WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:43 AM GMT

PDB ID : 2NZV
Title : Structural mechanism for the fine-tuning of CcpA function by the small molecule effectors G6P and FBP
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Deposited on : 2006-11-25
Resolution : 3.00 Å(reported)

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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 3.00 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		0.291
Clashscore		34
Ramachandran outliers		3.1%
Sidechain outliers		12.1%
RSRZ outliers		4.2%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
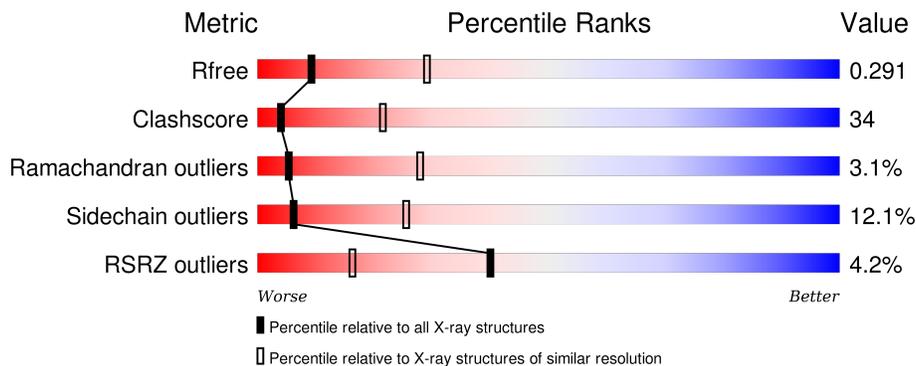
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	G	280	% 43% 46% 9% ·
2	L	88	14% 43% 49% 7% ·

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
3	FBP	G	2128	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2833 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 Catabolite control protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	275	Total	C	N	O	S	0	0	0
			2141	1349	356	428	8			

- Molecule 2 is a protein called Phosphocarrier protein HPr.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	87	Total	C	N	O	P	S	0	0	0
			632	386	104	138	1	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	46	SEP	SER	MODIFIED RESIDUE	UNP O69250

