	155.21	8.62	1.91
2	A	902	KEG	W5-O39	156.58	8.68	1.91
2	D	901	KEG	W5-O39	156.90	8.70	1.91
2	C	900	KEG	W2-O28	159.07	7.56	1.92
2	D	901	KEG	W1-O25	160.91	8.87	1.91
2	D	901	KEG	W4-O6	161.32	6.12	1.71
2	A	902	KEG	W3-O37	162.21	9.49	1.93
2	D	901	KEG	W10-O12	163.35	6.18	1.71
2	D	901	KEG	W3-O37	165.83	9.66	1.93
2	C	900	KEG	W7-O43	169.68	7.93	1.92
2	C	900	KEG	W4-O6	171.44	6.05	1.71
2	C	900	KEG	W10-O12	177.01	6.19	1.71
2	C	900	KEG	W8-O41	195.26	8.84	1.92
2	C	900	KEG	W3-O37	217.69	9.63	1.92

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	KEG	O21-P1-O17	-66.35	28.70	108.94
2	A	902	KEG	O21-P1-O17	-60.91	35.28	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	901	KEG	O21-P1-O19	-35.78	65.67	108.94
2	A	902	KEG	O21-P1-O19	-34.76	66.90	108.94
2	D	901	KEG	O19-P1-O17	-17.07	88.30	108.94
2	A	902	KEG	O19-P1-O17	-5.81	101.91	108.94
2	A	902	KEG	O18-P1-O17	9.94	120.96	108.94
2	A	902	KEG	O19-P1-O18	14.50	126.47	108.94
2	D	901	KEG	O21-P1-O18	23.98	137.94	108.94
2	D	901	KEG	O19-P1-O18	32.26	147.95	108.94
2	A	902	KEG	O21-P1-O18	33.74	149.74	108.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	KEG	12	1
2	C	900	KEG	8	0
2	D	901	KEG	9	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	180/195 (92%)	0.12	13 (7%)	18	25	14, 23, 49, 68	0
1	B	179/195 (91%)	-0.00	10 (5%)	28	36	14, 21, 45, 65	0
1	C	184/195 (94%)	0.07	10 (5%)	29	38	13, 21, 51, 66	0
1	D	172/195 (88%)	-0.25	6 (3%)	48	57	13, 20, 36, 52	0
All	All	715/780 (91%)	-0.01	39 (5%)	29	37	13, 21, 45, 68	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	11	SER	10.0
1	C	9	ILE	7.9
1	C	12	PRO	7.8
1	C	4	ARG	6.5
1	A	9	ILE	6.0
1	C	10	PRO	5.7
1	C	13	PRO	5.3
1	B	6	VAL	5.2
1	A	12	PRO	4.9
1	A	11	SER	4.4
1	C	186	ASP	3.8
1	A	5	GLN	3.8
1	B	9	ILE	3.7
1	B	11	SER	3.7
1	A	184	ARG	3.5
1	B	59	ASP	3.5
1	B	12	PRO	3.4
1	B	8	PRO	3.4
1	D	14	ALA	3.4
1	B	183	SER	3.1
1	A	23	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	10	PRO	3.0
1	C	5	GLN	2.9
1	A	26	TYR	2.8
1	D	48	SER	2.8
1	A	24	LEU	2.8
1	B	184	ARG	2.8
1	D	20	GLU	2.7
1	C	8	PRO	2.6
1	D	47	ILE	2.6
1	B	60	GLY	2.4
1	A	15	LYS	2.4
1	A	7	ILE	2.4
1	D	15	LYS	2.4
1	A	60	GLY	2.4
1	C	185	GLU	2.3
1	A	123	ARG	2.2
1	D	185	GLU	2.1
1	B	10	PRO	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	KEG	D	901	53/53	0.83	0.29	2.96	51,64,68,69	53
2	KEG	C	900	52/53	0.72	0.35	0.46	80,83,84,85	52
2	KEG	A	902	53/53	0.92	0.19	-0.27	41,53,60,63	53

6.5 Other polymers (i)

There are no such residues in this entry.