- Molecule 3 is SUGAR (FRUCTOSE-1,6-DIPHOSPHATE) (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).
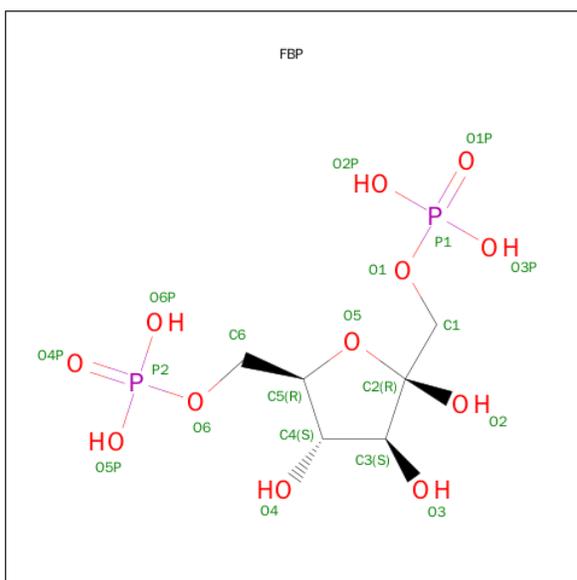
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total 20	C 6	O 12	P 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
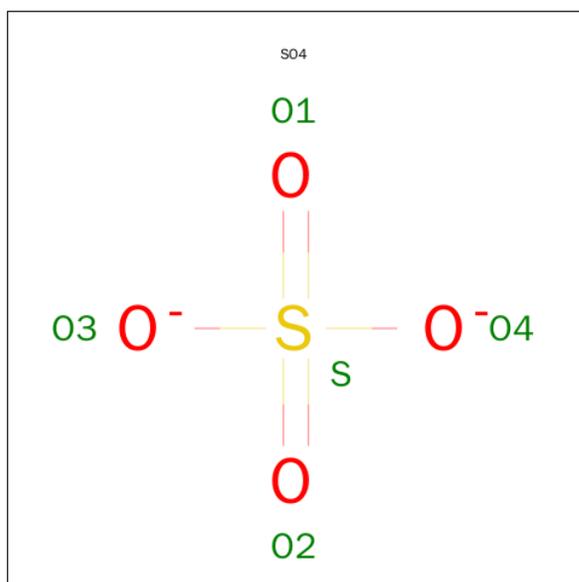
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total 5	O 4	S 1	0	0
4	G	1	Total 5	O 4	S 1	0	0
4	G	1	Total 5	O 4	S 1	0	0
4	G	1	Total 5	O 4	S 1	0	0
4	L	1	Total 5	O 4	S 1	0	0
4	L	1	Total 5	O 4	S 1	0	0
4	G	1	Total 5	O 4	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	4	Total 4	O 4	0	0
5	L	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Catabolite control protein
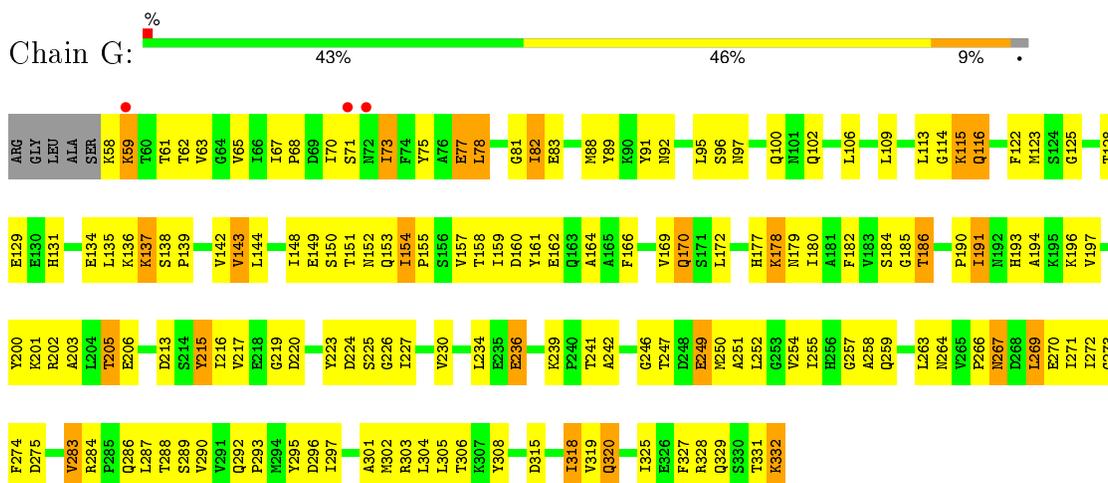
- Molecule 2: Phosphocarrier protein HPr
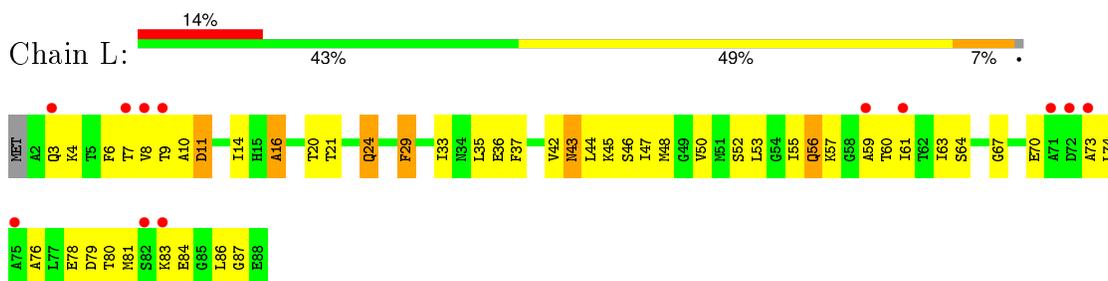
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	69.77Å 69.77Å 231.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.53 – 3.00 38.53 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.9 (38.53-3.00) 93.8 (38.53-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.298 0.253 , 0.291	Depositor DCC
R_{free} test set	1563 reflections (13.67%)	DCC
Wilson B-factor (Å^2)	82.6	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 100.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	3 of 11436 reflections (0.026%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2833	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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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: FBP, SO4, SEP

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	G	0.40	0/2174	0.70	0/2945
2	L	0.34	0/625	0.58	0/839
All	All	0.39	0/2799	0.68	0/3784

There are no bond length outliers.

There are no bond angle outliers.

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	G	2141	0	2147	150	0
2	L	632	0	624	42	0
3	G	20	0	10	4	0
4	G	25	0	0	0	0
4	L	10	0	0	0	0
5	G	4	0	0	1	0
5	L	1	0	0	0	0
All	All	2833	0	2781	191	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 34.

All (191) 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:G:62:THR:HG22	1:G:92:ASN:HB2	1.34	1.06
1:G:264:ASN:HB2	1:G:267:ASN:HB2	1.43	1.00
1:G:67:ILE:HD11	1:G:75:TYR:HB3	1.55	0.88
1:G:178:LYS:HG2	1:G:179:ASN:H	1.43	0.83
1:G:102:GLN:HG3	1:G:131:HIS:HE1	1.44	0.80
1:G:295:TYR:CD1	2:L:16:ALA:HA	2.17	0.80
1:G:154:ILE:HD12	1:G:154:ILE:H	1.48	0.79
1:G:164:ALA:HB1	1:G:290:VAL:HG11	1.66	0.76
1:G:178:LYS:H	1:G:178:LYS:HE2	1.51	0.76
3:G:2128:FBP:O4	3:G:2128:FBP:H12	1.87	0.75
1:G:159:ILE:HD11	1:G:293:PRO:HD2	1.68	0.74
3:G:2128:FBP:H61	3:G:2128:FBP:O3	1.86	0.74
1:G:230:VAL:HG11	1:G:258:ALA:HB2	1.70	0.73
1:G:274:PHE:O	1:G:275:ASP:HB2	1.90	0.72
1:G:264:ASN:HB3	1:G:267:ASN:HD22	1.54	0.72
1:G:230:VAL:HG21	1:G:254:VAL:HA	1.75	0.69
1:G:303:ARG:HG2	2:L:47:ILE:HG22	1.75	0.69
2:L:6:PHE:HZ	2:L:78:GLU:HG2	1.57	0.69
2:L:7:THR:HG22	2:L:60:THR:HG22	1.74	0.68
1:G:293:PRO:O	1:G:297:ILE:HG12	1.93	0.68
1:G:273:GLY:HA3	1:G:287:LEU:HD11	1.76	0.68
1:G:143:VAL:HG12	1:G:305:LEU:HD13	1.78	0.66
1:G:73:ILE:H	1:G:73:ILE:HD12	1.59	0.65
2:L:44:LEU:HD13	2:L:44:LEU:O	1.97	0.65
1:G:172:LEU:HD13	1:G:242:ALA:HB1	1.79	0.64
1:G:318:ILE:HB	5:G:993:HOH:O	1.98	0.64
3:G:2128:FBP:C1	3:G:2128:FBP:O4	2.46	0.63
1:G:266:PRO:HB2	1:G:270:GLU:HG2	1.79	0.63
1:G:227:ILE:HG23	1:G:257:GLY:HA3	1.81	0.63
1:G:178:LYS:H	1:G:178:LYS:CE	2.12	0.62
2:L:47:ILE:CG2	2:L:48:MET:N	2.62	0.62
1:G:230:VAL:CG2	1:G:254:VAL:HA	2.29	0.62
1:G:178:LYS:HE2	1:G:178:LYS:N	2.14	0.62
1:G:78:LEU:HD13	1:G:123:MET:HE3	1.82	0.62
1:G:67:ILE:CD1	1:G:75:TYR:HB3	2.29	0.61
1:G:190:PRO:HA	1:G:193:HIS:CE1	2.35	0.61
1:G:264:ASN:CB	1:G:267:ASN:HD22	2.14	0.61
1:G:331:THR:O	1:G:331:THR:HG23	2.01	0.61
1:G:202:ARG:O	1:G:206:GLU:HB2	2.01	0.61
1:G:234:LEU:O	1:G:239:LYS:HE3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:137:LYS:N	1:G:137:LYS:HE3	2.16	0.60
1:G:201:LYS:O	1:G:205:THR:HG23	2.01	0.60
1:G:152:ASN:HD22	1:G:318:ILE:HG13	1.68	0.59
2:L:46:SEP:O2P	2:L:48:MET:HB2	2.02	0.59
1:G:149:GLU:CG	1:G:154:ILE:HD11	2.33	0.59
2:L:21:THR:HG21	2:L:84:GLU:OE2	2.03	0.58
1:G:286:GLN:O	1:G:328:ARG:HB2	2.03	0.58
1:G:288:THR:OG1	1:G:331:THR:HG22	2.04	0.58
2:L:44:LEU:O	2:L:44:LEU:HD22	2.04	0.57
2:L:46:SEP:O	2:L:50:VAL:HG23	2.04	0.57
1:G:73:ILE:O	1:G:77:GLU:HB2	2.04	0.57
2:L:43:ASN:OD1	2:L:45:LYS:HE3	2.04	0.57
1:G:136:LYS:NZ	1:G:153:GLN:HE21	2.02	0.57
1:G:191:ILE:HD13	1:G:191:ILE:C	2.25	0.57
1:G:216:ILE:HG13	1:G:216:ILE:O	2.05	0.57
1:G:67:ILE:HG21	1:G:70:ILE:HG23	1.87	0.56
1:G:68:PRO:CG	1:G:100:GLN:HE21	2.17	0.56
1:G:227:ILE:HG23	1:G:257:GLY:CA	2.36	0.56
1:G:191:ILE:HD13	1:G:191:ILE:O	2.04	0.56
1:G:100:GLN:HE22	1:G:125:GLY:H	1.54	0.56
1:G:252:LEU:HG	1:G:283:VAL:HG13	1.88	0.56
1:G:302:MET:O	1:G:306:THR:HG23	2.05	0.56
2:L:9:THR:O	2:L:57:LYS:HE3	2.05	0.56
1:G:78:LEU:HD13	1:G:123:MET:CE	2.36	0.55
2:L:47:ILE:HG22	2:L:48:MET:H	1.71	0.55
2:L:8:VAL:CG1	2:L:59:ALA:H	2.20	0.55
1:G:109:LEU:O	1:G:109:LEU:HD23	2.07	0.55
2:L:37:PHE:HB3	2:L:53:LEU:HD22	1.89	0.55
1:G:179:ASN:HB3	1:G:215:TYR:CE2	2.42	0.54
1:G:252:LEU:HG	1:G:283:VAL:CG1	2.36	0.54
1:G:255:ILE:O	1:G:259:GLN:HG3	2.06	0.54
1:G:102:GLN:HG3	1:G:131:HIS:CE1	2.35	0.54
2:L:47:ILE:HG22	2:L:48:MET:N	2.21	0.54
2:L:48:MET:O	2:L:52:SER:HB3	2.08	0.54
1:G:142:VAL:O	1:G:155:PRO:HD2	2.08	0.54
2:L:8:VAL:HG12	2:L:59:ALA:O	2.08	0.54
1:G:95:LEU:HD12	1:G:96:SER:H	1.73	0.53
1:G:178:LYS:HG2	1:G:179:ASN:N	2.18	0.53
2:L:81:MET:HG3	2:L:86:LEU:HB2	1.90	0.53
2:L:63:ILE:N	2:L:63:ILE:HD12	2.22	0.53
2:L:67:GLY:H	2:L:70:GLU:HG2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:67:ILE:O	1:G:97:ASN:HA	2.08	0.53
1:G:190:PRO:O	1:G:194:ALA:HB3	2.08	0.52
1:G:114:GLY:C	1:G:116:GLN:H	2.12	0.52
1:G:59:LYS:HD2	1:G:59:LYS:H	1.74	0.52
1:G:319:VAL:HG12	1:G:320:GLN:H	1.74	0.52
1:G:70:ILE:HG21	1:G:95:LEU:HD21	1.92	0.52
1:G:318:ILE:HD13	1:G:318:ILE:O	2.10	0.52
1:G:246:GLY:O	1:G:247:THR:HB	2.09	0.52
1:G:193:HIS:HA	1:G:197:VAL:CG2	2.39	0.51
1:G:59:LYS:N	1:G:59:LYS:HD2	2.26	0.51
1:G:251:ALA:O	1:G:255:ILE:HG12	2.11	0.51
1:G:113:LEU:HD22	1:G:139:PRO:HD2	1.91	0.51
1:G:149:GLU:HG2	1:G:154:ILE:HD11	1.93	0.51
2:L:8:VAL:HA	2:L:87:GLY:HA2	1.92	0.51
2:L:10:ALA:HB2	2:L:86:LEU:HA	1.94	0.50
1:G:185:GLY:HA2	1:G:219:GLY:O	2.12	0.50
1:G:162:GLU:CD	1:G:202:ARG:HH21	2.15	0.50
1:G:287:LEU:HD13	1:G:288:THR:O	2.12	0.49
1:G:250:MET:O	1:G:254:VAL:HG23	2.12	0.49
1:G:157:VAL:HG21	1:G:301:ALA:HA	1.94	0.48
2:L:24:GLN:HE21	2:L:24:GLN:HB2	1.49	0.48
1:G:179:ASN:HB3	1:G:215:TYR:HE2	1.79	0.48
1:G:102:GLN:O	1:G:106:LEU:HD23	2.14	0.48
2:L:80:THR:O	2:L:84:GLU:HG2	2.14	0.48
1:G:319:VAL:HG12	1:G:320:GLN:N	2.29	0.48
2:L:79:ASP:O	2:L:83:LYS:HB2	2.13	0.48
1:G:89:TYR:O	1:G:91:TYR:HD1	1.96	0.48
1:G:193:HIS:HA	1:G:197:VAL:HG21	1.96	0.48
1:G:166:PHE:CE1	1:G:170:GLN:HG3	2.49	0.47
1:G:122:PHE:HB3	1:G:144:LEU:HD23	1.95	0.47
1:G:318:ILE:HG23	1:G:318:ILE:O	2.13	0.47
1:G:303:ARG:HG2	2:L:47:ILE:CG2	2.44	0.47
2:L:35:LEU:HD11	2:L:61:ILE:HB	1.97	0.47
2:L:29:PHE:CZ	2:L:76:ALA:HB3	2.49	0.47
1:G:159:ILE:HG13	1:G:292:GLN:HG3	1.95	0.47
1:G:216:ILE:CG1	1:G:216:ILE:O	2.63	0.47
1:G:135:LEU:HD22	1:G:142:VAL:HG11	1.97	0.46
1:G:159:ILE:HG22	1:G:160:ASP:N	2.29	0.46
1:G:136:LYS:HZ3	1:G:153:GLN:HE21	1.64	0.46
1:G:223:TYR:HB2	1:G:249:GLU:OE1	2.16	0.46
1:G:81:GLY:HA2	1:G:295:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:271:ILE:HG22	1:G:272:ILE:N	2.30	0.46
1:G:135:LEU:HD22	1:G:142:VAL:HG21	1.96	0.46
1:G:325:ILE:HG21	1:G:327:PHE:CZ	2.50	0.46
1:G:274:PHE:O	1:G:275:ASP:CB	2.62	0.46
1:G:191:ILE:HD11	1:G:196:LYS:HE3	1.98	0.46
1:G:100:GLN:HE22	1:G:125:GLY:N	2.12	0.46
2:L:9:THR:C	2:L:57:LYS:HE3	2.37	0.45
1:G:138:SER:HA	1:G:139:PRO:HD3	1.76	0.45
1:G:161:TYR:CD1	1:G:191:ILE:HG12	2.51	0.45
2:L:53:LEU:HD13	2:L:55:ILE:HD11	1.98	0.45
1:G:136:LYS:HZ1	1:G:153:GLN:HG3	1.81	0.45
1:G:329:GLN:C	1:G:331:THR:H	2.20	0.45
2:L:11:ASP:HA	2:L:57:LYS:HD2	1.99	0.45
1:G:266:PRO:HG3	1:G:332:LYS:HB3	1.98	0.45
1:G:154:ILE:HD12	1:G:154:ILE:O	2.16	0.45
1:G:166:PHE:CE2	1:G:203:ALA:HA	2.52	0.45
1:G:73:ILE:HD12	1:G:73:ILE:N	2.30	0.45
2:L:37:PHE:CE2	2:L:59:ALA:HB1	2.52	0.45
2:L:33:ILE:HA	2:L:64:SER:O	2.17	0.45
1:G:136:LYS:HE3	1:G:153:GLN:HB3	1.99	0.44
1:G:185:GLY:O	1:G:186:THR:C	2.55	0.44
1:G:67:ILE:CG2	1:G:95:LEU:HD11	2.48	0.44
1:G:223:TYR:CE1	1:G:227:ILE:HD11	2.52	0.44
2:L:14:ILE:HG22	2:L:14:ILE:O	2.16	0.44
1:G:287:LEU:HD12	1:G:289:SER:HB2	2.00	0.44
2:L:42:VAL:HG12	2:L:43:ASN:N	2.32	0.44
2:L:67:GLY:H	2:L:70:GLU:CG	2.31	0.44
1:G:154:ILE:CD1	1:G:154:ILE:O	2.66	0.44
1:G:151:THR:OG1	1:G:153:GLN:HG2	2.18	0.43
1:G:266:PRO:CB	1:G:270:GLU:HG2	2.47	0.43
1:G:263:LEU:HD23	1:G:269:LEU:CD2	2.49	0.43
1:G:129:GLU:CD	1:G:129:GLU:H	2.22	0.43
1:G:152:ASN:ND2	1:G:318:ILE:HG13	2.31	0.43
1:G:148:ILE:HG22	1:G:158:THR:HG21	2.00	0.43
1:G:177:HIS:CB	1:G:180:ILE:HD11	2.48	0.43
2:L:4:LYS:HB2	2:L:74:LEU:HD21	2.00	0.43
1:G:166:PHE:CE2	1:G:202:ARG:NH1	2.87	0.43
1:G:182:PHE:CE1	1:G:184:SER:HB3	2.54	0.43
1:G:331:THR:O	1:G:331:THR:CG2	2.67	0.43
1:G:58:LYS:HB3	1:G:59:LYS:HZ2	1.83	0.43
2:L:29:PHE:HZ	2:L:76:ALA:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:169:VAL:HG21	1:G:200:TYR:HA	2.00	0.42
1:G:164:ALA:HB1	1:G:290:VAL:CG1	2.43	0.42
1:G:136:LYS:HE3	1:G:153:GLN:CB	2.49	0.42
1:G:88:MET:HE2	2:L:24:GLN:HG3	2.00	0.42
1:G:128:THR:HG22	1:G:129:GLU:N	2.35	0.42
1:G:154:ILE:HD12	1:G:154:ILE:N	2.18	0.42
1:G:226:GLY:O	1:G:230:VAL:HG23	2.20	0.42
1:G:220:ASP:OD2	1:G:225:SER:HB3	2.20	0.42
1:G:293:PRO:HB2	1:G:296:ASP:HB2	2.00	0.42
1:G:287:LEU:O	1:G:328:ARG:HD2	2.20	0.42
1:G:236:GLU:O	1:G:239:LYS:HD2	2.20	0.42
1:G:65:VAL:O	1:G:65:VAL:HG23	2.20	0.41
1:G:78:LEU:O	1:G:82:ILE:HG12	2.21	0.41
2:L:29:PHE:CZ	2:L:73:ALA:HA	2.55	0.41
1:G:247:THR:HG22	1:G:250:MET:CE	2.50	0.41
1:G:114:GLY:O	1:G:116:GLN:N	2.51	0.41
1:G:241:THR:O	1:G:269:LEU:HA	2.21	0.41
1:G:271:ILE:N	1:G:271:ILE:HD12	2.36	0.41
1:G:73:ILE:H	1:G:73:ILE:CD1	2.25	0.41
1:G:135:LEU:HD23	1:G:135:LEU:HA	1.87	0.41
1:G:131:HIS:O	1:G:135:LEU:HB2	2.21	0.41
1:G:247:THR:OG1	3:G:2128:FBP:H62	2.21	0.41
2:L:44:LEU:HD13	2:L:44:LEU:C	2.42	0.40
1:G:65:VAL:HG22	1:G:95:LEU:HA	2.03	0.40
1:G:89:TYR:O	1:G:91:TYR:CD1	2.73	0.40
1:G:302:MET:O	1:G:305:LEU:HB3	2.21	0.40
1:G:67:ILE:HG22	1:G:95:LEU:HD11	2.04	0.40
1:G:109:LEU:HD11	1:G:135:LEU:HG	2.03	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	G	273/280 (98%)	219 (80%)	47 (17%)	7 (3%)	7	33
2	L	84/88 (96%)	69 (82%)	11 (13%)	4 (5%)	3	17
All	All	357/368 (97%)	288 (81%)	58 (16%)	11 (3%)	5	28

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	116	GLN
1	G	150	SER
1	G	186	THR
2	L	16	ALA
2	L	56	GLN
1	G	115	LYS
1	G	83	GLU
1	G	267	ASN
2	L	43	ASN
2	L	29	PHE
1	G	82	ILE

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	G	241/244 (99%)	210 (87%)	31 (13%)	5	23
2	L	66/67 (98%)	60 (91%)	6 (9%)	12	41
All	All	307/311 (99%)	270 (88%)	37 (12%)	6	25

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	59	LYS
1	G	61	THR
1	G	63	VAL
1	G	71	SER
1	G	73	ILE

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Mol	Chain	Res	Type
1	G	77	GLU
1	G	78	LEU
1	G	115	LYS
1	G	134	GLU
1	G	137	LYS
1	G	143	VAL
1	G	154	ILE
1	G	170	GLN
1	G	178	LYS
1	G	191	ILE
1	G	205	THR
1	G	213	ASP
1	G	215	TYR
1	G	217	VAL
1	G	224	ASP
1	G	236	GLU
1	G	249	GLU
1	G	269	LEU
1	G	283	VAL
1	G	284	ARG
1	G	304	LEU
1	G	308	TYR
1	G	315	ASP
1	G	318	ILE
1	G	320	GLN
1	G	332	LYS
2	L	3	GLN
2	L	11	ASP
2	L	20	THR
2	L	24	GLN
2	L	36	GLU
2	L	56	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	92	ASN
1	G	100	GLN
1	G	153	GLN
1	G	163	GLN
1	G	193	HIS
1	G	267	ASN

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Mol	Chain	Res	Type
1	G	292	GLN
1	G	310	ASN
1	G	323	HIS
2	L	15	HIS
2	L	24	GLN
2	L	38	ASN
2	L	56	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)

1 non-standard protein/DNA/RNA residue is 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	SEP	L	46	2	8,9,10	1.01	0	8,12,14	2.81	3 (37%)

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	SEP	L	46	2	-	0/6/8/10	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	46	SEP	O2P-P-O1P	-2.47	102.63	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	46	SEP	O3P-P-O1P	3.30	121.21	110.58
2	L	46	SEP	OG-CB-CA	6.42	113.75	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	46	SEP	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	FBP	G	2128	-	18,20,20	1.68	5 (27%)	21,32,32	1.83	7 (33%)
4	SO4	G	745	-	4,4,4	0.25	0	6,6,6	0.13	0
4	SO4	G	945	-	4,4,4	0.19	0	6,6,6	0.10	0
4	SO4	G	946	-	4,4,4	0.22	0	6,6,6	0.08	0
4	SO4	G	966	-	4,4,4	0.19	0	6,6,6	0.12	0
4	SO4	G	995	-	4,4,4	0.24	0	6,6,6	0.12	0
4	SO4	L	975	-	4,4,4	0.20	0	6,6,6	0.13	0
4	SO4	L	978	-	4,4,4	0.23	0	6,6,6	0.07	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	FBP	G	2128	-	-	0/13/32/32	0/1/1/1
4	SO4	G	745	-	-	0/0/0/0	0/0/0/0
4	SO4	G	945	-	-	0/0/0/0	0/0/0/0
4	SO4	G	946	-	-	0/0/0/0	0/0/0/0
4	SO4	G	966	-	-	0/0/0/0	0/0/0/0
4	SO4	G	995	-	-	0/0/0/0	0/0/0/0
4	SO4	L	975	-	-	0/0/0/0	0/0/0/0
4	SO4	L	978	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2128	FBP	O2-C2	2.11	1.44	1.41
3	G	2128	FBP	C4-C5	2.25	1.59	1.53
3	G	2128	FBP	O5-C2	2.65	1.47	1.43
3	G	2128	FBP	P1-O1P	3.12	1.61	1.51
3	G	2128	FBP	O5-C5	3.12	1.51	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	2128	FBP	O4-C4-C3	-2.70	103.44	112.01
3	G	2128	FBP	O5-C5-C6	-2.43	103.96	109.49
3	G	2128	FBP	O6-C6-C5	2.00	116.50	109.12
3	G	2128	FBP	O3P-P1-O2P	2.40	116.50	107.38
3	G	2128	FBP	O3P-P1-O1	2.49	113.72	106.56
3	G	2128	FBP	O4-C4-C5	2.77	119.36	111.05
3	G	2128	FBP	O2-C2-O5	3.94	117.51	109.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2128	FBP	4	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	G	275/280 (98%)	-0.12	3 (1%)	82	58	53, 79, 114, 146	0
2	L	86/88 (97%)	0.71	12 (13%)	4	1	76, 133, 151, 160	0
All	All	361/368 (98%)	0.08	15 (4%)	40	16	53, 86, 143, 160	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	59	LYS	3.4
2	L	9	THR	3.2
2	L	59	ALA	3.1
2	L	72	ASP	3.0
2	L	83	LYS	2.7
2	L	7	THR	2.6
1	G	71	SER	2.6
1	G	72	ASN	2.5
2	L	73	ALA	2.4
2	L	61	ILE	2.4
2	L	75	ALA	2.4
2	L	82	SER	2.4
2	L	71	ALA	2.2
2	L	8	VAL	2.1
2	L	3	GLN	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. 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	SEP	L	46	10/11	0.94	0.14	-	81,86,92,95	0

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
3	FBP	G	2128	20/20	0.72	0.45	1.89	52,65,74,76	0
4	SO4	G	946	5/5	0.67	0.27	1.63	153,153,155,155	0
4	SO4	G	945	5/5	0.96	0.14	-	114,115,118,120	0
4	SO4	L	978	5/5	0.78	0.26	-	169,169,170,170	0
4	SO4	G	966	5/5	0.57	0.36	-	193,193,193,194	0
4	SO4	L	975	5/5	0.76	0.26	-	193,193,194,194	0
4	SO4	G	745	5/5	0.72	0.21	-	162,163,165,165	0
4	SO4	G	995	5/5	0.42	0.35	-	189,190,191,191	0

6.5 Other polymers (i)

There are no such residues in this entry.